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**Essential Graduate Physics**  
*Lecture Notes and Problems*

## **Exercise Problems with Model Solutions**

# **Part QM: Quantum Mechanics**

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## Chapter 1. Introduction

**Problem 1.1.** The actual postulate made by N. Bohr in his original 1913 paper was not directly Eq. (1.8) of the lecture notes, but rather the assumption that at quantum leaps between adjacent electron orbits with  $n \gg 1$ , the hydrogen atom either emits or absorbs the energy  $\Delta E = \hbar\omega$ , where  $\omega$  is its classical radiation frequency – according to classical electrodynamics, equal to the angular velocity of the electron’s rotation.<sup>1</sup> Prove that this postulate, complemented with the natural requirement that  $L = 0$  at  $n = 0$ , is equivalent to Eq. (1.8).

*Solution:* Combining the classical Eqs. (1.9) and (1.11) written for the  $n^{\text{th}}$  circular orbit,

$$m_e \frac{v^2}{r_n} = \frac{e^2}{4\pi\epsilon_0 r_n^2}, \quad E_n = \frac{m_e v_n^2}{2} - \frac{e^2}{4\pi\epsilon_0 r_n},$$

with the well-known classical relations  $\omega_n = v_n/r_n$ ,  $L_n = m_e v_n r_n$ , we may readily express the energy and the rotation frequency of the electron via its angular momentum  $L_n$ :

$$E_n = -\frac{m_e}{2} \left( \frac{e^2}{4\pi\epsilon_0} \right)^2 \frac{1}{L_n^2}, \quad \omega_n = m_e \left( \frac{e^2}{4\pi\epsilon_0} \right)^2 \frac{1}{L_n^3}. \quad (*)$$

For large orbits, with for  $n \gg 1$  and  $L_n \rightarrow \infty$ , both  $E_n$  and  $\omega_n$  tend to zero, and hence the difference between the adjacent energy levels ( $\Delta n = 1$ ) may be well approximated as

$$\Delta E_n \equiv E_{n+1} - E_n \approx \frac{dE_n}{dn}.$$

From here and the first of Eqs. (\*),

$$\Delta E_n = m_e \left( \frac{e^2}{4\pi\epsilon_0} \right)^2 \frac{1}{L_n^3} \Delta L_n.$$

Comparing this expression with the second of Eqs. (\*), we get

$$\Delta L_n = \frac{\Delta E_n}{\omega_n}.$$

Hence the actual Bohr’s assumption ( $\Delta E_n = \hbar\omega_n$ ) yields  $\Delta L_n = \hbar$ . Together with the natural requirement  $L_0 = 0$ , this result is equivalent to Eq. (1.8).

**Problem 1.2.** Generalize Bohr’s theory for a hydrogen-like atom/ion with a nucleus of the electric charge  $Q = Ze$ , to the relativistic case.

*Solution:* According to classical relativity,<sup>2</sup> the non-relativistic equation of motion of a charged particle in an electromagnetic field retains its form even in the relativistic case, provided that the particle’s mass  $m$  is replaced with its relativistic, velocity-dependent value

<sup>1</sup> See, e.g., EM Sec. 8.2.

<sup>2</sup> See, e.g., EM Sec. 9.6, in particular Eq. (9.144).

$$M = \gamma m \equiv \frac{m}{(1 - v^2/c^2)^{1/2}}, \quad (*)$$

where  $m$  is now the rest mass, and  $c$  is the speed of light. With this replacement and the similar change of the particle's momentum,  $\mathbf{p} \rightarrow M\mathbf{v} \equiv \gamma m\mathbf{v}$ , Eqs. (1.8) and (1.9) for a circular orbit of an electron in a hydrogen-like atom/ion become

$$M_e v r = \hbar n, \quad M_e \frac{v^2}{r} = \frac{Ze^2}{4\pi\epsilon_0 r^2}.$$

Solving this simple system of two equations for  $v$  and  $r$ , for the former variable, we get formally the same result as in the non-relativistic case:

$$v = \frac{Ze^2 / 4\pi\epsilon_0}{\hbar n}; \quad (**)$$

however, Eq. (1.10) for the orbit's radius is now rescaled by the Lorentz factor  $\gamma$ :

$$r = \frac{n^2}{\gamma} r_B \equiv n^2 \left[ 1 - \left( \frac{v}{c} \right)^2 \right]^{1/2} r_B = n^2 \left[ 1 - \left( \frac{Z\alpha}{n} \right)^2 \right]^{1/2} r_B,$$

where  $\alpha \equiv e^2/4\pi\epsilon_0\hbar c \approx 1/137$  is the so-called fine structure constant.<sup>3</sup>

Most importantly, this formula gives imaginary values for  $r$  (indicating that Bohr's orbits do not exist) for  $n < Z\alpha \approx Z/137$ . The physical reason for this effect becomes clear from Eq. (\*\*) rewritten as  $v = (Z\alpha/n)c$ : for  $n < Z\alpha$ , it gives values of  $v$  larger than  $c$ , i.e. no realistic electron's speed can sustain Bohr's condition of the angular momentum quantization. In particular, for

$$Z > Z_{\max} \approx 137, \quad (***)$$

even the ground state (with  $n = 1$ ) does not exist. Remarkably, exactly the same restriction (\*\*\*) is given by the Dirac equation, i.e. by the most accurate quantum theory of electrons' motion in a classical (non-quantized) electromagnetic field – see Eq. (9.136) and its discussion in Sec. 9.7 of the lecture notes.

**Problem 1.3.** A hydrogen atom, initially in the lowest excited state, returns to its ground state by emitting a photon propagating in a certain direction. Use the same approach as in Sec. 1.1(iv) of the lecture notes to calculate the photon's frequency reduction due to atomic recoil.

*Solution:*<sup>4</sup> According to Eq. (1.12) of the lecture notes, the ground state of the hydrogen atom corresponds to  $n = 1$ , and its lowest-energy excited state, to  $n' = 2$ . So, according to Eqs. (1.7) and (1.12), in the absence of recoil, the emitted photon's energy is

$$\hbar\omega_0 = E_{n'} - E_n = \frac{E_H}{2} \left( \frac{1}{1^2} - \frac{1}{2^2} \right) \equiv \frac{3}{8} E_H.$$

<sup>3</sup> For its discussion, see, e.g., Sec. 6.3 of the lecture notes.

<sup>4</sup> This problem is essentially a variant of EM Problem 9.10.

Now let us calculate the atom's recoil momentum  $p$ , by using the laws of momentum and energy conservation. In the reference frame in that the atom was at rest before the photon emission, they read

$$0 = \frac{\hbar\omega}{c} - p,$$

$$mc^2 + \hbar\omega_0 = \hbar\omega + \left[ (mc^2)^2 + (pc)^2 \right]^{1/2},$$

where  $\omega$  is the photon's frequency with the account of the atomic recoil, and  $m$  is the rest mass of the atom in its ground state, dominated by that of a proton. Solving this system of two equations for  $p$  and  $\omega$ , we get, in particular:

$$\omega = \omega_0 \frac{1 + \hbar\omega_0 / 2mc^2}{1 + \hbar\omega_0 / mc^2} < \omega_0, \quad \text{i.e. } \Delta\omega \equiv \omega_0 - \omega = \omega_0 \frac{\hbar\omega_0 / 2mc^2}{1 + \hbar\omega_0 / mc^2}.$$

Due to the very large difference between  $\hbar\omega_0 \approx 10.2$  eV and  $mc^2 \approx m_p c^2 \approx 0.938 \times 10^9$  eV, this expression may be simplified:

$$\Delta\omega \approx \omega_0 \frac{\hbar\omega_0'}{2m_p c^2}, \quad \text{so } \frac{\Delta\omega}{\omega_0} \approx \frac{\hbar\omega_0}{2m_p c^2} \approx 5.43 \times 10^{-9}.$$

It is curious that the recoil velocity has a human scale:

$$v \approx \frac{p}{m_p} = \frac{\hbar\omega/c}{m_p} \approx 3.26 \frac{\text{m}}{\text{s}} \ll c.$$

Note, however, that the qualification “propagating in a certain direction” in this problem's assignment is very loaded. Indeed, as will be discussed later in this course, forming a photon (i.e. an electromagnetic wave packet) with virtually definite magnitude and direction of its momentum, resulting in a similarly definite recoil momentum  $\mathbf{p}$ , requires the involvement of not one but many sinusoidal waves with different (if close) frequencies corresponding to different (if close) energies. In the opposite limit, if one insists the emitted electromagnetic wave to be strictly monochromatic, the wave's propagation direction becomes completely uncertain, and the quantum-ensemble average (“expectation value”) of the resulting recoil velocity vector  $\mathbf{v}$  vanishes.<sup>5</sup>

Perhaps even more shockingly, which of these two approximations describes the real experimental situation better, and hence what the “real” recoil of the atom is, depends on the photon's detection conditions – even if this detection takes place long after the emission's moment! Thus, even this apparently simple situation touches deep issues of quantum mechanics including the rather counterintuitive *local reality* problem, which will be only discussed at the very end of this course (Chapter 10) because this discussion requires the course's full contents as the background.

**Problem 1.4.** Use Eq. (1.53) of the lecture notes to prove that the linear operators of quantum mechanics are commutative:  $\hat{A}_2 + \hat{A}_1 = \hat{A}_1 + \hat{A}_2$ , and associative:  $(\hat{A}_1 + \hat{A}_2) + \hat{A}_3 = \hat{A}_1 + (\hat{A}_2 + \hat{A}_3)$ .

*Solution:* These relations look obvious, but the reader should remember that in the operators, we face a mathematical entity different from the usual numbers, functions, and geometrical vectors, and

<sup>5</sup> Moreover, that strict requirement would also imply that the wave emission time is infinite – see, e.g., Sec. 2.5.

cannot take for granted any properties that have not been postulated or already proved. For example, for any two usual functions  $\Psi_1$  and  $\Psi_2$  (which, for given argument values, are just numbers), we may always write  $\Psi_1\Psi_2 = \Psi_2\Psi_1$ , but for similar operator “products”, such commutation is generally invalid – see, e.g., Eq. (2.14) of the lecture notes. This is why we should be careful.

First, let us use Eq. (1.53), with the index swap  $1\leftrightarrow 2$ , to write

$$(\hat{A}_2 + \hat{A}_1)\Psi = \hat{A}_2\Psi + \hat{A}_1\Psi.$$

The left-hand side of this equation, and each of the two terms of its right-hand side, are just functions (not operators!) and hence obey the rules of the “usual” algebra. In particular, these terms are commutative, so that side is equal to the right-hand side of the initial form of Eq. (1.53):

$$(\hat{A}_1 + \hat{A}_2)\Psi = \hat{A}_1\Psi + \hat{A}_2\Psi.$$

Hence, the left-hand sides of these relations (again, each of them is just a function!) have to be equal as well:

$$(\hat{A}_2 + \hat{A}_1)\Psi = (\hat{A}_1 + \hat{A}_2)\Psi.$$

Since this relation is valid for an arbitrary function  $\Psi$ , it gives the required proof that the operators are commutative as well.

Similarly, we may use Eq. (1.53) twice to write

$$\left[ (\hat{A}_1 + \hat{A}_2) + \hat{A}_3 \right] \Psi = (\hat{A}_1 + \hat{A}_2)\Psi + \hat{A}_3\Psi = \hat{A}_1\Psi + \hat{A}_2\Psi + \hat{A}_3\Psi.$$

Again, the operands on the right-hand side of this equation are just functions and may be regrouped as

$$\hat{A}_1\Psi + \hat{A}_2\Psi + \hat{A}_3\Psi = \hat{A}_1\Psi + (\hat{A}_2\Psi + \hat{A}_3\Psi).$$

Now we may apply Eq. (1.53) twice to the right-hand side of the above relation, to write

$$\hat{A}_1\Psi + (\hat{A}_2\Psi + \hat{A}_3\Psi) = \left[ \hat{A}_1 + (\hat{A}_2 + \hat{A}_3) \right] \Psi.$$

Comparing the initial and final expressions of our calculation, we get

$$\left[ (\hat{A}_1 + \hat{A}_2) + \hat{A}_3 \right] \Psi = \left[ \hat{A}_1 + (\hat{A}_2 + \hat{A}_3) \right] \Psi.$$

This equality is valid for any  $\Psi$  and hence the linear operators are indeed associative.

**Problem 1.5.** Prove that for any time-independent Hamiltonian operator  $\hat{H}$  and two arbitrary complex functions  $f(\mathbf{r})$  and  $g(\mathbf{r})$ ,

$$\int f(\mathbf{r})\hat{H}g(\mathbf{r})d^3r = \int \hat{H}f(\mathbf{r})g(\mathbf{r})d^3r.$$

*Solution:* Using the fact (discussed in Sec. 1.5 of the lecture notes) that the set of eigenfunctions  $\psi_n$  of the given Hamiltonian operator (i.e. the set of stationary states of the corresponding quantum system) is full, we may expand the function  $g(\mathbf{r})$  and the complex conjugate of the function  $f(\mathbf{r})$  into series over the set, just as it was done with the function  $\Psi(\mathbf{r}, 0)$  in Eq. (1.67):

$$g(\mathbf{r}) = \sum_n g_n \psi_n(\mathbf{r}), \quad f^*(\mathbf{r}) = \sum_n f_n \psi_n(\mathbf{r}), \quad \text{so that } f(\mathbf{r}) \equiv [f^*(\mathbf{r})]^* = \left[ \sum_n f_n \psi_n(\mathbf{r}) \right]^* \equiv \sum_n f_n^* \psi_n^*(\mathbf{r}),$$

where  $f_n$  and  $g_n$  are some (generally, complex) coefficients. Plugging these expressions (with one of the summation indices  $n$  denoted as  $n'$ ) into each side of the equality to be proved, and taking the constant coefficients out of the spatial integrals, we may transform them as

$$\begin{aligned} \int f(\mathbf{r}) \hat{H} g(\mathbf{r}) d^3 r &= \sum_{n,n'} f_n^* g_{n'} \int \psi_n^*(\mathbf{r}) \hat{H} \psi_{n'}(\mathbf{r}) d^3 r, \\ \int \hat{H} f(\mathbf{r}) g(\mathbf{r}) d^3 r &= \sum_{n,n'} f_n^* g_{n'} \int \hat{H} \psi_n^*(\mathbf{r}) \psi_{n'}(\mathbf{r}) d^3 r. \end{aligned}$$

Now using Eq. (1.60) with  $n$  replaced for  $n'$ ,  $\hat{H} \psi_{n'} = E_{n'} \psi_{n'}$ , in the first expression, and its complex conjugate,  $\hat{H} \psi_n^* = E_n \psi_n^*$ ,<sup>6</sup> in the second one, and then employing the orthonormality condition (1.66), we get

$$\begin{aligned} \int f(\mathbf{r}) \hat{H} g(\mathbf{r}) d^3 r &= \sum_{n,n'} f_n^* g_{n'} E_{n'} \int \psi_n^*(\mathbf{r}) \psi_{n'}(\mathbf{r}) d^3 r = \sum_{n,n'} f_n^* g_{n'} E_{n'} \delta_{nn'} = \sum_n f_n^* g_n E_n, \\ \int \hat{H} f(\mathbf{r}) g(\mathbf{r}) d^3 r &= \sum_{n,n'} f_n^* g_{n'} E_n \int \psi_n^*(\mathbf{r}) \psi_{n'}(\mathbf{r}) d^3 r = \sum_{n,n'} f_n^* g_{n'} E_n \delta_{nn'} = \sum_n f_n^* g_n E_n, \end{aligned}$$

so the left-hand sides of these two relations (i.e. both sides of the formula in question) are equal as well.

**Problem 1.6.** Prove that the Schrödinger equation (1.25) with the Hamiltonian operator given by Eq. (1.41) is Galilean form-invariant, provided that the wavefunction is transformed as

$$\Psi'(\mathbf{r}', t') = \Psi(\mathbf{r}, t) \exp \left\{ -i \frac{m\mathbf{v} \cdot \mathbf{r}}{\hbar} + i \frac{mv^2 t}{2\hbar} \right\},$$

where the prime sign marks the variables observed in the reference frame  $0'$  that moves, without rotation and with a constant velocity  $\mathbf{v}$ , relative to the “lab” frame  $0$ . Give a physical interpretation of this transformation.

*Solution:* The non-relativistic (“Galilean”) space/time transform between the two reference frames is expressed by the following relations:<sup>7</sup>

$$\mathbf{r}' = \mathbf{r} - \mathbf{v}t, \quad t' = t. \quad (*)$$

The Galilean form-invariance means that the wavefunctions  $\Psi'(\mathbf{r}', t')$  and  $\Psi(\mathbf{r}, t)$ , related as specified in the assignment, should satisfy similar Schrödinger equations in these reference frames:

$$i\hbar \frac{\partial \Psi'}{\partial t'} = -\frac{\hbar^2}{2m} \nabla'^2 \Psi' + U'(\mathbf{r}', t') \Psi', \quad \text{and} \quad i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + U(\mathbf{r}, t) \Psi. \quad (**)$$

<sup>6</sup> The eigenenergies  $E_n$  are real numbers, so they do not change at the complex conjugation, and neither are the Hamiltonians of the type (1.41).

<sup>7</sup> If needed, you may consult, e.g., EM Sec. 9.1, in particular, Fig. 9.1 and Eq. (9.2).

For proof of this fact, let us note that the functions  $U'(\mathbf{r}', t')$  and  $U(\mathbf{r}, t)$  describe the same potential energy of the particle, i.e. must give the same value at the same space-time point:

$$U'(\mathbf{r}', t') \equiv U'(\mathbf{r} - \mathbf{v}t, t) = U(\mathbf{r}, t).$$

(Note also that the wavefunction transform suggested in the assignment gives a similar relation for the probability density to find the particle at the same space-time point:

$$w'(\mathbf{r}', t') = |\Psi'(\mathbf{r}', t')|^2 = |\Psi'(\mathbf{r} - \mathbf{v}t, t)|^2 = |\Psi(\mathbf{r}, t)|^2 = w(\mathbf{r}, t),$$

just as it should.)

Next, considering  $t'$ , at fixed  $\mathbf{r}'$ , a function of arguments  $\mathbf{r}(t) \equiv \{r_1(t), r_2(t), r_3(t)\}$  and  $t$ , we may use the general rule of differentiation of a function of several variables<sup>8</sup> and then the first of Eqs. (\*) in the form  $\mathbf{r} = \mathbf{r}' + \mathbf{v}t'$  to write<sup>9</sup>

$$\frac{\partial}{\partial t'} = \frac{\partial}{\partial t} + \sum_{j=1}^3 \frac{\partial}{\partial r_j} \frac{\partial r_j}{\partial t'} \equiv \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla,$$

while at fixed  $t'$ , Eq. (\*) yields  $\nabla' = \nabla$ , so  $\nabla'^2 = \nabla^2$ . Let us also spell out the expression

$$(\mathbf{v} \cdot \nabla)(\mathbf{v} \cdot \mathbf{r}) = \sum_{j=1}^3 v_j \frac{\partial}{\partial r_j} \sum_{j'=1}^3 v_{j'} r_{j'} = \sum_{j=1}^3 v_j v_{j'} \delta_{jj'} = v^2.$$

With these relations, a straightforward differentiation of the suggested transform of the wavefunction, after it has been plugged into the first of Eqs. (\*\*), immediately yields the second of these equations, i.e. proves the form-invariance of the Schrödinger equation.

For the interpretation of the wavefunction's transform, let us apply it to the simplest case of a monochromatic plane de Broglie wave given by Eqs. (1.29) of the lecture notes, describing a free particle's state with its momentum  $\mathbf{p} = \hbar \mathbf{k}$  and (kinetic) energy  $E = \hbar \omega$  having definite values, i.e. being  $c$ -numbers:

$$\Psi(\mathbf{r}, t) = a \exp \left\{ i \frac{\mathbf{p} \cdot \mathbf{r}}{\hbar} - i \frac{Et}{\hbar} \right\}.$$

The proved transform shows that in the moving reference frame, the wavefunction is a similar plane wave:

$$\Psi'(\mathbf{r}', t') = a \exp \left\{ i \frac{\mathbf{p} \cdot \mathbf{r}}{\hbar} - i \frac{Et}{\hbar} - i \frac{m\mathbf{v} \cdot \mathbf{r}}{\hbar} + i \frac{mv^2 t}{2\hbar} \right\} \equiv a \exp \left\{ i \frac{\mathbf{p}' \cdot \mathbf{r}'}{\hbar} - i \frac{E't'}{\hbar} \right\},$$

where

$$\mathbf{p}' \equiv \mathbf{p} - m\mathbf{v}, \quad \text{and} \quad E' \equiv E - \mathbf{p}' \cdot \mathbf{v} - \frac{mv^2}{2} = E - \mathbf{p} \cdot \mathbf{v} + \frac{mv^2}{2}.$$

However, these are exactly the Galilean transform expressions for the momentum and the kinetic energy of the particle, given by the non-relativistic classical mechanics. Indeed, expressing the particle's momentum via its velocity  $\mathbf{u}$  (in the lab frame) as  $\mathbf{p} = m\mathbf{u}$ , so  $E = mu^2/2$ , we get

<sup>8</sup> See, e.g., MA Eq. (4.2).

<sup>9</sup> This expression is essentially the *convective derivative*, which was discussed several times in this course series – see especially CM Sec. 8.3.



$$\mathbf{p}' = m\mathbf{u} - m\mathbf{v} = m\mathbf{u}', \quad \text{and} \quad E' = \frac{m\mathbf{u}^2}{2} - m\mathbf{u} \cdot \mathbf{v} + \frac{m\mathbf{v}^2}{2} = \frac{m\mathbf{u}'^2}{2},$$

where  $\mathbf{u}' = \mathbf{u} - \mathbf{v}$  is the particle's velocity as observed from the moving reference frame. So, the wavefunction's transform we have proved is just a very natural wave-mechanical expression of the Galilean invariance.

**Problem 1.7.**\* Prove the so-called *Hellmann-Feynman theorem*:<sup>10</sup>

$$\frac{\partial E_n}{\partial \lambda} = \left\langle \frac{\partial H}{\partial \lambda} \right\rangle_n,$$

where  $\lambda$  is some  $c$ -number parameter, on which the time-independent Hamiltonian  $\hat{H}$ , and hence its eigenenergies  $E_n$ , depend.

*Solution:* By multiplying both parts of the basic Eq. (1.60) of the lecture notes,  $\hat{H}\psi_n = E_n\psi_n$ , by  $\psi_n^*$ , and integrating the result over space, we get

$$\int \psi_n^*(\mathbf{r})\hat{H}\psi_n(\mathbf{r})d^3r = \int \psi_n^*(\mathbf{r})E_n\psi_n(\mathbf{r})d^3r.$$

On the right-hand side of this relation, we may take the constant  $E_n$  out of the integral, and then use the orthonormality condition (1.66) to get the following expression for the eigenenergy:<sup>11</sup>

$$E_n = \int \psi_n^*(\mathbf{r})\hat{H}\psi_n(\mathbf{r})d^3r. \quad (*)$$

Let us differentiate both parts of this relation over the parameter  $\lambda$ , taking into account that not only  $\hat{H}$  and  $E_n$  but also the eigenfunctions  $\psi_n$  may depend on it:

$$\begin{aligned} \frac{\partial E_n}{\partial \lambda} &= \int \frac{\partial}{\partial \lambda} \left[ \psi_n^*(\mathbf{r})\hat{H}\psi_n(\mathbf{r}) \right] d^3r \\ &\equiv \int \left[ \frac{\partial \psi_n^*(\mathbf{r})}{\partial \lambda} \hat{H}\psi_n(\mathbf{r}) + \psi_n^*(\mathbf{r}) \frac{\partial \hat{H}}{\partial \lambda} \psi_n(\mathbf{r}) + \psi_n^*(\mathbf{r}) \hat{H} \frac{\partial \psi_n(\mathbf{r})}{\partial \lambda} \right] d^3r. \end{aligned} \quad (**)$$

Next, let us spell out the general equality whose proof was the task of Problem 5, for the particular case when  $f(\mathbf{r}) = \psi_n^*(\mathbf{r})$ , while  $g(\mathbf{r}) = \partial \psi_n(\mathbf{r})/\partial \lambda$ :

$$\int \psi_n^*(\mathbf{r})\hat{H} \frac{\partial \psi_n(\mathbf{r})}{\partial \lambda} d^3r = \int \hat{H}\psi_n^*(\mathbf{r}) \frac{\partial \psi_n(\mathbf{r})}{\partial \lambda} d^3r.$$

<sup>10</sup> Despite this common name, H. Hellmann (in 1937) and R. Feynman (in 1939) were not the first ones in the long list of physicists who had (apparently, independently) discovered this equality. Indeed, it has been traced back to a 1922 paper by W. Pauli and was carefully proved by P. Güttinger in 1931.

<sup>11</sup> Note that per Eq. (1.64) of the lecture notes, Eq. (\*) means that the Hamiltonian is nothing else than the operator corresponding to a very special observable, the system's energy – the fact which was already mentioned at its introduction in Sec. 1.2.

By applying this equality to the last term of Eq. (\*\*), using Eq. (1.60) again in the first term, and then its complex conjugate,  $\hat{H}\psi_n^* = E_n\psi_n^*$ ,<sup>12</sup> in the last term, we get

$$\frac{\partial E_n}{\partial \lambda} = \int \psi_n^*(\mathbf{r}) \frac{\partial \hat{H}}{\partial \lambda} \psi_n(\mathbf{r}) d^3r + E_n \int \left[ \frac{\partial \psi_n^*(\mathbf{r})}{\partial \lambda} \psi_n(\mathbf{r}) + \psi_n^*(\mathbf{r}) \frac{\partial \psi_n(\mathbf{r})}{\partial \lambda} \right] d^3r. \quad (***)$$

Now let us stop here for a minute, and differentiate over  $\lambda$  both sides of the wavefunctions' orthonormality condition (1.66), written for the particular case  $n' = n$ :

$$\frac{\partial}{\partial \lambda} \int \psi_n^*(\mathbf{r}) \psi_n(\mathbf{r}) d^3r \equiv \int \left[ \frac{\partial \psi_n^*(\mathbf{r})}{\partial \lambda} \psi_n(\mathbf{r}) + \psi_n^*(\mathbf{r}) \frac{\partial \psi_n(\mathbf{r})}{\partial \lambda} \right] d^3r.$$

However, per the normalization condition (1.22c), the left-hand side of this relation is  $\partial 1 / \partial \lambda = 0$ , so its right-hand side has to vanish as well. This means that Eq. (\*\*\*) reduces to

$$\frac{\partial E_n}{\partial \lambda} = \int \psi_n^*(\mathbf{r}) \frac{\partial \hat{H}}{\partial \lambda} \psi_n(\mathbf{r}) d^3r \equiv \left\langle \frac{\partial H}{\partial \lambda} \right\rangle_n,$$

thus proving the Hellmann-Feynman theorem.

**Problem 1.8.\*** Use Eqs. (1.73) and (1.74) of the lecture notes to analyze the effect of phase locking of Josephson oscillations on the dc current flowing through a weak link between two superconductors (frequently called the *Josephson junction*), assuming that an external source applies to the junction a sinusoidal ac voltage with frequency  $\omega$  and amplitude  $A$ .

*Solution:* Let us assume that the phase locking has happened, so our dc bias point is already on the  $n^{\text{th}}$  current step (1.76); then for the total voltage across the junction we may write

$$V(t) = n \frac{\hbar \omega}{2e} + A \cos \omega t,$$

and Eq. (1.73) yields the following differential equation for the Josephson phase evolution,

$$\frac{d\varphi}{d\tau} = n + a \cos \tau, \quad \text{with } \tau \equiv \omega t \quad \text{and } a \equiv \frac{2e}{\hbar \omega} A.$$

This equation may be easily integrated:

$$\varphi = a \sin \tau + n\tau + \varphi_0,$$

where  $\varphi_0$  is some (so far, arbitrary) integration constant. As a result, the Josephson supercurrent (1.74) is equal to

$$I = I_c \sin(a \sin \tau + n\tau + \varphi_0) \equiv I_c [\sin(a \sin \tau + n\tau) \cos \varphi_0 + \cos(a \sin \tau + n\tau) \sin \varphi_0].$$

Calculating its time average (i.e., the dc component of the current),

<sup>12</sup> See the footnote to the model solution of Problem 1.5.

$$\bar{I} = I_c \left[ \overline{\sin(a \sin \tau + n \tau)} \cos \varphi_0 + \overline{\cos(a \sin \tau + n \tau)} \sin \varphi_0 \right], \quad (*)$$

for example as

$$\bar{f} = \frac{1}{2\pi} \int_{-\pi}^{+\pi} f(\tau) d\tau,$$

we see that the first term in the square brackets vanishes due to the asymmetry of the function under the integral, while for the calculation of the second term, we may use the well-known integral representation of the Bessel functions of the first kind of an integer order  $m$ :<sup>13</sup>

$$J_m(a) = \overline{\exp\{i(a \sin \tau - m \tau)\}} \equiv \overline{\cos(a \sin \tau - m \tau)} + i \overline{\sin(a \sin \tau - m \tau)}.$$

As we have just discussed, the second of these averages equals zero and we get

$$J_m(a) = \overline{\cos(a \sin \tau - m \tau)},$$

where  $m$  is an arbitrary integer number. By taking  $m = -n$ , we see from Eq. (\*) that the dc current on the  $n^{\text{th}}$  step is

$$\bar{I} = I_n \sin \varphi_0, \quad \text{where } I_n \equiv I_c J_{-n}(a) \equiv I_c J_{-n}\left(\frac{2eA}{\hbar\omega}\right), \quad \text{so that } |I_n| \equiv I_c \left| J_n\left(\frac{2eA}{\hbar\omega}\right) \right|. \quad (**)$$

Let us assume that the external circuit fixes the dc current through the junction; then the phase shift  $\varphi_0$  may self-adjust to fit the external current only if it is in the range<sup>14</sup>

$$-|I_n| \leq \bar{I} \leq +|I_n|.$$

Hence the full size of the  $n^{\text{th}}$  current step is twice the  $|I_n|$  given by the last of Eqs. (\*\*); a look at the plot of the Bessel functions<sup>15</sup> shows that the size oscillates as a function of the ac voltage amplitude  $A$ , gradually diminishing at  $eA \gg n\hbar\omega$ . Exactly this behavior (predicted by B. Josephson in his Nobel-prize-winning 1962 paper<sup>16</sup>) was very soon observed experimentally by S. Shapiro;<sup>17</sup> as a result, one can frequently meet the term *Shapiro* (or “Josephson-Shapiro”) *steps*.

**Problem 1.9.** Calculate  $\langle x \rangle$ ,  $\langle p_x \rangle$ ,  $\delta x$ , and  $\delta p_x$  for the eigenstate  $\{n_x, n_y, n_z\}$  of a particle placed inside a rectangular hard-wall box described by Eq. (1.77) of the lecture notes and compare the product  $\delta x \delta p_x$  with the Heisenberg’s uncertainty relation.

**Solution:** Since the spatial factors  $X$ ,  $Y$ , and  $Z$  of wavefunctions, given by Eq. (1.84) of the lecture notes and by similar relations for  $Y$  and  $Z$ , are already normalized and real, we may use Eq. (1.23) to write

<sup>13</sup> See, e.g., the first of MA Eqs. (6.15a).

<sup>14</sup> Even without a quantitative analysis of the stability of such phase locking (for its example, see, e.g., CM Sec. 5.4), it is physically clear that one of the two different values of the phase difference  $\varphi_0$ , at which Eq. (\*) is satisfied ( $\varphi_0 = \sin^{-1}(\bar{I}/I_n)$  and  $\varphi_0' = \pi - \varphi_0$ ), has to be stable.

<sup>15</sup> See, e.g., EM Fig. 2.16.

<sup>16</sup> B. Josephson, *Phys. Lett.* **1**, 251 (1962).

<sup>17</sup> S. Shapiro, *Phys. Rev. Lett.* **11**, 80 (1963).

$$\langle x \rangle = \int_0^{a_x} X^*(x) x X(x) dx = \int_0^{a_x} X^2(x) x dx = \frac{2}{a_x} \int_0^{a_x} \left( \sin \frac{\pi n_x x}{a_x} \right)^2 x dx \equiv \frac{1}{a_x} \int_0^{a_x} \left( 1 - \cos \frac{2\pi n_x x}{a_x} \right) x dx.$$

Integrating the second term in the parentheses of the last expression by parts, we get

$$\begin{aligned} \langle x \rangle &= \frac{1}{a_x} \left[ \frac{a_x^2}{2} - \frac{a_x}{2\pi n_x} \int_{x=0}^{x=a_x} x d \left( \sin \frac{2\pi n_x x}{a_x} \right) \right] = \frac{a_x}{2} + \frac{1}{2\pi n_x} \int_0^{a_x} \sin \frac{2\pi n_x x}{a_x} dx \\ &= \frac{a_x}{2} + \frac{a_x}{(2\pi n_x)^2} \cos \frac{2\pi n_x x}{a_x} \Big|_{x=0}^{x=a_x} = \frac{a_x}{2}. \end{aligned}$$

This simple result is hardly surprising because the wavefunctions  $X(x)$  are either symmetric or antisymmetric with respect to the central point  $a_x/2$  – see Fig. 1.8 of the lecture notes. Acting absolutely similarly but repeating the integration by parts twice, we get

$$\langle x^2 \rangle = \frac{2}{a_x} \int_0^{a_x} \left( \sin \frac{\pi n_x x}{a_x} \right)^2 x^2 dx = a_x^2 \left( \frac{1}{3} - \frac{1}{2\pi^2 n_x^2} \right),$$

so, according to Eqs. (1.33)-(1.34),

$$\delta x = \left( \langle x^2 \rangle - \langle x \rangle^2 \right)^{1/2} = a_x \left( \frac{1}{12} - \frac{1}{2\pi^2 n_x^2} \right)^{1/2}.$$

Notice that neither  $\langle x \rangle$  nor  $\delta x$  depends on other quantum numbers ( $n_y$  and  $n_z$ ) and that the uncertainty of the coordinate is the smallest for  $n_x = 1$  (in particular, for the ground state), with  $\delta x_{\min} \approx 0.181 a_x$ , and increases with  $n_x$ , approaching the limit  $\delta x_{\max} = a_x/\sqrt{12} \approx 0.289 a_x$  at  $n_x \rightarrow \infty$ .

For the particle's momentum, the corresponding calculations are even simpler:

$$\begin{aligned} \langle p_x \rangle &= \int_0^{a_x} X^*(x) \hat{p}_x X(x) dx = \frac{2}{a_x} \int_0^{a_x} \sin \frac{\pi n_x x}{a_x} \left( -i\hbar \frac{\partial}{\partial x} \right) \sin \frac{\pi n_x x}{a_x} dx = -i\hbar \frac{2\pi n_x}{a_x^2} \int_0^{a_x} \sin \frac{\pi n_x x}{a_x} \cos \frac{\pi n_x x}{a_x} dx \\ &= -i\hbar \frac{\pi n_x}{a_x^2} \int_0^{a_x} \sin \frac{2\pi n_x x}{a_x} dx = -i\hbar \frac{1}{2a_x} \cos \frac{2\pi n_x x}{a_x} \Big|_{x=0}^{x=a_x} = 0. \end{aligned}$$

This result could be also predicted in advance, because, as was discussed in Sec. 1.7 of the lecture notes, the standing wave  $X(x)$  may be represented as a sum of two traveling waves with equal amplitudes and equal but opposite momenta  $p_x = \pm \hbar k_x = \pm \hbar \pi n_x / a_x$ , so the average momentum vanishes. This reasoning implies that  $\langle p_x^2 \rangle$  may be calculated from Eq. (1.37), with two possible states having equal probabilities:  $W_+ = W_- = 1/2$ :

$$\langle p_x^2 \rangle = p_+^2 W_+ + p_-^2 W_- = \frac{1}{2} (p_+^2 + p_-^2) = \left( \frac{\hbar \pi n_x}{a_x} \right)^2.$$

As a sanity check, this result may be confirmed directly from Eqs. (1.33)-(1.34):

$$\begin{aligned}\langle p_x^2 \rangle &= \int_0^{a_x} X^*(x) \hat{p}_x^2 X(x) dx = \frac{2}{a_x} \int_0^{a_x} \sin \frac{\pi n_x x}{a_x} \left( -\hbar^2 \frac{\partial^2}{\partial x^2} \right) \sin \frac{\pi n_x x}{a_x} dx = \frac{2}{a_x} \hbar^2 \left( \frac{\pi n_x}{a_x} \right)^2 \int_0^{a_x} \left( \sin \frac{\pi n_x x}{a_x} \right)^2 dx \\ &= \frac{1}{a_x} \hbar^2 \left( \frac{\pi n_x}{a_x} \right)^2 \int_0^{a_x} \left( 1 - \cos \frac{2\pi n_x x}{a_x} \right) dx = \left( \frac{\hbar \pi n_x}{a_x} \right)^2 + \hbar^2 \frac{\pi n_x}{2a_x^2} \sin \frac{2\pi n_x x}{a_x} \Big|_{x=0}^{x=a_x} = \left( \frac{\hbar \pi n_x}{a_x} \right)^2.\end{aligned}$$

Now we can calculate the momentum's uncertainty,

$$\delta p_x = \left( \langle p_x^2 \rangle - \langle p_x \rangle^2 \right)^{1/2} = \frac{\hbar \pi n_x}{a_x},$$

and the uncertainty product:

$$\delta x \delta p_x = \hbar \left( \frac{\pi^2 n_x^2}{12} - \frac{1}{2} \right)^{1/2}.$$

This expression shows that for the lowest quantum number,  $n_x = 1$ , the uncertainty product,  $(\delta x \delta p_x)_{\min} \approx 0.568 \hbar$ , is just slightly (by about 12%) larger than Heisenberg's minimum  $0.5 \hbar$ . On the other hand, at  $n_x \rightarrow \infty$  the product grows as  $(\pi/\sqrt{12})n_x \hbar \approx 0.907 n_x \hbar$ .

**Problem 1.10.** Looking at the lowest (red) line in Fig. 1.8 of the lecture notes, it seems plausible that the lowest-energy eigenfunction (84) of the 1D boundary problem (83) may be well approximated with an inverted parabola:  $X(x) \approx Cx(a_x - x)$ , where  $C$  is a normalization constant. Explore how good this approximation is.

*Solution:* A convenient “global” measure of the approximation quality is the proximity of the expectation value (1.23) of the system's Hamiltonian, given by the guessed approximation<sup>18</sup> ( ):

$$\langle H \rangle_{\text{trial}} = \int \psi_{\text{trial}}^*(\mathbf{r}) \hat{H} \psi_{\text{trial}}(\mathbf{r}) d^3 r, \quad (*)$$

where  $\psi_{\text{trial}}(\mathbf{r})$  is properly normalized,

$$\int \psi_{\text{trial}}^*(\mathbf{r}) \psi_{\text{trial}}(\mathbf{r}) d^3 r = 1,$$

to the genuine ground-state energy  $E_g$ , which, according to Eq. (1.60), satisfies a similar relation but with the genuine ground-state wavefunction  $\psi_g(\mathbf{r})$ :

$$\langle H \rangle_g = \int \psi_g^*(\mathbf{r}) \hat{H} \psi_g(\mathbf{r}) d^3 r = \int \psi_g^*(\mathbf{r}) E_g \psi_g(\mathbf{r}) d^3 r = E_g \int \psi_g^*(\mathbf{r}) \psi_g(\mathbf{r}) d^3 r = E_g.$$

In our 1D case with  $X_{\text{trial}}(x) = Cx(a_x - x)$ , the normalization condition is

$$\int_0^a X_{\text{trial}}^*(x) X_{\text{trial}}(x) dx \equiv |C|^2 \int_0^a x^2 (a - x)^2 dx = 1,$$

where, for the notation simplicity,  $a \equiv a_x$ . Working out this simple integral, we get

<sup>18</sup> In the variational method, to be discussed in Sec. 2.9 of the lecture notes, it is called the *trial function*.

$$|C|^{-2} = \int_0^a x^2 (a-x)^2 dx \equiv \int_0^a (a^2 x^2 - 2ax^3 + x^4) dx = a^2 \frac{a^3}{3} - 2a \frac{a^4}{4} + \frac{a^5}{5} \equiv \frac{a^5}{30}.$$

Now using the fact that inside our simple quantum-well,  $U(x) = 0$ , so  $\hat{H} = (-\hbar^2/2m)d^2/dx^2$  in the whole region where  $X_{\text{trial}} \neq 0$ , we get

$$\begin{aligned} \langle H \rangle_{\text{trial}} &= \int_0^a X_{\text{trial}}^*(x) \hat{H} X_{\text{trial}}(x) dx = -\frac{\hbar^2}{2m} \int_0^a X_{\text{trial}}^* \frac{d^2 X_{\text{trial}}}{dx^2} dx = -\frac{\hbar^2}{2m} |C|^2 \int_0^a x(a-x)(-2) dx \\ &= \frac{30}{a^5} \frac{\hbar^2}{m} \int_0^a (ax - x^2) dx = \frac{30}{a^5} \frac{\hbar^2}{m} \left( a \frac{a^2}{2} - \frac{a^3}{3} \right) \equiv 5 \frac{\hbar^2}{ma^2}. \end{aligned}$$

Comparing this result with the exact ground state energy given by Eq. (1.85) with  $n_x = 1$  and  $a_x = a$ ,

$$E_g = \frac{\pi^2}{2} \frac{\hbar^2}{ma^2} \approx 4.935 \frac{\hbar^2}{ma^2},$$

we see that the approximation given by this simple trial function is indeed pretty good, giving a  $\sim 1\%$  accuracy – even in the absence of adjustable parameters that are used in the genuine variational method.

**Problem 1.11.** A particle placed into a hard-wall rectangular box with sides  $\{a_x, a_y, a_z\}$  is in its ground state. Calculate the average force it exerts on each face of the box. Can these forces be characterized by a certain pressure?

*Solution:* Directing the coordinates axes along the corresponding sides of the box, we may describe the situation by the boundary problem described by Eq. (1.78b) of the lecture notes, so the ground state energy  $E_g$  of the particle is expressed by Eq. (1.86) with the lowest possible values of the quantum numbers,  $n_x = n_y = n_z = 1$ :

$$E_g \equiv E_{1,1,1} = \frac{\pi^2 \hbar^2}{2m} \left( \frac{1}{a_x^2} + \frac{1}{a_y^2} + \frac{1}{a_z^2} \right).$$

Since this energy (while being *kinetic* by its origin) is a function of the box dimensions only, it may be considered a contribution to the effective *potential* energy of the box-particle system. Hence the force acting on any of the two faces normal to the  $x$ -axis may be calculated as

$$F_x = -\frac{\partial E_g}{\partial a_x} = \frac{\pi^2 \hbar^2}{ma_x^3}.$$

Since the area of this face is  $A_x = a_y a_z$ , the force-to-area ratio is

$$\mathcal{P}_x \equiv \frac{F_x}{A_x} = \frac{\pi^2 \hbar^2}{a_x^3 a_y a_z}.$$

Since the calculations for two other face pairs may be done absolutely similarly, and give similar results (with the proper index replacements), this expression shows that generally

$$\mathcal{P}_x \neq \mathcal{P}_y \neq \mathcal{P}_z,$$

and hence the exerted forces *cannot* be characterized by a unique pressure  $\mathcal{P}$ , which by definition<sup>19</sup> should be isotropic. Only in the particular case when the box is cubic, with sides  $a_x = a_y = a_z \equiv a$  and volume  $V = a^3$ , we may speak of a certain pressure:

$$\mathcal{P}_x = \mathcal{P}_y = \mathcal{P}_z \equiv \mathcal{P} = \frac{\pi^2 \hbar^2}{ma^5} = \frac{\pi^2 \hbar^2}{mV^{5/3}}.$$

Note that the resulting “equation of state”,  $\mathcal{P}V^{5/3} = \text{const}$ , differs from that of the ideal classical gas ( $\mathcal{P}V = \text{const}$ ). As will be discussed in Chapter 8, this “quantum equation of state” remains the same even if the cubic box is filled with an arbitrary number  $N$  of non-interacting particles – either bosons or fermions – though the dependence of the pressure on  $N$  is different for these two cases.<sup>20</sup>

**Problem 1.12.** A 1D quantum particle was initially in the ground state of a very deep, flat-bottom potential well of width  $a$ :

$$U(x) = \begin{cases} 0, & \text{for } -a/2 < x < +a/2, \\ +\infty, & \text{otherwise.} \end{cases}$$

At some instant, the well’s width is abruptly increased to a new value  $a' > a$ , leaving the potential symmetric with respect to the point  $x = 0$ , and then is kept constant. Calculate the probability that after the change, the particle is still in the ground state of the system.

*Solution:* According to Eqs. (1.69) and (1.84) of the lecture notes with the appropriate shift of the origin, the normalized initial wavefunction of the system (before the well width’s change) is

$$\Psi(x,0) = \left(\frac{2}{a}\right)^{1/2} \times \begin{cases} \cos \frac{\pi x}{a}, & \text{for } |x| < \frac{a}{2}, \\ 0, & \text{otherwise,} \end{cases} \quad (*)$$

with the ground-state energy  $E_g$  given by Eq. (1.85) with  $a_x = a$  and  $n_x = 1$ :

$$E_g = \frac{\pi^2}{2ma^2}.$$

This initial state serves as the initial condition for the final state of the system,

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) \exp\left\{-i \frac{E_n}{\hbar} t\right\},$$

where  $\psi_n(x)$  are the normalized eigenfunctions of the expanded well. In particular, according to the same Eq. (1.84) with the proper replacement  $a \rightarrow a'$ , the new ground-state wavefunction is

<sup>19</sup> See, e.g., CM Secs. 7.2 and 8.1.

<sup>20</sup> As statistical mechanics shows (see, e.g., SM Chapter 3), at sufficiently high temperatures, the pressure becomes isotropic and classical (with  $\mathcal{P}V = \text{const}$ ) – regardless of the shape of the box, the number of the particles, and their quantum properties.

$$\psi_1(x) = \left(\frac{2}{a'}\right)^{1/2} \times \begin{cases} \cos \frac{\pi x}{a'}, & \text{for } |x| < \frac{a'}{2}, \\ 0, & \text{otherwise,} \end{cases}$$

The constant coefficient  $c_1$ , which in particular determines the probability  $W_1 = |c_1|^2$  of the particle to remain in the ground state, may be found by using the 1D version of Eq. (1.68):

$$c_1 = \int_{-\infty}^{+\infty} \psi_1^*(x) \Psi(x,0) dx,$$

giving

$$\begin{aligned} c_1 &= \frac{2}{(aa')^{1/2}} \int_{-a/2}^{+a/2} \cos \frac{\pi x}{a} \cos \frac{\pi x}{a'} dx = \frac{2}{(aa')^{1/2}} \int_0^{+a/2} \left[ \cos \pi x \left( \frac{1}{a} + \frac{1}{a'} \right) + \cos \pi x \left( \frac{1}{a} - \frac{1}{a'} \right) \right] dx \\ &= \frac{2}{\pi(aa')^{1/2}} \left[ \left( \frac{1}{a} + \frac{1}{a'} \right)^{-1} \sin \frac{\pi a}{2} \left( \frac{1}{a} + \frac{1}{a'} \right) + \left( \frac{1}{a} - \frac{1}{a'} \right)^{-1} \sin \frac{\pi a}{2} \left( \frac{1}{a} - \frac{1}{a'} \right) \right] \equiv \frac{4}{\pi} \frac{a^{1/2} a'^{3/2}}{(a'^2 - a^2)} \cos \frac{\pi a}{2a'}, \end{aligned}$$

so<sup>21</sup>

$$W_1 = |c_1|^2 = \frac{16}{\pi^2} \frac{aa'^3}{(a'^2 - a^2)^2} \cos^2 \frac{\pi a}{2a'}.$$

As a sanity check: if the well is virtually unchanged,  $a' = a + \varepsilon \rightarrow a$ , then  $\cos(\pi a/2a') \rightarrow \pi \varepsilon/2a$ ,  $(a'^2 - a^2) \rightarrow 2a\varepsilon$ , so  $c_1 \rightarrow 1$ , and  $W_1 \rightarrow 1$ , as it should be. On the other hand, if the final well is much wider than the initial one,  $a \ll a'$ , then  $\cos(\pi a/2a') \approx 1$ , and  $W_1 \approx (16/\pi^2) a/a' \ll 1$ . This is also reasonable, because the relatively sharp initial probability distribution gives contributions to many final eigenfunctions, with a small probability for the particle to be in any particular of them.

(Additional question for the reader: Could a similar problem be rationally formulated for  $a' < a$ , i.e. for a sudden well's *shrinkage* rather than its *extension*?)

**Problem 1.13.** At  $t = 0$ , a 1D particle of mass  $m$  is placed into a hard-wall, flat-bottom potential well

$$U(x) = \begin{cases} 0, & \text{for } 0 < x < a, \\ +\infty, & \text{otherwise,} \end{cases}$$

in a 50/50 linear superposition of the lowest-energy (ground) state and the first excited state. Calculate:

- (i) the normalized wavefunction  $\Psi(x, t)$  for an arbitrary time  $t \geq 0$ , and
- (ii) the time evolution of the expectation value  $\langle x \rangle$  of the particle's coordinate.

*Solutions:*

- (i) The described linear superposition is described by the wavefunction

$$\Psi(x,0) = c_1 \psi_1(x) + c_2 \psi_2(x),$$

<sup>21</sup> Note that this result would not be affected by adding an arbitrary phase to the wavefunction (\*), because this would just shift the phase of the complex coefficient  $c_1$ .



where  $\psi_1$  and  $\psi_2$  are the two lowest-energy eigenfunctions of this problem, which were by-products of the 3D calculation in Sec. 1.7 of the lecture notes – see Eqs. (1.84)-(1.85):

$$\psi_n(x) = \left(\frac{2}{a}\right)^{1/2} \sin \frac{\pi n x}{a}, \quad E_n = \frac{\pi^2 \hbar^2 n^2}{2m}, \quad \text{with } n = 1, 2, \dots,$$

and  $|c_1|^2 = |c_2|^2$ . Due to the last condition, we may take  $c_2 = c_1 \exp\{i(\varphi_2 - \varphi_1)\} \equiv C \exp\{i\varphi\}$ , i.e.

$$\Psi(x, 0) = C [\psi_1(x) + e^{i\varphi} \psi_2(x)].$$

The coefficient  $C$  (or rather its modulus) may be readily calculated from the normalization requirement:

$$W \equiv \int_0^a \Psi^*(x, 0) \Psi(x, 0) dx \equiv |C|^2 \int_0^a [\psi_1(x) + e^{i\varphi} \psi_2(x)]^* [\psi_1(x) + e^{i\varphi} \psi_2(x)] dx = 1. \quad (*)$$

Since the wavefunctions  $\psi_{1,2}$  are orthonormal,

$$\int_0^a \psi_{1,2}^*(x) \psi_{1,2}(x) dx = 1, \quad \int_0^a \psi_{1,2}^*(x) \psi_{2,1}(x) dx = 0,$$

Eq. (\*) yields  $|C|^2 = 2$ , i.e.  $|C| = 1/\sqrt{2}$ . So, the initial wavefunction may be represented as

$$\Psi(x, 0) = \frac{e^{i \arg C}}{a^{1/2}} \left( \sin \frac{\pi x}{a} + \sin \frac{2\pi x}{a} e^{i\varphi} \right).$$

Per Eq. (1.69) of the lecture notes, the further time evolution of this function may be described merely by the multiplication of each of these terms by  $\exp\{-i\omega_n t/\hbar\}$ , where  $\omega_n = E_n/\hbar$ , so

$$\Psi(x, t) = \frac{e^{i \arg C}}{a^{1/2}} \left[ \sin \frac{\pi x}{a} \exp\{-i\omega_1 t\} + \sin \frac{2\pi x}{a} \exp\{-i\omega_2 t + i\varphi\} \right], \quad \text{with } \omega_1 = \frac{E_1}{\hbar}, \quad \omega_2 = \frac{E_2}{\hbar} = 4 \frac{E_1}{\hbar}.$$

(ii) Now we may use this wavefunction and the basic Eq. (1.23) to calculate the expectation value of the particle's coordinate:

$$\begin{aligned} \langle x \rangle &= \int_0^a \Psi^*(x, t) \hat{x} \Psi(x, t) dx \\ &= \frac{1}{a} \int_0^a \left( \sin \frac{\pi x}{a} \exp\{i\omega_1 t\} + \sin \frac{2\pi x}{a} \exp\{i\omega_2 t - i\varphi\} \right) x \left( \sin \frac{\pi x}{a} \exp\{-i\omega_1 t\} + \sin \frac{2\pi x}{a} \exp\{-i\omega_2 t + i\varphi\} \right) dx \\ &\equiv \frac{1}{a} \int_0^a \left[ \sin^2 \frac{\pi x}{a} + \sin^2 \frac{2\pi x}{a} + 2 \sin \frac{\pi x}{a} \sin \frac{2\pi x}{a} \cos(\omega t - \varphi) \right] x dx, \quad \text{with } \omega \equiv \omega_2 - \omega_1. \end{aligned}$$

Transforming the product of the two sine functions into the difference of two cosine functions of combinational arguments,<sup>22</sup> and working out the resulting four integrals by parts,<sup>23</sup> we finally get

<sup>22</sup> See, e.g., MA Eq. (3.2c).

<sup>23</sup> See, e.g., MA Eq. (5.1).

$$\langle x \rangle = \frac{1}{2}a - \frac{16}{9\pi^2}a \cos(\omega t - \varphi). \quad (**)$$

Evidently, this formula describes sinusoidal oscillations of the particle, with the amplitude  $(16/9\pi^2)a \approx 0.18a$ , around the middle of the well ( $x_0 = a/2$ ).

At least three comments are due here. First, this problem is a good reminder that the quantum-mechanical averaging  $\langle \dots \rangle$  is by no means equivalent to the averaging over time, and its result may still be a function of time – as Eq. (\*\*) is. Second, recall that  $\langle x \rangle$  does not oscillate if the system is in just one of the involved two stationary states, so the oscillations (\*\*) are the result of the states' interference. The frequency  $\omega$  of the oscillations is proportional to the difference between the energies of the involved stationary states; in our case

$$\hbar\omega \equiv \hbar(\omega_2 - \omega_1) = E_2 - E_1 = \frac{4\pi^2}{2ma^2} - \frac{\pi^2}{2ma^2} = \frac{3\pi^2}{2ma^2},$$

i.e. to the frequency of the potential radiation at quantum transitions between the corresponding energy levels – see Eq. (1.7) of the lecture notes. Finally, note that while the argument of the complex coefficient  $C$ , i.e. the common phase of the wavefunction, drops out of all expectation values, the mutual phase shift  $\varphi$  between its components in the linear superposition can affect the expectation values – in our particular case, of the coordinate.

**Problem 1.14.** Calculate the potential profiles  $U(x)$  for which the following wavefunctions,

(i)  $\Psi = c \exp\{-ax^2 - ibt\}$ , and

(ii)  $\Psi = c \exp\{-a|x| - ibt\}$

(with real coefficients  $a > 0$  and  $b$ ), satisfy the 1D Schrödinger equation for a particle with mass  $m$ . For each case, calculate  $\langle x \rangle$ ,  $\langle p_x \rangle$ ,  $\delta x$ , and  $\delta p_x$ , and compare the product  $\delta x \delta p_x$  with Heisenberg's uncertainty relation.

*Solutions:* Each of these wavefunctions may be represented as the product  $\psi_n(x)\exp\{-iE_n t/\hbar\}$ , with  $E_n = \hbar b$ , so per the discussion in Secs. 1.5-1.6 of the lecture notes, we may calculate the corresponding functions  $U(x)$  from the stationary Schrödinger equation (1.65), which may be rewritten as

$$U(x) = E_n + \frac{1}{\psi_n} \frac{\hbar^2}{2m} \frac{d^2\psi_n}{dx^2}.$$

(i) In this case,  $\psi_n = c \exp\{-ax^2\}$ , so a direct differentiation yields

$$U(x) = E_n + \frac{\hbar^2}{2m} (4a^2 x^2 - 2a).$$

Now notice that if we introduce, instead of  $a$ , the following constant:

$$\omega_0 \equiv \frac{2\hbar a}{m}, \quad (*)$$

the above expression may be rewritten as

$$U(x) = \frac{m\omega_0^2 x^2}{2} + \left( E_n - \frac{\hbar\omega_0}{2} \right),$$

while the corresponding wavefunction becomes

$$\psi_n = c \exp\{-ax^2\} \equiv c \exp\left\{-\frac{m\omega_0 x^2}{2\hbar}\right\}.$$

Since, according to the stationary Schrödinger equation, the origins of  $E_n$  and  $U$  may be shifted (simultaneously) by an arbitrary constant, in our case, we may select this constant so that

$$E_n = \frac{\hbar\omega_0}{2},$$

and  $U(x)$  becomes the well-known expression for the potential energy of a *harmonic oscillator* of frequency  $\omega_0$  and mass  $m$ :

$$U(x) = \frac{m\omega_0^2 x^2}{2}.$$

Hence, “by chance” (actually, not quite so :-), we have found one of the eigenfunctions  $\psi_n$  of this very important 1D system. Later in the course, we will see that this is actually its most important, lowest-energy (*ground*) state, usually marked with the quantum number  $n = 0$ .

Now, after finding the constant  $c$  (or rather its modulus) from the normalization condition<sup>24</sup>

$$1 = \int_{-\infty}^{+\infty} \psi_n^* \psi_n dx \equiv |c|^2 \int_{-\infty}^{+\infty} \exp\{-2ax^2\} dx \equiv \left(\frac{\pi}{2a}\right)^{1/2} |c|^2,$$

we can use Eq. (1.23) of the lecture notes to calculate the following expectation values:<sup>25</sup>

$$\langle x \rangle = 0, \quad \langle p_x \rangle = 0, \quad \langle x^2 \rangle = \frac{1}{4a}, \quad \langle p_x^2 \rangle = \hbar^2 a,$$

so

$$\delta x = \frac{1}{2a^{1/2}}, \quad \delta p_x = \hbar a^{1/2}.$$

Hence, the product  $\delta x \delta p_x$  equals  $\hbar/2$  i.e. has the smallest value allowed by the uncertainty relation (1.35).<sup>26</sup> In the notation (\*), very common for the harmonic oscillator’s description, the above results for the coordinate and momentum variances read

$$\langle x^2 \rangle = \frac{\hbar}{2m\omega_0}, \quad \langle p_x^2 \rangle = \frac{\hbar m\omega_0}{2}.$$

Notice that the averages of the kinetic and potential energies of the oscillator are equal to each other:

$$\left\langle \frac{p_x^2}{2m} \right\rangle = \left\langle \frac{m\omega_0^2 x^2}{2} \right\rangle = \frac{\hbar\omega_0}{4},$$

<sup>24</sup> The last step uses the well-known Gaussian integral MA Eq. (6.9b).

<sup>25</sup> The calculation of the two last averages requires one more Gaussian integral, given by MA Eq. (6.9c).

<sup>26</sup> This relation also holds for more general Gaussian wave packets, to be discussed in Sec. 2.2.

just as they are at the classical oscillations of this system.

(ii) In this case,  $\psi_n = c \exp\{-a|x|\}$ , so a similar calculation of  $U(x)$  gives

$$U(x) = \hbar b + e^{a|x|} \frac{\hbar^2}{2m} \frac{d^2}{dx^2} e^{-a|x|}.$$

At  $x \neq 0$ , this expression gives a constant (equal to  $\hbar b + \hbar^2 a^2/2m$ ), but the point  $x = 0$  requires a special calculation, because here the wavefunction has a “cusp”, and is not analytically differentiable. However, using the notions of the sign function  $\text{sgn}(x)$  and Dirac’s delta function  $\delta(x)$ ,<sup>27</sup> we can still write formulas valid for all  $x$ :

$$\frac{d}{dx} e^{-a|x|} = -a \text{sgn}(x) e^{-a|x|}, \quad \frac{d^2}{dx^2} e^{-a|x|} = a[a - 2\delta(x)] e^{-a|x|}, \quad (**)$$

so, finally, we get the potential  $U(x)$  describing (besides the inconsequential constant  $U_0$ ) an ultimately narrow 1D potential well:

$$U(x) = \hbar b + \frac{\hbar^2}{2m} [a^2 - 2a\delta(x)] \equiv U_0 - \mathcal{W}\delta(x),$$

where

$$U_0 \equiv \hbar b + \frac{\hbar^2 a^2}{2m} \quad \text{and} \quad \mathcal{W} \equiv \frac{\hbar^2 a}{m} > 0.$$

In this notation, the eigenfunction and the eigenenergy of the system become

$$\psi = c \exp\{-a|x|\} \equiv c \exp\left\{-\frac{m\mathcal{W}}{\hbar^2}|x|\right\}, \quad E = \hbar b = U_0 - \frac{\hbar^2 a^2}{2m} \equiv U_0 - \frac{m\mathcal{W}^2}{2\hbar^2}.$$

In Chapter 2 of the lecture notes, we will see that these results describe the *only* localized eigenstate of such a well; they will be broadly used in this course as the basis for discussion of more complex problems.

Now after the wavefunction’s normalization, giving  $cc^* = a$ , Eq. (1.23) of the lecture notes, after a straightforward integration, yields<sup>28</sup>

$$\langle x \rangle = 0, \quad \langle x^2 \rangle = \frac{1}{2a^2}.$$

Calculating the expectation values of  $p_x$  and  $p_x^2$ , we should be careful not to lose the functions  $\text{sgn}(x)$  and  $\delta(x)$  – see Eq. (\*\*):

$$\hat{p}_x \psi = -i\hbar \frac{d}{dx} \left( c e^{-a|x|} \right) = ica \text{sgn}(x) e^{-a|x|}, \quad \hat{p}_x^2 \psi = -\hbar^2 \frac{d^2}{dx^2} \left( c e^{-a|x|} \right) = -\hbar^2 ca [a - 2\delta(x)] e^{-a|x|}.$$

Now the integration (1.23) is easy and yields

$$\langle p_x \rangle = 0, \quad \langle p_x^2 \rangle = \hbar^2 a^2, \quad \text{so} \quad \Delta x \Delta p_x = \frac{\hbar}{\sqrt{2}}.$$

<sup>27</sup> If you need a reminder, see, e.g., MA Sec. 14.

<sup>28</sup> For the second integration, we may use the table integral given by MA Eq. (6.7d) for  $n = 2$ .

We see that for this non-Gaussian eigenfunction, the uncertainty product is substantially (by  $\sim 40\%$ ) larger than its minimum possible value  $\hbar/2$ .

**Problem 1.15.** The wavefunction of an excited stationary state of a 1D particle moving in a potential profile  $U(x)$  is related to that of its ground state as  $\psi_e(x) \propto x\psi_g(x)$ . Calculate the function  $U(x)$ .

*Solution:* Both wavefunctions  $\psi_e(x)$  and  $\psi_g(x)$  have to satisfy the 1D version of the stationary Schrödinger equation (1.65), with the corresponding energy values  $E_e$  and  $E_g$ :

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_e}{dx^2} + U(x)\psi_e = E_e\psi_e, \quad -\frac{\hbar^2}{2m} \frac{d^2\psi_g}{dx^2} + U(x)\psi_g = E_g\psi_g. \quad (*)$$

With the given relation  $\psi_e(x) \propto x\psi_g(x)$ , the first of these equations becomes

$$-\frac{\hbar^2}{2m} \frac{d^2(x\psi_g)}{dx^2} + U(x)(x\psi_g) = E_e(x\psi_g), \quad \text{i.e.} \quad -\frac{\hbar^2}{2m} \left( 2\frac{d\psi_g}{dx} + x\frac{d^2\psi_g}{dx^2} \right) + U(x)x\psi_g = E_e x\psi_g.$$

The last form of this equation is close to the second of Eqs. (\*), with all terms multiplied by  $x$ :

$$-\frac{\hbar^2}{2m} x \frac{d^2\psi_g}{dx^2} + U(x)x\psi_g = E_g x\psi_g.$$

Subtracting them, we get a first-order differential equation

$$-\frac{\hbar^2}{m} \frac{d\psi_g}{dx} = (E_e - E_g)x\psi_g, \quad \text{i.e.} \quad \frac{d\psi_g}{\psi_g} = -\frac{m(E_e - E_g)}{\hbar^2} x dx,$$

which may be easily integrated, giving

$$\ln \psi_g = -\frac{m(E_e - E_g)}{2\hbar^2} x^2 + C, \quad \text{so} \quad \psi_g = C \exp\left\{-\frac{m(E_e - E_g)x^2}{2\hbar^2}\right\},$$

where  $C$  is the integration constant, playing the role of the normalization factor for this ground-state wavefunction.<sup>29</sup> Now we may either plug this result back into the second of Eqs. (\*) or just use the solution of the previous problem's Task (i) with  $a = m(E_e - E_g)/2\hbar^2$ ; the result is

$$U(x) = 2E_g - E_e + \frac{m(E_e - E_g)^2 x^2}{2\hbar^4}.$$

As was already noted in the model solution of the previous problem, this expression coincides with the potential energy of a 1D harmonic oscillator of frequency  $\omega_0$ :

$$U(x) = \frac{m\omega_0^2 x^2}{2}.$$

Hence our result is valid for such an oscillator if we take

<sup>29</sup> Since by the definition of state excitation,  $E_e > E_g$ , the calculated  $\psi_g(x)$  converges fast at  $x \rightarrow \pm\infty$ , and its normalization is uneventful.

$$2E_g - E_e = 0 \quad \text{and} \quad \frac{(E_e - E_g)^2}{\hbar^4} = \omega_0^2.$$

Solving this simple system of two equations with the condition  $E_e - E_g > 0$ , we get

$$E_g = \frac{\hbar\omega_0}{2}, \quad E_e = E_g + \hbar\omega_0.$$

As will be discussed in Sec. 2.9 of the lecture notes, these are indeed the energies of the ground state and the *first* excited state of the oscillator. (From the above solution, we could not determine its number.)

**Problem 1.16.** A 1D particle of mass  $m$ , moving in a potential well  $U(x)$ , has the following stationary eigenfunction:  $\psi(x) = C/\cosh \kappa x$ , where  $C$  is the normalization constant and  $\kappa$  is a given real constant. Calculate the function  $U(x)$  and the state's eigenenergy  $E$ .

*Solution:* After calculating the second derivative of the eigenfunction:

$$\frac{d\psi}{dx} = -\frac{C\kappa \sinh \kappa x}{\cosh^2 \kappa x}, \quad \frac{d^2\psi}{dx^2} = \frac{d}{dx} \left( -\frac{C\kappa \sinh \kappa x}{\cosh^2 \kappa x} \right) = \frac{C\kappa^2}{\cosh \kappa x} \left( \frac{2 \sinh^2 \kappa x}{\cosh^2 \kappa x} - 1 \right),$$

we may plug the result into the 1D version of the stationary Schrödinger equation (1.65):

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + U(x)\psi = E\psi,$$

getting

$$U(x) - E = \frac{\hbar^2 \kappa^2}{2m} \left( \frac{2 \sinh^2 \kappa x}{\cosh^2 \kappa x} - 1 \right). \quad (*)$$

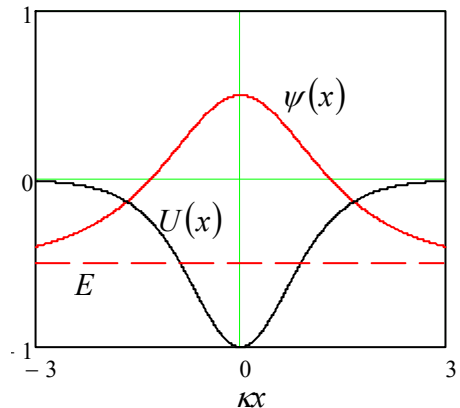
The function  $U(x)$  and the eigenenergy  $E$  are defined to an arbitrary constant (essentially the energy reference level), provided that their difference is definite – as specified by Eq. (\*). It is convenient to select this constant so that  $U(x) \rightarrow 0$  at  $x \rightarrow \pm\infty$ . Since in these limits, the expression in the parentheses of Eq. (\*) tends to 1, we have to associate the resulting constant level with  $(-E)$ , so

$$E = -\frac{\hbar^2 \kappa^2}{2m}.$$

Now plugging this value back into Eq. (\*), we get a result that may be recast into a very simple form:

$$\begin{aligned} U(x) &= \frac{\hbar^2 \kappa^2}{2m} \left( \frac{2 \sinh^2 \kappa x}{\cosh^2 \kappa x} - 1 \right) + E = \frac{\hbar^2 \kappa^2}{2m} \left( \frac{2 \sinh^2 \kappa x}{\cosh^2 \kappa x} - 1 \right) - \frac{\hbar^2 \kappa^2}{2m} \\ &\equiv -\frac{\hbar^2 \kappa^2}{2m} \frac{2(\cosh^2 \kappa x - \sinh^2 \kappa x)}{\cosh^2 \kappa x} \equiv -\frac{\hbar^2 \kappa^2}{m} \frac{1}{\cosh^2 \kappa x}. \end{aligned}$$

A plot of this function is shown with the black line in the figure on the right, together with the calculated eigenenergy (dashed horizontal line), both in the units of  $\hbar^2 \kappa^2/m$ , and the



eigenfunction  $\psi(x)$  (red line, in arbitrary units). Due to the simple eigenfunction describing the localized state of the particle (which may be proved to be its ground state), this potential is one of the convenient models for the description of “soft” confinement in one dimension.

**Problem 1.17.** Calculate the density  $dN/dE$  of the traveling-wave quantum states inside large hard-wall rectangular boxes of various dimensions:  $d = 1, 2$ , and  $3$ .

*Solution:* First, let us use the discussion of the 3D box in Sec. 1.7 of the lecture notes to calculate the number  $N_3$  of the states with the kinetic energy  $\hbar^2 k^2/2m$  below a certain value  $E$ . For that, we may integrate Eq. (1.90) over the  $\mathbf{k}$ -space region satisfying the requirement

$$k^2 < \frac{2mE}{\hbar^2},$$

i.e. over a sphere with the so-called *Fermi radius*  $k_F \equiv (2mE)^{1/2}/\hbar$ :

$$N_3 = \frac{V}{(2\pi)^3} \int_{k < k_F} d^3k = \frac{V}{(2\pi)^3} \frac{4\pi}{3} k_F^3 \equiv \frac{V}{(2\pi)^3} \frac{4\pi}{3} \frac{(2m)^{3/2}}{\hbar^3} E^{3/2}.$$

From here, the density of 3D states is

$$\frac{dN_3}{dE} = \frac{V}{(2\pi)^3} \frac{4\pi}{3} \frac{(2m)^{3/2}}{\hbar^3} \frac{3}{2} E^{1/2} \equiv V \frac{(2m)^{3/2}}{4\pi^2 \hbar^3} E^{1/2}.$$

Note that the density *grows* with energy.

An absolutely similar calculation for a rectangular 2D box, based on Eq. (1.92), yields

$$N_2 = \frac{A}{(2\pi)^2} \int_{k < k_F} d^2k = \frac{A}{(2\pi)^2} \pi k_F^2 \equiv \frac{A}{(2\pi)^2} \pi \frac{2m}{\hbar^2} E,$$

so the 2D density of states *does not depend* on energy:

$$\frac{dN_2}{dE} = \frac{A}{(2\pi)^2} \pi \frac{2m}{\hbar^2} \equiv A \frac{m}{2\pi\hbar^2}.$$

Finally, for 1D particles, Eq. (1.93) yields

$$N_1 = \frac{l}{2\pi} \int_{|k| < k_F} dk = \frac{l}{2\pi} 2k_F \equiv \frac{l}{2\pi} 2 \frac{(2m)^{1/2}}{\hbar} E^{1/2},$$

so the 1D density of states,

$$\frac{dN_1}{dE} = \frac{l}{2\pi} 2 \frac{(2m)^{1/2}}{\hbar} \frac{1}{2} E^{-1/2} \equiv l \frac{(2m)^{1/2}}{2\pi\hbar} E^{-1/2},$$

*decreases* with energy.

**Problem 1.18.\*** A 1D particle is confined in a potential well of width  $a$ , with a flat bottom and hard, infinitely high walls. Use the finite-difference method with steps  $a/2$  and  $a/3$  to find as many eigenenergies as possible. Compare the results with each other, and with the exact formula.<sup>30</sup>

*Solution:* The eigenproblem is described by the ordinary differential equation (1.83), which includes the second derivative of the wavefunction  $X(x)$ . In the finite-difference method, we are approximating the derivative with the following finite difference:<sup>31</sup>

$$\frac{d^2 X}{dx^2} \approx \frac{X(x-h) + X(x+h) - 2X(x)}{h^2},$$

where  $h$  (not to be confused with either  $\hbar$  or  $\hbar/2\pi!$ ) is the selected step along the  $x$ -axis.

For  $h = a/2$ , the only reasonable choice is to select the point  $x$  in the middle of the potential well (in the notation of Fig. 1.8 of the lecture notes, at  $x = a/2$ ), so the points  $(x-h)$  and  $(x+h)$  are on the well's walls, where  $X = 0$ . Thus Eq. (1.83) turns into a very simple relation

$$\frac{0 + 0 - 2X}{h^2} + k^2 X = 0,$$

where  $X \equiv X(a/2)$  and  $k \equiv k_x$ . This homogeneous equation cannot be used to calculate  $X$ , but assuming that  $X \neq 0$  (i.e. that the wavefunction is nonvanishing), it gives simple results for the eigenvalue of the standing wave's number  $k$  and hence for the eigenenergy  $E \equiv E_x \equiv (\hbar^2/2m)k^2$ :

$$k = \frac{\sqrt{2}}{h} \equiv \frac{2\sqrt{2}}{a} \approx \frac{2.83}{a}, \quad E = 2 \frac{\hbar^2}{2mh^2} \equiv 4 \frac{\hbar^2}{ma^2}.$$

These values should be compared with the exact analytical results (1.84)-(1.85) for the lowest (ground) eigenstate ( $n_x = 1$ ):

$$k_1 = \frac{\pi}{a} \approx \frac{3.14}{a}, \quad E_1 = \pi^2 \frac{\hbar^2}{2ma^2} \approx 4.93 \frac{\hbar^2}{ma^2}.$$

So, this large step (in the numerical-math lingo, "coarse mesh") makes the calculations very simple but allows the calculation of only one, ground eigenstate, and with a relatively large error:  $\sim 10\%$  for  $k$  and  $\sim 20\%$  for the eigenenergy. This could be expected because such mesh corresponds to the approximation of the genuine sinusoidal solutions (1.84) with a single quadratic parabola.

So it is only natural to explore a slightly finer mesh with  $h = a/3$ , making a similar approximation for two interleaved segments of the same length  $2h = 2a/3$ :  $x \in [0, 2a/3]$  and  $x \in [a/3, a]$ . Applying the finite-difference version of Eq. (1.83),

$$\frac{X(x-h) + X(x+h) - 2X(x)}{h^2} + k^2 X = 0,$$

to the central points  $x_- \equiv h = a/3$  and  $x_+ \equiv 2h = 2a/3$  of these two segments, we get two equations for the corresponding wavefunction's values  $X_-$  and  $X_+$ :

<sup>30</sup> You may like to start by reading about the finite difference method – see, e.g., CM Sec. 8.5 or EM Sec. 2.11.

<sup>31</sup> See, e.g., CM Eq. (8.65) or EM Eq. (2.220).



$$\frac{0 + X_+ - 2X_-}{h^2} + k^2 X_- = 0, \quad \frac{X_- + 0 - 2X_+}{h^2} + k^2 X_+ = 0.$$

This system of two homogeneous linear equations is consistent if its determinant equals zero:

$$\begin{vmatrix} \frac{1}{h^2} & -\frac{2}{h^2} + k^2 \\ -\frac{2}{h^2} + k^2 & \frac{1}{h^2} \end{vmatrix} = 0, \quad \text{i.e.} \quad \left(k^2 - \frac{2}{h^2}\right)^2 = \left(\frac{1}{h^2}\right)^2.$$

The resulting quadratic equation for  $k^2$  has two solutions:

$$k^2 = \frac{2}{h^2} \pm \frac{1}{h^2} \equiv (18 \pm 9) \frac{1}{a^2},$$

giving the following two eigenvalue sets:

$$k_- = (18 - 9)^{1/2} \frac{1}{a} \equiv \frac{3}{a}, \quad E_- = 4.5 \frac{\hbar^2}{ma^2};$$

$$k_+ = (18 + 9)^{1/2} \frac{1}{a} \approx \frac{5.20}{a}, \quad E_+ = 13.5 \frac{\hbar^2}{ma^2}.$$

The first of them is just a better approximation for the ground state, with a  $\sim 5\%$  accuracy for  $k$  and a  $\sim 10\%$  accuracy for energy. The second result is a much cruder description of the next (first excited) state, whose exact parameters are given by the same Eqs. (1.84)-(1.85) with  $n_x = 2$ :

$$k_2 = \frac{2\pi}{a} \approx \frac{6.27}{a}, \quad E_1 = 4\pi^2 \frac{\hbar^2}{2ma^2} \approx 19.7 \frac{\hbar^2}{ma^2}.$$

Obviously, even finer meshes with smaller  $h$  would allow a more precise description of more eigenstates, for the price of solving a larger system of homogeneous linear equations.<sup>32</sup> For this particular problem, which has a simple analytical solution, this numerical method makes sense only as a demonstration, but for eigenstates of particles moving in more complex potential profiles  $U(x)$ , this is one of the few possible approaches. (A different, frequently more efficient numerical approach to the eigenproblems of quantum mechanics will be described in Sec. 6.1 of the lecture notes – see Eq. (6.7) and its discussion.)

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<sup>32</sup> All popular public-domain and commercial software packages, including those listed in MA Sec. 16(iv), have efficient standard routines for such solutions.

## Chapter 2. 1D Wave Mechanics

**Problem 2.1.** As was stated in Sec. 2.1 of the lecture notes, Eq. (2.1) may be incorrect if the particle's potential energy depends on just one spatial coordinate:  $U = U(x, t)$ , and is much more reliable for particles strongly but uniformly confined in the transverse directions  $y, z$ . Explain why.

*Solution:* Naively, one may think that if the particle's potential energy depends on just one spatial coordinate, say  $U = U(x, t)$ , then its wavefunction has to be one-dimensional as well:  $\psi = \psi(x, t)$ . However, already the discussion of the particular case  $U(\mathbf{r}) = \text{const}$  (which is just a special case of a 1D potential) in Sec. 1.7 has shown that this assumption is wrong.<sup>33</sup> Indeed, its eigenfunctions, given by Eq. (1.88), do depend on the other two coordinates. So the solutions  $\Psi(x, t)$  of the 1D Schrödinger equation (2.1) that follows from Eq. (1.65) by assuming  $\partial\Psi/\partial y = \partial\Psi/\partial z = 0$ , are insufficient to form the general solution of that equation even in this simplest case.

Let us consider the slightly more general case of a 1D potential:  $U = U(x)$ , i.e. a potential profile that is flat in two directions,  $y$  and  $z$ . Repeating the arguments of Sec. 1.7 for this case, we see that the eigenfunctions of a particle in such a well have the form

$$\psi(\mathbf{r}) = X(x) \exp\{i(k_y y + k_z z)\}, \quad (*)$$

where  $X(x)$  is an eigenfunction of the following stationary 1D Schrödinger equation:

$$-\frac{\hbar^2}{2m} \frac{d^2 X}{dx^2} + U_{\text{ef}}(x)X = EX, \quad (**)$$

where  $U_{\text{ef}}(x)$  is *not* the full potential energy of the particle, as it would follow from Eq. (92), but rather its effective value including the kinetic energy of the lateral motion:

$$U_{\text{ef}} \equiv U + (E_y + E_z) = U + \frac{\hbar^2}{2m} (k_y^2 + k_z^2).$$

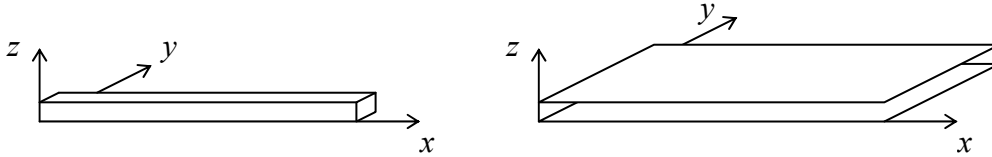
In plain English, the particle's partial wavefunction  $X(x)$  and its full energy depend on its transverse momenta, which have a continuous spectrum – see the discussion of Eq. (1.89). This means that Eq. (2.1) is adequate only if the condition  $k_y = k_z = 0$  is somehow enforced, and in the case  $U = U(x)$ , it is not. For example, if a de Broglie (or any other) plane wave  $\Psi(x, t)$  is incident on a potential step (see, e.g., Fig. 2.4) it is reflected exactly back, i.e. with  $k_y = k_z = 0$ , only if the wall's surface is perfectly plane and exactly normal to the axis  $x$ . Any imperfection (and there are so many of them in real physical systems) causes the induction of waves with non-zero values of  $k_y$  and  $k_z$ , due to the continuous character of the functions  $E_y(k_y)$  and  $E_z(k_z)$ .<sup>34</sup>

<sup>33</sup> Unfortunately, most textbooks on quantum mechanics jump to the formal solution of 1D problems without such a discussion.

<sup>34</sup> This problem is not specific to quantum mechanics. The reflection of plane acoustic and electromagnetic waves from plane mirrors is also unstable with respect to small imperfections. Even the classical motion of a particle in a 1D potential may be unstable with respect to lateral perturbations. This is why so many 1D problems of classical mechanics use formulations like “a bead slides along a wire”, etc., assuming rigid lateral confinement.

There is essentially one, perhaps a counter-intuitive way to make the 1D solutions “robust” to small perturbations: provide the particle’s *rigid lateral confinement*<sup>35</sup> in other directions. As the simplest example, consider a narrow *quantum wire* (see the left panel of the figure below) described by the following potential:

$$U(\mathbf{r}) = \begin{cases} U(x), & \text{for } 0 < y < a_y, \text{ and } 0 < z < a_z, \\ +\infty, & \text{otherwise.} \end{cases} \quad (***)$$



Performing the standard variable separation (1.79), we see that the corresponding stationary Schrödinger equation is satisfied if the partial wavefunction  $X(x)$  obeys Eqs. (\*)-(\*\*), but now with a discrete energy spectrum in the transverse directions:

$$U_{\text{ef}} = U + \frac{\pi^2 \hbar^2}{2m} \left( \frac{n_y^2}{a_y^2} + \frac{n_z^2}{a_z^2} \right).$$

If the lateral confinement is tight:  $a_y, a_z \rightarrow 0$ , then there is a large energy gap,

$$\Delta U \sim \frac{\pi^2 \hbar^2}{2ma_{y,z}^2},$$

between the ground-state energy of the lateral motion (with  $n_y = n_z = 1$ ) and that of its excited states. As a result, if the particle is initially placed into the ground lateral state, i.e. its energy  $E$  is much smaller than  $\Delta U$ , it would stay in such a state, i.e. may be described by a 1D Schrödinger equation similar to Eq. (2.1) – even in the time-dependent case, proved that the frequency scale of the potential’s change is much smaller than  $\Delta U/\hbar$ . Absolutely similarly, a strong lateral confinement in just one dimension (say,  $z$  – see the right panel of the figure above) enables systems with a robust 2D evolution of the particle’s wavefunction.

The tight lateral confinement may ensure the dimensionality reduction even if the potential well is not rectangular in the lateral direction(s), as described by Eq. (\*\*\*), but is described by some  $x$ - and  $t$ -independent profile providing a sufficiently large energy gap  $\Delta U$ . For example, many 2D quantum phenomena, such as the quantum Hall effect,<sup>36</sup> have been studied experimentally using electrons confined at semiconductor heterojunctions (e.g., epitaxial interfaces GaAs/Al<sub>x</sub>Ga<sub>1-x</sub>As), where the potential well in the direction perpendicular to the interface has a nearly triangular shape and provides an energy gap  $\Delta U$  of the order of  $10^{-2}$  eV.<sup>37</sup> Such a gap corresponds to  $k_B T$  with  $T \sim 100$  K, so careful experimentation at liquid helium temperatures (4K and below) may keep the electrons performing a purely 2D motion within the lowest “subband” ( $n_z = 1$ ).

<sup>35</sup> The term “quantum confinement”, sometimes used to describe this phenomenon, is as unfortunate as the “quantum well” term discussed in Sec. 1.7 of the lecture notes, because of the same reason: the confinement is a purely classical effect, and as we will repeatedly see in this course, the quantum-mechanical effects *reduce* rather than enable it.

<sup>36</sup> To be discussed in Sec. 3.2.

<sup>37</sup> See, e.g., P. Harrison, *Quantum Wells, Wires, and Dots*, 3<sup>rd</sup> ed., Wiley, 2010.

**Problem 2.2.** Prove that the final form of Eq. (2.23) of the lecture notes is correct even though  $x'$  has an ( $x$ -independent) imaginary part.

*Hint:* This is a good exercise in using the Cauchy theorem.<sup>38</sup>

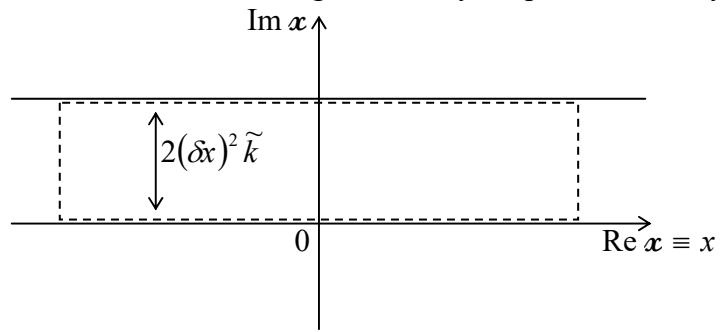
*Solution:* On the complex plane  $\alpha$ , the integral in the first form of Eq. (2.23) is along the horizontal line with

$$\text{Im } \alpha = 2(\delta x)^2 \tilde{k}, \quad (*)$$

while the standard form<sup>39</sup> of the Gaussian integral, used in the second form of that formula, is for real  $x$ , i.e. for the integration along a different horizontal line, with

$$\text{Im } \alpha = 0 \quad (**)$$

see the figure on the right. However, since the function under the integral is analytic, per the Cauchy theorem, its integral over any closed contour on the  $\alpha$ -plane, in particular the rectangular contour of the type shown with the dashed line in the figure on the right, has to equal zero. Let us tend the horizontal size of this contour to infinity. Since the function under the integral tends to zero at  $\text{Re } \alpha \equiv x \rightarrow \pm\infty$ , the contributions to the contour integral from the integration along the two vertical sides vanish.



Hence the integrals over the two horizontal sides of the contour (taken in the same direction of  $x$ ), i.e. the integrals along the lines (\*) and (\*\*), have to be equal.

By the way, this is a good reminder of the fact that due to the complex character of the wavefunction, many integrals met in wave mechanics are actually over the complex planes.

**Problem 2.3.** The initial wave packet of a free 1D particle is described by Eq. (2.20) of the lecture notes:

$$\Psi(x,0) = \int a_k e^{ikx} dk.$$

(i) Obtain a compact expression for the expectation value  $\langle p \rangle$  of the particle's momentum at an arbitrary moment  $t > 0$ .

(ii) Calculate  $\langle p \rangle$  for the case when the function  $|a_k|^2$  is symmetric with respect to some value  $k_0$ .

*Solutions:*

(i) Per the basic relation (1.23) and the explicit expression (1.26b) for the momentum operator, we may write

$$\langle p \rangle(t) = \int_{-\infty}^{+\infty} \Psi^*(x,t) \left( -i\hbar \frac{\partial}{\partial x} \right) \Psi(x,t) dx. \quad (*)$$

<sup>38</sup> See, e.g., MA Eq. (15.1).

<sup>39</sup> See, e.g., MA Eq. (6.9b).

According to Eq. (2.27), we may represent the wavefunction of a free particle, with the initial state given in the assignment, as

$$\Psi(x,t) = \int a_k \exp\{i[kx - \omega(k)t]\} dk, \quad \text{where } \hbar\omega(k) = E(k) = \frac{\hbar^2 k^2}{2m}, \quad (**)$$

and the integral is in infinite limits. Plugging this expression and its complex conjugate (with the replacement  $k \rightarrow k'$ ) into Eq. (\*), we may transform it as follows:

$$\begin{aligned} \langle p \rangle(t) &= \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dk' \int_{-\infty}^{+\infty} dk a_{k'}^* \exp\{-i[k'x - \omega(k')t]\} \left( -i\hbar \frac{\partial}{\partial x} \right) a_k \exp\{i[kx - \omega(k)t]\} \\ &= \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dk' \int_{-\infty}^{+\infty} dk a_{k'}^* \exp\{-i[k'x - \omega(k')t]\} (\hbar k) a_k \exp\{i[kx - \omega(k)t]\} \\ &\equiv \int_{-\infty}^{+\infty} dk' \int_{-\infty}^{+\infty} dk a_{k'}^* a_k (\hbar k) \exp\{i[\omega(k') - \omega(k)]t\} \int_{-\infty}^{+\infty} dx \exp\{i(k - k')x\}. \end{aligned}$$

The last integral is just the delta function (times  $2\pi$ ),<sup>40</sup> so we may continue as

$$\begin{aligned} \langle p \rangle(t) &= \int dk' \int dk (\hbar k) a_{k'}^* a_k \exp\{i[\omega(k') - \omega(k)]t\} 2\pi \delta(k - k') \\ &= 2\pi \int (\hbar k) a_k^* a_k dk \equiv 2\pi \int (\hbar k) |a_k|^2 dk. \end{aligned} \quad (***)$$

So, the average momentum of a free particle is time-independent (just as it is in classical mechanics) and, besides a numerical normalization factor, is expressed via the momentum envelope function  $a_k$  just as the average of a function  $f(x)$  is expressed via the wavefunction itself:

$$\langle f(x) \rangle(t) = \int_{-\infty}^{+\infty} f(x) |\Psi(x,t)|^2 dx.$$

As will be discussed in Sec. 4.7 of the lecture notes, the reason for this similarity is that the amplitude  $a_k$  (or rather a function  $\varphi(p) \equiv \varphi(\hbar k)$  proportional to  $a_k$ ) plays the role of the wavefunction in the so-called *momentum representation* – an alternative to the *coordinate representation* used in the wave-mechanics approach we are studying now.

(ii) If  $|a_k|^2$  is an even function of the difference  $(k - k_0)$ , we may recast the last form of Eq. (\*\*\*) as follows:

$$\langle p \rangle = 2\pi \int (\hbar k) |a_k|^2 dk \equiv 2\pi \int (\hbar k_0 + \hbar k - \hbar k_0) |a_k|^2 dk = 2\pi \hbar k_0 \int |a_k|^2 dk + 2\pi \hbar \int (k - k_0) |a_k|^2 dk.$$

Since the last integral has infinite limits, we may always represent the integration segment as a limit of  $[k_0 - \kappa, k_0 + \kappa]$  at  $\kappa \rightarrow \infty$ , i.e. the integral as

$$\lim_{\kappa \rightarrow \infty} \int_{-\kappa}^{+\kappa} (k - k_0) |a_k|^2 d(k - k_0) \equiv \lim_{\kappa \rightarrow \infty} \int_{-\kappa}^{+\kappa} \tilde{k} |a_k|^2 d\tilde{k}, \quad \text{where } \tilde{k} \equiv k - k_0.$$

<sup>40</sup> See, e.g., MA Eq. (14.4).

Since  $|a_k|^2$  is an even function of  $\tilde{k}$ , the whole function under the integral is odd, and the integral vanishes. So our result is reduced to

$$\langle p \rangle = \hbar k_0 2\pi \int |a_k|^2 dk. \quad (****)$$

In order to evaluate this integral, let us require the wavefunction to be normalized:

$$\int_{-\infty}^{+\infty} \Psi^*(x,t)\Psi(x,t)dx = 1.$$

Plugging in the expansions (\*\*), and transforming the integral exactly as this was done in Task (i), we get

$$2\pi \int |a_k|^2 dk = 1.$$

So, Eq. (\*\*\*\*) is reduced to the very simple and natural form  $\langle p \rangle = \hbar k_0$ , which corresponds to the physics discussed in Secs. 1.1 and 1.7 of the lecture notes – see, e.g., Eqs. (1.14) and the text before Eq. (1.88).

**Problem 2.4.** Calculate the function  $a_k$  defined by Eq. (2.20) of the lecture notes, for the wave packet with a rectangular spatial envelope:

$$\Psi(x,0) = \begin{cases} C \exp\{ik_0 x\}, & \text{for } -a/2 \leq x \leq +a/2, \\ 0, & \text{otherwise.} \end{cases}$$

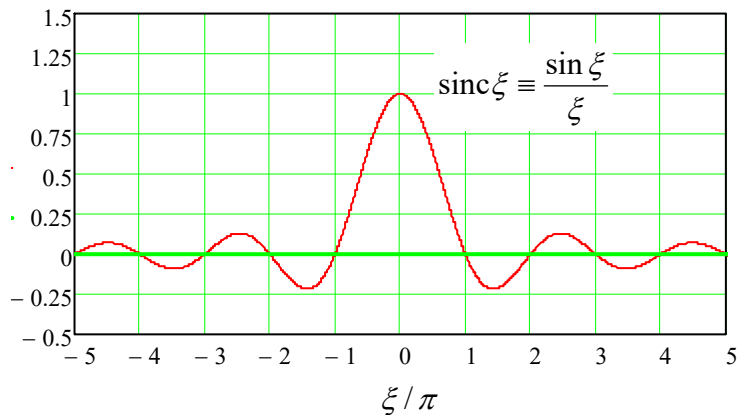
Analyze the result in the limit  $k_0 a \rightarrow \infty$ .

*Solution:* Using the Fourier transform reciprocal to Eq. (2.20), we get

$$\begin{aligned} a_k &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \Psi(x,0) e^{-ikx} dx = \frac{C}{2\pi} \int_{-a/2}^{+a/2} e^{ik_0 x} e^{-ikx} dx \equiv \frac{C}{2\pi} \int_{-a/2}^{+a/2} e^{i(k_0 - k)x} dx \\ &= \frac{C}{2\pi} \frac{1}{i(k_0 - k)} \left[ e^{i(k_0 - k)a/2} - e^{-i(k_0 - k)a/2} \right] \equiv \frac{C}{\pi} \frac{\sin[(k - k_0)a/2]}{k - k_0} \equiv \frac{Ca}{2\pi} \operatorname{sinc} \frac{(k - k_0)a}{2}, \end{aligned}$$

where  $\operatorname{sinc} \xi \equiv \sin(\xi)/\xi$  is the well-known function (see the figure on the right), which describes, in particular, the Fraunhofer diffraction on a narrow slit.<sup>41</sup>

The result shows that, in contrast to the delta-functional amplitude  $a_k$  of a sinusoidal (“monochromatic”) wavefunction, in our current case,  $a_k$  is a smooth function of  $k$ . (Physically this means that the monochromatic wavefunction restricted in space is not truly monochromatic but is a coherent superposition of an infinite number



<sup>41</sup> See, e.g., EM Sec. 8.4.

of de Broglie waves with different  $k$ .) It has a peak at  $k = k_0$ , with a finite height of  $Ca/2\pi$  and a width  $\Delta k \sim 1/a$ . At  $k_0 a \rightarrow \infty$ , this width becomes much smaller than  $k_0$ , while the peak's height grows, so  $a_k$  tends to the delta function of  $k$ , which we had for the space-unrestricted sinusoidal wavefunction.

**Problem 2.5.** Prove Eq. (2.49) of the lecture notes for the 1D propagator of a free quantum particle, by starting from Eq. (2.48).

*Solution:* Following the Gaussian integration routine discussed in Sec. 2.2 of the lecture notes, let us complement the contents of the square brackets in Eq. (2.48) to a full square of  $(k + \text{const})$ :

$$k\tilde{x} - \frac{\hbar k^2}{2m} \tilde{t} = -\frac{\hbar \tilde{t}}{2m} \left( k - \frac{m\tilde{x}}{\hbar \tilde{t}} \right)^2 + \frac{m\tilde{x}^2}{2\hbar \tilde{t}} \equiv -\frac{\hbar \tilde{t}}{2m} \tilde{k}^2 + \frac{m\tilde{x}^2}{2\hbar \tilde{t}},$$

where the following natural notation is used:

$$\tilde{x} \equiv x - x_0, \quad \tilde{t} \equiv t - t_0, \quad \text{and} \quad \tilde{k} \equiv k - \frac{m\tilde{x}}{\hbar \tilde{t}}. \quad (*)$$

With this replacement, Eq. (2.48) may be rewritten as

$$\begin{aligned} G &= \frac{1}{2\pi} \exp\left\{i \frac{m\tilde{x}^2}{2\hbar \tilde{t}}\right\} \int \exp\left\{-i \frac{\hbar \tilde{t}}{2m} \tilde{k}^2\right\} d\tilde{k} = \frac{1}{2\pi} \exp\left\{i \frac{m\tilde{x}^2}{2\hbar \tilde{t}}\right\} \left(\frac{2m}{\hbar \tilde{t}}\right)^{1/2} \int_{-\infty}^{+\infty} \exp\{-i\xi^2\} d\xi \\ &\equiv \frac{1}{2\pi} \exp\left\{i \frac{m\tilde{x}^2}{2\hbar \tilde{t}}\right\} \left(\frac{2m}{\hbar \tilde{t}}\right)^{1/2} \left[ \int_{-\infty}^{+\infty} \cos(\xi^2) d\xi - i \int_{-\infty}^{+\infty} \sin(\xi^2) d\xi \right]. \end{aligned}$$

Each of the *full Fresnel integrals*<sup>42</sup> in the last square brackets is equal to  $(\pi/2)^{1/2}$ ; hence we may write

$$\int_{-\infty}^{+\infty} \cos(\xi^2) d\xi - i \int_{-\infty}^{+\infty} \sin(\xi^2) d\xi = (\pi/2)^{1/2} (1 - i) \equiv \left(\frac{\pi}{i}\right)^{1/2},$$

so, finally:

$$G = \frac{1}{2\pi} \exp\left\{i \frac{m\tilde{x}^2}{2\hbar \tilde{t}}\right\} \left(\frac{2m}{\hbar \tilde{t}}\right)^{1/2} \left(\frac{\pi}{i}\right)^{1/2} = \left(\frac{m}{2\pi i \hbar \tilde{t}}\right)^{1/2} \exp\left\{-\frac{m\tilde{x}^2}{2i\hbar \tilde{t}}\right\}.$$

Taking into account the notation (\*), this is exactly Eq. (2.49).

**Problem 2.6.** Express the 1D propagator defined by Eq. (2.44) of the lecture notes via the eigenfunctions and eigenenergies of a particle moving in an arbitrary stationary potential  $U(x)$ .

*Solution:* As its definition shows, the 1D propagator  $G(x, t; x_0, t_0)$  is the solution of the 1D Schrödinger equation (2.1) with the delta-functional initial condition

$$\Psi(x, t_0) = \delta(x - x_0). \quad (*)$$

From Sec. 1.5, we know that if the potential energy  $U$  does not depend on time, the general solution of the equation is given by the 1D version of Eq. (1.69):

<sup>42</sup> See, e.g., MA Eq. (6.10).

$$\Psi(x, t) = \sum_n c_n \psi_n(x) \exp\left\{-i \frac{E_n}{\hbar}(t - t_0)\right\},$$

where  $\psi_n(x)$  are the eigenfunctions of the problem, and the coefficients  $c_n$  are given by the 1D version of Eq. (1.68):

$$c_n = \int \psi_n^*(x) \Psi(x, t_0) dx.$$

(Here, the initial moment of time is denoted as  $t_0$  rather than 0.) Plugging into the last equality the initial condition (\*), and integrating over  $x$ , we get  $c_n = \psi_n^*(x_0)$ , so, finally,

$$G(x, t; x_0, t_0) = \sum_n \psi_n(x) \psi_n^*(x_0) \exp\left\{-i \frac{E_n}{\hbar}(t - t_0)\right\}.$$

This result shows that in the general case, the propagator's dependences on  $x$  and  $x_0$  may be different from each other, and only if  $U(x) = \text{const}$ , it is a function of only the difference  $(x - x_0)$  – see, for example, Eqs. (2.48)-(2.49) – due to the space-translational invariance of the problem.

**Problem 2.7.** Calculate the change of a 1D particle's wavefunction, resulting from a short pulse of an external classical force that may be well approximated by a delta function:  $F(t) = P\delta(t)$ .

*Solution:* According to the well-known relation  $\mathbf{F} = -\nabla U$ , a space-independent classical force  $\mathbf{F}(t)$  may be described by the additional potential energy term  $U_F(\mathbf{r}, t) = -\mathbf{F}(t) \cdot \mathbf{r}$ , in the 1D case reduced to  $U_F(x, t) = -F(t)x$ . As a result, the full Hamiltonian of the particle is

$$\hat{H} = \hat{H}_0 + U_F(x, t) = \hat{H}_0 - F(t)x = \hat{H}_0 - Px\delta(t), \quad \text{where } \hat{H}_0 \equiv -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U(x, t),$$

so the Schrödinger equation (2.1) takes the form

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + U(x, t)\Psi - Px\delta(t)\Psi.$$

If the background potential energy  $U(x, t)$  is finite at  $t = 0$  for all  $x$  and the initial form of the wavefunction is smooth (so its second derivative over the coordinate is also finite for all  $x$ ), then during the short interval of the force pulse (which may be symbolically represented as  $-0 \leq t \leq +0$ ),<sup>43</sup> the first two terms on the right-hand side of the Schrödinger equation are much smaller than the last (diverging) one, and may be neglected:

$$i\hbar \frac{\partial \Psi}{\partial t} = -Px\delta(t)\Psi, \quad \text{i.e. } \frac{\partial \Psi}{\Psi} = i \frac{Px}{\hbar} \delta(t) \partial t, \quad \text{for } -0 \leq t \leq +0.$$

Integrating both sides of this equation over this infinitesimal time interval, we get

$$\ln \frac{\Psi(x, t = +0)}{\Psi(x, t = -0)} = i \frac{Px}{\hbar}, \quad \text{so } \Psi(x, t = +0) = \Psi(x, t = -0) \exp\left\{i \frac{Px}{\hbar}\right\}. \quad (*)$$

<sup>43</sup> If the reader is uneasy with this shorthand notation, they may consider a small time interval  $-\Delta t/2 \leq t \leq +\Delta t/2$ , and then pursue the limit  $\Delta t \rightarrow 0$ .



This is the requested change of the wavefunction. Its physical sense becomes more clear if we represent the initial wavefunction by its Fourier expansion (2.20):

$$\Psi(x, t = -0) = \int a_k e^{ikx} dk;$$

then Eq. (\*) yields

$$\Psi(x, t = +0) = \exp\left\{i \frac{Px}{\hbar}\right\} \int a_k e^{ikx} dk \equiv \int a_k e^{ik'x} dk, \quad \text{where } k' \equiv k + \frac{P}{\hbar}, \quad \text{i.e. } \hbar k' = \hbar k + P.$$

This result has a simple physical sense: the force pulse changes the effective momentum  $p = \hbar k$  of *each* monochromatic component of the particle's wave packet by the same constant, equal to the force's impulse  $P$ . This result is in full accordance with the correspondence principle, because in classical mechanics, the force pulse results in a similar change of the particle's momentum, from  $p$  to  $p' = p + P$ . (In higher dimensions, this relation is generalized as  $\mathbf{p}' = \mathbf{p} + \mathbf{P}$ , both in classical and quantum mechanics.)

Later in the course (in Sec. 5.5), we will see that the force-induced multiplier in Eq. (\*) is just a particular (coordinate) representation of the general momentum shift operator

$$\hat{\mathcal{G}}_P = \exp\left\{i \frac{P\hat{x}}{\hbar}\right\}.$$

(Please do not panic looking at this expression: in Sec. 4.6 we will discuss what is meant by the exponential function of an operator argument.)

**Problem 2.8.** Calculate the transparency  $\mathcal{T}$  of the rectangular potential barrier (2.68):

$$U(x) = \begin{cases} 0, & \text{for } x < -d/2, \\ U_0, & \text{for } -d/2 < x < +d/2, \\ 0, & \text{for } d/2 < x, \end{cases}$$

for a 1D particle with energy  $E > U_0$ . Analyze and interpret the result, taking into account that  $U_0$  may be either positive or negative. (In the latter case, we are speaking about the particle's passage over a rectangular potential well of a finite depth  $|U_0|$ .)

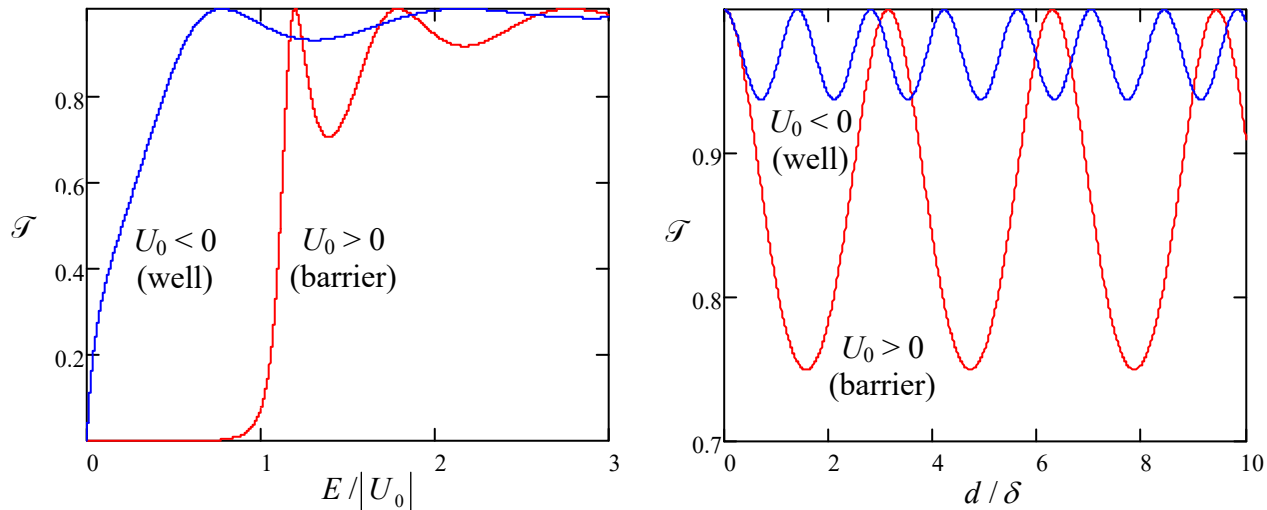
*Solution:* Just as has been done for the potential step, we can use the final result of the tunneling problem analysis in Sec. 2.3 of the lecture notes, in particular, Eqs. (2.71), by replacing  $\kappa$  with  $(-ik')$ , with  $k'$  defined by Eq. (2.65):

$$k'^2 \equiv \frac{2m(E - U_0)}{\hbar^2}.$$

The result, valid for both  $U_0 < 0 < E$  (a well) and  $0 < U_0 < E$  (a barrier), becomes

$$\mathcal{T} = \left| \cos k'd - \frac{i}{2} \left( \frac{k'^2 + k^2}{k'k} \right) \sin k'd \right|^{-2} \equiv \left[ 1 + \frac{U_0^2}{4E(E - U_0)} \sin^2 k'd \right]^{-1}. \quad (*)$$

The figure below shows typical results given by this formula.



The transparency  $\mathcal{T}$  as a function of (a) the particle's energy (for a fixed ratio  $d/\delta = 5$ , where  $\delta$  is defined by Eq. (2.59) of the lecture notes, with  $U_0 \rightarrow |U_0|$ ), and (b) the barrier/well width  $d$  (for  $E = 1.5|U_0|$ ).

A common feature of these plots is transparency oscillations whose period is clear from the term  $\sin^2 k'd$  in the last form of Eq. (\*):  $\Delta(k'd) = \pi$ . The origin of these oscillations is the (partial) reflection of the de Broglie waves at the particle's passage over a sharp potential cliff, which was been discussed in Sec. 2.3 of the lecture notes – in particular, see Eq. (2.71b) and Fig. 2.7a. The reflected wave travels back, is reflected from the opposite cliff, etc., thus forming a standing wave. The constructive interference condition is achieved when the barrier/well width  $d$  corresponds to an integer number of standing half-waves, i.e., at  $k'd = n\pi$ , with  $n = 0, 1, 2, \dots$ <sup>44</sup>

The remarkable fact that for any parameters,  $\mathcal{T} = 1$  at all constructive-interference points, was discussed, for a different particular case, in Sec. 2.5.

**Problem 2.9.** Prove Eq. (2.117) of the lecture notes, for the case  $\mathcal{F}_{\text{WKB}} \ll 1$ , by using the connection formulas (2.105).

**Solution:** Let us apply the mnemonic rule (i) formulated in Sec. 2.4 of the lecture notes just after Eq. (2.106), to a relatively thick potential barrier,<sup>45</sup> with the transparency  $\mathcal{T} \ll 1$ . In this case, the partial wave proportional to the coefficient  $d$  in Eq. (2.116) is negligibly small at both classical turning points,  $x_c$  and  $x_c'$  (see Fig. 2.11), and we may rewrite these formulas as

<sup>44</sup> An additional task for the reader: explain why in our current problem, in contrast to the resonances inside a potential well described by Eq. (1.77),  $n = 0$  is a meaningful value.

<sup>45</sup> Of course, it also has to be smooth, i.e. satisfy the WKB approximation conditions (2.96) and (2.107).

$$\psi_{\text{WKB}} = \begin{cases} \frac{a}{k^{1/2}(x)} \exp\left\{i \int_{x_c}^x k(x') dx'\right\} + \frac{b}{k^{1/2}(x)} \exp\left\{-i \int_{x_c}^x k(x') dx'\right\}, & \text{for } x < x_c, \\ \frac{c}{\kappa^{1/2}(x)} \exp\left\{-\int_{x_c}^x \kappa(x') dx'\right\} \equiv \frac{c}{\kappa^{1/2}(x)} \exp\left\{-\int_{x_c}^{x_c'} \kappa(x') dx'\right\} \exp\left\{-\int_{x_c'}^x \kappa(x') dx'\right\}, & \text{for } x_c < x < x_c', \\ \frac{f}{k^{1/2}(x)} \exp\left\{-\int_{x_c}^{x_c'} \kappa(x') dx'\right\} \exp\left\{i \left[ \int_{x_c'}^x k(x') dx' + \text{const} \right]\right\}, & \text{for } x_c' < x, \end{cases}$$

where for our current purposes, the second term in the top line and the constant phase shift in the last line are unimportant. According to the mnemonic rule applied to the classical turning points  $x_c$  and  $x_c'$ ,

$$|a| = |b| = |c|, \quad |c| \exp\left\{-\int_{x_c'}^x \kappa(x') dx'\right\} = |f|.$$

Now calculating the probability currents (2.95) corresponding to the de Broglie waves propagating to the right, in both classically allowed regions, we get

$$I_{x < x_c} = \frac{\hbar}{m} |a|^2, \quad I_{x > x_c'} = \frac{\hbar}{m} |f|^2 = \frac{\hbar}{m} |a|^2 \exp\left\{-2 \int_{x_c}^{x_c'} \kappa(x') dx'\right\},$$

so the barrier transparency is indeed described by Eq. (2.117):

$$\mathcal{T}_{\text{WKB}} \equiv \frac{I_{x > x_c'}}{I_{x < x_c}} = \exp\left\{-2 \int_{x_c}^{x_c'} \kappa(x') dx'\right\}.$$

**Problem 2.10.** Spell out the stationary wavefunctions of a harmonic oscillator in the WKB approximation, and use them to calculate  $\langle x^2 \rangle$  and  $\langle x^4 \rangle$  for an eigenstate number  $n \gg 1$ .

*Solution:* In the WKB approximation, the stationary wavefunctions  $\psi_n$  are given by Eq. (2.94) of the lecture notes. Taking the lower limit of both WKB integrals at  $x = 0$ , i.e. at the central point of the harmonic oscillator's potential (2.111),

$$U(x) = \frac{m\omega_0^2 x^2}{2},$$

we have to take  $a = b$  for symmetric wavefunctions, i.e. for even  $n$ , and  $a = -b$  for antisymmetric wavefunctions, i.e. for odd  $n$  – see, e.g., Fig. 2.35. For the  $n^{\text{th}}$  stationary state, this gives

$$\psi_n = \frac{C_n}{k_n^{1/2}(x)} \times \begin{cases} \cos \int_0^x k_n(x) dx, & \text{for } n = 0, 2, 4, \dots, \\ \sin \int_0^x k_n(x) dx, & \text{for } n = 1, 3, 5, \dots, \end{cases} \quad (*)$$

with  $k_n(x)$  given by Eq. (2.82):

$$k_n(x) = \frac{1}{\hbar} \{2m[E_n - U(x)]\}^{1/2} = \frac{1}{\hbar} [m(2E_n - m\omega_0^2 x^2)]^{1/2}.$$

According to Eq. (2.262), which coincides with the WKB result (2.114) with the replacement  $n' \rightarrow n$ ,

$$2E_n = \hbar\omega_0(2n+1),$$

so

$$k_n(x) = \frac{1}{\hbar} \{m[\hbar\omega_0(2n+1) - m\omega_0^2 x^2]\}^{1/2} \equiv \frac{m\omega_0}{\hbar} (x_n^2 - x^2)^{1/2} \equiv \frac{(x_n^2 - x^2)^{1/2}}{x_0^2},$$

where  $x_0 \equiv (\hbar/m\omega_0)^{1/2}$  is the length scale of the harmonic oscillator's wavefunctions (see Eq. (2.276) of the lecture notes) and  $\pm x_n$  are the classical turning points defined by the equality  $E_n = U(x_n)$ ; for our potential,

$$x_n = \left[ \frac{\hbar(2n+1)}{m\omega_0} \right]^{1/2} \equiv x_0(2n+1)^{1/2}.$$

The constant  $C_n$  (or rather its modulus) participating in Eq. (\*) should be calculated from the normalization condition

$$\int_{-\infty}^{+\infty} |\psi_n(x)|^2 dx = 1. \quad (**)$$

In the WKB approximation, strictly valid only for  $n \gg 1$ , the effective depth of the particle's penetration into the classically forbidden regions is much smaller than the distance,  $x_R - x_L$ , between these two classical turning points. So, the integration limits in this equation may be limited to the classically allowed interval  $[-x_n, +x_n]$ . Also, the squares of the rapidly oscillating sine and cosine functions in Eq. (\*) may be replaced with their average value,  $1/2$ . As a result, Eq. (\*\*) becomes

$$\frac{|C_n|^2}{2} \int_{-x_n}^{+x_n} \frac{dx}{k_n(x)} = 1, \quad \text{i.e.} \quad \frac{|C_n|^2 x_0^2}{2} \int_{-x_n}^{+x_n} \frac{dx}{(x_n^2 - x^2)^{1/2}} \equiv |C_n|^2 x_0^2 I = 1, \quad \text{with } I \equiv \int_0^1 \frac{d\xi}{(1 - \xi^2)^{1/2}},$$

where  $\xi \equiv x/x_n$ . The last integral may be readily worked out, for example, by the substitution  $\xi \equiv \sin\varphi$ , giving  $d\xi = \cos\varphi d\varphi$  and  $(1 - \xi^2)^{1/2} = \cos\varphi$ , so  $I = \pi/2$ . Thus, the normalization constant turns out to be independent of the state's number:

$$|C_n|^2 = \frac{2}{\pi x_0^2}.$$

Now, by the definition of the expectation values of the observables  $x^{2m}$  (where, for our tasks,  $m$  equals either 1 or 2), in the  $n^{\text{th}}$  stationary state

$$\langle x^{2m} \rangle = \int_{-\infty}^{+\infty} |\psi_n(x)|^2 x^{2m} dx.$$

Using the same approximations as have been used to calculate  $C_n$ , we get

$$\langle x^{2m} \rangle_{\text{WKB}} = \frac{|C_n|^2}{2} \int_{-x_n}^{+x_n} \frac{x^{2m} dx}{k_n(x)} = \frac{1}{\pi} \int_{-x_n}^{+x_n} \frac{x^{2m} dx}{(x_n^2 - x^2)^{1/2}} \equiv \frac{2x_n^{2m}}{\pi} I_m, \quad \text{where } I_m \equiv \int_0^1 \frac{\xi^{2m} d\xi}{(1 - \xi^2)^{1/2}}.$$

These integrals, for  $m = 1$  and  $m = 2$ , may be worked out using the same substitution  $\xi \equiv \sin \varphi$ , giving

$$I_1 \equiv \int_0^{\pi/2} \sin^2 \varphi d\varphi = \int_0^{\pi/2} \frac{1 - \cos 2\varphi}{2} d\varphi = \frac{\pi}{4},$$

$$I_2 = \int_0^{\pi/2} \sin^4 \varphi d\varphi \equiv \int_0^{\pi/2} (\sin^2 \varphi)^2 d\varphi = \int_0^{\pi/2} \left( \frac{1 - \cos 2\varphi}{2} \right)^2 d\varphi \equiv \int_0^{\pi/2} \frac{1 - 2\cos 2\varphi + \cos^2 2\varphi}{4} d\varphi$$

$$= \frac{1}{4} \int_0^{\pi/2} \left( \frac{3}{2} - 2\cos 2\varphi + \frac{1}{2} \cos 4\varphi \right) d\varphi = \frac{3\pi}{16},$$

so, finally,

$$\langle x^2 \rangle_{\text{WKB}} = \frac{2x_n^2}{\pi} I_1 = \frac{x_0^2(2n+1)}{2} \equiv x_0^2 \left( n + \frac{1}{2} \right),$$

$$\langle x^4 \rangle_{\text{WKB}} = \frac{2x_n^4}{\pi} I_2 = \frac{3x_0^4(2n+1)^2}{8} \equiv \frac{3}{2} x_0^4 \left( n^2 + n + \frac{1}{4} \right).$$

As will be shown by operator methods in Chapter 5,<sup>46</sup> the exact expression for the first of these expectation values is exactly the same, while the second one differs by just a constant:

$$\langle x^4 \rangle_{\text{exact}} = \frac{3}{2} x_0^4 \left( n^2 + n + \frac{1}{2} \right),$$

so the WKB approximation gives a result that is asymptotically correct result in the limit  $n \rightarrow \infty$ , as it should.

**Problem 2.11.** Use the WKB approximation to express the expectation value of the kinetic energy of a 1D particle confined in a soft potential well, in its  $n^{\text{th}}$  stationary state, via the derivative  $dE_n/dn$ , for  $n \gg 1$ .

*Solution:* We need to calculate

$$\langle T \rangle_n \equiv \left\langle \frac{p^2}{2m} \right\rangle_n = \int_{-\infty}^{+\infty} \psi_n^*(x) \frac{\hat{p}^2}{2m} \psi_n(x) dx = -\frac{\hbar^2}{2m} \int_{-\infty}^{+\infty} \psi_n^*(x) \frac{\partial^2 \psi_n(x)}{\partial x^2} dx. \quad (*)$$

As was discussed in Sec. 2.4 of the lecture notes and also in the solution of the previous problem, for higher stationary states with  $n \gg 1$ , we may limit the integration in Eq. (\*) to the classically allowed interval  $[x_L, x_R]$ . On this interval, we may use Eq. (2.94) with  $|a| = |b|$ , which may be rewritten as

$$\psi_n(x) = \frac{C_n}{k_n^{1/2}(x)} \sin \left( \int_{x_L}^x k_n(x') dx' + \varphi \right), \quad \text{with } k_n^2(x) \equiv \frac{2m[E_n - U(x)]}{\hbar^2}; \quad (**)$$

for our current purposes, the value of the constant phase shift  $\varphi$  is not important. Since the WKB approximation is valid only if the sine function in this expression changes much faster than the pre-exponential factor, we may limit the double differentiation in Eq. (\*) to this function, getting

<sup>46</sup> A brute-force calculation of the exact values, starting from Eqs. (2.276) and (2.284) and then using recurrence relations between the Hermite polynomials, is also possible, but much more cumbersome.

$$\langle T \rangle_n = \frac{\hbar^2}{2m} |C_n|^2 \int_{x_L}^{x_R} k_n(x) \sin^2 \left( \int_{x_L}^x k_n(x') dx' + \varphi \right) dx.$$

Just as in the solution of the previous problem, at each period of the rapidly oscillating sine function, its square may be replaced with its average value, equal to  $1/2$ , so we get

$$\langle T \rangle_n = \frac{\hbar^2}{4m} |C_n|^2 \int_{x_L}^{x_R} k_n(x) dx.$$

But as we know from Eq. (2.109) of the lecture notes, in the limit  $n \gg 1$ , this integral equals  $\pi n$ , so we get a very simple expression:

$$\langle T \rangle_n = \frac{\pi \hbar^2}{4m} |C_n|^2 n.$$

What remains is to calculate  $|C_n|^2$  from the normalization condition; with Eq. (\*\*), it is

$$\int_{-\infty}^{+\infty} \psi_n^*(x) \psi_n(x) dx \equiv |C_n|^2 \int_{x_L}^{x_R} \frac{1}{k_n(x)} \sin^2 \left( \int_{x_L}^x k_n(x) dx + \varphi \right) dx = 1.$$

With the similar approximation of the rapidly changing  $\sin^2(\dots)$  by  $1/2$ , we get

$$|C_n|^2 = \left[ \frac{1}{2} \int_{x_L}^{x_R} \frac{dx}{k_n(x)} \right]^{-1}.$$

In order to calculate this integral, we may spell out Eq. (2.109), in the limit  $n \gg 1$ , as

$$\int_{x_L}^{x_R} k_n(x) dx \equiv \frac{(2m)^{1/2}}{\hbar} \int_{x_L}^{x_R} [E_n - U(x)]^{1/2} dx = \pi n,$$

and differentiate both parts of the last equality over  $n$  – the operation legitimate at  $n \gg 1$  when the energy spectrum is quasi-continuous. In the same limit, the changes of  $x_L$  and  $x_R$  with  $n$  are negligible, and (at the last step, using the expression for  $k_n(x)$  again) we get

$$\begin{aligned} \frac{(2m)^{1/2}}{\hbar} \frac{d}{dn} \int_{x_L}^{x_R} [E_n - U(x)]^{1/2} dx &\equiv \frac{(2m)^{1/2}}{\hbar} \frac{dE_n}{dn} \frac{d}{dE_n} \int_{x_L}^{x_R} [E_n - U(x)]^{1/2} dx \\ &\equiv \frac{(2m)^{1/2}}{\hbar} \frac{dE_n}{dn} \frac{1}{2} \int_{x_L}^{x_R} \frac{dx}{[E_n - U(x)]^{1/2}} \equiv \frac{m}{\hbar^2} \frac{dE_n}{dn} \int_{x_L}^{x_R} \frac{dx}{k_n(x)} = \pi, \end{aligned}$$

Combining the above relations, we finally get a very simple result:

$$\langle T \rangle_n = \frac{n}{2} \frac{dE_n}{dn}.$$

For example, for the harmonic oscillator of frequency  $\omega_0$ ,  $E_n = \hbar \omega_0 (n + 1/2)$ , so  $dE_n/dn = \hbar \omega_0$ , and our WKB result yields  $\langle T_n \rangle = \hbar \omega_0 n/2$ . As will be shown in Sec. 5.4 of the lecture notes, the exact expression is given by Eq. (5.97):  $\langle T_n \rangle = E_n/2 = \hbar \omega_0 (n + 1/2)/2$ ; in the limit  $n \gg 1$ , the relative difference between these two results tends to zero.

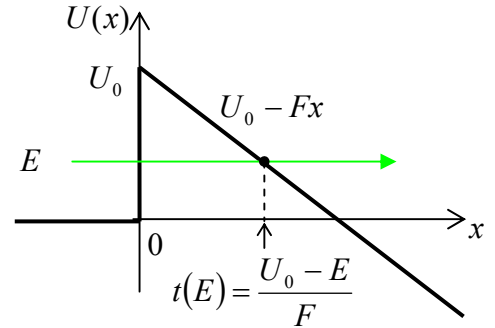
**Problem 2.12.** Use the WKB approximation to calculate the transparency  $\mathcal{T}$  of the following triangular potential barrier:

$$U(x) = \begin{cases} 0, & \text{for } x < 0, \\ U_0 - Fx, & \text{for } x > 0, \end{cases}$$

with  $F, U_0 > 0$ , as a function of the incident particle's energy  $E$ .

*Hint:* Be careful treating the sharp potential step at  $x = 0$ .

*Solution:* With the classical turning points for this specific potential (see the figure on the right), Eq. (2.117) of the lecture notes yields



$$\mathcal{T}_{\text{WKB}} = \exp\left\{-\frac{2}{\hbar} \int_0^{t(E)} [2m(U_0 - Fx - E)]^{1/2} dx\right\} \equiv \exp\left\{-\frac{2}{\hbar} (2mF)^{1/2} [t(E)]^{3/2} \int_0^1 \xi^{1/2} d\xi\right\},$$

where  $\xi \equiv 1 - x/t(E)$ , while  $t(E) \equiv (U_0 - E)/F$  is the potential barrier's thickness for a particle of energy  $E$  – see the figure above. The elementary integral in the last expression is equal to  $2/3$ , so we get

$$\mathcal{T}_{\text{WKB}} = \exp\left\{-\frac{2}{\hbar} (2mF)^{1/2} [t(E)]^{3/2} \frac{2}{3}\right\} \equiv \exp\left\{-\frac{4}{3} \frac{(2m)^{1/2}}{\hbar} \frac{(U_0 - E)^{3/2}}{F}\right\}. \quad (*)$$

This is an approximate version of a formula derived by H. Fowler and L. Nordheim at the very dawn of quantum mechanics, in 1928. In this form, it is used in solid-state physics and engineering (with  $F = -e\mathcal{E}$ , where  $\mathcal{E}$  is the applied electric field) so often that it even gave its name, the *Fowler-Nordheim tunneling*, to the very effect of electron transfer through a potential barrier of the triangular (or a nearly-triangular) shape formed by the field.<sup>47</sup>

Note, however, that at the sharp (step-like) left border of the barrier, the second condition (2.107) of the WKB approximation validity is not satisfied even in the low-field limit

$$F \ll \frac{1}{\hbar} (2mU_0^3)^{1/2}, \quad (**)$$

when  $\kappa t(E) \gg 1$  and hence its first condition (2.96) is satisfied for most energies of the interval  $0 < E < U_0$ . As a result, Eq. (\*) is *never* quantitatively correct. To rectify this deficiency, let us write explicit expressions for the wavefunction of a particle with energy  $E$ , in all three relevant spatial regions. If the condition (\*\*) is satisfied, the barrier's transparency, by the order of magnitude given by Eq. (\*), is very small, so inside the barrier, i.e. at  $0 \leq x \leq t(E) \equiv (U_0 - E)/F$ , we may not only use the WKB form of the wavefunction given by the second line of Eq. (2.116) of the lecture notes but also neglect the second term on its right-hand side (proportional to the coefficient  $d$ ) because the ratio  $d/c$  scales as  $\mathcal{T} \ll 1$ :

<sup>47</sup> In particular, this is exactly the effect used for writing and erasing bits of information (encoded by the amount of electric charge trapped in a nearly-insulated conducting electrode called the *floating gate*) in the now-ubiquitous flash memories, in particular in the so-called solid-state drives (SSD). In the case of electron tunneling into vacuum, the same effect is usually called the *field emission of electrons*.

$$\psi(x) = \begin{cases} A \exp\{ikx\} + B \exp\{-ikx\}, & \text{with } k = \frac{(2mE)^{1/2}}{\hbar}, & \text{for } x \leq 0, \\ \frac{c}{\kappa^{1/2}(x)} \exp\left\{-\int_0^x \kappa(x') dx'\right\}, & \text{with } \kappa(x) = \frac{\{2m[U(x) - E]\}^{1/2}}{\hbar}, & \text{for } 0 \leq x \leq t(E), \\ \frac{f}{k^{1/2}(x)} \exp\left\{i\int_0^x k(x') dx'\right\}, & \text{with } k(x) = \frac{\{2m[E - U(x)]\}^{1/2}}{\hbar}, & \text{for } t(E) \leq x. \end{cases}$$

Writing the usual boundary conditions of continuity of the wavefunction and its first derivative at the sharp border  $x = 0$ , we get a system of two equations for the coefficients  $A$ ,  $B$ , and  $c$ :<sup>48</sup>

$$A + B = \frac{c}{\kappa^{1/2}(0)}, \quad ik(A - B) = -c\kappa^{1/2}(0),$$

which yield, in particular,

$$\frac{c}{A} = \frac{2}{\kappa^{-1/2}(0) + i\kappa^{1/2}(0)/k}, \quad \text{so } \left|\frac{c}{A}\right|^2 = 4 \frac{\kappa(0)}{1 + \kappa^2(0)/k^2} \equiv \frac{4E}{\hbar U_0} [2m(U_0 - E)]^{1/2}.$$

On the other hand, at the border  $x = t(E)$ , where the WKB condition (2.107) is satisfied, we may use the connection formulas similar to Eqs. (2.106) of the lecture notes, in particular, giving

$$\left|\frac{f}{c}\right| = \exp\left\{-\int_0^{t(E)} \kappa(x') dx'\right\} \equiv \mathcal{F}_{\text{WKB}}^{1/2}, \quad \text{so } \left|\frac{f}{A}\right|^2 \equiv \left|\frac{c}{A}\right|^2 \left|\frac{f}{c}\right|^2 = \frac{4E}{\hbar U_0} [2m(U_0 - E)]^{1/2} \mathcal{F}_{\text{WKB}}.$$

Now, calculating the probability currents corresponding to the incident and passed de Broglie waves, we find the barrier's transparency<sup>49</sup>

$$\mathcal{T} \equiv \frac{I_f}{I_A} = \frac{(\hbar/m)|f|^2}{(\hbar/m)|A|^2 k} = \frac{4[E(U_0 - E)]^{1/2}}{U_0} \mathcal{F}_{\text{WKB}} \equiv \frac{4[E(U_0 - E)]^{1/2}}{U_0} \exp\left\{-\frac{4}{3} \frac{(2m)^{1/2}}{\hbar} \frac{(U_0 - E)^{3/2}}{F}\right\}. \quad (***)$$

For typical energies  $E \sim U_0/2$ , the pre-exponential factor in this expression is of the order of 2, i.e. is quite noticeable. However, for typical applications, its effect on the result is much smaller than the transparency's uncertainty due to those of parameters  $U_0$  and  $m$ .<sup>50</sup> ( ) This is why using the simpler Eq. (\*) may be justified for some applications.

Note also that in some textbooks discussing the Fowler-Nordheim tunneling of electrons from metals or degenerate semiconductors, the above potential profile is modified as

$$U(x) = \begin{cases} 0, & \text{for } x < 0, \\ U_0 - Fx - \frac{e^2}{16\pi\kappa\epsilon_0 x}, & \text{for } x > 0, \end{cases}$$

<sup>48</sup> Note that taking the first derivative of the wavefunction under the barrier, we may skip differentiating the pre-exponential factor because due to the condition (2.96), the exponential factor changes much faster.

<sup>49</sup> In their original work, H. Fowler and L. Nordheim derived this formula, in the low-field limit (\*\*), in a different way – using the Airy functions (which were discussed in Sec. 2.4 of the lecture notes).

<sup>50</sup> In solid-state systems,  $m$  in Eq. (\*\*\*) should be replaced with the effective mass  $m_{\text{ef}}$  of the charge carriers in the barrier's material – see the discussion in Sec. 2.8 of the lecture notes.



where  $\kappa$  is the dielectric constant of the barrier's material, with the corresponding modification (increase) of  $\mathcal{F}$ , to account for the potential barrier's suppression by the image charge effect.<sup>51</sup> However, this modification is quantitatively valid only if the so-called *traversal time*  $\tau_i$  of tunneling through the barrier (which will be discussed in Sec. 5.3 of the lecture notes) is much longer than the reciprocal plasma frequency  $\omega_p$  of the conductor,<sup>52</sup> because  $\omega_p^{-1}$  gives the time scale of the transients (surface plasmon propagation<sup>53</sup>) leading, in particular, to the image charge field formation.

**Problem 2.13.** Prove that Eq. (2.67) of the lecture notes is valid even if the potential  $U(x)$  changes, sufficiently slowly, on both sides of the potential step, provided that  $U(x) < E$  everywhere.

*Solution:* If the potential changes slowly, the characteristic length  $a$  of its variation is large. If it is so large that the first condition, Eq. (2.96), of the WKB approximation validity is satisfied, we may use for the wavefunction, both before and after the step, expressions similar to Eq. (2.94):

$$\psi_{\text{WKB}}(x) = \begin{cases} \frac{a}{k^{1/2}(x)} \exp\left\{i \int_0^x k(x') dx'\right\} + \frac{b}{k^{1/2}(x)} \exp\left\{-i \int_0^x k(x') dx'\right\}, & \text{for } x < 0, \\ \frac{c}{k^{1/2}(x)} \exp\left\{i \int_0^x k(x') dx'\right\}, & \text{for } x > 0, \end{cases}$$

with the local wave number  $k(x)$  defined by Eq. (2.82):

$$k^2(x) \equiv \frac{2m[E - U(x)]}{\hbar^2}.$$

Here the lower integration limits are chosen, for the convenience of what follows, at the step location point  $x = 0$ , and the back-propagating wave at  $x > 0$  is set to zero due to the reasons that were discussed in detail in Sec. 2.3 of the lecture notes. (Note again that they are valid only if  $U(x) < E$  in the whole region of the particle's propagation.)

The second condition of WKB approximation, Eq. (2.207), is not satisfied at  $x = 0$ , so instead, the relation between the coefficients  $a$ ,  $b$ , and  $c$  should be found by writing explicit boundary conditions (of the continuity of the wavefunction and its first derivative) at this point. The former condition is straightforward,

$$\frac{a}{k_-^{1/2}} + \frac{b}{k_-^{1/2}} = \frac{c}{k_+^{1/2}}, \quad \text{where } k_-^2 \equiv k^2(-0) = \frac{2mE}{\hbar^2}, \quad k_+^2 \equiv k^2(+0) = \frac{2m(E - U_0)}{\hbar^2},$$

while writing the second one, we should take into account that within the WKB approximation's validity domain, the pre-exponential factor changes much slower than the exponential function. As a result, at the calculation of the first derivatives, we may differentiate only the exponent. This approximation, used also in the solutions of the two previous problems, yields the boundary condition

<sup>51</sup> See, e.g., EM Sec. 2.9, in particular Eq. (2.193), with the replacement  $\varepsilon_0 \rightarrow \kappa\varepsilon_0$  (see EM Sec. 3.4).

<sup>52</sup> See, e.g., EM Sec. 7.2, in particular Eq. (7.37).

<sup>53</sup> See, e.g., the model solution of EM Problem 7.18.

$$ik_- \left[ \frac{a}{k_-^{1/2}} - \frac{b}{k_-^{1/2}} \right] = ik_+ \frac{c}{k_+^{1/2}}.$$

But these equations for normalized coefficients  $a/k_-^{1/2}$ ,  $b/k_-^{1/2}$ , and  $c/k_+^{1/2}$  are exactly the same as were obtained for coefficients  $A$ ,  $B$ , and  $C$  in Sec. 2.3, and their solution is also the same, giving, in particular,

$$\frac{b}{a} \equiv \frac{b/k_-^{1/2}}{a/k_-^{1/2}} = \frac{k_- - k_+}{k_- + k_+} \equiv \frac{E^{1/2} - (E - U_0)^{1/2}}{E^{1/2} + (E - U_0)^{1/2}}.$$

Now calculating the WKB probability currents (2.95) carried by the incident and reflected de Broglie waves at an arbitrary point  $x < 0$ , for the reflection coefficient, we get

$$\mathcal{R} \equiv \frac{|I_b|}{|I_a|} = \frac{(\hbar/m)|b|^2}{(\hbar/m)|a|^2} \equiv \left| \frac{b}{a} \right|^2 = \left[ \frac{E^{1/2} - (E - U_0)^{1/2}}{E^{1/2} + (E - U_0)^{1/2}} \right]^2. \quad (*)$$

Since according to Eq. (2.6), in any stationary state, the probability current has to be independent of  $x$ , the reflection and transmission coefficients have to satisfy the relation

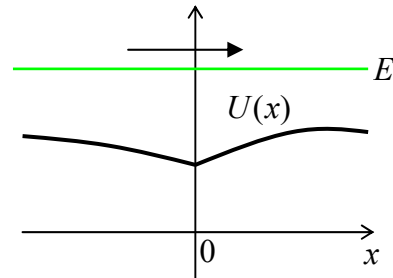
$$\mathcal{T} + \mathcal{R} = 1.$$

Using this relation together with Eq. (\*) to calculate the transmission coefficient,

$$\mathcal{T} = 1 - \mathcal{R} = 1 - \left[ \frac{E^{1/2} - (E - U_0)^{1/2}}{E^{1/2} + (E - U_0)^{1/2}} \right]^2 \equiv \frac{4E^{1/2}(E - U_0)^{1/2}}{\left[ E^{1/2} + (E - U_0)^{1/2} \right]^2},$$

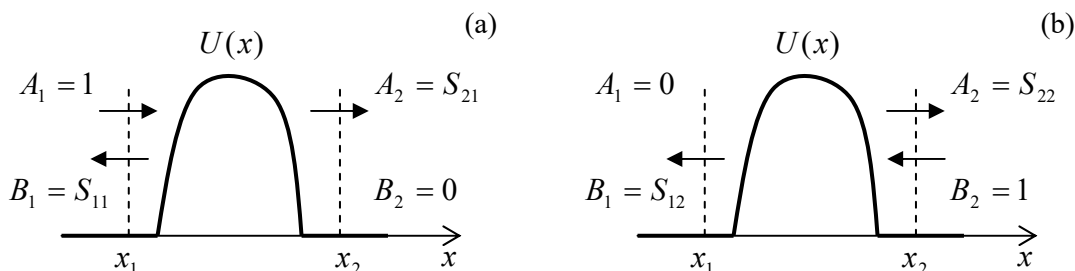
we see that it indeed coincides with Eq. (2.67) of the lecture notes.

In particular, this result gives  $\mathcal{T} = 1$  at  $U_0 = 0$ , i.e. shows that in the WKB approximation, a “cusp” in an otherwise slowly changing potential  $U(x) < E$  (see an example in the figure on the right) does not reflect the incident particle.



**Problem 2.14.\*** Prove that the symmetry of the 1D scattering matrix  $S$  describing an arbitrary time-independent scatterer allows its representation in the form (2.127) of the lecture notes.

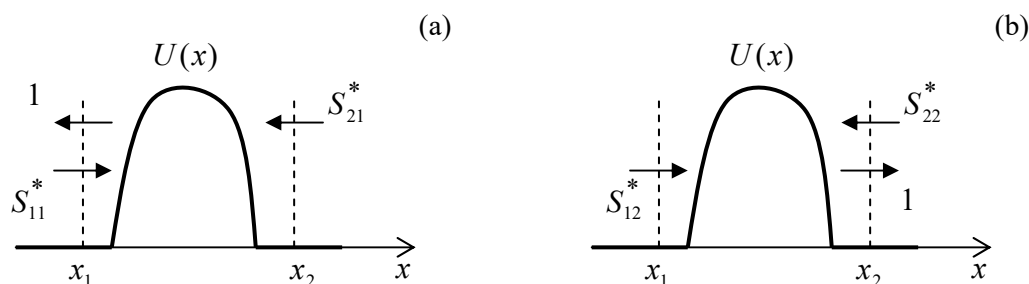
*Solution:* First of all, if the scattering potential does not depend on time, the probability density distribution (for an infinitely wide wave packet) should be also constant in time. In this case, according to Eq. (2.6) of the lecture notes, the values of the probability current  $I$  at the points  $x_1$  and  $x_2$  outside the scatterer (see Fig. 2.12 of the notes) should be equal, for any combination of the amplitudes  $A_1$ ,  $B_2$  of the incident waves. Let us consider two particular cases shown in the figure below.



In case (a), a unit-amplitude wave is incident from the left ( $A_1 = 1, B_2 = 0$ ), while in case (b), the situation is opposite ( $A_1 = 0, B_2 = 1$ ). According to Eqs. (2.123)-(2.124), we may express the amplitudes of the transmitted and reflected waves in these cases via the scattering matrix elements as shown by the labels in the figure above. Now using Eq. (2.5) to calculate the total probability currents:  $I(x_1) = I_{A1} + I_{B1} = (\hbar k/m)(|A_1|^2 - |B_1|^2)$ , and  $I(x_2) = I_{A2} + I_{B2} = (\hbar k/m)(|A_2|^2 - |B_2|^2)$ , and requiring them to be equal to each other in both situations (a) and (b), we get two relations:

$$\begin{aligned} \text{(a): } & 1 - |S_{11}|^2 = |S_{21}|^2 - 0, \\ \text{(b): } & 0 - |S_{12}|^2 = |S_{22}|^2 - 1. \end{aligned} \quad (*)$$

One more set of relations between the matrix elements may be obtained from the fact that all observable results of any Hamiltonian mechanics (including the wave mechanics) of a particle moving in a time-independent potential profile  $U(\mathbf{r})$  should be invariant with respect to the time reversal. According to Eq. (1.23) and (1.69), this invariance requires that at the reversal, the spatial components of 1D wavefunctions change as  $\psi(x) \rightarrow \psi^*(x)$ . At this complex conjugation, a 1D monochromatic traveling wave  $C\exp\{ikx\}$  turns into the wave  $C^*\exp\{-ikx\}$  propagating in the opposite direction. This means that the two particular cases considered above are now modified as shown in the figure below.



Comparing these cases with the general situation shown in Fig. 2.12 of the lecture notes, we see that they may be described by taking:

$$\begin{aligned} \text{case (a): } & A_1 = S_{11}^*, \quad B_1 = 1, \quad A_2 = 0, \quad B_2 = S_{21}^*, \\ \text{case (b): } & A_1 = S_{12}^*, \quad B_1 = 0, \quad A_2 = 1, \quad B_2 = S_{22}^*, \end{aligned}$$

Now applying the general Eq. (2.123) to these cases, we get four more relations:

$$\text{(a): } \begin{cases} 1 = S_{11}S_{11}^* + S_{12}S_{21}^*, \\ 0 = S_{21}S_{11}^* + S_{22}S_{21}^*, \end{cases} \quad \text{(b): } \begin{cases} 0 = S_{11}S_{12}^* + S_{12}S_{22}^*, \\ 1 = S_{21}S_{12}^* + S_{22}S_{22}^*. \end{cases} \quad (**)$$

Not all of the eight relations of the sets (\*) and (\*\*) are independent. Indeed, comparing the first equations of each set, we see that  $|S_{21}|^2 \equiv S_{21}S_{21}^*$  has to equal  $S_{12}S_{21}^*$ , so

$$S_{12} = S_{21},$$

i.e. the off-diagonal elements of the scattering matrix have to be equal to each other. Denoting this single complex number as  $t \exp\{i\theta\}$  (with real  $t$  and  $\theta$ ), and plugging it into the four *inhomogeneous* relations of the sets (\*)-(\*\*), we see that they give only two independent relations. The first of them,

$$|S_{11}|^2 = |S_{22}|^2,$$

allows the replacement of the two complex parameters  $S_{11}$  and  $S_{22}$  (i.e. of four real parameters) with just three real parameters  $r$ ,  $\varphi_1$ , and  $\varphi_2$ :  $S_{11} \equiv r \exp\{i(\theta + \varphi_1)\}$ ,  $S_{22} \equiv -r \exp\{i(\theta + \varphi_2)\}$ . With this notation,<sup>54</sup> the second independent relation may be indeed represented in the form of Eq. (2.127b):

$$r^2 + t^2 = 1,$$

evidently expressing the probability current conservation:  $\mathcal{R} + \mathcal{T} = 1$ .

Now plugging these results into the two *homogeneous* equations of the set (\*\*), we see that they give just one more new relation:

$$e^{i\varphi_1} = e^{-i\varphi_2}.$$

Besides the trivial cases when either  $t = 0$  or  $r = 0$  (when either the transmitted wave or the reflected wave vanishes, and hence its phase is undetermined), the last relation shows that, apart from a possible but inconsequential shift  $2\pi n$ , the phases  $\varphi_1$  and  $\varphi_2$  are equal and opposite, and may be denoted as  $\varphi_1 = \varphi$  and  $\varphi_2 = -\varphi$ . (This fact may be also expressed as  $S_{11} = -S_{22}^*$ .) Plugging these results into Eq. (2.124), we get Eq. (2.127a) proved as well.

**Problem 2.15.** Prove the universal relations between the elements of the 1D transfer matrix  $T$  of a stationary (but otherwise arbitrary) scatterer, mentioned in Sec. 2.5 of the lecture notes.

*Solution:* First of all, let us use the same argument as in the model solution of the previous problem: the total probability current should be the same at the external points  $x_1$  and  $x_2$ , for any combination of the amplitudes  $A_1$  and  $B_1$  on the right-hand side of the transfer matrix definition – see Eq. (2.125) of the lecture notes. Taking, first,  $A_1 = 0$ ,  $B_1 = 1$ , we get

$$|T_{22}|^2 - |T_{12}|^2 = 1,$$

while the second alternative,  $A_1 = 1$ ,  $B_1 = 0$ , gives

$$|T_{11}|^2 - |T_{21}|^2 = 1.$$

Two more relations may be obtained from the time-inversion arguments spelled out in the solution of the previous problem. They imply, in particular, that Eqs. (2.125) should be valid if we complex-conjugate all wave amplitudes  $A$  and  $B$ , and simultaneously swap them at each spatial point (to reflect the change of the sign of the wave number  $k$ ):

$$\begin{aligned} B_2^* &= T_{11} B_1^* + T_{12} A_1^*, \\ A_2^* &= T_{21} B_1^* + T_{22} A_1^*. \end{aligned}$$

Taking the complex conjugate of these equations, and changing the order of lines and columns, we get

<sup>54</sup> This notation is motivated by Eqs. (2.121)-(2.122) of the lecture notes, which allow one to interpret the off-diagonal elements of the scattering matrix as *transmission amplitudes*, and their diagonal elements, as *reflection amplitudes*, for two possible directions of the incident wave. (The *amplitudes*  $t$  and  $r$  should not be confused with the corresponding real *transparency*  $\mathcal{T} \equiv t^2$  and *reflectivity*  $\mathcal{R} \equiv r^2$ .)

$$A_2 = T_{22}^* A_1 + T_{21}^* B_1,$$

$$B_2 = T_{12}^* A_1 + T_{11}^* B_1.$$

Comparing this system with Eqs. (2.125), we see that the matrix elements should satisfy the conditions

$$T_{22}^* = T_{11}, \quad T_{21}^* = T_{12}.$$

An alternative way to obtain all these relations is to plug Eqs. (2.127) of the lecture notes (whose proof was the task of the previous problem) into Eqs. (2.126). The results may be merged into the following matrix form:

$$T = \frac{1}{t} \begin{pmatrix} e^{i\theta} & -re^{-i\varphi} \\ -re^{i\varphi} & e^{-i\theta} \end{pmatrix}, \quad \text{with } r^2 + t^2 = 1;$$

one can readily check that all the above relations between the matrix elements are indeed satisfied.

**Problem 2.16.\*** A  $k$ -narrow wave packet is incident on a finite-length 1D scatterer. Obtain a general expression for the time of its delay caused by the scatterer, and evaluate the time for the case of a very short but high potential barrier.

*Solution:* The initial packet may be represented by Eq. (2.20) of the lecture notes,

$$\Psi(x,0) = \int a_k e^{ikx} dk, \quad (*)$$

Then, generalizing Eq. (2.28) by applying Eq. (2.121) to each frequency component, we may use the linear superposition principle to represent the packet after its scattering as a sum of the transmitted and reflected parts:

$$\Psi(x,t) = \int a_k S_{21}(k) e^{i(kx-\omega t)} dk + \int a_k S_{11}(k) e^{i(-kx-\omega t)} dk,$$

where  $S$  is the scattering matrix (2.124).<sup>55</sup> In our case of a narrow wave packet, the magnitude of the Fourier amplitude  $a_k$  rapidly decreases with its argument's deviation from some central point  $k_0$ . This is why let us rewrite the first term, representing the transmitted component of the packet, as

$$\Psi_{\text{trans}}(x,t) = \int a_k |S_{21}(k_0 + \tilde{k})| \exp\left\{i\left[(k_0 + \tilde{k})x - \omega(k_0 + \tilde{k})t + \varphi(k_0 + \tilde{k})\right]\right\} dk,$$

where  $\varphi \equiv \arg S_{12}$  is the phase of this matrix element, and consider the Taylor expansion of the factors in this integral in relatively small  $\tilde{k} \equiv k - k_0$  – exactly as it was done in Eq. (2.29) but neglecting the quadratic term. (As was discussed in Sec. 2.2, that term describes the eventual broadening of the wave packet, and does not affect the time delay we are calculating.) For a small variation of  $k$ , the resulting variation of  $|S_{12}|$  (responsible for the change of the wave packet's shape) is also relatively small and for our purposes, may be neglected. However, as we will see in a minute, such variations of  $\omega$  and  $\varphi$ ,

<sup>55</sup> Generally, the off-diagonal element  $S_{12}$  of the scattering matrix  $S$  includes the factor  $\exp\{-ika\}$  resulting from the distance  $a \equiv x_2 - x_1$  between the reference points  $x_1$  and  $x_2$  – see Eq. (2.120) and its discussion. For our current purposes, it is convenient to take  $a = 0$ .

$$\omega - \omega_0 \approx \left. \frac{d\omega}{dk} \right|_{k=k_0} \tilde{k}, \quad \varphi - \varphi_0 \approx \left. \frac{d\varphi}{dk} \right|_{k=k_0} \tilde{k}, \quad \text{where } \omega_0 \equiv \omega(k_0) \text{ and } \varphi_0 \equiv \varphi(k_0),$$

describe contributions to the transmitted wave packet's delay, and hence have to be kept for its analysis:

$$\Psi_{\text{trans}}(x, t) \approx \exp\{i(k_0 x - \omega_0 t + \varphi_0)\} |S_{21}(k_0)| \int a_k \exp\left\{i\tilde{k}\left(x - \left. \frac{d\omega}{dk} \right|_{k=k_0} t + \left. \frac{d\varphi}{dk} \right|_{k=k_0}\right)\right\} dk. \quad (*)$$

Indeed, comparing this expression with Eq. (\*) rewritten as

$$\Psi(x, 0) = \exp\{ik_0 x\} \int a_k \exp\{i\tilde{k}x\} dk,$$

we see that besides changing its general phase shift and size, as described by the pre-integral factors, during the time interval  $[0, t]$ , the packet moves forward by

$$\Delta x = \left. \frac{d\omega}{dk} \right|_{k=k_0} t - \left. \frac{d\varphi}{dk} \right|_{k=k_0} \equiv v_{\text{gr}} \left( t - \frac{1}{v_{\text{gr}}} \left. \frac{d\varphi}{dk} \right|_{k=k_0} \right),$$

where  $v_{\text{gr}}$  is the group velocity of the particle in the absence of the scatterer— see the first of Eqs. (2.33a). This means the scatterer-induced additional time delay is

$$\Delta t = \frac{1}{v_{\text{gr}}} \left. \frac{d\varphi}{dk} \right|_{k=k_0}. \quad (**)$$

This is the result we were seeking for. For a particular case of a very short but high potential barrier that may be represented with Eq. (2.74), we may use the second of Eqs. (2.133) to write

$$S_{21} = \frac{1}{1+i\alpha} \equiv \frac{1}{1+\alpha^2} e^{i\varphi}, \quad \text{with } \varphi = -\tan^{-1}\alpha, \quad \text{where } \alpha \equiv \frac{m\omega}{\hbar^2 k},$$

so using the first of Eqs. (2.33b) for  $v_{\text{gr}}$ , we get

$$\Delta t = \frac{m}{\hbar k_0} \frac{d}{dk} \left( -\tan^{-1} \frac{m\omega}{\hbar^2 k} \right)_{k=k_0} = \frac{m}{\hbar k_0} \frac{m\omega/\hbar^2}{(m\omega/\hbar^2)^2 + k_0^2} \equiv \frac{\hbar}{2E} \frac{\alpha}{1+\alpha^2},$$

where the last expression also has to be evaluated at  $k = k_0$ . Interestingly, at  $\alpha = 1$ , i.e. at moderate transparency of the barrier, the delay reaches the largest fraction (a quarter) of the value  $\hbar/E$  that would follow from a naïve application of the energy-time uncertainty relation (2.155). The delay is even much smaller at both  $\alpha \ll 1$  and  $\alpha \gg 1$ , i.e. at any strong relation between the particle's energy  $E = \hbar^2 k_0^2 / 2m$  and its natural scale for this potential,  $E_0 \equiv m\omega^2 / 2\hbar^2$ — see Eq. (2.79).

Note also that one should resist the temptation to interpret this wave packet's delay by a potential barrier as “the time of tunneling” of the particle through the barrier. (Such interpretation is sound only in the limit of very long and low scattering profiles.) Generally, no single time of tunneling may rationally explain the results of all experiments that may be performed with the barrier.<sup>56</sup>

<sup>56</sup> See, e.g., the review paper by R. Landauer and Th. Martin, *Rev. Mod. Phys.* **66**, 217 (1994). See also the related brief discussion at the very end of Sec. 5.3 of the lecture notes

**Problem 2.17.** A 1D particle had been localized in a very narrow and deep potential well, with the “weight”  $\int U(x)dx$  equal to  $-\mathcal{W}$ , where  $\mathcal{W} > 0$ . Then (say, at  $t = 0$ ) the well’s bottom is suddenly lifted up, so the particle becomes completely free. Calculate the probability density to find the particle in a state with a certain wave number  $k$  at  $t > 0$  and the total final energy of the system.

*Solution:* As was discussed at the beginning of Sec. 2.6 of the lecture notes, such a well, located at  $x = 0$ , may be described by the delta-functional potential

$$U(x) = -\mathcal{W}\delta(x)$$

and the (only) localized state of a particle in the well is described by Eqs. (2.159), (2.161), and (2.162):

$$\Psi(x, t \leq 0) = A \exp\left\{-\kappa|x| - i\frac{E_{\text{ini}}}{\hbar}t\right\}, \quad \text{with } \kappa = \frac{m\mathcal{W}}{\hbar^2} \quad \text{and } E_{\text{ini}} = -\frac{\hbar^2\kappa^2}{2m} \equiv -\frac{m\mathcal{W}^2}{2\hbar^2}. \quad (*)$$

For this state, the normalization condition is

$$\int_{-\infty}^{+\infty} |\Psi(x, t \leq 0)|^2 dx \equiv |A|^2 2 \int_0^{\infty} e^{-2\kappa x} dx \equiv \frac{|A|^2}{\kappa} = 1, \quad \text{giving } |A| = \kappa^{1/2}.$$

After the well bottom’s lifting, the particle becomes free to move, so, as was discussed in Sec. 2.2, its wavefunction may be expanded into a sum over either traveling de Broglie waves (as given by Eq. (2.27) of the lecture notes) or, equivalently, standing waves:

$$\Psi(x, t \geq 0) = \sum_k (c_k C \cos kx + s_k S \sin kx) \exp\left\{-i\frac{E_k}{\hbar}t\right\}, \quad \text{with } E_k = \frac{\hbar^2 k^2}{2m}.$$

For our purposes, the latter form (spelled out above) is more convenient. If the coefficients  $C$  and  $S$  are selected so that each of the component wavefunctions,  $C\cos kx$  and  $S\sin kx$ , are normalized (see below), then the amplitudes  $c_k$  and  $s_k$  may be calculated from the 1D version of Eq. (1.68):

$$c_k = \int_{-\infty}^{+\infty} C \cos kx \Psi(x, 0) dx \equiv |A| C \int_{-\infty}^{+\infty} \cos kx e^{-\kappa|x|} dx, \quad s_k = \int_{-\infty}^{+\infty} C \sin kx \Psi(x, 0) dx \equiv |A| C \int_{-\infty}^{+\infty} \sin kx e^{-\kappa|x|} dx.$$

The second integral (of an odd function of  $x$ , in symmetric limits) equals zero, while the first one may be readily calculated

$$c_k = |A| C 2 \operatorname{Re} \int_0^{+\infty} e^{ikx} e^{-\kappa x} dx = 2|A| C \operatorname{Re} \frac{0-1}{ik-\kappa} \equiv 2|A| C \frac{\kappa}{k^2 + \kappa^2} = 2C \frac{\kappa^{3/2}}{k^2 + \kappa^2}. \quad (**)$$

What remains is to calculate the normalization coefficient  $C$ . The most transparent way<sup>57</sup> to do this is to introduce (as was already discussed in Chapter 1 of the lecture notes) an artificial, very large segment  $-l/2 \leq x \leq +l/2$ , with  $\kappa l \gg 1$ , requiring the wavefunction to equal zero everywhere outside it, and hence on its boundaries, i.e. at  $x = \pm l/2$ . For our eigenfunctions,  $C\cos kx$ , this gives the following spectrum of possible values,  $k_n$ , of the wave number:

<sup>57</sup> Another way is to recognize that, in a spatially unlimited system, this sum over  $k$  is actually an integral, and use the so-called delta-normalization of  $\Psi$ . This approach, to be discussed in Sec. 4.7 of the lecture notes, would give identical final results.

$$\cos \frac{k_n l}{2} = 0, \quad \text{i.e. } \frac{k_n l}{2} = \frac{\pi}{2} + \pi m, \quad \text{with } n = 0, 1, 2, \dots$$

If  $l$  is selected to be large enough, then for all essential wave numbers  $k_n \sim \kappa \gg 1/l$ , i.e.  $n \gg 1$ , the first term in the last expression is negligible, so the spectrum may be well approximated as<sup>58</sup>

$$k_n = \frac{2\pi}{l} n, \quad (***)$$

and the normalization condition becomes

$$\int_{-l/2}^{+l/2} |C \cos k_n x|^2 dx \equiv \frac{|C|^2 l}{2} = 1, \quad \text{giving } |C| = \left(\frac{2}{l}\right)^{1/2}.$$

With this, Eq. (\*\*) yields the following probability of finding the particle in the state with a wave number  $k$ :

$$W_k \equiv |c_k|^2 = \frac{8}{l} \frac{\kappa^3}{(k^2 + \kappa^2)^2}.$$

Now we may calculate the requested probability density  $w(k)$  as the ratio of the sum of all probabilities  $W_k$  within an elementary interval  $dk \ll k$ , to the width  $dk$  of this interval. Due to the small distance between the adjacent numbers  $k_n$ , the sum may be calculated just as  $W_k dn$ , where  $dn$  is the number of these modes in the interval  $dk$ . According to Eq. (\*\*\*),  $dk = (2\pi/l)dn$ , so

$$w(k) \equiv W_k \frac{dn}{dk} = \frac{8}{l} \frac{\kappa^3}{(k^2 + \kappa^2)^2} \frac{l}{2\pi} \equiv \frac{4}{\pi} \frac{\kappa^3}{(k^2 + \kappa^2)^2}. \quad (***)$$

Note the cancellation, in this final expression, of the length  $l$  of the artificial bounding segment; this is the necessary condition for the correctness of this normalization procedure. Another useful sanity check is the calculation of the total probability to find the released particle in the state with *some*  $k > 0$ :

$$W \equiv \int_0^{\infty} w(k) dk = \frac{4}{\pi} \int_0^{\infty} \frac{\kappa^3 dk}{(k^2 + \kappa^2)^2} = \frac{4}{\pi} \int_0^{\infty} \frac{d\xi}{(\xi^2 + 1)^2},$$

where  $\xi \equiv k/\kappa$ . This is a table integral,<sup>59</sup> equal to  $\pi/4$ , so (fortunately :- )  $W = 1$ , as it should be. Our result for  $w(k)$  shows that the probability density is finite but nonvanishing at  $k \rightarrow 0$ , and rapidly decreases as soon as  $k$  is increased beyond the reciprocal spatial extension,  $\kappa$ , of the initial wavefunction.

Now we may use Eq. (\*\*\*\*) to calculate the total energy<sup>60</sup> of the particle at  $t > 0$ .

$$\begin{aligned} E_{\text{fin}} &= \int_0^{\infty} E_k w(k) dk = \int_0^{\infty} \frac{\hbar^2 k^2}{2m} \frac{4}{\pi} \frac{\kappa^3}{(k^2 + \kappa^2)^2} dk = \frac{4}{\pi} \frac{\hbar^2 \kappa^3}{2m} \int_0^{\infty} \frac{\xi^2 d\xi}{(\xi^2 + 1)^2} \\ &\equiv \frac{4}{\pi} \frac{\hbar^2 \kappa^3}{2m} \left[ \int_0^{\infty} \frac{d\xi}{\xi^2 + 1} - \int_0^{\infty} \frac{d\xi}{(\xi^2 + 1)^2} \right], \end{aligned}$$

<sup>58</sup> This approximation corresponds to the general 1D mode counting rule – see Eq. (1.100) of the lecture notes.

<sup>59</sup> See, e.g., MA Eq. (6.5b) with  $n = 2$ .

<sup>60</sup> Since, per the problem's assignment,  $U = 0$  at  $t > 0$ , this energy has only the kinetic component:  $E_k = \hbar^2 k^2 / 2m$ .



where  $\xi \equiv k/\kappa$  again. The second integral is the same as the one above (and is equal to  $\pi/4$ ), while the first one is another well-known integral,<sup>61</sup> equal to  $\pi/2$ . As a result, we get an extremely simple formula:

$$E_{\text{fin}} = \frac{\hbar^2 \kappa^2}{2m} \equiv |E_{\text{ini}}| \equiv -E_{\text{ini}}.$$

It means, in particular, that the total work done on the system by the force lifting the potential well's bottom is

$$E_{\text{fin}} - E_{\text{ini}} = 2|E_{\text{ini}}|,$$

i.e. twice larger than that (just  $|E_{\text{ini}}|$ ) necessary to do this process very slowly – with a duration  $\Delta t$  much larger than the characteristic time constant  $\tau \sim \hbar/|E_{\text{ini}}|$ . This two-fold increase is the price for the high speed of the process: at a slow (“adiabatic”) well's bottom lift, the total energy of the resulting de Broglie waves with  $E_k > 0$  is vanishingly small.

**Problem 2.18.** Calculate the lifetime of the metastable localized state of a 1D particle in the potential

$$U(x) = -w\delta(x) - Fx, \quad \text{with } w > 0,$$

in the WKB approximation. Formulate the condition of validity of the result.

*Solution:* According to Eqs. (2.159), (2.161), and (2.162) of the lecture notes, and the normalization carried out at the beginning of the previous problem's solution, if  $F = 0$ , the normalized wavefunction of the (in this case, stable) localized state is

$$\psi_0 = \kappa_0^{1/2} \exp\{-\kappa_0|x|\}, \quad \text{where } \kappa_0 = \frac{m\omega}{\hbar^2},$$

and the corresponding energy is

$$E = -\frac{\hbar^2 \kappa_0^2}{2m} = -\frac{m\omega^2}{2\hbar^2}. \quad (*)$$

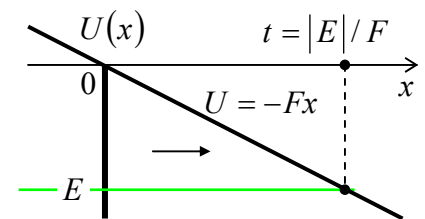
At  $F \neq 0$ ,<sup>62</sup> the potential's profile is tilted – see the figure on the right. As a result, the localized particle may escape into the classically allowed region  $x > t$ , where

$$t = \frac{|E|}{F} = \frac{m\omega^2}{2\hbar^2 F},$$

by tunneling through the classically forbidden region  $0 < x < t$ . If the force is sufficiently weak,

$$F \ll \frac{m^2 \omega^3}{\hbar^4}, \quad (**)$$

the barrier is relatively thick,  $\kappa_0 t \gg 1$ , the barrier's transparency is low, and we may carry out the lifetime calculation by using the WKB approximation.



<sup>61</sup> See, e.g. MA Eq. (6.5a).

<sup>62</sup> Physically,  $F$  is just an additional constant force applied to the particle.

According to Eq. (2.98) of the lecture notes, in this approximation, the wavefunction under the barrier is proportional to

$$\frac{1}{\kappa^{1/2}(x)} \exp\left\{-\int_0^{|x|} \kappa(x') dx'\right\}, \quad \text{with } \frac{\hbar^2 \kappa^2(x)}{2m} \equiv U(x) - E = -Fx - E = \frac{m\omega^2}{2\hbar^2} - Fx.$$

For the metastable state with the energy given by Eq. (\*), this wavefunction virtually coincides with  $\psi_0$  at  $|x| \sim 1/\kappa_0 \ll t$ , so the weak force does not change either the wavefunction's normalization factor or the energy  $E$  substantially. As a result, for the potential-barrier region,  $0 < x < t$ , we may write

$$\psi(x) = \frac{\kappa_0}{\kappa^{1/2}(x)} \exp\left\{-\int_0^x \kappa(x') dx'\right\} \equiv \frac{\kappa_0}{\kappa^{1/2}(x)} \exp\left\{-\int_0^t \kappa(x) dx\right\} \exp\left\{-\int_t^x \kappa(x') dx'\right\}.$$

Now using the first mnemonic rule of the WKB connection, we may write the outgoing de Broglie wave in the classically allowed region ( $t < x$ ) as

$$\psi(x) = \frac{\kappa_0}{k^{1/2}(x)} \exp\left\{-\int_0^t \kappa(x) dx\right\} \exp\left\{i\left[\int_t^x k(x') dx' + \text{const}\right]\right\}, \quad \text{with } \frac{\hbar^2 k^2(x)}{2m} \equiv Fx + E.$$

The probability current (2.95) corresponding to this wave is

$$I = \frac{\hbar}{m} \kappa_0^2 \exp\left\{-2\int_0^t \kappa(x) dx\right\} \equiv \frac{m\omega^2}{\hbar^3} \exp\left\{-2\int_0^t \kappa(x) dx\right\},$$

so according to Eq. (2.6) (with the localized wavefunction normalized to 1), the metastable state's lifetime is just  $1/I$ :<sup>63</sup>

$$\tau = \frac{\hbar^3}{m\omega^2} \exp\left\{2\int_0^t \kappa(x) dx\right\} = \frac{\hbar^3}{m\omega^2} \exp\left\{\frac{2}{\hbar} \int_{[\dots]>0} \left[2m\left(\frac{m\omega}{2\hbar^2} - Fx\right)\right]^{1/2} dx\right\} = \frac{\hbar^3}{m\omega^2} \exp\left\{\frac{2m^2\omega^3}{3\hbar^4 F}\right\}.$$

Note that we could also calculate the lifetime simpler, but more crudely, using the WKB formula (2.117) for the barrier's transparency,

$$\mathcal{T}_{\text{WKB}} = \exp\left\{-2\int_0^t \kappa(x) dx\right\} = \exp\left\{-\frac{2m^2\omega^3}{3\hbar^4 F}\right\},$$

and then Eq. (2.153) with the attempt time is  $t_a$  estimated as  $2\pi/\omega_a$ , with  $\hbar\omega_a \equiv |E|$ . This approach yields the following result,

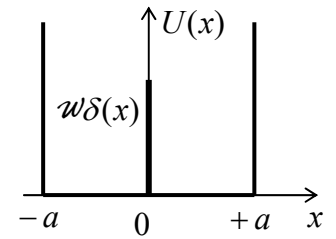
$$\tau_{\text{WKB}} = \frac{t_a}{\mathcal{T}_{\text{WKB}}} = \frac{2\pi\hbar}{|E|} \exp\left\{\frac{2m^2\omega^3}{3\hbar^4 F}\right\} = \frac{4\pi\hbar^3}{m\omega^2} \exp\left\{\frac{2m^2\omega^3}{3\hbar^4 F}\right\},$$

with exactly the same tunneling exponent, but a numerically different pre-exponential numerical factor. This is natural, because the left side of the potential barrier (at  $x = 0$ ) is sharp, so the WKB validity conditions are not satisfied for it. On the other hand, the first approach used above treats this sharpness

<sup>63</sup> This is the same integral as in Problem 2.10, with the replacement  $U_0 - E \rightarrow -E \equiv |E|$ , and  $E$  given by Eq. (\*).

explicitly, and hence yields the correct pre-exponential factor, though (as was discussed in Sec. 2.4 of the lecture notes) for most practical applications, this factor is of minor importance.

**Problem 2.19.** Calculate the energy levels and the corresponding eigenfunctions of a 1D particle placed into a flat-bottom potential well of width  $2a$ , with infinitely high hard walls and a narrow potential barrier in the middle – see the figure on the right. Discuss the particle's dynamics in the limit when  $w$  is very large but still finite.



*Solution:* With the origin of  $x$  in the middle of the well, its potential may be described as

$$U(x) = \begin{cases} +\infty, & \text{for } |x| > a, \\ w\delta(x), & \text{for } |x| < a, \end{cases} \quad \text{with } w > 0.$$

From Sec. 1.7 of the lecture notes, we know that the standing-wave eigenfunctions  $\psi_n$  of the Schrödinger equation in the regions with  $U(x) = 0$  (in our case, the segments  $-a < x < 0$  and  $0 < x < +a$ ) may be always represented as linear superpositions of the fundamental solutions  $\sin kx$  and  $\cos kx$ . To immediately satisfy the boundary conditions  $\psi = 0$  at  $x = \pm a$ , we may take these solutions in the form

$$\psi_n(x) = \begin{cases} C_- \sin k(x+a), & \text{for } -a < x < 0, \\ C_+ \sin k(x-a), & \text{for } 0 < x < +a. \end{cases}$$

What remains is to satisfy the boundary conditions at  $x = 0$ . Plugging the above solution into Eqs. (2.75) and (2.76) of the lecture notes, we get two equations for the coefficients  $C_{\pm}$ :

$$k(C_+ - C_-) \cos ka = \frac{2m\omega}{\hbar^2} C_- \sin ka, \quad (*)$$

$$C_- \sin ka = -C_+ \sin ka.$$

The second equation has two types of solutions, corresponding to antisymmetric and symmetric eigenfunctions (with the lowest-energy functions sketched in the figure on the right):

(i) *Antisymmetric solutions* (index A), with

$$(C_+)_A = (C_-)_A, \quad \text{i.e. } \psi_A = C_A \sin k_A x,$$

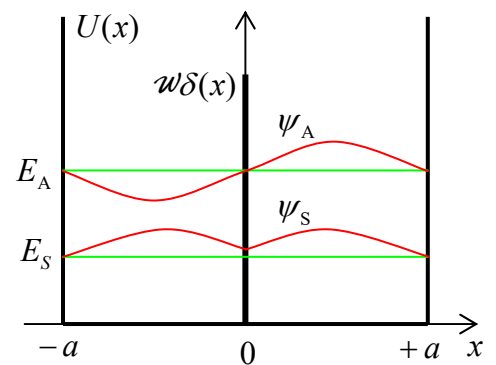
and the eigenvalues independent of  $w$ :

$$\sin k_A a = 0, \quad \text{i.e. } k_A a = k_n a \equiv \pi n, \quad n = 1, 2, \dots$$

Note that these values of  $k$ , and hence the eigenenergies  $E = \hbar^2 k^2 / 2m$  of these antisymmetric states,

$$E_A = E_n \equiv \frac{\hbar^2 k_n^2}{2m} \equiv \frac{\pi^2 n^2}{2ma^2},$$

coincide with those of a single sub-well of width  $a$  – see Fig. 1.8 and its discussion.



(ii) *Symmetric solutions* (index S):

$$(C_+)_S = -(C_-)_S, \quad \text{i.e. } \psi_S = C_S \sin k_S(|x| - a),$$

together with Eq. (\*) giving the following characteristic equation for the eigenvalue  $k_S$ :

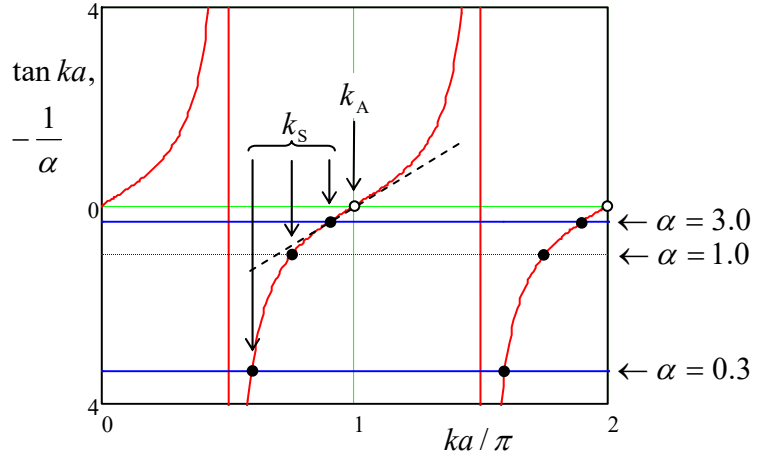
$$\tan k_S a = -\frac{1}{\alpha}, \quad (**)$$

where the parameter  $\alpha$  is given by Eq. (2.78) of the lecture notes, with  $k = k_S$ :

$$\alpha \equiv \frac{m\omega}{\hbar^2 k_S}.$$

The figure on the right shows the graphical solution of Eq. (\*\*) for three representative values of this parameter, i.e. of the sub-well coupling strength.<sup>64</sup> It shows that the equation has an infinite set of solutions that may be also indexed with integer numbers  $n = 1, 2, \dots$ ; for the  $n^{\text{th}}$  of them,  $k_S a$  is within the interval

$$\pi n - \frac{\pi}{2} < k_S a < \pi n,$$



so the values of  $k$  (and hence of the energy  $E = \hbar^2 k^2/2m$ ) for the antisymmetric and symmetric states alternate, with the difference  $k_A - k_S$ , for each pair of adjacent states, being positive but smaller than  $\pi/2a$ , for any  $\alpha$ .

In the limit  $\alpha \rightarrow 0$  (i.e.  $\omega \rightarrow 0$ , meaning virtually no partition between the two sub-wells),  $k_S \rightarrow \pi(n - 1/2)/a$ , i.e. the symmetric eigenfunctions and eigenenergies approach those of the symmetric states of the full potential well of width  $2a$ . In the opposite limit of weak sub-well coupling,  $\alpha \rightarrow \infty$ , we have  $k_S a \rightarrow \pi n$ . In the vicinity of each such point, we may approximate  $\tan k_S a$  with the difference  $(k_S a - \pi n)$  – see the dashed line in the figure above, drawn for  $n = 1$ . As a result, the characteristic equation (\*\*), in this limit, is reduced to

$$k_S a \approx \pi n - \frac{1}{\alpha},$$

so the splitting between the wave numbers and eigenenergies of the adjacent symmetric and antisymmetric states is small:

$$k_A - k_S \approx \frac{1}{\alpha a} \ll k_n, \quad 2\delta_n \equiv E_A - E_S \approx \frac{dE}{dk}(k_A - k_S) = \frac{\pi\hbar^2}{ma} \frac{1}{\alpha a} \equiv \frac{2E_n}{\pi n \alpha} \ll E_n.$$

The dynamics of the particle placed into such a split well, even in the weak coupling limit  $\omega \rightarrow \infty$ , i.e.  $\alpha \rightarrow \infty$ , depends on its initial state. In the simplest case when the state corresponds to just one

<sup>64</sup> For the eigenvalue classification using this plot, the fact that  $\alpha$  depends on  $k$  is not essential. (For example, one may view the argument  $ka$  as a normalized well's width  $2a$ , which does not affect  $\alpha$ .)

(say, the  $n^{\text{th}}$ ) couple of the adjacent symmetric and antisymmetric eigenstates, with close values of the wave number:  $k_A \approx k_S \approx k_n$  and energy:  $E_A \approx E_S \approx E_n$ , the above expressions for the eigenfunctions may be approximated just as in Eq. (2.169) of the lecture notes (obtained in Sec. 2.6 for a different system – see Fig. 2.19):

$$\psi_S(x) \approx \frac{1}{\sqrt{2}} [\psi_R(x) + \psi_L(x)], \quad \psi_A(x) \approx \frac{1}{\sqrt{2}} [\psi_R(x) - \psi_L(x)],$$

where  $\psi_{R,L}$  are the normalized ground states of the completely insulated wells:

$$\psi_R(x) = \left(\frac{2}{a}\right)^{1/2} \times \begin{cases} 0, & \text{for } -a < x < 0, \\ \sin k_n |x|, & \text{for } 0 < x < +a, \end{cases} \quad \psi_L(x) = \left(\frac{2}{a}\right)^{1/2} \times \begin{cases} \sin k_n |x|, & \text{for } -a < x < 0, \\ 0, & \text{for } 0 < x < +a. \end{cases}$$

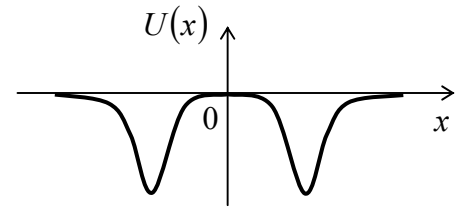
As a result, repeating all the arguments of Sec. 2.6, we arrive at the same picture of sinusoidal quantum oscillations of the particle between the two sub-wells (i.e. of the probability of finding on either side of the partition) with the frequency  $\omega_n = 2\delta_n/\hbar$ . Note that just as in the example analyzed in Sec. 2.6, the time period of these oscillations,

$$\tau_n \equiv \frac{2\pi}{\omega_n} = \frac{\pi\hbar}{\delta_n} \approx \frac{2ma^2}{n\hbar} \alpha,$$

is a factor of  $\alpha/2\pi \gg 1$  shorter than the lifetime  $\tau$  (2.152) of the metastable state of the particle in a potential well limited by two delta-functional walls (see Fig. 2.15) with the same parameter  $\alpha$ .

However, in contrast to the system analyzed in the lecture notes (see Fig. 2.19), which has just one pair of localized symmetric-antisymmetric states, our current system may have many such pairs. As a result, for an arbitrary initial state of the particle, the system may exhibit many simultaneous quantum oscillations, with incommensurate frequencies  $\omega_n$ .

**Problem 2.20.\*** Consider a symmetric system of two potential wells of the type shown in Fig. 2.21 of the lecture notes, but now with  $U(0) = U(\pm\infty) = 0$  – see the figure on the right. Derive a general expression for the well interaction force due to their sharing a quantum particle of mass  $m$ , and determine its sign for the cases when the particle is in:



- (i) a symmetric localized eigenstate, with  $\psi_S(-x) = \psi_S(x)$ , and
- (ii) an antisymmetric localized eigenstate, with  $\psi_A(-x) = -\psi_A(x)$ .

Use a different approach to verify your conclusions for the particular case of delta-functional wells.

**Solution:** In classical mechanics, a potential field described by a 1D potential  $U(x)$  exerts the force  $F_p = -dU/dx$  on the particle moving in this field. According to the 3<sup>rd</sup> Newton law, the force  $F$  exerted by the particle on the potential well (physically, on the source of the field) is equal and opposite:

$$F = -F_p = \frac{dU(x)}{dx}.$$

Due to the correspondence principle, in quantum mechanics, this force is described by the corresponding operator, in the coordinate representation equal to  $dU/dx$ , whose expectation value  $\langle F \rangle$

may be calculated using the general Eq. (2.4) of the lecture notes. However, if we want to calculate the force exerted just on just one potential well (say, the right one, with  $x > 0$  – see the figure above), we need to limit the integration by the corresponding semi-axis:

$$\langle F \rangle(t) = \int_0^{\infty} \Psi^*(x,t) \frac{dU}{dx} \Psi(x,t) dx.$$

In the  $n^{\text{th}}$  stationary state, with its simple time dependence (1.62), this force is time-independent:

$$\langle F \rangle = \int_0^{\infty} \psi_n^*(x) \frac{dU}{dx} \psi_n(x) dx \equiv \int_0^{\infty} |\psi_n(x)|^2 \frac{dU}{dx} dx.$$

Since in a localized stationary state of a 1D system, the probability current (2.5) has to vanish for all  $x$ ,<sup>65</sup> i.e. the wavefunction's phase  $\varphi$  has to be constant, for the notation simplicity, we may always set the phase (which, according to Eq. (2.4), does not affect the expectation value of any physical observable, including  $F$ ) to zero, and write

$$\langle F \rangle = \int_0^{\infty} \psi_n^2(x) \frac{dU}{dx} dx \equiv \int_{x=0}^{x=\infty} \psi_n^2(x) dU.$$

Integrating the last expression by parts, we get

$$\langle F \rangle = \psi_n^2(x) U(x) \Big|_{x=0}^{x=\infty} - \int_{x=0}^{x=\infty} U(x) d(\psi_n^2).$$

The first term of the last expression vanishes due to the condition imposed in this problem on the function  $U(x)$ . Plugging into its second term the expression for  $U(x)$  following from the stationary Schrödinger equation (2.53) for the  $n^{\text{th}}$  eigenstate we are considering,

$$U(x) = E_n + \frac{\hbar^2}{2m} \frac{d^2 \psi_n}{d^2 x} \frac{1}{\psi_n},$$

we get

$$\langle F \rangle = - \int_0^{\infty} \left[ E_n + \frac{\hbar^2}{2m} \frac{d^2 \psi_n}{d^2 x} \frac{1}{\psi_n} \right] d(\psi_n^2) \equiv -E_n \int_{x=0}^{x=\infty} d(\psi_n^2) - \frac{\hbar^2}{m} \int_0^{\infty} \frac{d^2 \psi_n}{d^2 x} \frac{d\psi_n}{dx} dx.$$

In the second term of the last expression, we may write

$$\frac{d^2 \psi_n}{d^2 x} \frac{d\psi_n}{dx} dx \equiv \frac{d}{dx} \left( \frac{d\psi_n}{dx} \right) \frac{d\psi_n}{dx} dx \equiv \frac{d\psi_n}{dx} d \left( \frac{d\psi_n}{dx} \right) \equiv \frac{1}{2} d \left[ \left( \frac{d\psi_n}{dx} \right)^2 \right],$$

so for the average force, we get

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<sup>65</sup> Otherwise, according to Eq. (2.6), with say  $x = x_1$ , and  $x_2 \rightarrow \infty$ , the probability  $W$  to find the particle to the right of point  $x$  would change with time. Note that (as we already know from a discussion in Sec. 2.2), this statement is not necessarily true for infinite 1D systems, such as a fully free particle, because the probability there may “flow from  $-\infty$  to  $+\infty$ ” without accumulation at any finite  $x$ . Later in the course, we will also see that even in finite systems of higher dimensions, the probability current density may not vanish in a stationary state, because the probability may “flow in circles”.

$$\langle F \rangle = -E_n \int_{x=0}^{x=\infty} d(\psi_n^2) - \frac{\hbar^2}{2m} \int_{x=0}^{x=\infty} d \left[ \left( \frac{d\psi_n}{dx} \right)^2 \right] = -E_n \psi_n^2 \Big|_{x=0}^{x=\infty} - \frac{\hbar^2}{2m} \left( \frac{d\psi_n}{dx} \right)^2 \Big|_{x=0}^{x=\infty} .$$

Since we are discussing localized eigenfunctions  $\psi_n(x)$ , which vanish at  $x \rightarrow \infty$  together with their derivatives, only the second substitutions (at  $x = 0$ ) in the above expression may be different from zero, and we finally get

$$\langle F \rangle = E_n \psi_n^2 \Big|_{x=0} + \frac{\hbar^2}{2m} \left[ \left( \frac{d\psi_n}{dx} \right)^2 \right]_{x=0} . \quad (*)$$

This general formula enables us to answer the problem's questions.

(i) For any *symmetric* eigenfunction, the derivative  $d\psi_n/dx$  vanishes at  $x = 0$ , so the second term in Eq. (\*) equals zero, while the first one is negative because for any localized state,  $E_n < U(\pm\infty) = 0$ . Hence for such an eigenstate,  $\langle F \rangle < 0$ . Since the above calculation was for the force exerted on the right well, we may conclude that sharing a particle in a symmetric eigenstate produces an *attractive* force between the wells.

(ii) On the other hand, for any *antisymmetric* eigenstate, the wavefunction  $\psi_n$  itself has to vanish at  $x = 0$ , so  $\langle F \rangle > 0$ , meaning that in this case, the wells' interaction is *repulsive*.

Now note that an alternative way to calculate the wells' interaction force is to write

$$\langle F \rangle = -\frac{\partial E_n}{\partial a} , \quad (**)$$

where  $a$  is the distance between the wells, with the partial derivative meaning that the shape of each well is kept constant at the distance variation. This requirement limits the strict applicability of Eq. (\*\*) to the potential profiles with nonvanishing intervals with  $U(x) = \text{const}$  between the wells. In particular, it may be applied to the system of two delta-functional potential wells considered in Sec. 2.6 of the lecture notes (see Fig. 2.19):

$$U(x) = -w \left[ \delta \left( x - \frac{a}{2} \right) + \delta \left( x + \frac{a}{2} \right) \right], \quad \text{with } w > 0 .$$

As a reminder, in the limit of distant wells ( $\kappa_0 a \gg 1$ , where  $\kappa_0 \equiv 2m w / \hbar^2$ ), that analysis gave, for the only pair of localized eigenstates (one antisymmetric and the other one, symmetric), the following expressions:

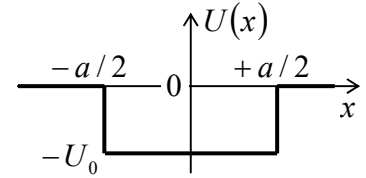
$$E_A = E_0 + \delta, \quad E_S = E_0 - \delta, \quad \text{where } \delta \equiv \frac{2m w^2}{\hbar^2} \exp\{-\kappa_0 a\} > 0 ,$$

and  $E_0$  does not depend on  $a$ . Since  $\delta$  grows (and hence  $E_A$  grows as well, while  $E_S$  decreases) as  $a$  is reduced, the wells sharing a quantum particle in the antisymmetric state repulse each other, while if the particle is in an antisymmetric state, the wells attract each other – in full agreement with the conclusions following from Eq. (\*).<sup>66</sup>

<sup>66</sup> As may be readily shown from Eqs. (2.166) and (2.172) (and their graphical solution shown in Fig. 2.20) of the lecture notes, this qualitative conclusion is valid for *any* distance between the wells – besides that the antisymmetric localized state does not exist at all if  $a$  is lower than the critical value  $a_{\min}$  given by Eq. (2.167).

**Problem 2.21.** Derive and analyze the characteristic equation for localized eigenstates of a 1D particle in a rectangular potential well of a finite depth (see the figure on the right):

$$U(x) = \begin{cases} -U_0, & \text{for } |x| \leq a/2, \\ 0, & \text{otherwise,} \end{cases} \quad \text{with } U_0 > 0.$$



In particular, calculate the number of the localized states as a function of the well's width  $a$  and explore the limit  $U_0 \ll \hbar^2/2ma^2$ .

*Solution:* This problem is conceptually similar to the two-well problems analyzed in Sec. 2.6 of the lecture notes, as well as to Problems 19-20 above, though the quantitative results are different.

(i) The *antisymmetric* eigenfunctions satisfying the requirement of the wavefunction's continuity at  $x = \pm a/2$  have the form

$$\psi_A = C_A \times \begin{cases} \sin kx, & \text{for } |x| \leq \frac{a}{2}, \\ \text{sgn}(x) \sin \frac{ka}{2} \exp\left\{-\kappa\left(|x| - \frac{a}{2}\right)\right\}, & \text{for } |x| \geq \frac{a}{2}, \end{cases}$$

where the real parameters  $k$  and  $\kappa$  are defined as in, respectively, Eqs. (2.65) and (2.162):

$$\frac{\hbar^2 k^2}{2m} \equiv E - U \equiv E + U_0 > 0, \quad \frac{\hbar^2 \kappa^2}{2m} \equiv -E > 0,$$

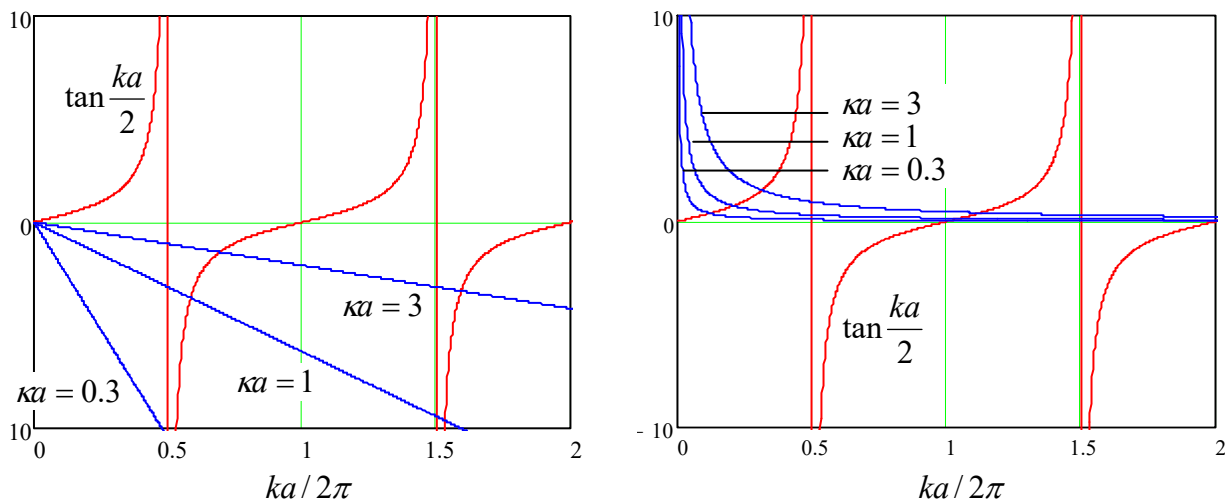
so, in particular,

$$k^2 + \kappa^2 = K^2, \quad \text{where } K^2 \equiv \frac{2mU_0}{\hbar^2} > 0. \quad (*)$$

From here, by using the second pair of boundary conditions (of the continuity of the derivative  $d\psi/dx$  at  $x = \pm a/2$ ), we get the following characteristic equation:

$$\tan \frac{ka}{2} = -\frac{k}{\kappa}, \quad \text{i.e. } \tan \frac{ka}{2} = -\frac{ka}{\kappa a} < 0, \quad (**)$$

whose graphical solution is shown on the left panel of the figure below, for several representative values of the dimensionless parameter  $\kappa a$ .





As the plots show, the solutions  $k$  of Eq. (\*\*), besides the physically unacceptable solution  $k = 0$  (which gives vanishing  $\psi$ ), may be numbered by integer numbers  $n = 1, 2, 3, \dots$ , with

$$n - \frac{1}{2} \leq \frac{k_n a}{2\pi} \leq n.$$

The lower end of this interval, i.e.  $k_n a / 2\pi \rightarrow n - 1/2$ , corresponds to  $\kappa \rightarrow 0$ . This means that the  $n^{\text{th}}$  eigenfunction becomes delocalized, with  $k_n = K$ , at the following value  $a_n$  of the well's width:

$$a = a_n \equiv \frac{2\pi}{K} \left( n - \frac{1}{2} \right),$$

so the number of antisymmetric states in the well is

$$N_A = \text{floor} \left( \frac{Ka}{2\pi} - \frac{1}{2} \right),$$

where  $\text{floor}(\xi)$  is the *floor function* (frequently denoted as  $\lfloor \xi \rfloor$ ), defined as the largest integer not greater than the function's argument  $\xi$  – whose values may be continuous. In particular, at  $a < a_{\min}$ , where

$$a_{\min} \equiv a_1 = \frac{\pi}{K} \equiv \frac{\pi \hbar}{(2mU_0)^{1/2}},$$

the well does not have any antisymmetric localized states at all.

(ii) The *symmetric* eigenfunctions,

$$\psi_s = C_s \times \begin{cases} \cos kx, & \text{for } |x| \leq \frac{a}{2}, \\ \cos \frac{ka}{2} \exp \left\{ -\kappa \left( |x| - \frac{a}{2} \right) \right\}, & \text{for } |x| \geq \frac{a}{2}, \end{cases}$$

lead, in an absolutely similar way, to a different characteristic equation:

$$\tan \frac{ka}{2} = \frac{\kappa}{k} \equiv \frac{\kappa a}{ka} > 0, \quad (***)$$

whose graphical solution is shown on the right panel of the figure above. As the plots show, Eq. (\*\*\*) has one solution  $k_n$  in each of the complementary intervals:

$$n - 1 \leq \frac{k_n a}{2\pi} \leq n - \frac{1}{2}.$$

Each of these solutions, besides  $k_1$  (i.e. for  $n = 2, 3, \dots$ ), gives  $\kappa \rightarrow 0$  and hence  $k_n = K$  (i.e. becomes non-localized) at  $k_n a = 2\pi(n - 1)$ . Hence, such a solution is impossible at

$$a < a'_n \equiv \frac{2\pi n'}{K}, \quad \text{where } n' \equiv n - 1 = 1, 2, \dots,$$

so the number of remaining symmetric states

$$N_S = \text{floor} \left( \frac{Ka}{2\pi} \right).$$

Notice that since  $U_0 > 0$ , i.e.  $K > 0$ , this result shows that  $N_S > 0$  for any  $a > 0$ . This means that the lowest localized symmetric eigenfunction (with  $k = k_1$ ) exists in *any* potential well of nonvanishing width and depth. According to the first of Eqs. (\*), for very shallow wells with  $U_0 \ll \hbar^2/2ma^2$ , i.e.  $Ka \ll 1$ , both  $ka$  and  $\kappa a$  have to be much less than 1, and for  $n = 1$ , the characteristic equation (\*\*\*) is reduced to

$$\frac{k_1 a}{2} = \frac{\kappa}{k_1} \ll 1, \quad \text{i.e. } \kappa = \frac{k_1^2 a}{2} \ll k_1,$$

giving the following equation for the only remaining energy level:

$$|E_1| \equiv \frac{\hbar^2}{2m} \kappa^2 = \frac{\hbar^2}{2m} \left( \frac{k_1^2 a}{2} \right)^2 \equiv \frac{ma^2}{2\hbar^2} \left( \frac{\hbar^2 k_1^2}{2m} \right)^2 \equiv \frac{ma^2}{2\hbar^2} (U_0 - |E_1|)^2.$$

In this limit,  $\kappa \ll k \leq K$ , and hence  $|E_1| \ll U_0$ , so we may neglect  $|E_1|$  on the right-hand side of the last expression, thus arriving at the following approximate (but asymptotically correct) result:

$$|E_1| = \frac{m}{2\hbar^2} U_0^2 a^2, \quad \text{for } U_0 \ll \frac{\hbar^2}{2ma^2}. \quad (****)$$

Note that for the (only) localized state of the particle in a delta-functional, i.e. very deep and narrow well, this formula coincides with Eq. (2.162):

$$|E| = \frac{m}{2\hbar^2} w^2.$$

Indeed, for the rectangular potential well, the “weight”  $w$  of the delta function is just the product  $U_0 a$ .

The task of the next problem is to generalize Eq. (\*\*\*\*) to the case of an arbitrary (but very shallow) potential well.

**Problem 2.22.** Calculate the energy of a 1D particle localized in a potential well of an arbitrary shape  $U(x)$ , provided that its width  $a$  is finite, and the average depth is very small:

$$|\bar{U}| \ll \frac{\hbar^2}{2ma^2}, \quad \text{where } \bar{U} \equiv \frac{1}{a} \int_{\text{well}} U(x) dx.$$

*Solution:* Let us select the origin of  $x$  in the middle of the well, and integrate both sides of the stationary Schrödinger equation, rewritten as

$$\frac{d^2 \psi}{dx^2} = \frac{2m}{\hbar^2} [U(x) - E] \psi,$$

over an interval  $[-x_0, +x_0]$  with  $x_0 > a/2$ . The result is

$$\left. \frac{d\psi}{dx} \right|_{x=+x_0} - \left. \frac{d\psi}{dx} \right|_{x=-x_0} = \frac{2m}{\hbar^2} \int_{-x_0}^{+x_0} [U(x) - E] \psi(x) dx. \quad (*)$$

As we already know from Secs. 2.3-2.6 of the lecture notes, near the points  $x = \pm x_0$ , i.e. outside the potential well, the wavefunction changes as  $\exp\{-\kappa|x|\}$ , where  $\kappa$  is defined by the relation

$$\frac{\hbar^2 \kappa^2}{2m} \equiv |E| = -E, \quad \text{i.e. } \kappa = \frac{(2m|E|)^{1/2}}{\hbar},$$

so we may rewrite Eq. (\*) as

$$-\kappa[\psi(+x_0) + \psi(-x_0)] \equiv -\frac{(2m|E|)^{1/2}}{\hbar} [\psi(+x_0) + \psi(-x_0)] = \frac{2m}{\hbar^2} \int_{-x_0}^{+x_0} [U(x) - E] \psi(x) dx. \quad (**)$$

So far, this is an exact result, valid for any  $x_0 > a/2$ . Now let us suppose that if  $|U|$  satisfies the condition specified in the assignment, then  $|E|$  is even much smaller. (This assumption, implied by Eq. (\*\*\*) of the previous problem's solution, will be confirmed by our final result.) This means that  $1/\kappa$  is much larger than  $a$ , so if we select  $x_0$  somewhere within the following wide range,

$$a \ll x_0 \ll 1/\kappa,$$

then within the interval  $[-x_0, +x_0]$ , the wavefunction is virtually constant. Hence we may cancel it on both sides of Eq. (\*\*), getting simply

$$-\frac{(2m|E|)^{1/2}}{\hbar} 2 = \frac{2m}{\hbar^2} \int_{-x_0}^{+x_0} [U(x) - E] dx \equiv -\frac{2m}{\hbar^2} \int_{-a/2}^{+a/2} |U(x)| dx + \frac{2m}{\hbar^2} 2x_0 |E|.$$

Moreover, since at our choice,  $x_0 \ll 1/\kappa \equiv \hbar/(2m|E|)^{1/2}$ , the last term on the right-hand side of this relation is negligible in comparison with its left-hand side, and the formula may be reduced to just

$$-\frac{(2m|E|)^{1/2}}{\hbar} 2 = -\frac{2m}{\hbar^2} \int_{-a/2}^{+a/2} |U(x)| dx,$$

giving us the final result<sup>67</sup>

$$|E| = \frac{m}{2\hbar^2} \left[ \int_{\text{well}} |U(x)| dx \right]^2, \quad \text{so } \frac{|E|}{|\bar{U}|} = \frac{ma^2}{2\hbar^2} |\bar{U}| \ll 1,$$

confirming our assumption that  $|E|$  is much smaller than the average value of  $|U|$ .

Just one warning: this scaling of the localized state's energy (as the square of the average confinement potential) is only valid for 1D systems. As we will see in Chapter 3, in a similar 2D problem,  $|E|$  is exponentially low, while the 3D localization has a threshold: the confining potential  $|U|$  has to reach a certain non-zero value before it can house a localized state.

**Problem 2.23.** A particle of mass  $m$  is moving in a field with the following potential:

$$U(x) = U_0(x) + w\delta(x),$$

where  $U_0(x)$  is a smooth symmetric function with  $U_0(0) = 0$ , growing monotonically at  $x \rightarrow \pm\infty$ . Use the WKB approximation to:

<sup>67</sup> In the particular case of a rectangular well, this formula is immediately reduced to Eq. (\*\*\*) of the previous problem's solution (obtained in the same limit).

(i) derive the characteristic equation for the particle's energy spectrum, and  
(ii) semi-quantitatively describe the spectrum's evolution at the increase of  $|\omega|$ , for both signs of this parameter.

Spell out both results for the quadratic-parabolic potential (2.111):  $U_0(x) = m\omega_0^2 x^2/2$ .

*Solutions:*

(i) As was demonstrated in Sec. 2.4 of the lecture notes, the "soft" potential  $U_0(x)$  alone may be handled with the WKB approximation very successfully,<sup>68</sup> but this approximation is not directly applicable to such "hard" potentials as the delta-functional peak – please have one more look at the condition expressed by Eq. (2.96). However, we may solve this problem by combining the WKB approach with the delta-functional potential treatment discussed in Sec. 2.3, based on the boundary conditions (2.75)-(2.76). For the delta-functional potential located at  $x = 0$ , they read

$$\psi_+(0) = \psi_-(0) \equiv \psi(0), \quad \frac{d\psi_+}{dx}(0) - \frac{d\psi_-}{dx}(0) = \frac{2m}{\hbar^2} \omega \psi(0), \quad (*)$$

where  $\psi_{\pm}(x)$  are the wavefunctions at  $x \geq 0$  and  $x \leq 0$ , respectively.

Due to the symmetry of our current potential  $U(x)$ , the eigenfunctions of our problem have to be either symmetric:  $\psi(-x) = \psi(x)$ , or antisymmetric:  $\psi(-x) = -\psi(x)$ . According to the latter of Eqs. (\*), the *antisymmetric* eigenfunctions are not affected by the delta-functional potential peak at all, because, for them,  $\psi(0)$  has to vanish. Hence for these eigenstates, corresponding to even values of the integer  $n$  in Eq. (2.109), we still may use the general Wilson-Sommerfeld result (2.110) for an arbitrary smooth potential  $U_0(x)$ , and the specific result (2.114) for the quadratic potential (2.111):

$$E_n = \hbar\omega_0 \left( n' + \frac{1}{2} \right), \quad \text{for } n' \equiv n - 1 = 1, 3, 5, \dots$$

On the other hand, for *symmetric* eigenfunctions, for which the first of Eqs. (\*) is satisfied automatically, and  $d\psi_-/dx = -d\psi_+/dx$  at  $x = 0$ , the second of the boundary conditions may be rewritten as

$$\frac{d\psi_+}{dx}(0) = \frac{m}{\hbar^2} \omega \psi_+(0). \quad (**)$$

For  $x > 0$ , where  $U(x) = U_0(x)$ , we may use the connection formulas (2.105), obtained for exactly this situation: the total reflection of a monochromatic de Broglie wave from the classical turning point  $x_c$  of a soft potential well – in our current case, of  $U_0(x)$ . With these formulas, Eq. (2.94) takes the form

$$\psi_+(x) = \frac{a}{k^{1/2}(x)} \left[ e^{-i\varphi(x)} - e^{i\varphi(x) + i\pi/2} \right], \quad \text{with } \varphi(x) \equiv \int_x^{x_c} k(x') dx' \geq 0, \quad k^2(x) \equiv \frac{2m}{\hbar^2} [E - U_0(x)].$$

Now calculating the wavefunction's derivative,

$$\frac{d\psi_+}{dx} = \frac{a}{k^{1/2}(x)} i \frac{d\varphi}{dx} \left[ -e^{-i\varphi(x)} - e^{i\varphi(x) + i\pi/2} \right] - \frac{1}{2} \frac{a}{k^{3/2}(x)} \frac{dk}{dx} \left[ e^{-i\varphi(x)} - e^{i\varphi(x) + i\pi/2} \right],$$

<sup>68</sup> As a reminder, this approximation gives the *exact* result (2.114) for the energy spectrum of the harmonic oscillator.

we should note that since  $d\varphi/dx = -k$ , and  $|dk/dx| \sim k/a$ , where  $a$  is the potential's change length scale, the first term on the right-hand side is by the factor  $\sim ka$  larger than the second one. However, the WKB approximation is strictly valid only at  $ka \gg 1$ , so the second term is negligible unless the first one vanishes.<sup>69</sup> As a result, after the cancellation of  $a/k^{1/2}(0)$ , Eq. (\*\*\*) yields

$$ik \left[ e^{-i\varphi} + e^{i(\varphi + \pi/2)} \right] = \frac{m}{\hbar^2} \mathcal{W} \left[ e^{-i\varphi} - e^{i(\varphi + \pi/2)} \right],$$

where

$$\varphi \equiv \varphi(0) = \frac{1}{\hbar} \int_0^{x_c} p dx \equiv \frac{1}{\hbar} \int_0^{x_c} \{2m[E - U(x)]\}^{1/2} dx \geq 0, \quad \text{and} \quad k \equiv k(0) = \frac{1}{\hbar} (2mE)^{1/2}, \quad (***)$$

because  $k(0)$  should be understood as a limit of  $k(x > 0)$  at  $x \rightarrow 0$ , i.e. calculated taking into account only the "soft" part  $U_0(x)$  – which, in our case, vanishes at  $x = 0$ .

The system of the last three relations defines the eigenenergies  $E$  of the symmetric modes. Since

$$i \frac{e^{-i\varphi} + e^{i(\varphi + \pi/2)}}{e^{-i\varphi} - e^{i(\varphi + \pi/2)}} \equiv i \frac{e^{-i(\varphi + \pi/4)} + e^{i(\varphi + \pi/4)}}{e^{-i(\varphi + \pi/4)} - e^{i(\varphi + \pi/4)}} \equiv -\cotan\left(\varphi + \frac{\pi}{4}\right),$$

the first of them may be rewritten in a more compact form,

$$\cotan\left(\varphi + \frac{\pi}{4}\right) = -\frac{m\mathcal{W}}{\hbar^2 k}. \quad (***)$$

Together with Eqs. (\*\*\*), this is the required characteristic equation – for symmetric eigenfunctions.

(ii) Since, according to Eqs. (\*\*\*), both  $\varphi$  and  $k$  are functions of  $E$ , the characteristic equation (\*\*\*) does not allow an analytical solution for an arbitrary potential  $U_0(x)$ . For its semi-quantitative analysis, we may notice that since in the region  $\varphi \geq 0$ , the function  $\cotan(\varphi + \pi/4)$  turns to 0 at points  $\varphi_l = (l + 1/4)\pi$ , with  $l = 0, 1, 2, \dots$ , then if  $\mathcal{W} = 0$  (no delta function at origin), Eq. (\*\*\*) is satisfied at

$$4\varphi \equiv \frac{4}{\hbar} \int_0^{x_c} p(x) dx = (4l + 1)\pi \equiv 2\pi \left( n - \frac{1}{2} \right), \quad \text{with} \quad n \equiv 2l + 1 = 1, 3, 5, \dots,$$

thus returning us to the odd- $n$  subset of the Wilson-Sommerfeld series (2.110). In the particular case of the quadratic potential, we may rewrite Eq. (2.113) of the lecture notes as

$$\varphi \equiv \frac{1}{2\hbar} \int_{+x_c}^{+x_c} p(x) dx = \frac{\pi}{2} \frac{E}{\hbar\omega_0},$$

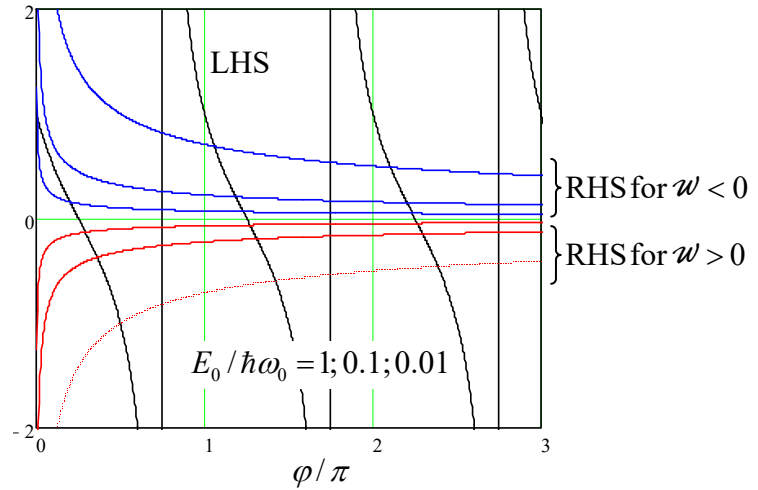
so for the energy, we get the following eigenvalues:

$$E_l = \hbar\omega_0 \frac{2}{\pi} \varphi_l = \hbar\omega_0 \frac{2}{\pi} \left( l + \frac{1}{4} \right) \pi \equiv \hbar\omega_0 \left( 2l + \frac{1}{2} \right),$$

i.e. the subset of the spectrum (2.114), with even  $n' \equiv n - 1 = 2l = 0, 2, 4, \dots$

<sup>69</sup> Besides that, in our current problem, the derivatives  $dU_0/dx$ , and hence  $dk/dx$ , vanish at the point of our interest,  $x = 0$ , so the second contribution to  $d\psi_+/dx$  vanishes exactly.

The situations with  $\omega \neq 0$  may be analyzed graphically, by plotting both sides of Eq. (\*\*\*\*) as functions of  $\varphi$ . Each continuous branch of the function  $\cotan(\varphi + \pi/4)$  is descending with the growth of  $\varphi$ , spanning the values from  $+1$  to  $-\infty$  in the interval  $0 \leq \varphi \leq \pi - \pi/4$ , and from  $+\infty$  to  $-\infty$  within intervals  $(l - 1/4)\pi \leq \varphi \leq (l + 3/4)\pi$ , with  $l = 1, 2, \dots$  – see the black lines in the figure on the right. The red and blue lines in this figure show the right-hand side of Eq. (\*\*\*\*) for the particular case of the quadratic potential, for the positive and negative  $\omega$ ,



respectively, and for several values of the dimensionless parameter  $E_0/\hbar\omega_0$ , where  $E_0 \equiv m\omega^2/2\hbar^2$  is the energy scale imposed by the delta-functional potential – see Eqs. (2.79) and (2.162) of the lecture notes. Semi-quantitatively, these plots are also valid for any smooth symmetric potential  $U_0(x)$ , monotonically growing at  $x \rightarrow \infty$ .

As the plots show, an increase of the positive “weight”  $\omega$  leads to the shift of each eigenvalue toward larger  $\varphi$  and hence larger  $E$ , and vice versa, while for  $\omega < 0$  (corresponding to a narrow potential well at  $x = 0$ ), each eigenvalue is shifted down as  $|\omega|$  is increased. In the former case ( $\omega > 0$ ), this trend is unlimited but saturated: at  $\omega \rightarrow +\infty$  we get

$$\varphi \rightarrow \left(l + \frac{3}{4}\right)\pi, \quad \text{for } l = 0, 1, 2, \dots$$

For the particular case of the quadratic potential, this formula yields

$$E_l = \hbar\omega_0 \frac{2}{\pi} \varphi_l \rightarrow \hbar\omega_0 \frac{2}{\pi} \left(l + \frac{3}{4}\right)\pi \equiv \hbar\omega_0 \left(2l + \frac{3}{2}\right) \equiv \hbar\omega_0 \left(n' + 1 + \frac{1}{2}\right),$$

with even values of  $n' = 2l = 0, 2, \dots$ . This means that due to the barrier, the even-numbered energy levels approach (from below) the odd-numbered levels, with higher  $n'$ , of the system without the central barrier. (In the figure above, these values correspond to the vertical black lines.)

In the opposite limit of a very deep potential well ( $\omega \rightarrow -\infty$ ), there is a similar saturation of the phase shifts  $\varphi$ , and hence of the eigenenergies:

$$\varphi \rightarrow \left(l - \frac{1}{4}\right)\pi,$$

so for the quadratic potential,

$$E_l \rightarrow \hbar\omega_0 \frac{2}{\pi} \left(l - \frac{1}{4}\right)\pi \equiv \hbar\omega_0 \left(2l - \frac{1}{2}\right) \equiv \hbar\omega_0 \left(n' - 1 + \frac{1}{2}\right), \quad \text{for } l = 1, 2, 3, \dots$$

This expression shows that the even-numbered energy levels approach the odd-numbered levels, now with *lower*  $n'$ , of the system without the central well. Note that this trend is not valid for the ground state – the symmetric state with  $l = 0$ . As the figure above shows, the corresponding solution of Eq. (\*\*\*\*)

exists only for relatively small values of  $|\mathcal{W}|$  – for the quadratic potential, only for the ratio  $E_0/\hbar\omega_0$  smaller than  $\sim 0.058$ ). However, this particular prediction of the WKB approximation is unreliable, because, as was discussed in Sec. 2.4, its validity condition (2.96) is strictly fulfilled only for  $n' \gg 1$ . Physically, it is evident that as  $-\mathcal{W}$  grows, the ground-state energy should become negative at  $E_0/\hbar\omega_0 \sim 1$ , and at  $E_0/\hbar\omega_0 \gg 1$  (i.e. when the potential  $U_0(x)$  has a negligible effect on this state) should approach the value (2.162):

$$E_g \rightarrow -E_0 \equiv -\frac{m\mathcal{W}^2}{2\hbar^2}.$$

**Problem 2.24.** Prove Eq. (2.189) of the lecture notes.

*Solution:* According to Eqs. (2.94), (2.98), and (2.105) of the lecture notes, within the WKB approximation, the localized wavefunction inside one of the wells, say  $\psi_L(x)$ , may be represented as

$$\psi_L(x) = \begin{cases} \frac{2c}{[k(x)]^{1/2}} \sin\left(\int_{x_c}^x k(x')dx' + \frac{\pi}{4}\right), & \text{for } x \leq x_c, \\ \frac{c}{[\kappa(x)]^{1/2}} \exp\left\{-\int_{x_c}^x \kappa(x')dx'\right\}, & \text{for } x_c \leq x \leq x_c', \end{cases} \quad (*)$$

where  $x_c$  and  $x_c'$  are the classical turning points at the state's energy  $E$  – see Fig. 2.21.<sup>70</sup> As we know from the derivation of the WKB formulas, the derivative  $d\psi_L/dx$  is dominated, in this approximation, by the exponential function – see, e.g., Eq. (2.90). (See also the solution of the previous problem.) As the result, in the under-barrier region (where the symmetry point  $x = 0$  resides), we may write

$$\left.\frac{d\psi_L}{dx}\right|_{x_c \leq x \leq 0} = -\kappa(x) \frac{c}{[\kappa(x)]^{1/2}} \exp\left\{-\int_{x_c}^x \kappa(x')dx'\right\}.$$

As a result, the last form of Eq. (2.188) yields

$$\delta = \frac{\hbar^2}{m} c^2 \exp\left\{-2 \int_{x_c}^0 \kappa(x')dx'\right\} = \frac{\hbar^2}{m} c^2 \exp\left\{-\int_{x_c}^{x_c'} \kappa(x')dx'\right\},$$

where the last step uses the barrier's symmetry.

The coefficient  $c^2$  in this relation should be found from the normalization condition,

$$\int_{\text{left well}} |\psi_L|^2 dx = 1.$$

Since the WKB approximation is strictly valid only when the well houses many ( $n \gg 1$ ) de Broglie wavelengths  $\lambda$ , at this calculation, we can neglect the wavefunction's penetration into the classically forbidden regions (by distances of the order of  $\lambda$ ) and thus limit the integration to the classically accessible segment, where the first of Eqs. (\*) is applicable:

<sup>70</sup> For a stationary state with no probability current, the coefficient  $c$  may be always taken to be real.

$$1 = 4c^2 \int_{k^2(x)>0} \frac{1}{k(x)} \sin^2 \left( \int_{x_c}^x k(x') dx' + \frac{\pi}{4} \right) dx'.$$

Since  $k(x')$  changes little on each de Broglie wavelength, the sine squared in this integral may be replaced with the average of  $\sin^2 kx'$  over one wavelength, i.e. with the factor  $1/2$ . We may also use Eq. (2.33b) for the group velocity to write  $k(x') = (m/\hbar)v_{gr}(x')$ . As a result, the normalization condition becomes

$$1 = \frac{2c^2 \hbar}{m} \int_{k^2(x)>0} \frac{dx'}{v_{gr}(x')} \equiv \frac{2c^2 \hbar}{m} \int_{k^2(x)>0} \frac{dx'}{(dx_0/dt)_{x_0=x'}}.$$

But the last integral is just the time of the classical motion of the wave packet's center  $x_0$  (i.e. of the classical position of the particle) from one wall limiting the well to the opposite one, i.e. the half of its oscillation period at the energy  $E$ , i.e. of the tunneling attempt time  $t_a$ . As a result, the normalization condition yields  $c^2 = m/\hbar t_a$ , and for the energy splitting, we get Eq. (2.189):

$$\delta = \frac{\hbar}{t_a} \exp \left\{ - \int_{x_c}^{x'_c} \kappa(x') dx' \right\}.$$

**Problem 2.25.** For the problem discussed at the beginning of Sec. 2.7 of the lecture notes, i.e. the 1D particle's motion in an infinite Dirac comb potential (Fig. 2.24), write explicit expressions for the eigenfunctions at the very bottom and at the very top of the lowest energy band. Sketch both functions.

*Solution:* According to Eq. (2.193b) of the lecture notes, at the *bottom* of the lowest energy band (i.e. in the ground state of the particle), where  $e^{iqa} = 1$ , the wavefunction is purely periodic:

$$\psi(x+a) = \psi(x).$$

Moreover, due to the mirror symmetry of the potential profile  $U(x)$  with respect to any point  $(ja + a/2)$ , where  $j$  is the comb period's number, the wavefunction also must have the same symmetry, in particular

$$\psi(x) = \psi(a-x).$$

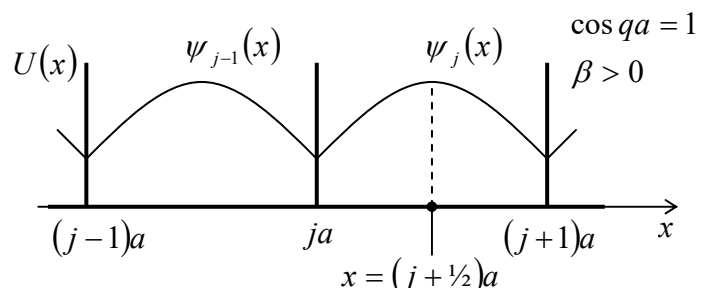
Finally, at each segment  $ja < x < (j+1)a$ , where  $U(x) = 0$ , the fundamental solutions of the stationary Schrödinger equation are  $\sin kx$  and  $\cos kx$ . Hence we may make an educated guess that at such a segment, the eigenfunction has the following simple form:

$$\psi(x) = \psi_j(x) = C \cos k \left( x - ja - \frac{a}{2} \right), \quad \text{for } \left| x - ja - \frac{a}{2} \right| < \frac{a}{2}, \quad (*)$$

(see the figure on the right), so on this segment,

$$\frac{d\psi_j}{dx} = -Ck \sin k \left( x - ja - \frac{a}{2} \right). \quad (**)$$

In order to confirm this solution, we may calculate the wave number  $k$  following from Eq. (\*) and the boundary condition (2.75) at any





point  $x = ja$ .<sup>71</sup> Plugging into that relation the expressions following from Eqs. (\*) and (\*\*),

$$\psi(ja) = C \cos \frac{ka}{2}, \quad \frac{d\psi_+(ja)}{dx} \equiv \frac{d\psi_j(ja)}{dx} = Ck \sin \frac{ka}{2}, \quad \frac{d\psi_-(ja)}{dx} \equiv \frac{d\psi_{j-1}(ja)}{dx} = -Ck \sin \frac{ka}{2},$$

and dividing both parts of the resulting equation by  $2Ck$ , we get

$$\sin \frac{ka}{2} = \frac{m\mathcal{W}}{\hbar^2 k} \cos \frac{ka}{2}, \quad \text{i.e.} \quad \sin \frac{ka}{2} = \frac{\beta}{ka} \cos \frac{ka}{2}, \quad (***)$$

where  $\beta$  is the (only) dimensionless parameter of the problem, given by Eq. (2.197) of the lecture notes:

$$\beta \equiv \frac{m\mathcal{W}a}{\hbar^2}.$$

Multiplying both parts of Eq. (\*\*\*) by  $2\sin(ka/2)$ , and then using the trigonometric identities<sup>72</sup>  $2\sin^2\xi = 1 - \cos 2\xi$  and  $2\sin\xi\cos\xi = \sin 2\xi$ , we may rewrite it in the form

$$1 - \cos ka = \frac{\beta}{ka} \sin ka.$$

But this is exactly the result given by the general characteristic equation (2.198) of the system,

$$\cos qa = \cos ka + \frac{\beta}{ka} \sin ka, \quad (***)$$

for our particular set of quasimomentum values, with  $\cos qa = 1$ .

Next, according to the same Eq. (2.193b), the wavefunction corresponding to the *top* of the lowest energy band, i.e. to  $e^{iqa} = -1$ , changes its sign each lattice period:

$$\psi(x+a) = -\psi(x).$$

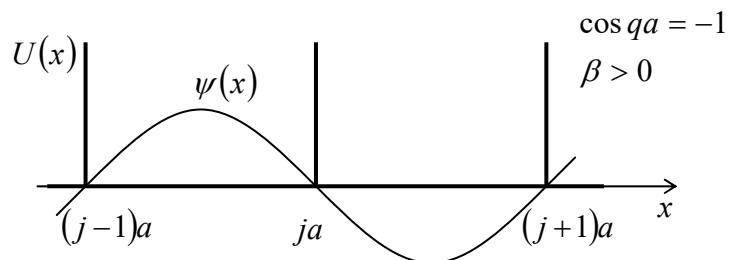
Besides that, as the dispersion relation (\*\*\*) shows (see its plot, for a fixed  $\alpha$ , in Fig. 2.25 of the lecture notes), at the top points of the lowest band,  $\cos qa = -1$  regardless of the parameter  $\beta$ . This is only possible if the wavefunction does not interact with delta-functional potential peaks, i.e.  $\psi(ja) = 0$ . The only linear combination of  $\sin ka$  and  $\cos ka$  satisfying these conditions is a pure sine function with its nodes at points  $x = ja$ :

$$\psi(x) = C \sin kx, \quad \text{with } ka = \pi n, \quad \text{for } n = 1, 2, \dots$$

At the lowest energy band,  $n = 1$ , i.e.  $ka = \pi$ . This function, shown in the figure on the right, has  $\psi(ja) = 0$  and

$$\frac{d\psi_+(ja)}{dx} = \frac{d\psi_-(ja)}{dx},$$

so it satisfies both boundary conditions (2.75) and (2.76), for any value of  $\mathcal{W}$ .



<sup>71</sup> Eq. (\*) automatically satisfies the boundary condition given by Eq. (2.76).

<sup>72</sup> See, e.g., MA Eqs. (3.3d).

**Problem 2.26.** A 1D particle of mass  $m$  moves in an infinite periodic system of very narrow and deep potential wells that may be described by delta functions:

$$U(x) = w \sum_{j=-\infty}^{+\infty} \delta(x - ja), \quad \text{with } w < 0.$$

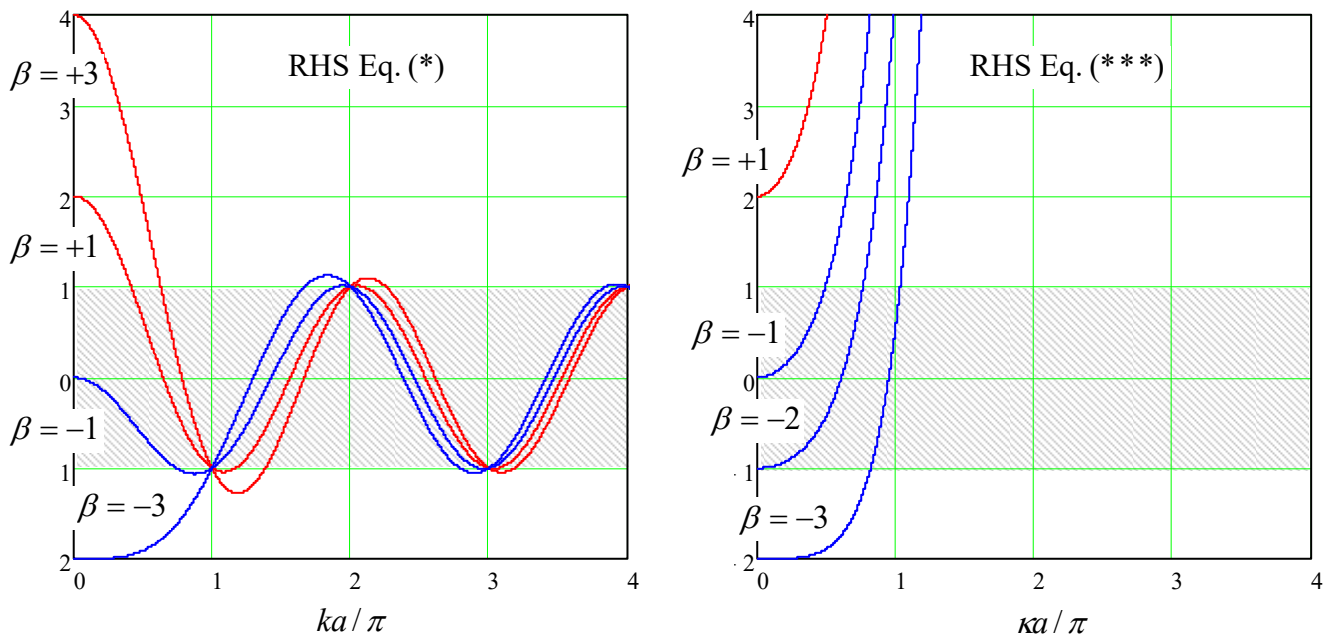
- (i) Sketch the energy band structure of the system for very small and very large values of the potential well's "weight"  $|w|$ , and  
 (ii) calculate explicitly the ground-state energy of the system in these two limits.

*Solutions:*

(i) This system is similar to the Dirac comb potential analyzed at the beginning of Sec. 2.7 of the lecture notes (see Fig. 2.24 and its discussion), but with the negative sign of  $w$ , and hence of the parameter  $\beta \equiv ma w / \hbar^2$  – see Eq. (2.197). As a result, its characteristic equation has the same form (2.198),

$$\cos qa = \cos ka + \beta \frac{\sin ka}{ka}, \quad (*)$$

but now should be analyzed for the case  $\beta < 0$ . For a comparison of these two cases, the left panel of the first figure below shows the plots of the right-hand side of Eq. (\*) for two representative values of  $|\beta|$ , each for two opposite signs of this parameter.



For  $\beta > 0$ , i.e. for the Dirac comb, these plots (which are similar to those shown in Fig. 2.25 of the lecture notes, but now with the parameter  $\beta$  rather than  $\alpha \equiv \beta/(ka)$  considered fixed) give the picture of the energy bands (with  $-1 < \cos qa < +1$ ) and gaps, that was discussed in detail in Sec. 2.7, with all energies  $E_n(q) > 0$  – see the first and the third top panels of the second figure below.<sup>73</sup> However, for our

<sup>73</sup> Just to save space, these plots are limited to one-half of the first Brillouin zone. In these plots, as in Fig. 2.26(b) of the lecture notes,  $E_0 \equiv \hbar^2/2ma^2$  – the natural energy scale of this problem.

current case  $\beta < 0$ , only the higher energy bands are (qualitatively) similar – see the second and the fourth top panels in that figure, while the lowest energy band is either completely absent (for  $\beta < -2$ ), or hits the horizontal axis ( $E = 0$ ) at a certain value of the quasimomentum  $q$ .

The explanation of this behavior is straightforward. In contrast with the case  $\mathcal{W} > 0$ , when  $U(x) \geq 0$  at any  $x$ , so the total (potential plus kinetic) energy cannot be negative, in the case  $\mathcal{W} < 0$ , the potential energy  $U(x) \leq 0$  at all points, so  $E_n(q)$  can be negative for some  $\beta$ ,  $n$ , and  $q$ . According to the definition of the parameter  $k$  (see Eq. (2.54) of the lecture notes),

$$k^2 \equiv \frac{2mE}{\hbar^2},$$

in order to calculate the dispersion curve branches with  $E_n(q) < 0$ , we have to take  $k = \pm i\kappa$ , with

$$\kappa^2 \equiv -\frac{2mE}{\hbar^2} \equiv \frac{2m|E|}{\hbar^2}. \quad (**)$$

With this substitution, Eq. (\*) takes the form

$$\cos qa = \cosh \kappa a + \beta \frac{\sinh \kappa a}{\kappa a}. \quad (***)$$

The right-hand side of this equation is plotted, as a function of  $\kappa a$ , on the right panel of the figure above, for several values of  $\beta$ . The plots show that for any positive  $\beta$ , this function is always larger than +1, so the equation does not have any real solutions for the quasimomentum  $q$ . Hence, in agreement with the above argument, the dispersion curves cannot spill into the negative energy region. However, for each  $\beta < 0$ , there is a (single!) range of the argument  $\kappa a$  where the right-hand side is in the range from  $-1$  to  $+1$ , giving either (for  $\beta < -2$ ) the whole lowest branch of the dispersion relation, or (for  $-2 < \beta < 0$ ) just its part – see the plots in the lower two subpanels of the figure below, which have been calculated numerically from Eqs. (\*\*) and (\*\*\*).

(ii) The lowest point  $E_1(0)$  of the lowest band, i.e. the ground state energy of the system, may be found from Eqs. (\*\*) and (\*\*\*) with  $q$  equal to any multiple of  $2\pi/a$ , i.e. with  $\cos qa = 1$ :

$$E_g \equiv E_1(0) = -\frac{\hbar^2 \kappa^2}{2m}, \quad \text{with } \cosh \kappa a + \beta \frac{\sinh \kappa a}{\kappa a} = 1, \quad \text{for } \beta \leq 0. \quad (***)$$

Since  $\sinh \kappa a > \kappa a$ , and  $\cosh \kappa a > 1$  for any  $\kappa a > 0$ , the (only) solution of this characteristic equation is real, and hence  $E_g < 0$ , for any  $\beta < 0$ . In particular, if  $\mathcal{W} \rightarrow 0$ , i.e.  $\beta \rightarrow 0$ , then  $\kappa a \rightarrow 0$ , and we may use the Taylor expansions  $\sinh \kappa a \approx \kappa a$  and  $\cosh \kappa a \approx 1 + (\kappa a)^2/2$  to find:

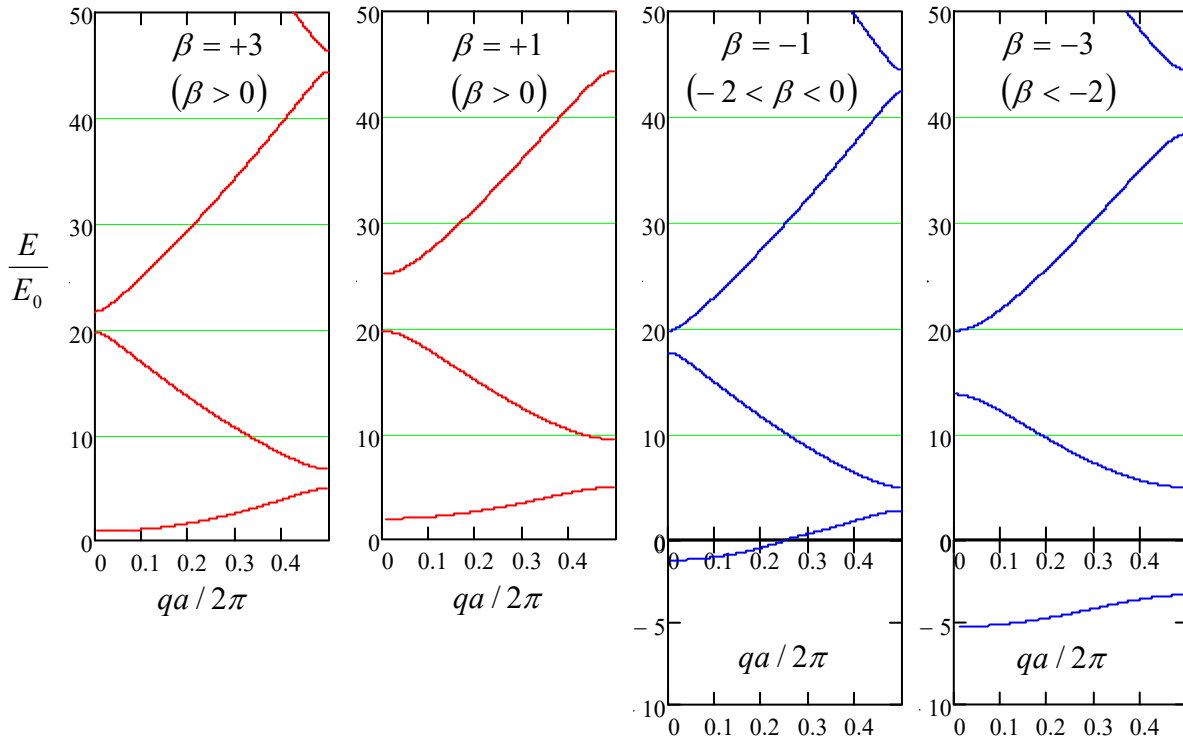
$$\frac{(\kappa a)^2}{2} \approx -\beta, \quad E_g \approx -2\beta E_0 \equiv -\frac{\mathcal{W}}{a}.$$

Note that this  $E_g$  is just the spatial-average potential energy,  $\bar{U} = -\mathcal{W}/a$ , of the system. As Eq. (\*) with  $k = 0$  shows, in this limit, the lowest energy band spills into the negative-energy region only at very small values of the quasimomentum,  $qa < (2|\beta|)^{1/2} \ll 1$ .

On the other hand, in the opposite limit  $\beta \rightarrow -\infty$ , both hyperbolic functions of  $\kappa a$  may be well approximated with  $\exp\{\kappa a/2\}/2 \gg 1$ , and the unity on the right-hand side of the characteristic equation (\*\*\*\*) is negligible. This approximation yields

$$\kappa a \approx -\beta, \quad E_g \approx -\beta^2 E_0 \equiv -\frac{\omega^2 m}{2\hbar^2}.$$

This is exactly the energy of the (only) localized eigenstate of a single well – see Eq. (2.162) of the lecture notes. This is natural because the limit  $\beta \rightarrow -\infty$  corresponds to a system of very deep and hence virtually uncoupled potential wells. (As Eq. (\*\*\*) shows, in this limit, the lowest allowed energy band is exponentially narrow.)



**Problem 2.27.** For the system discussed in the previous problem, write explicit expressions for the eigenfunctions of the system, corresponding to:

- (i) the bottom of the lowest energy band,
- (ii) the top of that band, and
- (iii) the bottom of each higher energy band.

Sketch these functions.

*Solutions:*

(i) As the solution of the previous problem has shown, the wave number  $k$  corresponding to the ground state energy of the system is imaginary,  $k = \pm i\kappa$ , for any  $\omega < 0$ , and hence the wavefunction at any segment  $ja < x < (j+1)a$  has to be a linear combination of  $\sinh\kappa a$  and  $\cosh\kappa a$ . Next, according to the Bloch theorem (2.193), at the bottom points of the lowest energy band (i.e. in the ground state of the system), where  $e^{iqa} = 1$ , the wavefunction has to be periodic:

$$\psi(x+a) = \psi(x).$$

Moreover, due to the mirror symmetry of the potential profile  $U(x)$  with respect to any point  $(ja + a/2)$ , the wavefunction also should have the same symmetry, in particular

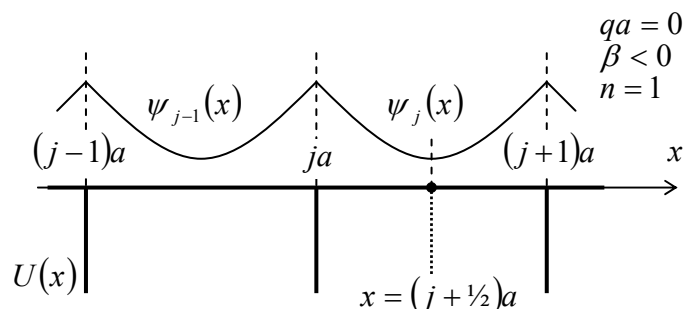
$$\psi(x) = \psi(a - x).$$

Hence we may conjecture that the eigenfunction has the following form:

$$\psi(x) = \psi_j(x) = C \cosh \kappa \left( x - ja - \frac{a}{2} \right), \quad \text{at } ja < x < (j+1)a, \quad (*)$$

(see the figure on the right), so

$$\begin{aligned} \frac{d\psi_j}{dx}(x) &= C\kappa \sinh \kappa \left( x - ja - \frac{a}{2} \right), \\ \frac{d\psi_j}{dx}(ja) &= -\frac{d\psi_{j-1}}{dx}(ja) = -C\kappa \sinh \frac{\kappa a}{2}, \\ \psi(ja) &= C \cosh \frac{\kappa a}{2}. \end{aligned}$$



Plugging these expressions into the only remaining<sup>74</sup> boundary condition (2.75),

$$\frac{d\psi_j}{dx} - \frac{d\psi_{j-1}}{dx} = \frac{2m}{\hbar^2} \omega \psi_j, \quad \text{at } x = ja,$$

we get, after the division of both parts by  $2C\kappa$ , the following characteristic equation:

$$-\sinh \frac{\kappa a}{2} = \frac{m\omega}{\hbar^2 k} \cosh \frac{\kappa a}{2}, \quad \text{i.e. } -\sinh \frac{\kappa a}{2} = \frac{\beta}{\kappa a} \cosh \frac{\kappa a}{2}, \quad (**)$$

where  $\beta$  is the system's dimensionless parameter defined by Eq. (2.197) of the lecture notes:

$$\beta \equiv \frac{m\omega a}{\hbar^2}.$$

Now multiplying both parts of Eq. (\*\*) by  $2\sinh(\kappa a/2)$ , and then using the identities<sup>75</sup>  $2\sinh^2 \xi = \cosh 2\xi - 1$  and  $2\sinh \xi \cosh \xi = \sinh 2\xi$ , we may rewrite this characteristic equation in the form

$$1 = \cosh \kappa a + \frac{\beta}{\kappa a} \sinh \kappa a.$$

But this is exactly the result given by the general characteristic equation of the system, obtained in the solution of the previous problem,

$$\cos qa = \cosh \kappa a + \frac{\beta}{\kappa a} \sinh \kappa a, \quad \text{for } \beta < 0, E < 0, \quad (***)$$

for our particular case  $\cos qa = +1$ . This agreement confirms our conjecture (\*).

(ii) At the top points of the lowest energy band,  $\exp\{iqa\} = -1$ , so, according to the Bloch theorem, the eigenfunctions at each period of the system are similar, but with alternating signs:

$$\psi(x+a) = -\psi(x).$$

Also, the eigenfunctions should be, at all points  $x \neq ja$ , the solutions of the Schrödinger equation with  $U(x) = 0$ , i.e. be linear superpositions of either  $\sin kx$  and  $\cos kx$  (for  $E > 0$ ) or  $\sinh \kappa x$  and  $\cosh \kappa x$  (for at  $E$

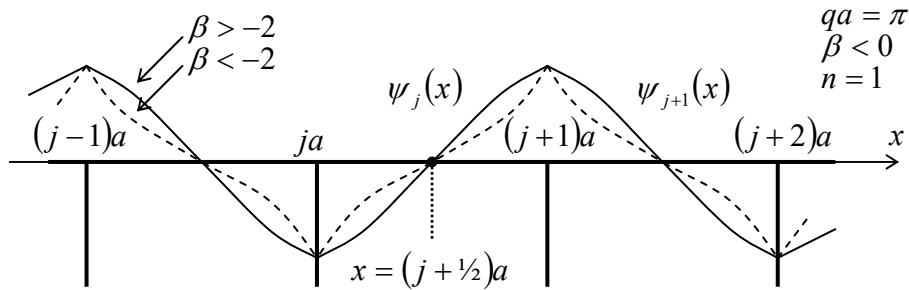
<sup>74</sup> Indeed, our solution (\*), by construction, satisfies the boundary condition (2.76):  $\psi_{j+1}(x) - \psi_j(x) = 0$  at  $x = ja$ .

<sup>75</sup> They may be readily proved using either the definition of hyperbolic functions or MA Eqs. (3.3d) and (3.5).

$< 0$ ). (As was discussed in the previous problem, at the top of this band (i.e. at  $\cos qa = -1$ ), the sign of the eigenenergy  $E$  depends on whether the parameter  $\beta$  is larger or smaller than  $-2$ .)

Moreover, as the general characteristic equations for  $E < 0$  and  $E > 0$  show (see the plots of their right-hand sides in the solution of the previous problem), for  $\beta < 0$ , at the top points of the lowest band,  $ka$  is not equal to  $qa$  (as it is at for  $\beta > 0$ ), so the states do “interact” with the delta-functional potential wells located at  $x = ja$ , i.e. their wavefunctions cannot be equal to zero at these points. As a result, we may conjecture that the wavefunction has one of the following forms (see sketches in the figure below):

$$\psi(x) = \psi_j(x) = (-1)^j C \times \begin{cases} \sin k \left( x - ja - \frac{a}{2} \right), & \text{for } \beta > -2, \\ \sinh \kappa \left( x - ja - \frac{a}{2} \right), & \text{for } \beta < -2, \end{cases} \quad (****)$$



so

$$\frac{d\psi_j}{dx}(x) = (-1)^j C \times \begin{cases} k \cos k \left( x - ja - \frac{a}{2} \right), & \text{for } \beta > -2, \\ \kappa \cosh \kappa \left( x - ja - \frac{a}{2} \right), & \text{for } \beta < -2. \end{cases} \quad \text{at } ja < x < (j+1)a.$$

We may readily verify this picture by using the same boundary condition as in Task (i),

$$\frac{d\psi_j}{dx} - \frac{d\psi_{j-1}}{dx} = \frac{2m}{\hbar^2} \omega \psi_j, \quad \text{at } x = ja,$$

with an arbitrary integer  $j$ . For our wavefunctions (\*\*\*\*) this condition yields, respectively,

$$(-1)^j Ck \cos \frac{ka}{2} - (-1)^{j-1} Ck \cos \frac{ka}{2} = -\frac{2m}{\hbar^2} \omega (-1)^j C \sin \frac{ka}{2}, \quad \text{for } \beta > -2,$$

$$(-1)^j C\kappa \cosh \frac{\kappa a}{2} - (-1)^{j-1} C\kappa \cosh \frac{\kappa a}{2} = -\frac{2m}{\hbar^2} \omega (-1)^j C \sinh \frac{\kappa a}{2}, \quad \text{for } \beta < -2.$$

After the division of all terms by  $2(-1)^j Ck$ , and using the definition of the parameter  $\beta$ , these equations are reduced to

$$\cos \frac{ka}{2} = -\frac{\beta}{ka} \sin \frac{ka}{2}, \quad \text{for } \beta > -2,$$

$$\cosh \frac{\kappa a}{2} = -\frac{\beta}{\kappa a} \sinh \frac{\kappa a}{2}, \quad \text{for } \beta < -2.$$

Multiplying these characteristic equations, respectively, by  $2\cos(ka/2)$  and  $2\cosh(\kappa a/2)$ , and using the well-known identities

$$2 \cos^2 \xi = 1 + \cos 2\xi, \quad 2 \sin \xi \cos \xi = \sin 2\xi; \quad 2 \cosh^2 \xi = 1 + \cosh 2\xi, \quad 2 \sinh \xi \cosh \xi = \sinh 2\xi,$$

we may recast them in the form

$$-1 = \cos ka + \beta \frac{\sin ka}{ka}, \quad \text{for } \beta > -2,$$

$$-1 = \cosh \kappa a + \beta \frac{\sin \kappa a}{\kappa a}, \quad \text{for } \beta < -2.$$

But these are exactly the general characteristic equations derived in Sec. 2.7 of the lecture notes and in the solution of the previous problem, taken for our current case:  $\cos qa = -1$ . Hence Eqs. (\*\*\*\*) indeed give the required eigenfunctions.

(iii) A bit counter-intuitively, the wavefunctions corresponding to the bottom points of the higher energy bands (with  $n > 1$ ) differ substantially from those given by both Eq. (\*) and Eqs. (\*\*\*\*), valid for  $n = 1$  only. Indeed, as was discussed in the model solution of the previous problem, at those points  $E > 0$ , so we have to look at the dispersion relation (2.198) derived in Sec. 2.7 of the lecture notes for this case:

$$\cos qa = \cos ka + \beta \frac{\sin ka}{ka},$$

but with  $\beta < 0$ .

As the blue-line plots of the right-hand side of this characteristic equation in the figure on the right<sup>76</sup> show, the allowed energy minima for  $n > 1$  correspond to  $\sin ka = 0$  (but  $ka \neq 0$ ) independently of the parameter  $\beta$ . This is only possible if the eigenstate does not interact with delta-functional potential peaks, i.e. if  $\psi(ja) = 0$ . The only linear combination of  $\sin ka$  and  $\cos ka$  satisfying this condition is a pure sine function, with its nodes at points  $x = ja$ :<sup>77</sup>

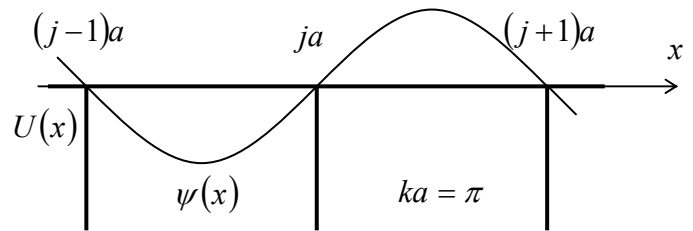
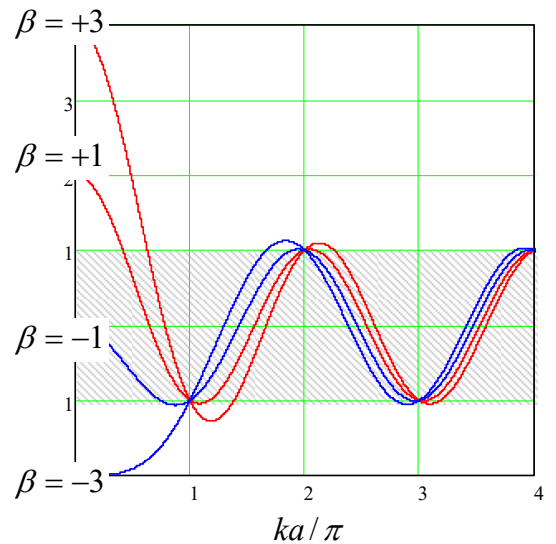
$$\psi(x) = C \sin kx; \quad \text{with } ka = \pi(n-1), \quad \text{for } n = 2, 3, \dots$$

(For example, at the lowest of such energy bands, with  $n = 2$ , this relation yields  $ka = \pi$ , giving the wavefunction sketched in the figure on the right.)

Such functions, with  $\psi(ja) = 0$  and

$$\frac{d\psi_+(ja)}{dx} = \frac{d\psi_+(ja)}{dx},$$

automatically satisfy both boundary conditions (2.75) and (2.176), for any value of  $\beta$ .



<sup>76</sup> These plots were already discussed in the model solution of the previous problem, and are reproduced here just for the reader's convenience.

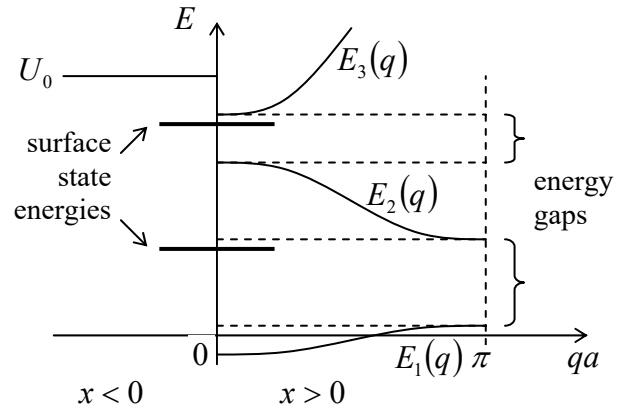
<sup>77</sup> As the red lines in the figure above show (and as was discussed in the solution of Problem 25), in a similar system, but with  $\beta > 0$ , such simple solutions, with  $ka = n\pi$ , are implemented at the top rather than bottom points of each energy band.

**Problem 2.28.\*** The 1D “crystal” analyzed in the last two problems, now extends only to  $x > 0$ , with a sharp potential step to a flat potential plateau at  $x < 0$ :

$$U(x) = \begin{cases} w \sum_{j=1}^{+\infty} \delta(x - ja), & \text{with } w < 0, & \text{for } x > 0, \\ U_0 > 0, & & \text{for } x < 0. \end{cases}$$

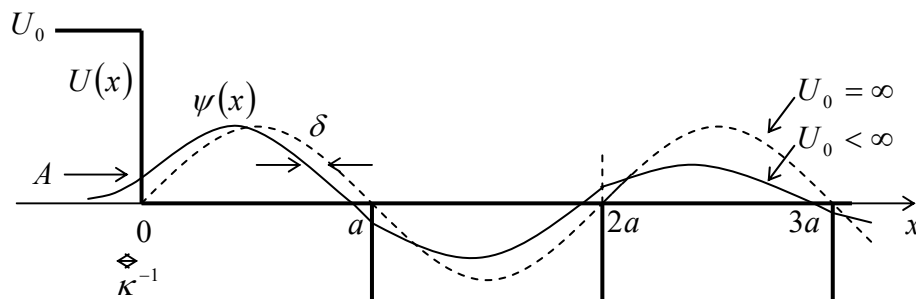
Prove that the system has a set of the so-called *Tamm states* localized near the “surface”  $x = 0$ , and calculate their energies in the limit when  $U_0$  is very large but finite. (Quantify this condition.)<sup>78</sup>

*Solution:* Let us start with a semi-qualitative observation. A localized wavefunction should be unable to propagate to either  $x \rightarrow -\infty$  or  $x \rightarrow +\infty$ . This means that the corresponding eigenenergy  $E$  should be, first, lower than  $U_0$ , and also inside one of the energy gaps of an infinite “crystal” with the same parameters as our semi-infinite one – see the figure on the right.<sup>79</sup>



For a quantitative analysis of the Tamm states, let us notice that in the limit  $U_0 = \infty$ , the simple bottom-of-the-band states discussed in Task (iii) of the previous problem (see the dashed line in the figure below, drawn here for the particular case of the second energy band) are not affected by the crystal termination at  $x = 0$ . Indeed, their wavefunctions vanish at  $x = 0$ , and hence their parts located at  $x \geq 0$  are exactly the same as in a similar but infinite crystal. Now, if  $U_0$  is large but finite, then, as we know from Sec. 2.3 of the lecture notes (see in particular Eq. (2.58) and Fig. 2.4), the wavefunction penetrates the classically forbidden region  $x < 0$  by a small distance  $\sim \kappa^{-1}$  – see the solid line in the figure below:

$$\psi(x \leq 0) \equiv \psi_-(x) \equiv Ae^{\kappa x}, \quad \frac{d\psi_-}{dx} = A\kappa e^{\kappa x}, \quad \text{where } \frac{\hbar^2 \kappa^2}{2m} = U_0 - E,$$



<sup>78</sup> In applications to electrons in solid-state crystals, such delta-potential wells model the attractive potentials of the atomic nuclei, while  $U_0$  represents the workfunction, i.e. the energy necessary for the extraction of an electron from the crystal to the free space – see, e.g., lecture notes QM Sec. 1.1(ii), and also EM Sec. 2.6 and SM Sec. 6.3.

<sup>79</sup> This figure uses a somewhat strange but very common (and hopefully, self-explanatory) format, displaying the system’s energy not only as a function of the quasimomentum  $q$  (for the bulk states), but also (very crudely) as a function of the wavefunction’s location in space.



so

$$\psi_-(0) = A, \quad \frac{d\psi_-}{dx}(0) = A\kappa. \quad (*)$$

Since the function and its first derivative have to be continuous at  $x = 0$ , this shift to the left “pulls” the wavefunction in the allowed regions  $x > 0$  to the left by a comparable distance  $\delta \sim 1/\kappa$ . This shift leads to some interaction of the wavefunction, now not vanishing at  $x = ja$ , with the delta-functional potential wells at these points, creating, according to Eq. (2.75) of the lecture notes, “cusps” (derivative jumps) of the initially smooth wavefunction. These cusps, in turn, result in the decrease of the sinusoidal wavefunction’s amplitude, by some factor  $0 < \lambda < 1$  (see the solid-line sketch in the figure above), eventually resulting in its full decay at  $x \rightarrow \infty$ , i.e. to the state’s localization near the “surface”.

These arguments allow us to guess that the wavefunction at  $x \geq 0$  has the following form:

$$\psi(x) = \psi_j(x) = C(-1)^j \lambda^j \sin k(x - ja + \delta), \quad \text{for } ja < x < (j+1)a,$$

so

$$\begin{aligned} \psi_j(ja) &= C(-1)^j \lambda^j \sin k\delta, & \psi_{j-1}(ja) &= C(-1)^{j-1} \lambda^{j-1} \sin k(a + \delta) \\ \frac{d\psi_j}{dx}(x) &= C(-1)^j \lambda^j k \cos k(x - ja + \delta), \\ \frac{d\psi_j}{dx}(ja) &= C(-1)^j \lambda^j k \cos k\delta, & \frac{d\psi_{j-1}}{dx}(ja) &= C(-1)^{j-1} \lambda^{j-1} k \cos k(a + \delta), \end{aligned}$$

This wavefunction, with the wave number  $k$  simply related to the state’s energy  $E$ :

$$\frac{\hbar^2 k^2}{2m} = E,$$

is an exact solution of the Schrödinger equation between the delta-functional wells, so we need only to satisfy all boundary conditions at the special points  $x = ja$  with  $j \geq 0$ . With the account of Eqs. (\*), the boundary conditions at  $x = 0$ :

$$\psi_0(0) - \psi_-(0) = 0, \quad \frac{d\psi_0}{dx}(0) - \frac{d\psi_-}{dx}(0) = 0,$$

yield, after the exclusion of the  $C/A$  ratio, one equation for three so-far unknown parameters  $\delta$ ,  $\lambda$ , and  $k$ :

$$k \cos k\delta = \kappa \sin k\delta. \quad (**)$$

Two other equations for these parameters may be found from the boundary conditions (2.75)-(2.76) written for any point  $x = ja$  with  $j > 0$ :

$$\psi_j(ja) - \psi_{j-1}(ja) = 0, \quad \frac{d\psi_j}{dx}(ja) - \frac{d\psi_{j-1}}{dx}(ja) = \frac{2m\omega}{\hbar^2} \psi_j(ja).$$

After the substitution of the assumed form of  $\psi_j$  and the cancellation of the common factors  $C(-1)^j \lambda^{j-1}$ , these two equalities become

$$\lambda \sin k\delta + \sin k(a + \delta) = 0, \quad \lambda k \cos k\delta + k \cos k(a + \delta) = \frac{2m\omega}{\hbar^2} \lambda \sin k\delta.$$

From these two relations,  $\lambda$  may be readily eliminated, reducing them to just one equation,

$$\sin ka = \frac{2\beta}{ka} \sin k(a + \delta) \sin k\delta, \quad (***)$$

where  $\beta$  is the dimensionless parameter of the “crystal”, defined by Eq. (2.197) of the lecture notes:

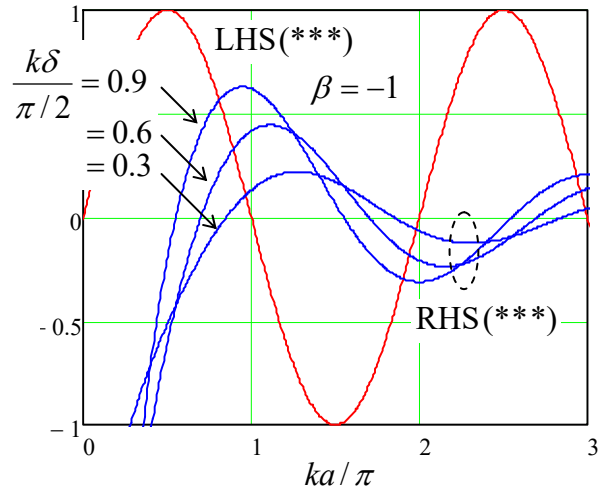
$$\beta \equiv \frac{m\omega a}{\hbar^2}.$$

(In our current problem,  $\omega < 0$ , and hence  $\beta < 0$ , though the Tamm states may also exist at  $\omega > 0$ .) The fact that our wavefunction assumption has led to two  $j$ -independent characteristic equations (\*\*) and (\*\*\*) for two unknown parameters  $\delta$  and  $k$  (assuming that  $\kappa$  is known<sup>80</sup>) proves that this guess was indeed correct – for arbitrary  $U_0$  and for any energy band number  $n$ .

Proceeding to the analysis of these equations, let us notice that Eq. (\*\*), rewritten as

$$\tan k\delta = \frac{k}{\kappa} \equiv \left( \frac{E}{U_0 - E} \right)^{1/2}, \quad (***)$$

shows that for any energy within the range of our interest,  $0 \leq E \leq U_0$ , the product  $k\delta$  is a monotonic function of  $E$ , and is confined to the interval  $[0, +\pi/2]$ . The figure on the right shows the plots of the left-hand and right-hand sides of Eq. (\*\*\*) as functions of the product  $ka$ , for several values of  $k\delta$  from that interval, and a modest negative value of  $\beta$ . (The variation of this parameter does not change the topological properties of the equation’s solutions.) The plots show that the equation has just one solution for  $ka$  somewhat below each value  $\pi(n - 1)$  corresponding to the bottom of the  $n^{\text{th}}$  energy band – see the solution of the previous problem. This means that the system has just one Tamm state inside each energy gap – see the energy scheme at the very beginning of this solution.



The plots also indicate the way to solve this equation analytically when  $U_0 \gg E$ , so  $k\delta \rightarrow 0$ , and as a result, the product  $ka$  is only slightly below  $\pi(n - 1)$ , i.e. the Tamm state’s energy is right below the  $n^{\text{th}}$  energy band’s bottom,<sup>81</sup>

$$(E_n)_{\min} = \frac{\pi^2 \hbar^2}{2ma^2} (n - 1)^2.$$

Indeed, in this limit, we may take  $ka = \pi[(n - 1) - \eta]$ , and expand both parts of Eq. (\*\*\*) in the Taylor series in small parameters  $(k\delta)^2$  and  $\eta$ , dropping all the terms but the leading ones. Such expansion, after the cancellation of the common multiplier  $\cos \pi(n - 1)$ , reduces Eq. (\*\*\*) to

<sup>80</sup> An explicit relation between  $k \equiv (2mE)^{1/2}/\hbar$  and  $\kappa \equiv [2m(U_0 - E)]^{1/2}/\hbar$  enables finding the state’s energy  $E$ , and hence all other characteristics of the system.

<sup>81</sup> In the similar limit, but at  $\omega > 0$ , the Tamm state’s energy, inside the same bandgap, is close to the *top* of the previous,  $(n - 1)^{\text{th}}$  energy band.

$$\eta \approx -\frac{2\beta}{\pi^2(n-1)}(k\delta)^2.$$

Now by using Eq. (\*\*\*\*), which in this limit  $U_0 \gg E$  is reduced to  $k\delta \approx (E/U_0)^{1/2}$ , we may continue as

$$\eta \approx -\frac{2\beta}{\pi^2(n-1)} \frac{(E_n)_{\min}}{U_0} \equiv \frac{(n-1)|w|}{aU_0},$$

so the distance between the Tamm level and the bottom of the  $n^{\text{th}}$  energy band is

$$\Delta E_n \equiv (E_n)_{\min} - E = \frac{\hbar^2}{2ma^2} \left\{ \pi^2(n-1)^2 - \pi^2[(n-1) - \eta]^2 \right\} \approx \frac{\hbar^2}{ma^2} \eta \pi^2(n-1) \approx 2(E_n)_{\min} \frac{|w|}{aU_0}.$$

Note also that in this limit, the wavefunction decay parameter  $\lambda$  is very close to 1:

$$\lambda = -\frac{\sin k(a+\delta)}{\sin k\delta} \approx \frac{-\pi\eta + k\delta}{k\delta} \equiv 1 - \frac{\pi\eta}{k\delta} \approx 1 - \frac{2|\beta|}{\pi(n-1)} k\delta \approx 1 - \frac{2|\beta|}{\pi(n-1)} \left( \frac{E}{U_0} \right)^{1/2},$$

so the scale  $\Delta x \equiv a/(1-\lambda)$  of the Tamm state's extension into the "crystal" is much larger than  $a$ .

These results are quantitatively valid if the dimensionless parameters  $k\delta$  and  $\eta$  are much smaller than 1, i.e. when

$$U_0 \gg \frac{(n-1)|w|}{a}, (E_n)_{\min}.$$

In conclusion, note that these states, named after I. Tamm (who was the first to predict them in 1932), are just one species of a general class of *surface states*. (Another important member of this class is the so-called *Shockley states*, described by a different theoretical model.)<sup>82</sup>

**Problem 2.29.** Calculate the transfer matrix of the rectangular potential barrier specified by Eq. (2.68) of the lecture notes, for particle energies both below and above  $U_0$ .

*Solution:* By either acting exactly as in Sec. 2.3 but with the account of an additional wave incident from the right or, even easier, using Eq. (2.71a) together with the universal relations mentioned in Sec. 2.5 (and derived in the model solution of Problem 15), we get the following transfer matrices

$$\mathbf{T}_d = \begin{pmatrix} \cosh \kappa d + \frac{i}{2} \left( \frac{k}{\kappa} - \frac{\kappa}{k} \right) \sinh \kappa d & -\frac{i}{2} \left( \frac{k}{\kappa} + \frac{\kappa}{k} \right) \sinh \kappa d \\ \frac{i}{2} \left( \frac{k}{\kappa} + \frac{\kappa}{k} \right) \sinh \kappa d & \cosh \kappa d - \frac{i}{2} \left( \frac{k}{\kappa} - \frac{\kappa}{k} \right) \sinh \kappa d \end{pmatrix}, \quad \text{for } 0 \leq E \leq U_0,$$

$$\mathbf{T}_d = \begin{pmatrix} \cos k'd + \frac{i}{2} \left( \frac{k}{k'} + \frac{k'}{k} \right) \sin k'd & -\frac{i}{2} \left( \frac{k}{k'} - \frac{k'}{k} \right) \sin k'd \\ \frac{i}{2} \left( \frac{k}{k'} - \frac{k'}{k} \right) \sin k'd & \cos k'd - \frac{i}{2} \left( \frac{k}{k'} + \frac{k'}{k} \right) \sin k'd \end{pmatrix}, \quad \text{for } 0, U_0 \leq E.$$

<sup>82</sup> For more on this topic, see, e.g., S. Davison and M. Stęślicka, *Basic Theory of Surface States*, Clarendon, 1992.

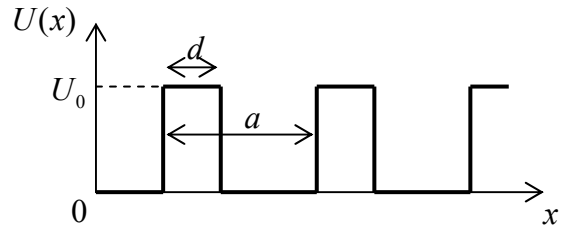
(If you use the second approach, the algebraic identity

$$\left[ \frac{1}{2} \left( \frac{k}{k'} + \frac{k'}{k} \right) \right]^2 - \left[ \frac{1}{2} \left( \frac{k}{k'} - \frac{k'}{k} \right) \right]^2 = 1,$$

is very handy for doing the calculations.)

As useful sanity checks, the top left elements ( $T_{11}$ ) of these expressions agree with Eq. (2.71b) of the lecture notes for  $\mathcal{F} = |T_{11}|^{-2}$ , and the matrices are reduced to Eq. (2.135) for the particular case of a very thin and high barrier ( $kd \ll \kappa d \ll 1$ ).

**Problem 2.30.** Use the results of the previous problem to calculate the transfer matrix of one period of the periodic Kronig-Penney potential shown in Fig. 2.31b of the lecture notes (reproduced on the right).



*Solution:* According to Eq. (2.132) of the lecture notes, in order to calculate the transfer matrix  $T$  of one potential's period starting from the potential barrier, it is sufficient to multiply the matrix  $T_d$  calculated in the previous problem by the transfer matrix (2.138) of the free-motion interval of the length  $(a-d)$ ,

$$T_{d-a} = \begin{pmatrix} e^{ik(a-d)} & 0 \\ 0 & e^{-ik(a-d)} \end{pmatrix}.$$

The result, for  $E < U_0$ , is

$$T = \begin{pmatrix} \left[ \cosh \kappa d + \frac{i}{2} \left( \frac{k}{\kappa} - \frac{\kappa}{k} \right) \sinh \kappa d \right] e^{ik(a-d)} & -\frac{i}{2} \left( \frac{k}{\kappa} + \frac{\kappa}{k} \right) \sinh \kappa d e^{-ik(a-d)} \\ \frac{i}{2} \left( \frac{k}{\kappa} + \frac{\kappa}{k} \right) \sinh \kappa d e^{ik(a-d)} & \left[ \cosh \kappa d - \frac{i}{2} \left( \frac{k}{\kappa} - \frac{\kappa}{k} \right) \sinh \kappa d \right] e^{-ik(a-d)} \end{pmatrix};$$

for  $E > U_0$ , it is sufficient to make the usual replacement (2.65):  $\kappa \rightarrow -ik$ .

At the alternative choice of the starting and ending points of the period (the free-motion interval first and the barrier next), the exponents in  $T_{12}$  and  $T_{21}$  would be complex-conjugated, with no effect on any observable result.

**Problem 2.31.** Using the results of the previous problem, derive the characteristic equations for a particle's motion in the periodic Kronig-Penney potential, for both  $E < U_0$  and  $E > U_0$ . Try to bring the equations to a form similar to that obtained in Sec. 2.7 of the lecture notes for the delta-functional barriers – see Eq. (2.198). Use the equations to formulate the conditions of applicability of the tight-binding and weak-potential approximations, in terms of the system's parameters and the particle's energy  $E$ .

*Solution:* Requiring the difference between the matrix  $T$  calculated in the previous problem for the case  $E < U_0$  and the diagonal Bloch matrix

$$\begin{pmatrix} e^{iqa} & 0 \\ 0 & e^{iqa} \end{pmatrix},$$

to have zero determinant, we get the following characteristic equation

$$\cos qa = \cosh \kappa d \cos k(a-d) + \frac{1}{2} \left( \frac{\kappa}{k} - \frac{k}{\kappa} \right) \sinh \kappa d \sin k(a-d). \quad (*)$$

Following the analysis of the periodic system of delta-functional barriers (see Fig. 2.25 and its discussion), we may notice that the right-hand side of this equation is a sinusoidal function of  $ka$ , and rewrite Eq. (\*) in the following equivalent form:

$$\cos qa = A \cos[k(a-d) + \varphi],$$

where  $\varphi$  is independent of  $a$  (and unimportant for our current purposes), while

$$A^2 = \cosh^2 \kappa d + \left[ \frac{1}{2} \left( \frac{k}{\kappa} - \frac{\kappa}{k} \right) \right]^2 \sinh^2 \kappa d \equiv 1 + \left[ \frac{1}{2} \left( \frac{k}{\kappa} + \frac{\kappa}{k} \right) \sinh \kappa d \right]^2, \quad (**)$$

so the characteristic diagram is topologically similar to that shown in Fig. 2.25 of the lecture notes – see the figure on the right.

The *tight-binding* approximation is applicable when an allowed energy band (with  $-1 \leq \cos qa \leq +1$ ) is much narrower than the adjacent energy gaps. As the figure on the right shows, this condition may be represented as  $A \gg 1$ , giving

$$\frac{1}{2} \left( \frac{k}{\kappa} + \frac{\kappa}{k} \right) \sinh \kappa d \gg 1, \quad (***)$$

or, in dimensional units,

$$\frac{U_0}{2[E(U_0 - E)]^{1/2}} \sinh \frac{[2m(U_0 - E)]^{1/2} d}{\hbar} \gg 1,$$

where  $E$  is close to one of the eigenvalues  $E^{(n)}$  of isolated potential wells – see Eq. (1.85):

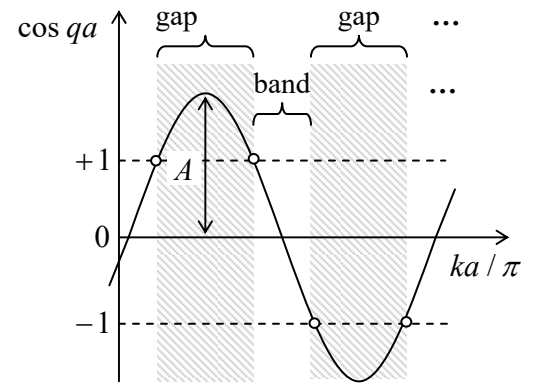
$$E \approx E^{(n)} \equiv \frac{\pi^2 \hbar^2}{2m(a-d)^2} n^2.$$

For analysis of the opposite case  $U_0 < E$ , we may use Eq. (\*\*) with the replacement (2.65):  $\kappa \rightarrow -ik'$ , getting

$$A^2 = \cos^2 k'd + \left[ \frac{1}{2} \left( \frac{k}{k'} + \frac{k'}{k} \right) \right]^2 \sin^2 k'd \equiv 1 + \left[ \frac{1}{2} \left( \frac{k}{k'} - \frac{k'}{k} \right) \sin k'd \right]^2,$$

so instead of Eq. (\*\*\*), we have to require

$$\frac{1}{2} \left( \frac{k}{k'} - \frac{k'}{k} \right) |\sin k'd| \gg 1, \quad \text{i.e.} \quad \frac{U_0}{2[E(E - U_0)]^{1/2}} \left| \sin \frac{[2m(E - U_0)]^{1/2} d}{\hbar} \right| \gg 1.$$



Let us analyze these conditions. If  $E < U_0$  ( $\kappa$  is real), virtually the only way to satisfy Eq. (\*\*\*) is to have sufficiently thick barriers,  $\kappa d \gg 1$ . (The only other option is to have a very low  $E \ll U_0$ , which requires an extremely large  $a - d \gg d$ .) In the opposite case,  $U_0 < E$ , since  $|\sin k'd|$  cannot exceed 1, the tight-binding approximation is only possible when  $E_n$  is almost exactly equal to  $U_0$ .

The *weak-potential* approximation requires, on the opposite, the parameter  $A$  to be very close to 1 – see the last figure above again. This requirement may be rewritten as  $(A^2 - 1)^{1/2} \ll 1$ , and if  $E < U_0$ , it reads

$$\frac{1}{2} \left( \frac{k}{\kappa} + \frac{\kappa}{k} \right) \sinh \kappa d \ll 1, \quad \text{i.e.} \quad \frac{U_0}{2[E(U_0 - E)]^{1/2}} \sinh \frac{[2m(U_0 - E)]^{1/2} d}{\hbar} \ll 1,$$

where now  $E$  is close to the branch anticrossing point – see Figs. 2.28 and its discussion in Sec. 2.7:

$$E \approx E^{(n)} \equiv \frac{\pi^2 \hbar^2}{2ma^2} n^2.$$

This condition may be only satisfied for very thin barriers,  $\kappa d \ll 1$ .

In the opposite case,  $U_0 < E$ , the weak-potential condition becomes

$$\frac{1}{2} \left( \frac{k}{k'} - \frac{k'}{k} \right) |\sin k'd| \ll 1, \quad \text{i.e.} \quad \frac{U_0}{2[E(E - U_0)]^{1/2}} \sin \left| \frac{[2m(E - U_0)]^{1/2} d}{\hbar} \right| \ll 1,$$

and, if  $E \gg U_0$ , is satisfied even for thick barriers because the magnitude of  $\sin k'd$  can never be larger than one.

To summarize these conditions, if the relative thickness of the barrier is appreciable ( $d \sim a$ ), the tight-binding approximation typically works well at  $E < U_0$ , while at  $U_0 \ll E$ , the weakly-potential limit is typically applicable. Semi-quantitatively, this is exactly the behavior visible at the characteristic curves of the Mathieu equation – see Fig. 2.32 in the lecture notes.

**Problem 2.32.** For the Kronig-Penney potential, use the tight-binding approximation to calculate the widths of the allowed energy bands. Compare the results with those of the previous problem (in the corresponding limit).

*Solution:* According to Eq. (2.206) of the lecture notes, in the tight-binding limit, the allowed energy band's width  $\Delta E_n$  equals  $4 |\delta_n|$ , where  $\delta_n$  is given by Eq. (2.204):

$$\delta_n = \frac{\hbar^2}{m} u_n(x_0) \frac{du_n}{dx}(a - x_0), \quad (*)$$

where  $u_n$  are the localized wavefunctions of an isolated potential well. For the Kronig-Penney potential, the wells are rectangular and their eigenfunctions were calculated in the solution of Problem 21. In that solution, the well's width was denoted as  $a$ , and should be replaced with  $(a - d)$  in our current notation – see Fig. 2.31b. With this replacement (but still keeping the origin of  $x$  in the well's middle), the solution takes the following form:

(i) Antisymmetric eigenfunctions, implemented at odd  $n = 1, 3, \dots$ :

$$u_n = C \times \begin{cases} \sin kx, & \text{for } |x| \leq \frac{a-d}{2}, \\ \operatorname{sgn}(x) \sin \frac{k(a-d)}{2} \exp\left\{-\kappa\left(|x| - \frac{a-d}{2}\right)\right\}, & \text{for } \frac{a-d}{2} \leq |x|, \end{cases}$$

with the following relation between  $k$  and  $\kappa$ :

$$\tan \frac{k(a-d)}{2} = -\frac{k}{\kappa}, \quad \text{giving} \quad \sin \frac{k(a-d)}{2} = -\frac{k}{K}, \quad \cos \frac{k(a-d)}{2} = \frac{\kappa}{K}, \quad (**)$$

where  $K^2 \equiv k^2 + \kappa^2 = 2mU_0/\hbar^2$ .

(ii) Symmetric eigenfunctions, corresponding to even  $n = 0, 2, 4, \dots$ :

$$u_n = C \times \begin{cases} \cos kx, & \text{for } |x| \leq \frac{a-d}{2}, \\ \cos \frac{k(a-d)}{2} \exp\left\{-\kappa\left(|x| - \frac{a-d}{2}\right)\right\}, & \text{for } \frac{a-d}{2} \leq |x|, \end{cases}$$

with a different relation between  $k$  and  $\kappa$ ,

$$\tan \frac{k(a-d)}{2} = \frac{\kappa}{k},$$

which may be rewritten as

$$\sin \frac{k(a-d)}{2} = \frac{\kappa}{(k^2 + \kappa^2)^{1/2}} = \frac{\kappa}{K}, \quad \cos \frac{k(a-d)}{2} = \frac{k}{K}. \quad (***)$$

From here, we can readily spell out the  $\delta_n$  given by Eq. (\*) with the points  $x_0$  and hence  $(a - x_0)$  somewhere under the barrier, i.e. with  $(a - d)/2 < x_0 < [a - (a - d)/2] \equiv (a + d)/2$ , because the result is independent of the choice:<sup>83</sup>

$$\delta_n = (-1)^n \frac{\hbar^2 \kappa}{m} |C|^2 e^{-\kappa d} \times \begin{cases} \sin^2 \frac{k(a-d)}{2}, & \text{for } n = 1, 3, \dots, \\ \cos^2 \frac{k(a-d)}{2}, & \text{for } n = 0, 2, \dots, \end{cases} = (-1)^n \frac{\hbar^2 k^2 \kappa}{mK^2} |C|^2 e^{-\kappa d},$$

so our task is reduced to the calculation of the normalization coefficients  $C$ .

For the symmetric modes, the normalization condition, with an account of Eqs. (\*\*\*), gives

$$\begin{aligned} 1 &= \int_{-\infty}^{+\infty} u_n u_n^* dx = 2|C|^2 \left[ \int_0^{(a-d)/2} \cos^2 kx dx + \cos^2 \frac{k(a-d)}{2} \int_0^{\infty} \exp\{-2\kappa\tilde{x}\} d\tilde{x} \right] \\ &= 2|C|^2 \left[ \frac{(a-d)}{4} + \frac{\sin k(a-d)}{4k} + \cos^2 \frac{k(a-d)}{2} \frac{1}{2\kappa} \right] \equiv |C|^2 \left[ \frac{(a-d)}{2} + \frac{1}{\kappa} \right]; \end{aligned}$$

a similar calculation for the antisymmetric modes, with an account of Eqs. (\*\*), gives exactly the same result (though we should not forget that the values of  $k$  and  $\kappa$  are specific for each  $n$ ), so, finally, we get

<sup>83</sup> Note that the alternation of the  $\delta_n$ 's sign confirms the results of the general discussion of Eq. (2.204) in Sec. 2.7.

$$\Delta E_n = 4|\delta_n| = \frac{4\hbar^2 k^2 \kappa^2}{mK^2} \left[ \frac{\kappa(a-d)}{2} + 1 \right]^{-1} e^{-\kappa d}, \quad (****)$$

i.e., as we could expect, the allowed energy band is exponentially narrow.

Let us compare this result with that following from the exact characteristic equation derived in the previous problem (for the most natural case  $E < U_0$ ):

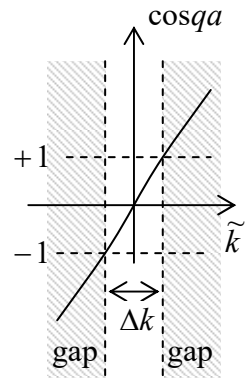
$$\cos qa = A \cos[k(a-d) + \varphi], \quad \text{with } A^2 = 1 + \left[ \frac{1}{2} \left( \frac{k}{\kappa} + \frac{\kappa}{k} \right) \sinh \kappa d \right]^2.$$

To solve this transcendental equation in the tight-binding limit, in which  $A \gg 1$ , we may linearize its right-hand side within the narrow interval of  $k$  in which the right-hand side ranges from  $-1$  to  $+1$ :

$$\cos qa \approx \frac{d}{dk} \{A \cos[k(a-d) + \varphi]\}_{\tilde{k}=0} \tilde{k},$$

where  $\tilde{k}$  is the deviation of  $k$  from the point where the cosine function equals zero – see the figure on the right. For the distance  $\Delta k$  between the edges of this interval (on which  $\cos qa = \pm 1$ ), this gives the expression

$$\Delta k = 2 \left| \frac{d}{dk} \{A \cos[k(a-d) + \varphi]\} \right|_{\max}^{-1}.$$



Generally, the required differentiation is a bit tedious because  $A$  and  $\varphi$  are also functions of  $k$ , but in the most interesting case when  $\kappa(a-d) \gg 1$  (meaning that the penetration of the wavefunction under the potential barrier is small), the derivative over  $k$  is dominated by the explicit dependence of cosine function of this parameter, and is simple:

$$\Delta k = 2 \left| \frac{d}{dk} \{A \cos[k(a-d) + \varphi]\} \right|_{\max}^{-1} \approx \frac{2}{A} \left| \frac{d}{dk} \{\cos[k(a-d) + \varphi]\} \right|_{\max}^{-1} = \frac{2}{A(a-d)},$$

where in our limit  $A \gg 1$ ,

$$A \equiv \left\{ 1 + \left[ \frac{1}{2} \left( \frac{k}{\kappa} + \frac{\kappa}{k} \right) \sinh \kappa d \right]^2 \right\}^{1/2} \approx \frac{1}{2} \left( \frac{k}{\kappa} + \frac{\kappa}{k} \right) \sinh \kappa d \equiv \frac{K^2}{2\kappa k} \sinh \kappa d \approx \frac{K^2}{4\kappa k} e^{\kappa d},$$

where the last approximate equality is valid at the same condition,  $\kappa d \gg 1$ , which was used in our calculation of  $\Delta E_n$  from the tight-binding limit formula.

What remains is to recalculate this (small) difference of the wave vector's values into the difference of the energies. We can do that by differentiating the relation  $E = (\hbar^2 k^2 / 2m + \text{const})$  over  $k$ :

$$\Delta E_n \approx \left| \frac{dE}{dk} \right| \Delta k = \frac{\hbar^2 k}{m} \Delta k = \frac{2\hbar^2 k}{mA(a-d)} = \frac{8\hbar^2 k^2 \kappa}{mK^2(a-d)} e^{-\kappa d}.$$

This is the same result as given by Eq. (\*\*\*\*) in the same limit  $\kappa(a-d) \gg 1$ .



**Problem 2.33.** For the same Kronig-Penney potential, use the weak-potential limit formulas to calculate the energy gap widths. Again, compare the results with those of Problem 31, in the corresponding limit.

*Solution:* In this limit, we may use Eq. (2.224) of the lecture notes to write

$$\Delta_n = 2|U_n|,$$

where  $U_n$  is the  $n^{\text{th}}$  Fourier coefficient of the function  $U(x)$  defined by the Fourier expansion (2.207). The coefficient may be calculated using the reciprocal Fourier transform:

$$U_n = \frac{1}{a} \int U(x) \exp\left\{i \frac{2\pi x}{a} n\right\} dx,$$

Where the integral is over one period of the function  $U(x)$ . For the Kronig-Penney potential, with the origin of the  $x$ -axis aligned with the middle of the potential barrier,<sup>84</sup> this integration gives

$$U_n = \frac{U_0}{a} \int_{-d/2}^{+d/2} \exp\left\{i \frac{2\pi n x}{a}\right\} dx = \frac{U_0}{2\pi i n} \left[ \exp\left\{i \frac{2\pi n x}{a}\right\} \right]_{-d/2}^{+d/2} \equiv \frac{U_0}{\pi n} \sin \frac{\pi n d}{a}, \quad \text{i.e. } \Delta_n = \frac{2U_0}{\pi n} \left| \sin \frac{\pi n d}{a} \right|. \quad (*)$$

Besides the monotonic decrease of the gap with the growth of number  $n$ , this expression describes an interesting commensurate effect of the gap suppression at  $nd \approx ma$ , where  $m$  is another integer. At such a relation of the parameters  $a$  and  $d$ , the gap location,  $\pi n/a$ , on the wave-vector axis coincides with value  $k' \approx k_m = \pi m/d$  corresponding to one of the over-barrier resonances (see the solution of Problem 8), which enhances the traveling wave transmission and hence suppresses its interaction with the lattice – which, as was discussed in Sec. 2.7 of the lecture notes, is responsible for the energy gap formation.

Now let us write the general characteristic equation of the system for the relevant case  $U_0 < E$ . It may be either derived exactly as this was done in the solution of Problem 31 for the opposite case or just obtained from Eq. (\*) of that solution with the usual replacement  $\kappa \rightarrow -ik'$ . The result<sup>85</sup> is

$$\cos qa = \cos k'd \cos k(a-d) - \frac{1}{2} \left( \frac{k}{k'} + \frac{k'}{\kappa} \right) \sin k'd \sin k(a-d). \quad (**)$$

In the weak-potential limit  $U_0 \ll E$ , we may approximate the front factor in the last term with two leading terms in its Taylor expansion in the small parameter  $U_0/E$ :

$$\frac{1}{2} \left( \frac{k}{k'} + \frac{k'}{\kappa} \right) \equiv \frac{1}{2} \left[ \frac{E^{1/2}}{(E-U_0)^{1/2}} + \frac{(E-U_0)^{1/2}}{E^{1/2}} \right] \approx 1 + \frac{1}{8} \left( \frac{U_0}{E} \right)^2,$$

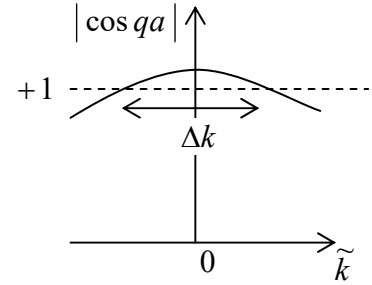
so Eq. (\*\*) reduces to

$$\begin{aligned} \cos qa &= \cos k'd \cos k(a-d) - \sin k'd \sin k(a-d) - \frac{U_0^2}{8E^2} \sin k'd \sin k(a-d) \\ &\equiv \cos[k'd - k(a-d)] - \frac{U_0^2}{8E^2} \sin k'd \sin k(a-d). \end{aligned} \quad (***)$$

<sup>84</sup> The origin's choice affects the phase of the complex coefficient  $U_n$ , but not its magnitude (the only parameter defining the energy gap's width), so for our purposes, we may select it in any way we like.

<sup>85</sup> In the model solution of Problem 31, only the resulting formula for  $A^2$  was given.

The difference  $\Delta k$  corresponding to the energy gap  $\Delta_n$  may be calculated as the distance between two close roots of the equation  $|\cos qa| = 1$  – see the figure on the right. To find it, we need to expand the right-hand side of Eq. (\*\*\*) into the Taylor series in the small parameter  $\tilde{k} \equiv k - k_n$ , where  $k_n$  is the value of  $k$  corresponding to the  $n^{\text{th}}$  maximum of the magnitude of the right-hand side of Eq. (\*\*\*). Since in our limit  $U_0 \ll E$ , the last term on that side and the difference between  $k$  and  $k'$  are small, the main contribution to this expansion is given by the first term:



$$\left| \cos[k'd - k(a-d)] - \frac{1}{8} \left( \frac{U_0}{E} \right)^2 \sinh k'd \sin k(a-d) \right| \approx 1 - \frac{1}{2} \left( \frac{\Delta k a}{2} \right)^2 + \frac{1}{8} \left( \frac{U_0}{E} \right)^2 |\sinh k'd \sin k(a-d)|.$$

From here, at the  $n^{\text{th}}$  gap position ( $k' \approx k \approx k_n = \pi n/a$ , with  $\sin k a \approx 0$ ), we get

$$|\Delta k| = \frac{U_0}{E} \left| \sin \frac{\pi n d}{a} \right|,$$

so that the recalculation of this result to the energy gap at  $E \approx E^{(n)} = \hbar^2 k_n^2 / 2m = \pi^2 n^2 \hbar^2 / 2ma^2$ :

$$\Delta_n \approx \left| \frac{dE}{dk} \Big|_{k=\pi n/a} \Delta k \right| = \frac{\pi \hbar^2 n}{ma} |\Delta k| = \frac{\pi \hbar^2 n}{ma} \frac{U_0}{E^{(n)}} \left| \sin \frac{\pi n d}{a} \right| = \frac{2U_0}{\pi n} \left| \sin \frac{\pi n d}{a} \right|,$$

brings us back to Eq. (\*).

**Problem 2.34.** 1D periodic chains of atoms may exhibit what is called the *Peierls instability*,<sup>86</sup> leading to the *Peierls transition* to a phase in which the atoms are slightly displaced, from the exact periodicity, by equal but sign-alternating shifts  $\Delta x_j = (-1)^j \Delta x$ , with  $\Delta x \ll a$ , where  $j$  is the atom's number in the chain, and  $a$  is its initial period. These displacements lead to an alternation of the coupling amplitudes  $\delta_n$  (see Eq. (2.204) of the lecture notes) between close values  $\delta_n^+$  and  $\delta_n^-$ . Use the tight-binding approximation to calculate the resulting change of the  $n^{\text{th}}$  energy band, and discuss the result.

*Solution:* In order to describe the band structure, we may use an equation similar to Eq. (2.203) of the lecture notes, but with alternating coupling constants:

$$i\hbar \dot{a}_j = -\delta_n^- a_{j-1} - \delta_n^+ a_{j+1}, \quad i\hbar \dot{a}_{j+1} = -\delta_n^+ a_j - \delta_n^- a_{j+2}. \quad (*)$$

The Bloch solution of the type (2.205) now has to accommodate alternating complex amplitudes  $a$ :

$$a_j(t) = \begin{cases} a^+, & \text{for } j \text{ odd,} \\ a^-, & \text{for } j \text{ even,} \end{cases} \times \exp \left\{ iqx_j - i \frac{\epsilon_n}{\hbar} t + \text{const} \right\}.$$

(Another way to express the same fact is to say that since the potential profile  $U(x)$  is now  $2a$ -periodic, the Bloch theorem is only valid for this larger period.) Plugging the last expression into Eq. (\*), we get a system of two linear equations for two complex amplitudes  $a^\pm$ :

<sup>86</sup> Named after Rudolf Peierls (1907-1995), a theorist most famous for the introduction of the notion of holes in semiconductors (and also as one of the main initiators of the Manhattan Project).

$$\varepsilon_n a^+ = -\left(\delta_n^- e^{-iqa} + \delta_n^+ e^{iqa}\right) a^-, \quad \varepsilon_n a^- = -\left(\delta_n^+ e^{-iqa} + \delta_n^- e^{iqa}\right) a^+.$$

The condition of consistency of this homogeneous system of linear equations,

$$\begin{vmatrix} \varepsilon_n & \delta_n^- e^{-iqa} + \delta_n^+ e^{iqa} \\ \delta_n^+ e^{-iqa} + \delta_n^- e^{iqa} & \varepsilon_n \end{vmatrix} = 0,$$

solved for the energy's deviation  $\varepsilon_n$  from the uncoupled-limit value  $E_n$ , gives the following dispersion relation:

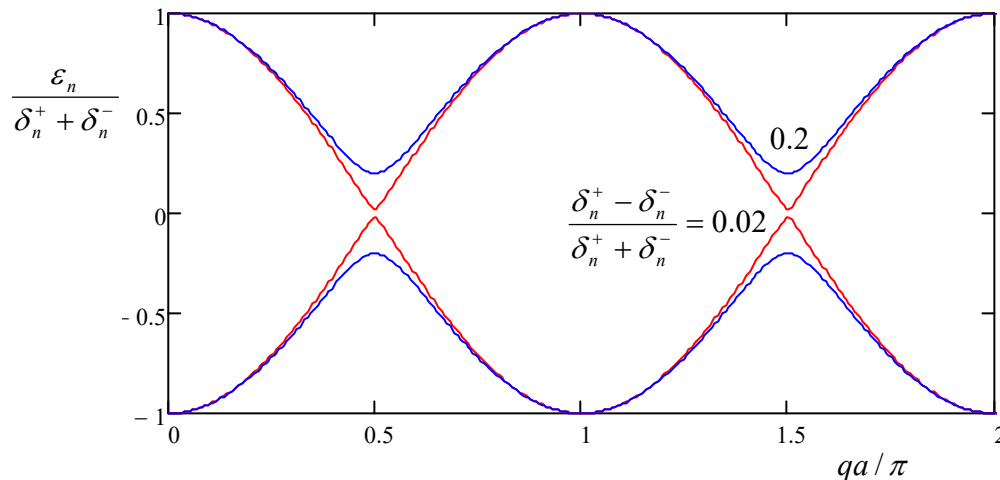
$$\varepsilon_n = \pm \left[ (\delta_n^+)^2 + (\delta_n^-)^2 + 2\delta_n^+ \delta_n^- \cos 2qa \right]^{1/2}.$$

A more revealing form of the same result may be obtained by using the trigonometric identity  $\cos 2qa = \cos^2 qa - \sin^2 qa$ , and then noticing that the terms under the square root form two full squares:

$$\varepsilon_n = \pm \left[ (\delta_n^+ + \delta_n^-)^2 \cos^2 qa + (\delta_n^+ - \delta_n^-)^2 \sin^2 qa \right]^{1/2}. \quad (**)$$

This equality shows that if the coupling alternation is negligible ( $\delta_n^+ - \delta_n^- \rightarrow 0$ ), the energy band tends to the sinusoidal form (2.206) with the “usual” period  $\Delta q = 2\pi/a$ . However, even a small but nonvanishing alternation of  $\delta_n$  results in the formation of an additional energy gap (see the numerical plots of Eq. (\*\*), for two alternation amplitudes, in the figure below), so the quasimomentum period decreases to  $(\Delta q)' = \pi/a$ . (Again, this is very natural from the point of spatial period's doubling:  $a' = 2a$ , leading to the quasimomentum's period  $(\Delta q)' = 2\pi/a' = \pi/a$ .)<sup>87</sup> The gap's minimum (reached at  $qa = \pi/2 + m\pi$ , with  $m$  integer) is

$$\Delta \varepsilon_n = 2(\delta_n^+ - \delta_n^-). \quad (***)$$



This effect may take place in highly anisotropic (quasi-1D) crystals (such as organic compounds TTF-TCNQ) of atoms with an odd number of electrons in incomplete energy shells (see, e.g., Sec. 3.7 of the lecture notes), and has rather dramatic consequences for their transport properties. Indeed, due to

<sup>87</sup> Note that such a gap opening is not an exclusively quantum phenomenon, but takes place at the propagation of waves of any nature in nearly-periodic systems – see, e.g., CM Problem 6.12.

the Fermi statistics of electrons, their states fill exactly the lower half of the usual conduction energy band. Such an “open” Fermi surface enables ready activation of electrons above the surface by even weak applied electric field, and hence their high electric conductivity.<sup>88</sup> However, the Peierls transition separates the lower half-band, completely filled with electrons, from the completely depleted upper half-band with the energy gap (\*\*\*) , suppressing the electron activation, and hence the crystal’s conductivity. As a result, the conductor turns into what is called the *Peierls dielectric*.

It is curious that the conductivity electrons are not only *affected* by the Peierls instability but also may *cause* it. Indeed, as the figure above shows, the Peierls transition leads to the *reduction* of electron energies in the lower (filled) half-band and hence can make the transition energy-favorable. Note that such self-supporting instabilities of the initial symmetry are very common in physics – another prominent example is the Cooper pairing of electrons in superconductors.

**Problem 2.35.\*** Use Eqs. (1.73)-(1.74) of the lecture notes to derive Eq. (2.252), and discuss the relation between these Bloch oscillations and the Josephson oscillations of frequency (1.75).

*Solution:* First, let us combine Eqs. (1.73) and (1.74) to calculate the work of an external voltage source at the Josephson phase’s change between some arbitrary initial ( $\varphi_{\text{ini}}$ ) and final ( $\varphi_{\text{fin}}$ ) values, as the integral of its power  $IV$  over the time interval  $\Delta t$  of the change:

$$\text{Work} = \int_{\Delta t} IV dt = \int_{\Delta t} (I_c \sin \varphi) \left( \frac{\hbar}{2e} \frac{d\varphi}{dt} \right) dt = \frac{\hbar I_c}{2e} \int_{\varphi_{\text{ini}}}^{\varphi_{\text{fin}}} \sin \varphi d\varphi = -\frac{\hbar I_c}{2e} (\cos \varphi_{\text{fin}} - \cos \varphi_{\text{ini}}).$$

We see that the work depends only on the initial and final values of  $\varphi$  (but not on the law of the phase evolution in time), and hence may be represented as the difference  $U(\varphi_{\text{fin}}) - U(\varphi_{\text{ini}})$ , where the function

$$U(\varphi) = -E_J \cos \varphi + \text{const}, \quad \text{with } E_J \equiv \frac{\hbar I_c}{2e}, \quad (*)$$

may be interpreted as the potential energy of the junction – if we consider the Josephson phase as a generalized coordinate.

Besides this energy, the Josephson junction, as a system of two close, nearly isolated (super)conductors, has a certain mutual capacitance  $C$  and the associated electrostatic energy  $E_C = CV^2/2$ . Using Eq. (1.73) again, we may represent it as

$$E_C = \frac{C}{2} V^2 = \frac{C}{2} \left( \frac{\hbar}{2e} \right)^2 \left( \frac{d\varphi}{dt} \right)^2.$$

This expression means that considering the phase  $\varphi$  the generalized coordinate of our system,  $E_C$  should be taken for its kinetic energy, whose dependence on the generalized velocity  $d\varphi/dt$  is similar to that of a 1D mechanical particle, with an effective mass<sup>89</sup>

$$m_J = C \left( \frac{\hbar}{2e} \right)^2.$$

<sup>88</sup> See, e.g., SM Sec. 6.3.

<sup>89</sup> Since the dimensionality of the generalized coordinate  $\varphi$  is different from [m], that of  $m_J$  is different from [kg].

Hence the total energy of the junction,  $E_C + U(\varphi)$ , is formally similar to that of a 1D non-relativistic particle of the mass  $m_J$ , moving along the  $\varphi$ -axis in the sinusoidal potential (\*) with the period  $a_J = 2\pi$ .

However, before using the results of the 1D band theory discussed in Secs. 2.6-2.7 of the lecture notes, to this system, we have to resolve one paradox – which, in the mid-1980s, was the subject of a lively scientific discussion. In Sec. 2.6, we (or rather Dr. F. Bloch :-)) implied that the particle's translation by the potential's period  $a$  is in principle measurable, i.e. the particle's positions  $x$  and  $(x + a)$  are distinguishable – otherwise Eq. (2.193) with  $q \neq 0$  would not have much sense. For the Josephson phase  $\varphi$ , a similar assumption is less plausible. Indeed, for example, if we change  $\varphi$  by  $a_J = 2\pi$  via changing the phase of one of the superconductors, say  $\varphi_1$  (see Fig. 1.7 of the lecture notes) by  $2\pi$ , then its wavefunction becomes  $|\psi| \exp\{i(\varphi_1 + 2\pi)\} = |\psi| \exp\{i\varphi_1\}$ , and it is not immediately clear whether these two states may be distinguished.

In order to resolve this contradiction, it is sufficient to have a look at Eq. (1.73). It shows that if  $\varphi$  changes in time by  $2\pi$ , the voltage  $V$  across the junction exhibits a pulse with the following “area”:

$$\int V(t)dt = \frac{\hbar}{2e} \int \frac{d\varphi}{dt} dt = \frac{\hbar}{2e} \int d\varphi = \frac{\hbar}{2e} 2\pi \equiv \frac{\pi\hbar}{e} \approx 2 \times 10^{-15} \text{ V} \cdot \text{s}. \quad (**)$$

Such *single-flux-quantum* (SFQ) pulses<sup>90</sup> have been not only observed experimentally but even used to demonstrate fast signaling and ultrafast (sub-THz) computation.<sup>91</sup>

Hence, the  $2\pi$ -shifts of phase  $\varphi$  are measurable, and in the absence of dissipation, the Josephson junction dynamics is indeed similar to that of a 1D particle in a periodic (sinusoidal) potential (\*). As this formula implies, the energy spectrum of this system forms the energy bands and gaps described by the Mathieu equation – see Fig. 2.31a and Eqs. (2.227)-(2.229) of the lecture notes. Experimentally, the easiest way to verify this picture is to measure the corresponding Bloch oscillations induced by an external current  $I_{\text{ex}}(t)$ . To find the frequency of these oscillations, it is sufficient to replace Eq. (2.237), which expresses the 2<sup>nd</sup> Newton law for the quasimomentum  $\hbar q$ , with the charge balance equation

$$\frac{dQ}{dt} = I_{\text{ex}}(t), \quad (***)$$

for the corresponding variable  $Q$ , called the *quasicharge*. This relation tells us that the quasicharge  $Q$  has the simple physical sense of the external electric charge being inserted into the junction by the external current  $I_{\text{ex}}$  – just like the physical sense of the quasimomentum  $\hbar q$  of a mechanical particle, according to Eq. (2.237), is the contribution into the average particle's momentum, due to the external force  $F$ . (Notice that at such quantum-mechanical averaging of the electric charge, the supercurrent (1.74) drops out from the equation, affecting the phenomena “only” via its contribution to the energy band structure.)

Since the Josephson-junction analog of the usual wave number  $k = (m/\hbar)(dx/dt)$  of a particle is

<sup>90</sup> This term has originated from the fact that the right-hand side of Eq. (\*\*) equals the single quantum unit ( $\Phi_0$ ) of the magnetic flux in superconductors – see Sec. 3.1 of the lecture notes (and/or EM Sec. 6.4-6.5).

<sup>91</sup> To the best of my knowledge, this technology (dubbed RSFQ) still holds the absolute records for the highest speed and smallest energy consumption at an elementary computation – see, e.g., P. Bunyk *et al.*, *Int. J. on High Speed Electronics and Systems* **11**, 257 (2001) and references therein.

$$k_j = \frac{m_j}{\hbar} \frac{d\varphi}{dt} = \frac{m_j}{\hbar} \frac{2e}{\hbar} V = \frac{CV}{2e},$$

and  $CV$  is the genuine charge on the capacitor, the analog of  $q$  (the quasimomentum divided by  $\hbar$ ) may be obtained just by the replacement of that product with the quasicharge  $Q$ :

$$q_j = \frac{Q}{2e}.$$

Comparing this expression with Eq. (\*\*\*), we see that  $q_j$  obeys the following equation of motion:

$$\frac{dq_j}{dt} = \frac{I_{\text{ex}}(t)}{2e}.$$

so the role of the mechanical force  $F$  is now played by  $F_j = \hbar I_{\text{ex}}/2e$ . Hence if  $I_{\text{ex}}(t) = \text{const} = \bar{I}$ , we can use Eq. (2.244) with that replacement and also with  $a \rightarrow a_j = 2\pi$ , to get Eq. (2.252) of the lecture notes:

$$f_B \equiv \frac{\omega_B}{2\pi} = \frac{1}{2\pi} \frac{F_j a_j}{\hbar} = \frac{\bar{I}}{2e}.$$

This very simple result has the following physical sense.<sup>92</sup> In the quantum operation mode, the junction is recharged by the external current, following Eq. (\*\*\*), until its electric charge reaches  $e$  (i.e. until the normalized quasimomentum  $q_j a_j = (Q/2e)2\pi$  reaches  $\pi$  – see Fig. 2.33a of the lecture notes); then one Cooper pair passes through the junction changing its charge to  $e - (2e) = -e$ , with the same charging energy  $Q^2/2C$  – the process corresponding to crossing the border of the 1<sup>st</sup> Brillouin zone; then the process repeats again and again.<sup>93</sup> It is paradoxical that Eq. (2.252), describing the frequency of such a *quantum* property of the Josephson phase  $\varphi$  as its Bloch oscillations, does not include the Planck's constant, while Eq. (1.75), describing the *classical* motion of  $\varphi$ , does.<sup>94</sup>

In this context, one may wonder which of these two types of oscillations would a dc-biased Josephson junction generate. For the dissipation-free (OK, *virtually* dissipation-free :-)) junction, the answer is: the Bloch oscillations (2.252) with the frequency proportional to the dc *current*. However, any practical junction has some energy losses that may be approximately described by a certain Ohmic conductance  $G$  connected in parallel to the junction. Very luckily for Dr. Josephson and his Nobel Prize, it turns up much easier to fabricate and test junctions with  $G \gg 1/R_Q$ , where  $R_Q$  is the so-called *quantum unit of resistance*

$$R_Q \equiv \frac{\pi\hbar}{2e^2} \approx 6.45 \text{ k}\Omega,$$

<sup>92</sup> D. Averin *et al.*, *Sov. Phys. – JETP* **61**, 407 (1985).

<sup>93</sup> Note that the qualitatively similar effect of the single-electron-tunneling (SET) oscillations, with twice higher frequency  $f_{\text{SET}} = I/e$ , takes place, at sufficiently low temperatures, in small “normal” (non-superconducting) tunnel junctions – see, e.g., EM Sec. 2.9 and references therein. However, the quantitative descriptions of these effects are rather different, because, in contrast to the Cooper pairs, the electrons in “normal” conductors do not form a coherent Bose-Einstein condensate.

<sup>94</sup> The phase locking of the Bloch oscillations, as well as that of the SET oscillations, by an external signal of a well-characterized frequency, may enable fundamental standards of dc current. The experimentally achieved relative accuracy of such standards is close to  $10^{-8}$ , just a few times worse than that of a less direct way toward such standards – by using a Josephson voltage standard combined with a resistance standard based on the quantum Hall effect.

the fundamental constant that comes up at analyses of several other effects as well – see, e.g., Sec. 3.2 below. As will be discussed in Chapter 7, the dissipation so high provides what is called *dephasing* – the suppression of the quantum coherence between different quantum states of the system (in our current case, between the wavefunctions  $u(\varphi - 2\pi j)$  localized at different minima of the potential energy  $U$ ), and thus make the dynamics of the Josephson phase  $\varphi$  virtually classical, obeying equations (1.73) and (1.74). As was discussed in Sec. 1.6 of the lecture notes, dc biasing of such a junction leads to Josephson oscillations with the frequency (1.75), which is proportional to the applied dc *voltage*, rather than the current.

**Problem 2.36.\*** A 1D particle of mass  $m$  is placed into the following triangular potential well:

$$U(x) = \begin{cases} +\infty, & \text{for } x < 0, \\ Fx, & \text{for } x > 0, \end{cases} \quad \text{with } F > 0.$$

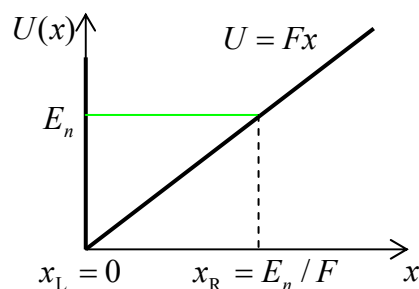
- (i) Calculate its energy spectrum using the WKB approximation.
- (ii) Estimate the ground state energy using the variational method, with two different trial functions.
- (iii) Calculate the three lowest energy levels, and also the 10<sup>th</sup> level, with an accuracy better than 0.1%, from the exact solution of the problem.
- (iv) Compare and discuss the results.

*Hint:* The values of the first few zeros of the Airy function, necessary for Task (iii), may be found in many math handbooks, for example, in Table 9.9.1 of the open-access online version of the collection edited by Abramowitz and Stegun.<sup>95</sup>

*Solutions:*

(i) Acting just as in Sec. 2.4 of the lecture notes (see, in particular, Fig. 2.10 and its discussion), let us calculate the total roundtrip phase shift of a traveling de Broglie wave of energy  $E_n$ . The quasiclassical motion from the left classical turning point  $x_L = 0$  to the right point  $x_R = E_n/F$  (see the figure on the right) yields the shift

$$\Delta\varphi_{\rightarrow} = \int_{x_L}^{x_R} k(x) dx = \frac{1}{\hbar} \int_0^{E_n/F} [2m(E_n - Fx)]^{1/2} dx = \frac{2}{3} (2m)^{1/2} \frac{E_n^{3/2}}{\hbar F}.$$



The total phase change of the wave's roundtrip (including also the way back from  $x_L$  and  $x_R$ ) consists of twice that shift, plus two shifts due to the wave reflection from the classical turning points. One of these reflections (at  $x = x_R$ ) may be treated quasiclassically, giving the additional shift (in comparison with the "hard", vertical wall) equal to  $\Delta\varphi = \pi/2$ . The reflection from the left, vertical potential wall at  $x = 0$  does not give such an additional shift.<sup>96</sup> As a result, the total phase change on the roundtrip is

$$\Delta\varphi_{\text{total}} = 2\Delta\varphi_{\rightarrow} + \frac{\pi}{2} = \frac{4}{3} (2m)^{1/2} \frac{E_n^{3/2}}{\hbar F} + \frac{\pi}{2}.$$

<sup>95</sup> See <https://dlmf.nist.gov/9.9>.

<sup>96</sup> Note that by this direct (non-WKB) treatment of the potential wall, we avoid violation of the condition (2.107).

Requiring this change to equal  $2\pi n$ , with  $n = 1, 2, \dots$ , we get the WKB spectrum

$$E_n|_{\text{WKB}} = E_0 \left[ \frac{3\pi}{2} \left( n - \frac{1}{4} \right) \right]^{2/3}, \quad \text{with } E_0 \equiv \left( \frac{\hbar^2 F^2}{2m} \right)^{1/3}.$$

(ii) Looking at the potential profile of the problem (see the figure above), it is clear that the following simple trial function:

$$\psi_1(x) = \begin{cases} 0, & \text{for } x < 0, \\ Cxe^{-\lambda x}, & \text{for } x > 0, \end{cases} \quad \text{with } \lambda > 0,$$

may give a reasonable approximation for the ground state of the system. (In particular, it yields the exact, zero values of the wavefunction for  $x \leq 0$  and  $x = +\infty$ , and also ensures the function's continuity at all points.) Its normalization condition is

$$\int_0^{\infty} |\psi_1|^2 dx \equiv |C|^2 \int_0^{\infty} x^2 e^{-2\lambda x} dx = 1.$$

Using the table integral MA (6.7d) with  $n = 2$ , we readily get

$$|C|^{-2} = \int_0^{\infty} x^2 e^{-2\lambda x} dx = \frac{1}{(2\lambda)^3} \int_0^{\infty} \xi^2 e^{-\xi} d\xi = \frac{1}{4\lambda^3}.$$

The expectation value of the Hamiltonian in this trial state is

$$\begin{aligned} \langle H \rangle_1 &\equiv \int_{-\infty}^{+\infty} \psi_1^* \hat{H} \psi_1 dx \equiv \int_{-\infty}^{+\infty} \psi_1^* \left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U(x) \right] \psi_1 dx \equiv \int_0^{\infty} C^* x e^{-\lambda x} \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + Fx \right) C x e^{-\lambda x} dx \\ &\equiv |C|^2 \left\{ -\frac{\hbar^2}{2m} \left[ \lambda^2 \int_0^{\infty} x^2 e^{-2\lambda x} dx - 2\lambda \int_0^{\infty} x e^{-2\lambda x} dx \right] + F \int_0^{\infty} x^3 e^{-2\lambda x} dx \right\}. \end{aligned}$$

All these integrals are of the same type MA (6.7d), with  $n = 2, 1$ , and  $3$ , respectively. Using the above expression for the normalization constant, we finally get

$$\langle H \rangle_1 = \frac{\hbar^2 \lambda^2}{2m} + \frac{3F}{2\lambda}.$$

This expectation value is positive for all  $\lambda > 0$  and diverges both at  $\lambda \rightarrow 0$  and  $\lambda \rightarrow \infty$ , so it certainly has a minimum at some optimum value  $\lambda_{\text{opt}}$ , for which

$$\frac{\partial}{\partial \lambda} \langle H \rangle_1 \Big|_{\lambda=\lambda_{\text{opt}}} = 0.$$

Performing the simple differentiation, we get

$$\lambda_{\text{opt}} = \left( \frac{3mF}{2\hbar^2} \right)^{1/3}, \quad E_{\text{var1}} \equiv \min_{\lambda} \langle H \rangle_1 \equiv \frac{\hbar^2 \lambda_{\text{opt}}^2}{2m} + \frac{3F}{2\lambda_{\text{opt}}} = \left( \frac{3}{2} \right)^{5/3} \left( \frac{\hbar^2 F^2}{m} \right)^{1/3} \approx 2.476 E_0.$$

Now let us try a somewhat different trial function:



$$\psi_2(x) = \begin{cases} 0, & \text{for } x < 0, \\ Cxe^{-\lambda x^2/2}, & \text{for } x \geq 0, \end{cases}$$

also having the proper (zero) boundary values at  $x \leq 0$  and  $x = +\infty$ . (Since the factor  $1/2$  in the exponent may be always absorbed into the fitting parameter  $\lambda$ , it is not necessary but convenient for calculations.) For this function, the normalization condition is

$$\int_0^{\infty} |\psi_2|^2 dx \equiv |C|^2 \int_0^{\infty} x^2 e^{-\lambda x^2} dx \equiv |C|^2 \lambda^{-3/2} \int_0^{\infty} \xi^2 e^{-\xi^2} d\xi = 1,$$

where  $\xi \equiv \lambda^{1/2}x$ . The last dimensionless integral<sup>97</sup> equals  $\pi^{1/2}/4$ , so

$$|C|^2 = \frac{4\lambda^{3/2}}{\pi^{1/2}}.$$

With this normalization, the expectation value of the Hamiltonian in the trial state is

$$\begin{aligned} \langle H \rangle_2 &\equiv \int_{-\infty}^{+\infty} \psi_2^* \hat{H} \psi_2 dx = |C|^2 \int_0^{\infty} x e^{-\lambda x^2/2} \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + Fx \right) x e^{-\lambda x^2/2} dx \\ &= \frac{4\lambda^{3/2}}{\pi^{1/2}} \left[ -\frac{\hbar^2}{2m} \left( -3\lambda \int_0^{\infty} x^2 e^{-\lambda x^2} dx + \lambda^2 \int_0^{\infty} x^4 e^{-\lambda x^2} dx \right) + F \int_0^{\infty} x^3 e^{-\lambda x^2} dx \right] \\ &\equiv \frac{4\lambda^{3/2}}{\pi^{1/2}} \left[ -\frac{\hbar^2}{2m} \left( -3\lambda^{-1/2} \int_0^{\infty} \xi^2 e^{-\xi^2} d\xi + \lambda^{-1/2} \int_0^{\infty} \xi^4 e^{-\xi^2} d\xi \right) + F\lambda^{-2} \int_0^{\infty} \xi^3 e^{-\xi^2} d\xi \right], \end{aligned}$$

where the same substitution as above,  $\xi \equiv \lambda^{1/2}x$ , was used. The first dimensionless integral is the same as above (equal to  $\pi^{1/4}/4$ ), and the remaining two are of the same type,<sup>98</sup> equal, respectively, to  $(3/8)\pi^{1/2}$  and  $1/2$ , so

$$\langle H \rangle_2 = \frac{4\lambda^{3/2}}{\pi^{1/2}} \left[ -\frac{\hbar^2}{2m} \left( -3\lambda^{-1/2} \frac{\pi^{1/2}}{4} + \lambda^{-1/2} \frac{3\pi^{1/2}}{8} \right) + F\lambda^{-2} \frac{1}{2} \right] \equiv \frac{3\hbar^2\lambda}{4m} + \frac{2F}{\pi^{1/2}\lambda^{1/2}}.$$

This expectation value is also positive and diverges both at  $\lambda \rightarrow 0$  and  $\lambda \rightarrow \infty$ , so it certainly has a minimum at some optimum value  $\lambda_{\text{opt}}$ , for which

$$\left. \frac{\partial}{\partial \lambda} \langle H \rangle_2 \right|_{\lambda=\lambda_{\text{opt}}} = 0.$$

Performing the differentiation, we get

$$\lambda_{\text{opt}} = \left( \frac{16m^2 F^2}{9\pi\hbar^4} \right)^{1/3}, \quad E_{\text{var } 2} \equiv \frac{3\hbar^2\lambda_{\text{opt}}}{4m} + \frac{2F}{\pi^{1/2}\lambda_{\text{opt}}^{1/2}} = \left( \frac{81}{2\pi} \right)^{1/3} E_0 \approx 2.345 E_0.$$

The fact that  $E_{\text{var } 2} < E_{\text{var } 1}$  shows that the second trial function provides a better approximation, though the difference is not that large (below 6%).

<sup>97</sup> See, e.g., MA Eq. (6.9c).

<sup>98</sup> See, e.g., MA Eq. (6.9d) and Eq. (6.9e) for  $n = 1$ .

(iii) In order to obtain the exact solution to the problem, we can solve the stationary Schrödinger equation

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + Fx\psi = E_n\psi, \quad (*)$$

at  $x > 0$ , with the boundary conditions  $\psi(0) = \psi(+\infty) = 0$ . By normalizing, just as it was done in Sec. 2.4 of the lecture notes, the coordinate  $x$  to the constant

$$x_0 \equiv \left( \frac{\hbar^2}{2m dU/dx} \right)^{1/3} \equiv \left( \frac{\hbar^2}{2mF} \right)^{1/3},$$

we can reduce Eq. (\*) to the canonical form (2.101) of the Airy equation, with the general solution

$$\psi(\zeta) = C_A \text{Ai}(\zeta) + C_B \text{Bi}(\zeta),$$

where  $\zeta \equiv (x - x_R)/x_0$ . One of the boundary conditions (at  $x \rightarrow \infty$ ) may be satisfied only by taking  $C_B = 0$ , so the second one (at  $x = 0$ , i.e. at  $\zeta = -x_R/x_0$ ) is reduced to the requirement  $\text{Ai}(-x_R/x_0) = 0$ ,<sup>99</sup> i.e.

$$-\frac{x_R}{x_0} \equiv -\frac{E_n}{Fx_0} = \zeta_n, \quad \text{i.e. } E_n = -Fx_0\zeta_n = -\left( \frac{\hbar^2 F^2}{2m} \right)^{1/3} \zeta_n = -E_0\zeta_n,$$

where  $\zeta_n$  is the  $n^{\text{th}}$  root of the Airy function  $\text{Ai}(\zeta)$ . Using the values of  $\zeta_n$  from any math handbook (see the *Hint*), we get the results shown in the rightmost column of the table below.

$n$	$E_n/E_0 \big _{\text{WKB}}$ $= [(3\pi/2)(n - 1/4)]^{2/3}$	$E_{\text{var1}}/E_0$ $= \min_{\lambda} \langle H \rangle_1$	$E_{\text{var2}}/E_0$ $= \min_{\lambda} \langle H \rangle_2$	$E_n/E_0 \big _{\text{exact}}$ $= -\zeta_n$
1	2.320	2.476	2.345	2.338
2	4.081	-	-	4.088
3	5.517	-	-	5.520
10	12.8281	-	-	12.8287

(iv) The table shows that the variational method results for the ground state depend much on the trial function. Indeed, our second attempt gave an error of just  $\sim 0.3\%$  – pretty good for virtually any practical application. Looking at the asymptotic behavior of the Airy functions (see, e.g., the first line of Eq. (2.102) of the lecture notes), we may guess that an even better trial function could be

$$\psi_{\text{trial}} = Cx \exp\left\{-\frac{2}{3}\zeta^{3/2}\right\}, \quad \text{with } \zeta \equiv \frac{x - x_c}{x_0}, \quad x_0 \equiv \left( \frac{\hbar^2}{2mF} \right)^{1/3},$$

with the classical turning point  $x_c$  treated as an adjustable parameter. The reader is invited to explore this option (running into less common integrals) as an additional exercise.

On the other hand, even for the ground level ( $n = 1$ ), which is always the hardest task for the WKB approximation, for this particular problem, it works surprisingly well, with a relative error of

<sup>99</sup> Note that the above WKB result could be also obtained by using this equation with the asymptotic form given by the second of Eqs. (2.106).

~1%; the error decreases fast as we go up the energy level ladder, dropping below  $10^{-4}$  for  $n = 10$ . Please remember, however, that while with the variational method, we may be always sure that the genuine ground state energy is below the estimated value, this is not true for the WKB method.

**Problem 2.37.** Use the variational method to estimate the ground state energy  $E_g$  of a 1D particle in the potential well

$$U(x) = -U_0 \exp\{-\alpha x^2\}, \quad \text{with } \alpha > 0, \text{ and } U_0 > 0.$$

Spell out the results in the limits of small and large  $U_0$ , and give their interpretation.

*Solution:* Since any smooth, symmetric potential well  $U(x)$  may be Taylor-approximated, near its bottom, with a quadratic parabola, the calculation at the beginning of Sec. 2.9 of the lecture notes indicates that a Gaussian function similar to that given by Eq. (2.270),<sup>100</sup>

$$\psi_{\text{trial}}(x) = C \exp\left\{-\frac{\lambda x^2}{2}\right\}, \quad \text{with } \lambda > 0,$$

is a reasonable choice for the trial function for our potential. The calculation of the expectation value of the corresponding Hamiltonian,

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} - U_0 \exp\{-\alpha x^2\},$$

is almost similar to that in Sec. 2.9 and in Task (ii) of the previous problem:

$$\begin{aligned} \langle H \rangle_{\text{trial}} &= \int_{-\infty}^{+\infty} \psi_{\text{trial}}^* \hat{H} \psi_{\text{trial}} dx = |C|^2 \int_{-\infty}^{+\infty} \exp\left\{-\frac{\lambda x^2}{2}\right\} \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} - U_0 \exp\{-\alpha x^2\} \right) \exp\left\{-\frac{\lambda x^2}{2}\right\} dx \\ &= \left(\frac{\lambda}{\pi}\right)^{1/2} \left[ \frac{\hbar^2 \lambda}{2m} \int_{-\infty}^{+\infty} \exp\{-\lambda x^2\} dx - U_0 \int_{-\infty}^{+\infty} \exp\{-(\lambda + \alpha)x^2\} dx - \frac{\hbar^2 \lambda^2}{2m} \int_{-\infty}^{+\infty} x^2 \exp\{-\lambda x^2\} dx \right] \\ &= \left(\frac{\lambda}{\pi}\right)^{1/2} \left[ \frac{\hbar^2 \lambda}{2m} \frac{\pi^{1/2}}{\lambda^{1/2}} - U_0 \frac{\pi^{1/2}}{(\lambda + \alpha)^{1/2}} - \frac{\hbar^2 \lambda^2}{2m} \frac{\pi^{1/2}}{2\lambda^{3/2}} \right] \equiv \frac{\hbar^2 \lambda}{4m} - U_0 \left(\frac{\lambda}{\lambda + \alpha}\right)^{1/2}. \end{aligned}$$

The last expression is negative at  $\lambda \rightarrow 0$ , with a negative derivative  $\partial \langle H \rangle_{\text{trial}} / \partial \lambda$  at  $\lambda = 0$ , while it is positive and diverges at  $\lambda \rightarrow \infty$ . Hence,  $\langle H \rangle_{\text{trial}}$  as a function of  $\lambda > 0$  has a minimum, corresponding to a localized ("bound") ground state of the system. For an arbitrary  $U_0$ , the condition of this minimum,

$$\frac{\partial \langle H \rangle_{\text{trial}}}{\partial \lambda} \Big|_{\lambda=\lambda_{\text{opt}}} \equiv \frac{\hbar^2}{4m} - U_0 \frac{\alpha}{2\lambda_{\text{opt}}^{1/2} (\lambda_{\text{opt}} + \alpha)^{3/2}} = 0,$$

gives a rather unpleasant 4<sup>th</sup>-degree-polynomial equation for the dimensionless variable  $\xi \equiv \lambda_{\text{opt}}/\alpha$ :

$$\xi(\xi + 1)^3 = \left(\frac{U_0}{T_0}\right)^2, \quad \text{where } T_0 \equiv \frac{\hbar^2 \alpha}{2m}, \quad (*)$$

with an extremely bulky general solution.<sup>101</sup>

<sup>100</sup> Just as in the previous problem, the factor  $1/2$  is unnecessary but makes calculations a bit less bulky.

However, we may readily spell out the result in the limits when the depth  $U_0$  of the potential well is much smaller or much larger than the scale  $T_0$  of the kinetic energy of the particle in it. In the former case, we should have  $\xi \ll 1$ , so the left-hand side of Eq. (\*) may be approximated with  $\xi$ , and this equation yields

$$\xi = \left(\frac{U_0}{T_0}\right)^2, \quad \text{i.e. } \lambda_{\text{opt}} = \alpha \left(\frac{U_0}{T_0}\right)^2 \ll \alpha, \quad \text{so } \langle H \rangle_{\text{min}} = -\frac{U_0^2}{2T_0}, \quad \text{i.e. } |\langle H \rangle_{\text{min}}| \ll U_0.$$

This result has a simple physical meaning: if the well is shallow, its particle-localization effect is weak, so the localized wavefunctions are spread far beyond the effective well's width  $1/\alpha^{1/2}$ . On the scale of this spread, the potential well potential may be well approximated with the delta function,

$$U(x) \approx -w\delta(x),$$

whose "weight"  $w$  may be calculated from the delta function's definition:

$$\int_{-\infty}^{+\infty} \delta(x) dx \equiv -\frac{1}{w} \int_{-\infty}^{+\infty} U(x) dx \equiv -\frac{1}{w} \int_{-\infty}^{+\infty} [-U_0 \exp\{-\alpha x^2\}] dx \equiv \frac{U_0}{w} \left(\frac{\pi}{\alpha}\right)^{1/2} = 1, \quad \text{giving } w = \left(\frac{\pi}{\alpha}\right)^{1/2} U_0.$$

If we now plug this value into Eq. (2.165) of the lecture notes, for the ground-state energy in such a delta-functional potential,  $E_g = -m w^2 / 2\hbar^2$ , we get

$$E_g = -\frac{\pi m U_0^2}{2 \hbar^2 \alpha} = -\frac{\pi U_0^2}{4 T_0} \approx -0.785 \frac{U_0^2}{T_0}.$$

So, in this limit, the variational method captures the correct functional dependence of the ground-state energy but is  $\sim 60\%$  off the exact result.<sup>102</sup>

In the opposite limit of a very deep potential well,  $U_0 \gg T_0$ , the left-hand side of Eq. (\*) may be well approximated with  $\xi^4$  and this equation yields

$$\xi \equiv \frac{\lambda_{\text{opt}}}{\alpha} = \left(\frac{U_0}{T_0}\right)^{1/2} \gg 1, \quad \text{giving } \langle H \rangle_{\text{min}} = -U_0 + (U_0 T_0)^{1/2}.$$

In order to interpret this result, let us use the fact that in this limit the wavefunction's spread is much smaller than the well's width scale  $1/\alpha^{1/2}$ , so it "feels" only the very bottom of the well, where the confining potential may be approximated with just two leading terms of its Taylor expansion:

$$U(x) = -U_0 \exp\{-\alpha x^2\} \approx -U_0 + U_0 \alpha x^2.$$

But this is exactly the potential of a harmonic oscillator (offset by  $-U_0$ ):

<sup>101</sup> Mercifully, since in the physically acceptable range  $\xi \geq 0$ , the left-hand side of Eq. (\*) is a monotonically growing function of  $\xi$ , starting from 0 at  $\xi = 0$ , this particular equation has just one root of our interest, for any ratio  $U_0/T_0$ .

<sup>102</sup> The reason for this difference is clear from the comparison of our Gaussian trial function with the exact ground state wavefunction (2.159):  $\psi_g \propto \exp\{-\kappa|x|\}$ .

$$U(x) = -U_0 + \frac{m\omega_0^2}{2}x^2, \quad \text{with } \frac{m\omega_0^2}{2} = \alpha U_0, \quad \text{i.e. } \omega_0 = \left(\frac{2\alpha U_0}{m}\right)^{1/2},$$

whose exact ground state energy is

$$E_g = -U_0 + \frac{\hbar\omega_0}{2} = -U_0 + \frac{\hbar}{2} \left(\frac{2\alpha U_0}{m}\right)^{1/2} \equiv -U_0 + (U_0 T_0)^{1/2}.$$

Thus, as might be expected, in this limit, the Gaussian trial function yields the exact ground-state energy.

**Problem 2.38.** For a 1D particle of mass  $m$ , in a potential well with the following profile,

$$U(x) = ax^{2s}, \quad \text{with } a > 0 \text{ and } s > 0,$$

- (i) calculate its energy spectrum using the WKB approximation, and
- (ii) estimate the ground-state energy using the variational method.

Compare the ground-state energy results.

*Solutions:*

- (i) Let us use the Wilson-Sommerfeld quantization rule (2.110),

$$\oint p(x) dx \equiv 2 \int_{x_L}^{x_R} p(x) dx = 2\pi\hbar \left( n - \frac{1}{2} \right), \quad \text{with } n = 1, 2, \dots, \quad (*)$$

where in our current case

$$p(x) = \{2m[E_n - U(x)]\}^{1/2} = [2m(E_n - ax^{2s})]^{1/2} \equiv (2mE_n)^{1/2} [1 - (x/x_n)^{2s}]^{1/2}.$$

Here  $x_n \equiv x_R = -x_L$  is the distance of the classical turning points from  $x = 0$ , related to the energy  $E = E_n$  by the condition

$$E_n = U(x_n) = ax_n^{2s}, \quad \text{giving } x_n = \left(\frac{E_n}{a}\right)^{1/2s}.$$

Introducing the dimensionless variable  $\xi \equiv x/x_n$ , so  $dx = x_n d\xi$ , and using the potential's symmetry with respect to the origin, we get

$$\int_{x_L}^{x_R} p(x) dx = 2 \int_0^{x_n} p(x) dx = 2(2mE_n)^{1/2} x_n \int_0^1 (1 - \xi^{2s})^{1/2} d\xi \equiv (8mE_n)^{1/2} \left(\frac{E_n}{a}\right)^{1/2s} \int_0^1 (1 - \xi^{2s})^{1/2} d\xi.$$

This is a table integral<sup>103</sup> equal to  $(\pi^{1/2}/4s)\Gamma(1/2s)/\Gamma(3/2 + 1/2s)$ , so Eq. (\*) yields the following energy spectrum:

$$E_n = E_{\text{WKB}} (2n-1)^{2s/(s+1)}, \quad \text{for } n = 1, 2, \dots, \quad (**)$$

where  $E_{\text{WKB}} \equiv E_1$  is the WKB result for ground-state energy:

<sup>103</sup> See, e.g., MA Eq. (6.6b).

$$E_{\text{WKB}} = \left\{ \left( \frac{\hbar^2}{2m} \right)^s a \left[ \pi^{1/2} s \frac{\Gamma(3/2 + 1/2s)}{\Gamma(1/2s)} \right]^{2s} \right\}^{1/(s+1)}. \quad (***)$$

As Eq. (\*\*) shows, for the quadratic-parabolic potential, i.e. for  $s = 1$ ,  $2s/(s + 1) = 1$ , the energy levels are equidistant:

$$E_n = E_1(2n - 1), \quad \text{i.e. } E_{n+1} - E_n = 2E_1 = \text{const},$$

as they should be for a harmonic oscillator – see, e.g., Eq. (2.114). However, as the parameter  $s$  grows, i.e. as the particle confinement becomes more rigid, the ratio  $2s/(s + 1)$  tends to 2, i.e. the dependence of  $E_n$  on  $n$  gradually approaches the quadratic one,  $E_n \propto n^2$ , pertinent to the hard-wall well discussed in Sec. 1.7 – see Eq. (1.85).

(ii) Since the potential is symmetric with respect to point  $x = 0$  and continuous at this (and all other) points, the simplest natural selection of the ground-state trial function is a Gaussian, for example

$$\psi_{\text{trial}}(x) = C \exp\left\{-\frac{\lambda^2 x^2}{4}\right\},$$

with some real  $\lambda$ . The normalization coefficient  $C$  may be immediately found either from the standard Gaussian integration of  $|\psi_{\text{trial}}(x)|^2$  over all  $x$ , or just from the comparison of this expression with Eq. (2.16) of the lecture notes, in which  $\lambda = 1/\delta x$ , i.e.  $\delta x = 1/\lambda$ , giving

$$|C|^2 = \frac{1}{(2\pi)^{1/2} \delta x} = \frac{\lambda}{(2\pi)^{1/2}}.$$

Now the expectation value of the particle's Hamiltonian,

$$\hat{H} = \frac{\hat{p}^2}{2m} + U(x) = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + ax^{2s},$$

in the trial state, may be calculated as

$$\begin{aligned} \langle H \rangle_{\text{trial}} &\equiv \int_{-\infty}^{+\infty} \psi_{\text{trial}}^* \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + ax^{2s} \right) \psi_{\text{trial}} dx = \int_{-\infty}^{\infty} C^* \exp\left\{-\frac{\lambda^2 x^2}{4}\right\} \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + ax^{2s} \right) C \exp\left\{-\frac{\lambda^2 x^2}{4}\right\} dx \\ &= 2 \frac{\lambda}{(2\pi)^{1/2}} \left( \frac{\hbar^2 \lambda^2}{4m} \frac{2^{1/2}}{\lambda} \int_0^{\infty} e^{-\xi^2} d\xi - \frac{\hbar^2 \lambda^4}{8m} \frac{2^{3/2}}{\lambda^3} \int_0^{\infty} \xi^2 e^{-\xi^2} d\xi + a \frac{2^{s+1/2}}{\lambda^{2s+1}} \int_0^{\infty} \xi^{2s} e^{-\xi^2} d\xi \right). \end{aligned}$$

All these three integrals are of the same well-known type,<sup>104</sup> yielding

$$\begin{aligned} \langle H \rangle_{\text{trial}} &= 2 \frac{\lambda}{(2\pi)^{1/2}} \left[ \frac{\hbar^2 \lambda^2}{4m} \frac{2^{1/2}}{\lambda} \frac{\pi^{1/2}}{2} - \frac{\hbar^2 \lambda^4}{8m} \frac{2^{3/2}}{\lambda^3} \frac{\pi^{1/2}}{4} + a \frac{2^{s+1/2}}{\lambda^{2s+1}} \frac{1}{2} \Gamma\left(s + \frac{1}{2}\right) \right] \\ &\equiv \frac{\hbar^2}{8m} \lambda^2 + a \frac{2^s}{\pi^{1/2}} \Gamma\left(s + \frac{1}{2}\right) (\lambda^2)^{-s}. \end{aligned}$$

<sup>104</sup> See, e.g., MA Eq. (6.9).

Since for  $s > 0$  this expression is positive for any  $\lambda^2$  and diverges at both  $\lambda^2 \rightarrow 0$  (due to the second term) and  $\lambda^2 \rightarrow \infty$  (due to the first term), it always has a minimum at some  $\lambda^2 = \lambda_{\text{opt}}^2$ , which may be found from the requirement

$$\frac{\partial \langle H \rangle_{\text{trial}}}{\partial (\lambda^2)} \Big|_{\lambda=\lambda_{\text{opt}}} \equiv \frac{\hbar^2}{8m} - a \frac{2^s}{\pi^{1/2}} \Gamma\left(s + \frac{1}{2}\right) s (\lambda^2)^{-s-1} \Big|_{\lambda=\lambda_{\text{opt}}} = 0,$$

giving

$$\lambda_{\text{opt}}^2 = \left[ \frac{8m}{\hbar^2} a \frac{2^s}{\pi^{1/2}} \Gamma\left(s + \frac{1}{2}\right) \right]^{\frac{1}{s+1}}, \quad E_{\text{var}} \equiv \langle H \rangle_{\text{trial}} \Big|_{\lambda=\lambda_{\text{opt}}} = \left[ \left( \frac{\hbar^2}{2m} \right)^s a \frac{s}{\pi^{1/2} 2^s} \Gamma\left(s + \frac{1}{2}\right) \right]^{\frac{1}{s+1}} \left( 1 + \frac{1}{s^s} \right).$$

For the quadratic potential, with  $s = 1$ , and hence  $\Gamma(s + 1/2) = \Gamma(3/2) = \pi^{1/2}/2$ ,<sup>105</sup> both the last expression and Eq. (\*\*\*) yield the same (and exact!) result

$$E_{\text{g}} = \hbar \left( \frac{a}{2m} \right)^{1/2} \equiv \frac{\hbar \omega_0}{2}, \quad \text{(*****)}$$

where  $\omega_0 \equiv (2a/m)^{1/2}$  is the classical frequency of this harmonic oscillator. However, with the growth of parameter  $s$ , the variational method starts to give higher ground-state energy than the WKB result. This is only natural because, for harder-wall potential wells with higher values of  $s$ , the Gaussian becomes an increasingly inadequate choice for the trial function. However, we should remember that the WKB approximation does not give accurate ground-state results either. (As was noted in Sec. 2.4 of the lecture notes, the validity of Eq. (\*\*\*) in this approximation is occasional.) Moreover, plugging the above WKB results for  $x_n$  and  $E_n$  into Eq. (2.107) spelled out for our potential, we see that it is fulfilled only if

$$2n - 1 \gg \left[ \frac{|2s - 1|^3}{2s} \right]^{1/2},$$

so that at  $s \gg 1$ , this approximation gives accurate results only for very high energy levels.

**Problem 2.39.** Use the variational method to estimate the 1<sup>st</sup> excited state of the 1D harmonic oscillator.

*Solution:* As was mentioned in Sec. 2.9 of the lecture notes, this may be done by requiring the new trial function to be orthogonal to the previously calculated ground state's eigenfunction, in our current case given by Eq. (2.275):

$$\psi_{\text{g}} = \frac{1}{\pi^{1/4} x_0^{1/2}} \exp\left\{-\frac{x^2}{2x_0^2}\right\}, \quad \text{with } x_0 \equiv \left(\frac{\hbar}{m\omega_0}\right)^{1/2}. \quad (*)$$

This wavefunction is symmetric, and has no zeros; hence, in the light of the Sturm oscillation theorem mentioned in Sec. 2.9, it is very natural to look for the first excited state's wavefunction in the form

$$\psi_{\text{trial}} = Cx \exp\{-\lambda x^2\}, \quad \text{with } \lambda > 0,$$

<sup>105</sup> See, e.g., MA Eq. (6.7e).

because it is antisymmetric (and hence automatically orthogonal to  $\psi_g$ ), and has just one zero. The normalization requirement,

$$\int_{-\infty}^{+\infty} \psi_{\text{trial}}^* \psi_{\text{trial}} dx \equiv |C|^2 \int_{-\infty}^{+\infty} x^2 \exp\{-2\lambda x^2\} dx \equiv \frac{|C|^2}{(2\lambda)^{3/2}} 2 \int_0^{+\infty} \xi^2 \exp\{-\xi^2\} d\xi = 1,$$

with  $\xi \equiv (2\lambda)^{1/2}x$ , includes a well-known table integral<sup>106</sup> equal to  $\pi^{1/2}/4$ , and hence yields

$$|C|^2 = \frac{2(2\lambda)^{3/2}}{\pi^{1/2}}.$$

With this normalization, the Hamiltonian's expectation value is

$$\begin{aligned} \langle H \rangle_{\text{trial}} &\equiv \int_{-\infty}^{+\infty} \psi_{\text{trial}}^* \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{m\omega_0^2 x^2}{2} \right) \psi_{\text{trial}} dx \\ &= |C|^2 \int_{-\infty}^{+\infty} x \exp\{-\lambda x^2\} \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{m\omega_0^2 x^2}{2} \right) x \exp\{-\lambda x^2\} dx \\ &\equiv \frac{2(2\lambda)^{3/2}}{\pi^{1/2}} \left[ 6\lambda \frac{\hbar^2}{2m} \frac{1}{(2\lambda)^{3/2}} 2 \int_0^{\infty} \xi^2 e^{-\xi^2} d\xi + \left( -4\lambda^2 \frac{\hbar^2}{2m} + \frac{m\omega_0^2}{2} \right) \frac{1}{(2\lambda)^{5/2}} 2 \int_0^{\infty} \xi^4 e^{-\xi^2} d\xi \right], \end{aligned}$$

with the same notation  $\xi \equiv (2\lambda)^{1/2}x$ . The former of these two dimensionless integrals is the same as above, and the latter one is of the same type,<sup>107</sup> equal to  $3\pi^{1/2}/8$ . As a result, we get

$$\langle H \rangle_{\text{trial}} = 3 \left( \lambda \frac{\hbar^2}{2m} + \frac{1}{4\lambda} \frac{m\omega_0^2}{2} \right).$$

The (only) minimum of this function of  $\lambda$  is achieved, not quite surprisingly, at the same value

$$\lambda_{\text{opt}} = \frac{m\omega_0}{2\hbar} \equiv \frac{1}{2x_0^2},$$

as for the ground-state wavefunction (\*), so the resulting 1<sup>st</sup> excited state's wavefunction is proportional to the same exponent:

$$\psi_1 \equiv (\psi_{\text{trial}})_{\lambda=\lambda_{\text{opt}}} = \frac{2^{1/2}}{\pi^{1/4} x_0^{3/2}} x \exp\left\{-\frac{x^2}{2x_0^2}\right\}.$$

Comparing this expression with Eq. (2.284) of the lecture notes for  $n = 1$ , and taking into account Eq. (2.282) for  $H_1$ , we see that for the harmonic oscillator, the variational method yields the *exact* expression for  $\psi_1(x)$ , and hence for the corresponding eigenenergy:

$$E_1 \equiv \langle H_{\text{trial}} \rangle_{\lambda=\lambda_{\text{opt}}} = \frac{3\hbar\omega_0}{2}.$$

Note, however, that the further development of this success would require a rapidly increasing volume of calculations. Indeed, as Eqs. (2.282) and (2.284) show, the next exact eigenfunction,  $\psi_2(x)$ , is

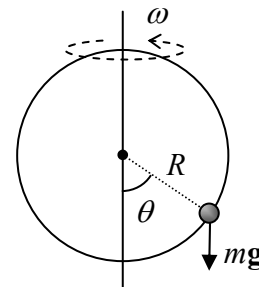
<sup>106</sup> See, e.g., MA Eq. (6.9c).

<sup>107</sup> See, e.g., MA Eq. (6.9d).



proportional to the Hermite polynomial  $H_2(x/x_0) = (4x^2/x_0^2 - 2)$  rather than just to some power of  $x$  as  $\psi_1(x)$  is, so finding it by using the variational approach would require at least two adjustable parameters, for example,  $\psi_{\text{trial}} \propto (x^2 + \lambda_1)\exp\{-\lambda_2 x^2\}$ .

**Problem 2.40.** Assuming the quantum effects to be small, calculate the lower part of the energy spectrum of the following system: a small bead of mass  $m$ , free to move without friction along a ring of radius  $R$ , which is rotated about its vertical diameter with a constant angular velocity  $\omega$  – see the figure on the right. Formulate a quantitative condition of validity of your results.



*Hint:* This system was used as the “testbed problem” in the CM part of this series, and the reader is welcome to use any relations derived there.

*Solution:* As was discussed in the CM part of this series, the classical Hamiltonian function of the system has the form<sup>108</sup>

$$H = \frac{p_\theta^2}{2mR^2} + U_{\text{ef}}(\theta),$$

with

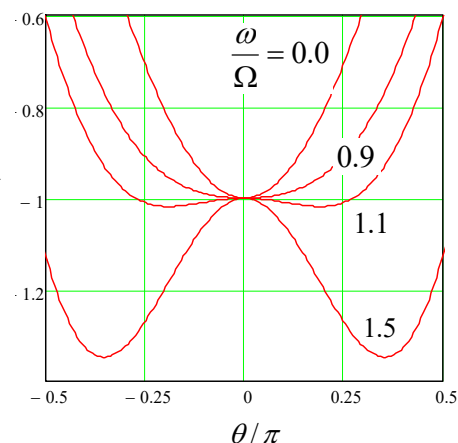
$$U_{\text{ef}}(\theta) = -mgR \cos \theta - \frac{m}{2} R^2 \omega^2 \sin^2 \theta \equiv -mgR \left( \cos \theta + \frac{\omega^2}{2\Omega^2} \sin^2 \theta \right),$$

where  $p_\theta$  is the generalized momentum corresponding to the generalized coordinate  $\theta$  (the angle of the bead’s deviation from the lowest point of the ring – see the figure above), and  $\Omega \equiv (g/R)^{1/2}$  is the frequency of small oscillations of the bead near that point in the case  $\omega = 0$  (no ring rotation).

The transition to quantum mechanics may be achieved, as was discussed in Chapter 1, by using the corresponding Hamiltonian operator,

$$\hat{H} = \frac{\hat{p}_\theta^2}{2mR^2} + U_{\text{ef}}(\theta), \quad \text{with } \hat{p}_\theta = -i\hbar \frac{\partial}{\partial \theta}. \quad (*)$$

Since the function  $U_{\text{ef}}(\theta)$  is not quite trivial (see the figure on the right), in the general case, the eigenvalues of this



<sup>108</sup> This result may be readily obtained by using either the Lagrangian formalism in an inertial (“lab”) reference frame or the effective 2<sup>nd</sup> Newton law with the additional centrifugal “inertial force”  $\mathbf{F}_c = -m\mathbf{a}_c \equiv -m\boldsymbol{\omega} \times (\boldsymbol{\omega} \times \mathbf{r})$  in the rotating (non-inertial) reference frame rotating with the ring – see, e.g., CM Secs. 2.2 and 4.6, respectively. At the latter approach, the second term in the above expression for  $U_{\text{ef}}$  is just the additional potential energy of the bead in the field of this “force”. Note also that is  $H$  the *effective* energy  $E_{\text{ef}}$  of the bead in the rotating reference frame rather than its “genuine” mechanical energy in an inertial reference frame. (The latter energy is *not* an integral of motion because of the bead’s strong interaction with the ring, and its minima do *not* correspond to stationary values of  $\theta$ . The reader to whom this point is not clear is strongly advised to review a discussion of this issue in classical mechanics – see, for example, the cited sections of the CM part of this series, in particular, CM Eq. (4.103) and the accompanying discussion.)

Hamiltonian cannot be calculated analytically. However, if the quantum-mechanical contributions to the system's lowest energies are small, it is sufficient for our task to consider only small vicinities of the minima of this effective potential.

If the ring's rotation is slow,  $\omega^2 \leq \Omega^2 \equiv g/R$ , the function  $U_{\text{ef}}(\theta)$  has only one minimum, at the lower point of the ring:  $\theta_0 = 0$ .<sup>109</sup> On the other hand, if the rotation velocity  $\omega$  exceeds the threshold value equal to  $\Omega$ , there are two similar minima of  $U_{\text{ef}}(\theta)$  at two symmetric points  $\theta_1 = \pm \sin^{-1}(\Omega^2/\omega^2) > 0$ , corresponding to the bead's rotation at the opposite sides of the ring. Taylor-expanding the effective potential energy near these points, and keeping only two first leading terms of the series, we get

$$U_{\text{ef}}(\theta) - U_{\text{min}} = \frac{mR^2 \tilde{\theta}^2}{2} \times \begin{cases} (\Omega^2 - \omega^2) > 0, & \text{for } \omega^2 < \Omega^2, \text{ where } \tilde{\theta} \equiv \theta - \theta_0, \\ (\omega^2 - \Omega^2) > 0, & \text{for } \Omega^2 < \omega^2, \text{ where } \tilde{\theta} \equiv \theta - \theta_1. \end{cases} \quad (**)$$

In this approximation, the Hamiltonian (\*) is reduced to that of a harmonic oscillator with a frequency equal to either  $\Omega_0 \equiv (\Omega^2 - \omega^2)^{1/2}$  (if  $\omega^2 < \Omega^2$ ), or  $\Omega_1 \equiv (\omega^2 - \Omega^2)^{1/2}$  (if  $\Omega^2 < \omega^2$ ). Hence the lower part of the effective energy's spectrum is well described, in both cases, by Eq. (2.262) of the lecture notes:

$$(E_{\text{ef}})_n = U_{\text{min}} + \left(n + \frac{1}{2}\right) \times \begin{cases} \hbar\Omega_0, & \text{for } \omega^2 < \Omega^2, \\ \hbar\Omega_1, & \text{for } \Omega^2 < \omega^2. \end{cases} \quad (***)$$

These expressions are only correct when this energy is within the range where the expansion (\*\*) is valid, i.e. only if  $(E_{\text{ef}})_n - U_{\text{min}} \ll U_{\text{max}} - U_{\text{min}}$ , giving the following validity condition:

$$n \ll n_{\text{max}} \equiv \frac{mR^2}{\hbar} \max[\Omega, \omega].$$

If the  $n_{\text{max}}$  so defined is less than or even of the order of 1, quantum effects are strong for all  $n$ , and the harmonic-oscillator approximation is not valid at all. Note, however, that in the opposite limit of *very* strong quantum effects, when  $n_{\text{max}} \ll 1$ , i.e. when  $\hbar^2/mR^2 \gg U_{\text{max}} - U_{\text{min}}$ , the system's properties become very simple again. (The *planar rotor* model valid in this limit will be discussed in Sec. 3.5.)

**Problem 2.41.** A 1D harmonic oscillator with mass  $m$  and frequency  $\omega_0$  was in its ground state. At  $t = 0$ , an additional force  $F$  is suddenly exerted on it and then that is kept constant. Calculate the probability of the oscillator staying in its ground state.

**Solution:** The ground-state wavefunction of the initial oscillator is given by Eq. (2.275) of the lecture notes, which may be recast as

$$\psi_{\text{ini}}(x) = \frac{1}{\pi^{1/4} x_0^{1/2}} \exp\left\{-\frac{x^2}{2x_0^2}\right\},$$

where  $x_0 \equiv (\hbar/m\omega_0)^{1/2}$ . Since the wavefunction does not have time to change during the abrupt application of the force,  $\psi_{\text{ini}}(x)$  plays the role of the initial condition,  $\Psi(x,0)$ , for the final system, described by the modified Hamiltonian

<sup>109</sup> For our current task, all the bead's positions that differ by a multiple of  $2\pi$  may be considered identical, and it is sufficient to consider just one of them.

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{m\omega_0^2}{2} x^2 - Fx \equiv -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{m\omega_0^2}{2} (x - X)^2 + \text{const}, \quad \text{with } X \equiv \frac{F}{m\omega_0^2}.$$

The last expression shows that the modified Hamiltonian differs from the initial one only by the shift  $X$  of the argument – which of course is just the classically-calculated static extension  $F/\kappa$  of the oscillator's spring, with the elastic constant  $\kappa = m\omega_0^2$ , by the applied force  $F$ . Hence the ground-state wavefunction of the final system differs from the initial one only by this shift:

$$\psi_{\text{fin}}(x) = \frac{1}{\pi^{1/4} x_0^{1/2}} \exp\left\{-\frac{(x - X)^2}{2x_0^2}\right\}.$$

Now we can calculate the requested probability as  $W_0 = |c_0|^2$ , where the coefficient  $c_0$  is given by the 1D version of Eq. (1.68):

$$c_0 = \int \psi_{\text{fin}}^*(x) \psi_{\text{ini}}(x) dx = \frac{1}{\pi^{1/2} x_0} \int_{-\infty}^{+\infty} \exp\left\{-\frac{x^2 + (x - X)^2}{2x_0^2}\right\} dx \equiv \frac{1}{\pi^{1/2}} \int_{-\infty}^{+\infty} \exp\left\{-\xi^2 + \xi \xi_X - \frac{1}{2} \xi_X^2\right\} d\xi,$$

where  $\xi \equiv x/x_0$  and  $\xi_X \equiv X/x_0 \equiv (F/m\omega_0^2)/(\hbar/m\omega_0)^{1/2}$ . This is a Gaussian integral, which may be readily worked out by the same completion to the full square as was repeatedly used in Chapter 2:

$$c_0 = \frac{1}{\pi^{1/2}} \int_{-\infty}^{+\infty} \exp\left\{-\left(\xi - \frac{1}{2} \xi_X\right)^2 - \frac{1}{4} \xi_X^2\right\} d\xi = \exp\left\{-\frac{\xi_X^2}{4}\right\}.$$

so, finally,

$$W_0 = \exp\left\{-\frac{\xi_X^2}{2}\right\} \equiv \exp\left\{-\frac{X^2}{2x_0^2}\right\} \equiv \exp\left\{-\frac{F^2}{2\hbar m \omega_0^3}\right\}.$$

The probability is very small if the force is larger than the so-called *standard quantum limit*

$$F_0 \equiv (\hbar m \omega_0^3)^{1/2} \equiv \kappa x_0;$$

this constant serves as a natural scale for the force effect's masking by quantum uncertainty.

**Problem 2.42.** A 1D particle of mass  $m$  was placed into a quadratic potential well (2.111),

$$U(x) = \frac{m\omega_0^2 x^2}{2},$$

and allowed to relax into the ground state. At  $t = 0$ , the well is fast accelerated to move with velocity  $v$ , without changing its profile, so at  $t \geq 0$  the above formula for  $U$  is valid with the replacement  $x \rightarrow x' \equiv x - vt$ . Calculate the probability for the system to still be in the ground state at  $t > 0$ .

*Solution:* Due to the invariance of the Schrödinger equation with respect to the Galilean transform (whose proof was the task of Problem 1.6), in the reference frame moving together with the potential profile,  $U$  is the function of the relative coordinate  $x' = x - vt$  only, but not of time. As was discussed in Sec. 1.5 of the lecture notes, in such time-independent potentials, the stationary state probabilities, in particular that of the ground state ( $W_0$ ), cannot change. Hence the system's exit from its ground state can arise only at the moment of its abrupt acceleration,  $t = 0$ .

For this short transient process, the ground state that existed at  $t \leq 0$ , with the wavefunction given by Eq. (2.275) of the lecture notes,

$$\Psi(x,0) = \psi_0(x) = \frac{1}{\pi^{1/4} x_0^{1/2}} \exp\left\{-\frac{x^2}{2x_0^2}\right\}, \quad \text{where } x_0 = \left(\frac{\hbar}{m\omega_0}\right)^{1/2}, \quad (*)$$

serves as the initial condition, so to calculate the requested probability  $W_0$ , we may apply Eq. (1.68) written in the moving reference frame:

$$W_0 = |c_0|^2, \quad \text{with } c_0 = \int_{-\infty}^{+\infty} \psi_0^*(x') \Psi'(x',0) dx'.$$

Here  $\psi_0(x')$  is given by the same Eq. (\*), with the replacement  $x \rightarrow x'$ , because in the moving reference frame the potential  $U(x')$ , and hence the ground state wavefunction, are exactly the same as they are in the lab frame at  $t \leq 0$ . However, the initial wavefunction  $\Psi'(x',0)$  has to be recalculated from  $\Psi(x,0)$  using the wavefunction transform whose proof was the subject of the same Problem 1.6; for the 1D case

$$\Psi'(x',t') = \Psi(x,t) \exp\left\{-i\frac{mvx}{\hbar} + i\frac{mv^2t}{2\hbar}\right\}.$$

For  $t = 0$ , when  $x' = x$ , this transform is reduced to

$$\Psi'(x',0) = \Psi(x,0) \exp\left\{-i\frac{mvx}{\hbar}\right\} = \psi_0(x') \exp\left\{-i\frac{mvx'}{\hbar}\right\}$$

so

$$c_0 = \int_{-\infty}^{+\infty} \psi_0^*(x') \psi_0(x') \exp\left\{-i\frac{mvx'}{\hbar}\right\} dx' = \frac{1}{\pi^{1/2} x_0} \int_{-\infty}^{+\infty} \exp\left\{-\frac{x'^2}{x_0^2} - i\frac{mvx'}{\hbar}\right\} dx'.$$

This is a standard Gaussian integral, with a structure similar to that, for example, of Eq. (2.21) of the lecture notes, which was worked out in detail in Sec. 2.2. An absolutely similar calculation yields

$$c_0 = \exp\left\{-\frac{v^2}{4v_0^2}\right\}, \quad \text{so } W_0 = |c_0|^2 = \exp\left\{-\frac{v^2}{2v_0^2}\right\}, \quad \text{where } v_0 \equiv \omega_0 x_0 = \left(\frac{\hbar\omega_0}{m}\right)^{1/2}.$$

This result shows that if the motion's velocity  $v$  is much lower than the natural quantum-mechanical scale  $v_0$  of the particle's velocity in its ground state,<sup>110</sup> then  $W_0 \rightarrow 1$ , i.e. the oscillator remains in its ground state with an almost 100% probability. If, on the contrary,  $v \gg v_0$ , then  $W_0 \rightarrow 0$ , meaning that the abrupt acceleration of the potential well almost certainly (with the probability  $1 - W_0 \rightarrow 1$ ) "shakes up" the oscillator into a linear superposition of its excited states.

**Problem 2.43.** Initially, a 1D harmonic oscillator was in its ground state. At a certain moment of time, its spring constant  $\kappa$  is abruptly increased so that its frequency  $\omega_0 = (\kappa/m)^{1/2}$  is increased by a factor of  $\alpha$ , and then is kept constant at the new value. Calculate the probability that after the change, the oscillator is still in its ground state.

<sup>110</sup> For example, it is easy (and hence left for the reader :-)) to use Eq. (\*) to prove that the expectation value of the observable  $(p/m)^2$ , i.e., of the square of the particle's velocity, in the ground state equals  $v_0^2/2$ .

*Solution:* According to Eq. (2.275) of the lecture notes, the ground state's wavefunction of the initial system is

$$\psi_{\text{ini}}(x) = \left(\frac{m\omega_0}{\pi\hbar}\right)^{1/4} \exp\left\{-\frac{m\omega_0 x^2}{2\hbar}\right\}.$$

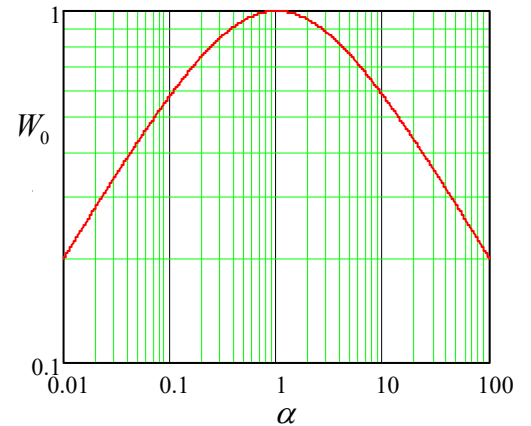
Since this wavefunction does not have time to change during the abrupt parameter's change, it plays the role of the initial condition,  $\Psi(x,0)$ , for the new system (the oscillator with the new spring constant). Hence we can use the 1D version of Eq. (1.68) to calculate the overlap integral  $c_0$  of this function with the similar ground state eigenfunction of the finite system (in which we have to make the replacement  $\omega_0 \rightarrow \alpha\omega_0$ ):

$$\begin{aligned} c_0 &= \int_{-\infty}^{+\infty} \psi_{\text{fin}}^*(x) \psi_{\text{ini}}(x) dx = \int_{-\infty}^{+\infty} \left(\frac{m\omega_0}{\pi\hbar}\right)^{1/4} \exp\left\{-\frac{m\omega_0 x^2}{2\hbar}\right\} \left(\frac{m\alpha\omega_0}{\pi\hbar}\right)^{1/4} \exp\left\{-\frac{m\alpha\omega_0 x^2}{2\hbar}\right\} dx \\ &\equiv \alpha^{1/4} \left(\frac{m\omega_0}{\pi\hbar}\right)^{1/2} \int_{-\infty}^{+\infty} \exp\left\{-(1+\alpha)\frac{m\omega_0 x^2}{2\hbar}\right\} dx \equiv \frac{\alpha^{1/4}}{\pi^{1/2}(1+\alpha)^{1/2}} \int_{-\infty}^{+\infty} \exp\left\{-\frac{\xi^2}{2}\right\} d\xi = \frac{2^{1/2} \alpha^{1/4}}{(1+\alpha)^{1/2}}. \end{aligned}$$

From this result, the probability that the oscillator remains in its ground state is:

$$W_0 = |c_0|^2 = \frac{2\alpha^{1/2}}{1+\alpha}.$$

This function is plotted in the figure on the right, in the most revealing log-log scale. As a sanity check, at  $\alpha = 1$  (i.e. no parameter change at all),  $W_0 = 1$ , just as it should be. If the spring constant *has* been changed, then  $W_0 < 1$  both for  $\alpha > 1$  (as in the problem's assignment), and for  $\alpha < 1$ , i.e. for the spring constant's *reduction*.



**Problem 2.44.** A 1D particle is in the following potential well:

$$U(x) = \begin{cases} +\infty, & \text{for } x < 0, \\ m\omega_0^2 x^2 / 2, & \text{for } x \geq 0. \end{cases}$$

- (i) Find its eigenfunctions and eigenenergies.
- (ii) The particle was allowed to relax into its ground state, and then the infinite potential wall at  $x < 0$  is rapidly removed so that the system is instantly turned into the usual harmonic oscillator (with the same  $m$  and  $\omega_0$ ). Find the probability for the particle to remain in the ground state.

*Solutions:*

(i) The stationary Schrödinger equation of the initial system at  $x > 0$  coincides with that of the usual harmonic oscillator and is hence satisfied by any of its eigenfunctions – see Eq. (2.284) of the lecture notes. However, the infinite potential at  $x < 0$  imposes the boundary condition  $\psi_n(0) = 0$ , which is satisfied only by the antisymmetric eigenfunctions with odd quantum numbers  $n = 2m + 1$  (with  $m = 0, 1, 2, \dots$ ). Taking into account that the wavefunctions should be now normalized on the segment  $0 < x < +\infty$  rather than  $-\infty < x < +\infty$ , we may write

$$\psi_m(x) = \begin{cases} 0, & \text{for } x < 0, \\ \frac{1}{[2^{2m}(2m+1)!]^{1/2} \pi^{1/4} x_0^{1/2}} \exp\left\{-\frac{x^2}{2x_0^2}\right\} H_{2m+1}\left(\frac{x}{x_0}\right), & \text{for } x > 0, \end{cases}$$

where  $x_0$  is given by Eq. (2.276), and the Hermite polynomials  $H_n(\xi)$  may be defined by Eq. (2.281).

(ii) Taking into account that, according to Eq. (2.282),  $H_1(\xi) = 2\xi$ , for the ground state of the initial system, with  $m = 0$ , the above result is reduced to

$$\psi_0(x) = \begin{cases} 0, & \text{for } x < 0, \\ \frac{1}{\pi^{1/4} x_0^{1/2}} \frac{2x}{x_0} \exp\left\{-\frac{x^2}{2x_0^2}\right\}, & \text{for } x > 0. \end{cases}$$

After the fast removal of the wall, this function plays the role of the initial condition  $\Psi(x, 0)$  for the resulting harmonic oscillator, so we may calculate the requested probability as  $W_g = |c_g|^2$ , with the coefficient  $c_g$  calculated by using the 1D version of Eq. (1.68):

$$c_g = \int \psi_g^*(x) \psi_0(x) dx,$$

where  $\psi_g(0)$  is the ground-state wavefunction of the usual harmonic oscillator, given by Eq. (2.275):

$$\psi_g(x) = \frac{1}{\pi^{1/4} x_0^{1/2}} \exp\left\{-\frac{x^2}{2x_0^2}\right\}.$$

As a result, we get

$$c_g = \frac{1}{\pi^{1/2} x_0} \int_0^\infty \frac{2x}{x_0} \exp\left\{-\frac{x^2}{x_0^2}\right\} dx \equiv \frac{1}{\pi^{1/2}} \int_0^\infty e^{-\xi} d\xi = \frac{1}{\pi^{1/2}},$$

so, finally,  $W_g = 1/\pi \approx 0.318$ .

**Problem 2.45.** Prove the following formula for the propagator of the 1D harmonic oscillator:

$$G(x, t; x_0, t_0) = \left( \frac{m\omega_0}{2\pi i \hbar \sin[\omega_0(t-t_0)]} \right)^{1/2} \exp\left\{ \frac{i m \omega_0}{2\hbar \sin[\omega_0(t-t_0)]} \left[ (x^2 + x_0^2) \cos[\omega_0(t-t_0)] - 2xx_0 \right] \right\}.$$

Discuss the relation between this formula and the propagator of a free 1D particle.

*Solution:* According to its definition given by Eq. (2.44) of the lecture notes (see also Eqs. (2.45)-(2.46) and their discussion), the propagator  $G(x, t; x_0, t_0)$  of a 1D quantum system has to satisfy two conditions:

- (i) if considered as a function of  $x$  and  $t$  only, it should obey the Schrödinger equation of the system, and
- (ii) it has to approach  $\delta(x - x_0)$  at  $t \rightarrow t_0$ .

For our case, condition (i) may be checked by direct differentiation of  $G$  over  $x$  (twice) and  $t$ , and plugging the results into the Schrödinger equation (2.261):

$$i\hbar \frac{\partial G}{\partial t} = \hat{H}G \equiv -\frac{\hbar^2}{2m} \frac{\partial^2 G}{\partial x^2} + \frac{m\omega_0^2 x^2}{2} G.$$

In order to check condition (ii), we may notice that in the limit  $(t - t_0) \ll 1/\omega_0$ , the propagator coincides with that of the free particle, given by Eq. (2.49) of the lecture notes, for which the condition (ii) is satisfied by construction – see Sec. 2.2.

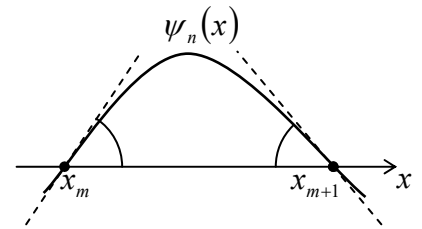
**Problem 2.46.** In the context of the Sturm oscillation theorem mentioned in Sec. 2.9 of the lecture notes, prove that the number of eigenfunction's zeros of a particle confined in an arbitrary but finite potential well always increases with the corresponding eigenenergy.

*Hint:* You may like to use the suitably modified Eq. (2.186).

*Solution:* Repeating the simple calculation that has led to Eq. (2.186), but now for two stationary states with such numbers  $n$  and  $n'$  that  $E_{n'} > E_n$  and for the  $x$ -segment limited by two adjacent zeros  $x_m$  and  $x_{m+1}$  of the stationary wavefunction  $\psi_n(x)$  corresponding to the lower energy, we get

$$(E_{n'} - E_n) \int_{x_m}^{x_{m+1}} \psi_n \psi_{n'} dx = \frac{\hbar^2}{2m} \left[ \frac{d\psi_n}{dx} \psi_{n'} \right]_{x_m}^{x_{m+1}}, \quad \text{where } \psi_n(x_m) = \psi_n(x_{m+1}) = 0. \quad (*)$$

Since, by construction, the zero points  $x_m$  and  $x_{m+1}$  are adjacent, the function  $\psi_n(x)$  does not change its sign between them. Since the wavefunctions are defined to an arbitrary complex multiplier  $\exp\{i\varphi\}$  with a real and constant phase  $\varphi$ ,<sup>111</sup> let us select this constant so that  $\psi_n(x)$  is real and positive on the interval  $x_m < x < x_{m+1}$ . Then  $d\psi_n/dx$  has to be positive (or equal zero) at  $x = x_m$  and negative (or equal zero) at  $x = x_{m+1}$  – see the figure on the right.



Let us assume for a minute that the function  $\psi_{n'}(x)$  corresponding to the larger energy  $E_{n'} > E_n$  also does not have a zero on this interval; in this case, we may also make this function real and positive on the whole interval  $[x_m, x_{m+1}]$  by the appropriate choice of its phase. Then the left-hand side of Eq. (\*) is positive, while its right-hand side is either negative or equal to zero. Hence our assumption has been wrong, i.e., the function  $\psi_{n'}(x)$  has at least one zero on the interval  $x_m < x < x_{m+1}$ . (It may be useful for the reader to revisit Figs. 1.8 and 2.35 of the lecture notes to see how spectacularly this general result works for the particular cases of hard and soft confinement.)

Now let us apply this result to each inter-zero interval of the function  $\psi_n(x)$ , noticing that it is also valid for infinite intervals, with  $x_m \rightarrow -\infty$  and/or  $x_{m+1} \rightarrow +\infty$ . (In these cases, the product  $(d\psi_n/dx)\psi_{n'}$  in Eq. (\*) equals zero at the corresponding end of the interval; note that the zero(s) of the function  $\psi_{n'}$  at such an interval still have to be finite.) If the function  $\psi_n(x)$  has  $M$  finite zeros  $x_m$ , there are  $(M + 1)$  of such intervals, and hence the function  $\psi_{n'}(x)$  has at least  $(M + 1)$  finite zeros. So the statement in the assignment is indeed correct.<sup>112</sup>

<sup>111</sup> According to Eq. (2.5) of the lecture notes, the phase  $\varphi$  of a stationary wavefunction of a confined 1D state, with the probability current  $I = 0$ , cannot depend on  $x$ .

<sup>112</sup> Other facts necessary for the full proof of the Sturm oscillation theorem, namely that  $M$  grows *exactly* by 1 at each step of the energy spectrum ladder and equals zero for the ground state, require more refined arguments.

**Problem 2.47.\*** Use the WKB approximation to calculate the lifetime of the metastable ground state of a 1D particle of mass  $m$  in the “pocket” of the potential profile

$$U(x) = \frac{m\omega_0^2}{2}x^2 - \alpha x^3.$$

Contemplate the significance of this problem.

*Solution:* This potential profile, sketched in the figure on the right for the case  $\alpha > 0$ ,<sup>113</sup> forms a soft potential well at  $x \sim 0$ , from which the particle may tunnel into the unrestricted half-space  $x > x_0$ . As a result, even the ground state of the particle in the well is metastable.

As was discussed in Sec. 2.5 of the lecture notes, the very notion of lifetime  $\tau$  of such a state is valid only if the potential barrier’s transparency  $\mathcal{T}$  calculated at the state’s energy  $E$  is much less than 1. For a smooth potential like ours, we may estimate the transparency by using the WKB-approximation-based Eq. (2.117), as

$$-\ln \mathcal{T} \sim \frac{2}{\hbar} \{2m[U_{\max} - E]\}^{1/2} x_1,$$

where  $x_1$  is the point where  $U(x) = 0$ . Calculating  $x_1$  and  $U_{\max}$  for our potential,

$$x_1 = \frac{m\omega_0^2}{2\alpha}, \quad x_m = \frac{m\omega_0^2}{3\alpha} \equiv \frac{2}{3}x_1, \quad \text{so } U_{\max} \equiv U(x_m) = \frac{(m\omega_0^2)^3}{54\alpha^2} \equiv \frac{2}{27}m\omega_0^2x_1^2,$$

and plugging these results into the above estimate, we see that the condition  $\mathcal{T} \ll 1$  requires that

$$E \ll U_{\max}.$$

(In this limit, we may use Eq. (2.274) to write

$$E = \frac{\hbar\omega_0}{2},$$

because for the small distances from the potential well’s bottom where the ground-state wavefunction is localized, the cubic term of the potential is negligible.) Due to this condition, the WKB expression,

$$-\ln \mathcal{T} = \frac{2(2m)^{1/2}}{\hbar} \int_{(\ )_{\geq 0}} \left( \frac{m\omega_0^2}{2}x^2 - \alpha x^3 - \frac{\hbar\omega_0}{2} \right)^{1/2} dx, \quad (*)$$

which follows from the general Eq. (2.117) for our potential profile, may be simplified.

In the crudest approximation, in which the ground-state energy  $E = \hbar\omega_0/2$  is neglected completely in comparison with  $U(x)$ , the integral is simple:

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However, they are virtually evident from the WKB-based Wilson-Sommerfeld quantization rule (2.110). Indeed, each new half-wave of the wavefunction corresponds to the increase of  $\Delta\varphi_{\rightarrow}$ , defined by Eq. (2.108), by  $\pi$ , and hence of  $\Delta\varphi_{\leftarrow} = \Delta\varphi_{\rightarrow}$  also by  $\pi$ , i.e. to the increase of the total wave change (2.109) by  $2\pi$ , i.e. to the increase of the quantum number  $n$  by 1.

<sup>113</sup> This choice of sign makes the notation simpler. (All final results for negative  $\alpha$ , i.e. for the potential  $U(x) = m\omega_0^2x^2/2 + \alpha x^3$ , with  $\alpha' = -\alpha > 0$ , are evidently similar, with the coordinate inversion  $x \rightarrow -x$ .)



$$-\ln \mathcal{F}_0 \equiv \frac{2(2m)^{1/2}}{\hbar} \int_0^{x_1} \left( \frac{m\omega_0^2}{2} x^2 - \alpha x^3 \right)^{1/2} dx \equiv \frac{27U_{\max}}{\hbar\omega_0} \int_0^1 \xi(1-\xi)^{1/2} d\xi,$$

where  $\xi \equiv x/x_1$ . The last integral may be readily worked out (for example, using the new substitution  $\alpha \equiv 1 - \xi$ ) and is equal to  $4/15$ , so we get

$$-\ln \mathcal{F}_0 = \frac{36 U_{\max}}{5 \hbar \omega_0}, \quad \text{i.e. } \mathcal{F}_0 = \exp\left\{-\frac{36 U_{\max}}{5 \hbar \omega_0}\right\},$$

proving that, indeed,  $\mathcal{F}_0 \ll 1$  only if  $\hbar\omega_0 \ll U_{\max}$ . Now, using Eq. (2.153) of the lecture notes, we can estimate the metastable lifetime  $\tau$  as  $t_a/\mathcal{F}_0$ , where  $t_a$  is the period between the classical particle's "attempts" to pass through the potential barrier.<sup>114</sup> In our case,  $t_a$  is the period  $2\pi/\omega_0$  of the classical oscillations at the bottom of the potential well, so

$$\tau_0 \equiv \frac{t_a}{\mathcal{F}_0} = \frac{2\pi}{\omega_0} \exp\left\{\frac{36 U_{\max}}{5 \hbar \omega_0}\right\}. \quad (**)$$

This expression is satisfactory for most practical applications because, as will be shown below, it gives the correct exponent – which, in our case  $\hbar\omega_0 \ll U_{\max}$ , dominates the value (\*\*).<sup>115</sup> To make a more exact calculation, we need to take into account the small ground-state energy  $E = \hbar\omega_0/2 \ll U_{\max}$ , at least in the first nonvanishing approximation. Looking at the figure above, it is clear the effect of non-zero  $E$  on the WKB integral (\*) is strongest at  $x \sim 0$  where the function  $U(x)$  grows most slowly. In this region,  $x_0 \leq x \leq x_{\text{int}}$ , where  $x_0$  is the left classical turning point defined by the condition

$$E = U(x_0), \quad \text{i.e. } \frac{\hbar\omega_0}{2} = \frac{m\omega_0^2 x_0^2}{2}, \quad \text{so } x_0 = \left(\frac{\hbar}{m\omega_0}\right)^{1/2},$$

and  $x_{\text{int}}$  is some intermediate point (see the figure above again) satisfying two strong conditions:

$$x_0 \ll x_{\text{int}} \ll x_m, \quad \text{so that } \frac{\hbar\omega_0}{2} \ll \frac{m\omega_0^2 x_{\text{int}}^2}{2} \ll \alpha x_{\text{int}}^3, \quad (***)$$

we may ignore the potential's anharmonic term  $\alpha x^3$ . On the other hand, in the complementary region  $x_{\text{int}} \leq x \leq x_0$ , the anharmonic term has to be treated exactly but the effects of non-zero energy  $E = \hbar\omega_0/2$  may be described in the linear approximation. As a result, the leading correction to our baseline result (\*\*) may be calculated as

<sup>114</sup> One may wonder whether this expression (which, for the lifetime problem considered in Sec. 2.5 of the lecture notes, was proved rather than conjectured, and is very intuitive for any nearly-classical motion) is quantitatively correct for the essentially quantum motion of the particle in the ground state of our current problem. However, its use is justified by the fact that, as was shown in Sec. 2.4, the WKB approximation gives the exact result of the ground-state energy of the harmonic oscillator and hence provides a perfect "stitching" of its exact wavefunction (2.275) with the WKB expression for it at  $x \gg x_0$ . (As the calculation below shows, for our current system with  $\hbar\omega_0 \ll U_{\max}$ , this stitching may be performed within the broad range  $x_0 \ll x \ll x_m$ , and is hence unaffected by the potential's anharmonicity at  $x \sim x_m$ .)

<sup>115</sup> Note the proximity of the numerical coefficient under the exponent,  $36/5 = 7.20$  for this cubic-parabolic barrier, to that for the quadratic-parabolic barrier,  $2\pi \approx 6.28$  – see Eq. (2.119) of the lecture notes, which is correctly described by the WKB approximation at  $(U_{\max} - E) \gg \hbar\omega_0$ .

$$\Delta(-\ln \mathcal{F}) \equiv (-\ln \mathcal{F}) - (-\ln \mathcal{F}_0)$$

$$\approx \frac{2(2m)^{1/2}}{\hbar} \left\{ \left[ \int_{x_0}^{x_{\text{int}}} \left( \frac{m\omega_0^2}{2} x^2 - \frac{\hbar\omega_0}{2} \right)^{1/2} dx - \int_{x_0}^{x_{\text{int}}} \left( \frac{m\omega_0^2}{2} x^2 \right)^{1/2} dx \right] + \int_{x_{\text{int}}}^{x_{\text{cl}}} \frac{\partial}{\partial E} \left[ \left( \frac{m\omega_0^2}{2} x^2 - \alpha x^3 - E \right)^{1/2} \right]_{E=0} \frac{\hbar\omega_0}{2} dx \right\}.$$

Performing the differentiation inside the last integral, and using the notation introduced above to bring the integrals to dimensionless forms, we get

$$\Delta(-\ln \mathcal{F}) \approx 2 \left[ \int_1^{x_{\text{int}}/x_0 \gg 1} (\zeta^2 - 1)^{1/2} d\zeta - \int_1^{x_{\text{int}}/x_0 \gg 1} \zeta d\zeta \right] - \int_{x_{\text{int}}/x_1 \ll 1}^1 \frac{d\xi}{\xi(1-\xi)^{1/2}},$$

where  $\zeta \equiv x/x_0$ , and  $\xi \equiv x/x_{\text{int}}$ . The second of these integrals is elementary, while the other two may be also readily worked out: the first one, by using the substitution  $\zeta \equiv \cosh \alpha$ , and the last one, by using the substitution  $\beta \equiv (1 - \xi)^{1/2}$ . The result,

$$\Delta(-\ln \mathcal{F}) \approx -\ln \frac{2x_{\text{int}}}{x_0} - \ln \frac{4x_1}{x_{\text{int}}} \equiv -\ln \frac{8x_1}{x_0} \equiv -\ln \left[ \left( \frac{864U_{\text{max}}}{\hbar\omega_0} \right)^{1/2} \right],$$

is independent of the exact choice of the auxiliary parameter  $x_{\text{int}}$  (as it has to be for the correctness of our “stitching” procedure), and we get the corrected WKB expression

$$\mathcal{F} = \left( \frac{864U_{\text{max}}}{\hbar\omega_0} \right)^{1/2} \exp \left\{ -\frac{36}{5} \frac{U_{\text{max}}}{\hbar\omega_0} \right\},$$

so the corrected lifetime of the metastable state is

$$\tau = \frac{2\pi}{\omega_0} \mathcal{F}^{-1} = \frac{2\pi}{\omega_0} \left( \frac{\hbar\omega_0}{864U_{\text{max}}} \right)^{1/2} \exp \left\{ \frac{36}{5} \frac{U_{\text{max}}}{\hbar\omega_0} \right\}, \quad \text{for } \hbar\omega_0 \ll U_{\text{max}}.$$

We see that the lifetime correction due to the ground-state energy leads not to just a different numerical factor in the pre-exponential coefficient; it makes this factor dependent on the system’s parameters.

Finally, let us discuss why this problem is very important. Let a 1D particle be confined at a minimum of an *arbitrary* but smooth potential  $U_0(x)$ . Let us gradually deform this potential, for example by application of an additional force  $F$ , which “tilts” its profile as

$$U(x) = U_0(x) - Fx,$$

so at some critical value  $F_c$  of the force, the minimum finally disappears. At  $F$  below but very close to this critical value, the “pocket” of energies  $U_{\text{min}} < E < U_{\text{max}}$  is very shallow, and the spatial extension of the pocket is very small, so the potential  $U(x)$  in its vicinity may be expanded into the Taylor series at its minimum, with only a few leading terms being essential. The linear term of the expansion, by definition, disappears at the minimum of the potential energy (say,  $x = 0$ ), so the leading term is quadratic and may

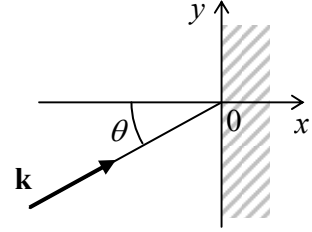
be always represented as  $m\omega_0^2 x^2/2$ , as in the potential of the solved problem. However, this term cannot describe the potential barrier – and hence the finite lifetime of the metastable state. For the minimal description of this effect, we need to keep the next, cubic term in the Taylor series, thus arriving at the model analyzed above.

Hence, our result for  $\tau$  is valid for the metastable ground state in virtually any sufficiently smooth potential  $U(x)$ , near the critical point of the potential well's disappearance. (The exception would be a very special function  $U(x)$  whose third derivative vanishes exactly at the point where the first one does.)

### Chapter 3. Higher Dimensionality Effects

**Problem 3.1.** A particle of energy  $E$  is incident (in the figure on the right, within the plane of the drawing) on a sharp potential step:

$$U(\mathbf{r}) = \begin{cases} 0, & \text{for } x < 0, \\ U_0, & \text{for } 0 < x. \end{cases}$$



Calculate the particle reflection probability  $\mathcal{R}$  as a function of the incidence angle  $\theta$ , and discuss this function for various magnitudes and signs of  $U_0$ .

*Solution:* As was discussed in Chapter 1, in wave mechanics, a particle with a definite energy, propagating in a definite direction (as implied by the assignment), is described by a monochromatic plane de Broglie wave (1.88) with a  $c$ -number wave vector  $\mathbf{k}$ . In our current case of the planar boundary ( $x = 0$ ) between two internally uniform regions, the vectors  $\mathbf{k}$  of the incident, reflected, and transmitted waves may have only two ( $x$ - and  $y$ -) components. In order to satisfy the boundary conditions at all points along the boundary's plane, the  $y$ -dependence of the waves at  $x \leq 0$  and  $0 \leq x$  should be the same. Thus the appropriate plane-wave solutions of the Schrödinger equation in these two regions are<sup>116</sup>

$$\psi(\mathbf{r}) = \begin{cases} (A \exp\{ik_x x\} + B \exp\{-ik_x x\}) \exp\{ik_y y\}, & \text{for } x \leq 0, \\ C \exp\{ik_x x\} \exp\{ik_y y\}, & \text{for } 0 \leq x, \end{cases}$$

where the wave vector components are related by a natural generalization of Eqs. (2.54) and (2.57):

$$\frac{\hbar^2 (k_x^2 + k_y^2)}{2m} = E, \quad \frac{\hbar^2 (k_x'^2 + k_y^2)}{2m} = E - U_0. \quad (*)$$

These expressions are valid even if  $E$  is so low that  $k_x'^2 < 0$  (for  $U_0 > E$ , this is the case for any angle  $\theta$ ); in this case, we may take  $k_x' = i\kappa$ , with real  $\kappa > 0$ , so toward the bulk of the region with  $0 < x$ , the wavefunction decays as  $\exp\{-\kappa x\}$ .

Thus the problem is reduced to the similar 1D problem that was solved in Sec. 2.3 of the lecture notes (see Fig. 2.4 and its discussion), and we can use the first of Eqs. (2.63), which, in our current notation, reads

$$\frac{B}{A} = \frac{k_x - k_x'}{k_x + k_x'}, \quad \text{so } \mathcal{R} \equiv \left| \frac{B}{A} \right|^2 = \left| \frac{k_x - k_x'}{k_x + k_x'} \right|^2. \quad (**)$$

However, due to Eqs. (\*), and the evident geometric relation (see the figure above)

$$\frac{k_y}{k_x} = \tan \theta, \quad (***)$$

<sup>116</sup> In classical mechanics, the fact that  $k_y$  is the same at  $x < 0$  and  $x > 0$ , corresponds to the conservation of the  $y$ -component of the particle's momentum, due to the absence of a force in this direction:  $F_y = -\partial U(\mathbf{r})/\partial y = 0$ .

we may see that if  $k_y \neq 0$  (i.e.  $\theta \neq 0$ ), the energy dependence of the x-component of the wave number is now different from the 1D case. Indeed, from Eqs. (\*) and (\*\*), we can readily get

$$\hbar k_x = (2mE)^{1/2} \cos \theta, \quad \hbar k_x' = [2m(E \cos^2 \theta - U_0)]^{1/2},$$

so Eq. (\*\*) yields

$$\mathcal{R} = \left| \frac{\cos \theta - (\cos^2 \theta - U_0/E)^{1/2}}{\cos \theta + (\cos^2 \theta - U_0/E)^{1/2}} \right|^2, \quad \text{for } \frac{U_0}{E} < \cos^2 \theta. \quad (****)$$

The figure on the right shows this reflection probability as a function of the incidence angle  $\theta$ , for several values of the  $U_0/E$  ratio. If  $U_0$  is negative, then Eq. (\*\*\*\*) is valid for any angle and describes a gradual increase of the reflection from such a potential “step-down” with the growth of  $\theta$  – see the dashed lines. (Note that the reflection always becomes almost total at  $\theta \rightarrow \pi/2$ , i.e. at the “grazing-angle” incidence.) Another visible trend is that the reflection is generally lower for smaller steps, and vanishes at  $U_0 \rightarrow 0$ .

As the solid lines show, both these trends are also valid for the potential “step-up”, i.e. if  $U_0$  is positive but still less than the particle’s energy  $E$ . Here Eq. (\*\*\*\*) also describes a reflection probability’s growth with the incidence angle, but now the increase is faster, and the reflection becomes total at a final “critical” value  $\theta_c = \arccos (U_0/E)^{1/2}$ . At larger angles (and also at any angle for  $U_0 > E$ ),  $k_x'$  is purely imaginary, and Eq. (\*\*) yields

$$\mathcal{R} = 1, \quad \text{for } \cos^2 \theta < \frac{U_0}{E},$$

describing the so-called *total internal reflection*, completely similar to that of electromagnetic waves.<sup>117</sup>

Moreover, Eq. (\*\*\*\*) is an analog of the well-known Fresnel formulas. However, due to the scalar nature of the de Broglie waves, there is only one such formula in wave mechanics, rather than two in electrodynamics – for two possible electromagnetic wave polarizations.<sup>118</sup>

**Problem 3.2.** For a charged particle moving in a magnetic field  $\mathcal{B}$ , calculate the commutation relations between Cartesian components of the kinetic (“ $m\mathbf{v}$ –”) momentum operator defined by Eq. (3.20). Can the result be represented in a vector form?

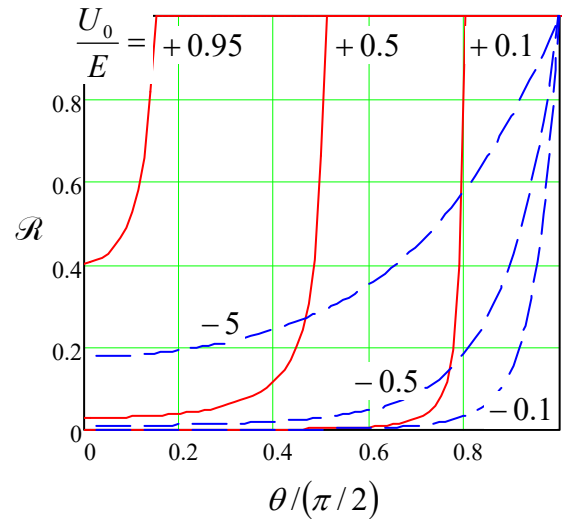
*Solution:* The operator form of Eq. (3.20), with the canonical momentum operator given by Eq. (3.25), is<sup>119</sup>

$$\hat{\mathbf{p}} = -i\hbar\nabla - q\mathbf{A}, \quad (*)$$

<sup>117</sup> See, e.g., EM Sec. 7.4.

<sup>118</sup> See, e.g., EM Eqs. (7.91) and (7.95).

<sup>119</sup> Implicitly, this expression was already used in Eq. (3.26) of the lecture notes.



where  $q$  is the particle's electric charge, so the  $j^{\text{th}}$  Cartesian component of the operator is

$$\hat{p}_j = -i\hbar \frac{\partial}{\partial r_j} - qA_j,$$

where the index  $j$  may take any value of the set  $\{1, 2, 3\}$ . Let us calculate the commutator of two such components, with  $j' \neq j$ :

$$\begin{aligned} [\hat{p}_j, \hat{p}_{j'}] &= \left[ \left( -i\hbar \frac{\partial}{\partial r_j} - qA_j \right), \left( -i\hbar \frac{\partial}{\partial r_{j'}} - qA_{j'} \right) \right] \\ &\equiv -\hbar^2 \left[ \frac{\partial}{\partial r_j}, \frac{\partial}{\partial r_{j'}} \right] + q^2 [A_j, A_{j'}] + i\hbar q \left( \left[ \frac{\partial}{\partial r_j}, A_{j'} \right] + \left[ A_j, \frac{\partial}{\partial r_{j'}} \right] \right). \end{aligned} \quad (**)$$

The first of the four commutators in the last expression equals zero because of the well-known rule of double partial differentiation of any function:

$$\frac{\partial^2 \psi}{\partial r_j \partial r_{j'}} = \frac{\partial^2 \psi}{\partial r_{j'} \partial r_j}, \quad \text{so} \quad \left( \frac{\partial}{\partial r_j} \frac{\partial}{\partial r_{j'}} - \frac{\partial}{\partial r_{j'}} \frac{\partial}{\partial r_j} \right) \psi \equiv \left( \frac{\partial^2}{\partial r_j \partial r_{j'}} - \frac{\partial^2}{\partial r_{j'} \partial r_j} \right) \psi = 0.$$

The second of the commutators in Eq. (\*\*) also vanishes because all Cartesian components of the vector operator  $\mathbf{A}$  are functions of  $\mathbf{r}$  (and maybe time), and hence, in the coordinate representation we are studying now, act upon any function just like the operator  $\hat{\mathbf{r}}$  (see the first of Eqs. (1.26) of the lecture notes), i.e. just as simple multipliers, which may be swapped:

$$A_j A_{j'} \psi = A_{j'} A_j \psi, \quad \text{so} \quad [A_j, A_{j'}] \psi \equiv (A_j A_{j'} - A_{j'} A_j) \psi = 0.$$

However, the last two commutators in Eq. (\*\*) do not vanish. Indeed, we may consider their action upon a function just as it was done with the operators of  $x$  and  $p_x$  in Eq. (2.14):

$$\left[ \frac{\partial}{\partial r_j}, A_{j'} \right] \psi \equiv \frac{\partial}{\partial r_j} (A_{j'} \psi) - A_{j'} \frac{\partial \psi}{\partial r_j} = \left( \frac{\partial A_{j'}}{\partial r_j} \psi + A_{j'} \frac{\partial \psi}{\partial r_j} \right) - A_{j'} \frac{\partial \psi}{\partial r_j} \equiv \frac{\partial A_{j'}}{\partial r_j} \psi.$$

Since this equality is valid for any  $\psi$ , we may represent it as the following operator identity:

$$\left[ \frac{\partial}{\partial r_j}, A_{j'} \right] = \frac{\partial A_{j'}}{\partial r_j}.$$

The last commutator in Eq. (\*\*) differs from this one only by the operand order (i.e. by the sign) and the index swap. As a result, Eq. (\*\*) yields

$$[\hat{p}_j, \hat{p}_{j'}] = i\hbar q \left( \frac{\partial A_{j'}}{\partial r_j} - \frac{\partial A_j}{\partial r_{j'}} \right). \quad (***)$$

However according to vector algebra,<sup>120</sup> if the indices  $j$  and  $j'$  run in any "correct" order:  $1 \rightarrow 2 \rightarrow 3 \rightarrow 1 \rightarrow 2 \dots$ , the expression in the parentheses is just the  $(j'')^{\text{th}}$  component of the vector  $\nabla \times \mathbf{A}$ , where

<sup>120</sup> See, e.g., MA Eq. (8.5).

the index  $j''$  is complementary to  $j$  and  $j'$ . On the other hand, classical electrodynamics<sup>121</sup> tells us that the vector  $\nabla \times \mathbf{A}$  is just the magnetic field  $\mathcal{B}$ , so we get a very simple result:

$$[\hat{p}_j, \hat{p}_{j'}] = i\hbar q \mathcal{B}_{j''}.$$

In the opposite case when the indices  $j$  and  $j'$  run in an “incorrect” order, this equality is still valid but with the opposite sign. Finally, if  $j = j'$ , the right-hand side of Eq. (\*\*\*) vanishes. All these facts may be represented by using the Levi-Civita symbol:<sup>122</sup>

$$[\hat{p}_j, \hat{p}_{j'}] = i\hbar q \sum_{j''=1}^3 \mathcal{B}_{j''} \varepsilon_{jj'j''}, \quad (****)$$

where the choice of the indices  $j, j'$ , and  $j''$  is now arbitrary. In particular, since this symbol may be used to rewrite the well-known relation<sup>123</sup> between the Cartesian components of the vector product and its operands as

$$a_j b_{j'} - b_j a_{j'} = \sum_{j''=1}^3 (\mathbf{a} \times \mathbf{b})_{j''} \varepsilon_{jj'j''},$$

the set of Eqs. (\*\*\*\*) for all Cartesian components may be represented in the following compact vector form:<sup>124</sup>

$$\hat{\mathbf{p}} \times \hat{\mathbf{p}} = i\hbar q \mathcal{B}.$$

Note that according to this formula, the vector product of the kinetic momentum operator by itself vanishes only in the absence of a magnetic field, while for the corresponding  $c$ -number vector of classical mechanics, this is always the case.

**Problem 3.3.** In the classical mechanics version of the Landau-level problem discussed in Sec. 3.2 of the lecture notes, the geometric center of the particle’s orbit is an integral of motion, determined by initial conditions. Calculate the commutation relation between the quantum-mechanical operators corresponding to the Cartesian coordinates of the center.

*Solution:* The Landau problem is that of a non-relativistic 2D particle of mass  $m$ , with electric charge  $q$ , moving in a uniform magnetic field  $\mathcal{B} = \mathcal{B} \mathbf{n}_z$  normal to the particle’s confinement plane  $[x, y]$ . Its solution in classical mechanics is simple and well-known:<sup>125</sup> since the magnetic Lorentz force  $\mathbf{F} = q[\mathbf{v} \times \mathcal{B}]$  exerted on the particle is perpendicular to the vector of its velocity  $\mathbf{v}$ , it causes the particle’s rotation within the confinement plane, with the radius  $r$  that may be readily calculated from 2<sup>nd</sup> Newton law for the circular motion:

<sup>121</sup> Just as a reminder, in this course until Chapter 9, we consider *quantum* properties of particles moving in the fields described *classically*.

<sup>122</sup> See, e.g., MA Eq. (13.2). Note that in some texts, the sum on the right-hand side of this (and other similar relations) is dropped. This is only correct if this omission is compensated by adding the condition  $j'' \neq j, j'$ .

<sup>123</sup> See, e.g., MA Eq. (7.3).

<sup>124</sup> A direct derivation of this formula from Eq. (\*) is a useful additional exercise, highly recommended to the reader.

<sup>125</sup> If necessary, see, e.g., EM Sec. 9.6 – which also discusses the relativistic version of the problem.

$$m \frac{v^2}{r} = |qv\mathcal{B}|, \quad \text{giving } r = m \left| \frac{v}{q\mathcal{B}} \right|.$$

In contrast, according to the same equation, the “cyclotron” frequency  $\omega_c \equiv d\varphi/dt$  of the particle’s rotation does not depend on its speed  $v$ , i.e. on the initial conditions:<sup>126</sup>

$$\omega_c = -\frac{q\mathcal{B}}{m}.$$

However, the coordinates  $\{X, Y\}$  of the rotation center, participating in the circular motion’s description,

$$x = X + r \cos \varphi, \quad y = Y + r \sin \varphi, \quad \text{where } \varphi = \omega_c t + \varphi_0,$$

(as well as the orbit’s radius  $r$  and the initial angle  $\varphi_0$ ), are constants determined by initial conditions. Since the Cartesian components of the particle’s velocity are

$$v_x \equiv \frac{dx}{dt} = -\omega_c r \sin \varphi, \quad v_y \equiv \frac{dy}{dt} = \omega_c r \cos \varphi,$$

these constants may be expressed as time-independent combinations of the coordinate and velocity components:

$$X = x - \frac{1}{\omega_c} v_y, \quad Y = y + \frac{1}{\omega_c} v_x. \quad (*)$$

Now in quantum mechanics, as was discussed in Sec. 3.1 of the lecture notes,<sup>127</sup> in the presence of a magnetic field, the operator of the particle’s velocity is

$$\hat{\mathbf{v}} = \frac{\hat{\mathbf{p}}}{m} = \frac{\hat{\mathbf{P}} - q\hat{\mathbf{A}}}{m}, \quad (**)$$

where  $\mathbf{P}$  is the canonical momentum whose operator may be expressed by Eq. (3.25) of the lecture notes, so it commutes in the standard way (2.14) with the Cartesian components of the radius vector:

$$[\hat{x}, \hat{P}_x] = i\hbar, \quad [\hat{y}, \hat{P}_y] = i\hbar, \quad [\hat{x}, \hat{P}_y] = 0, \quad [\hat{y}, \hat{P}_x] = 0, \quad [\hat{P}_x, \hat{P}_y] = 0. \quad (***)$$

Let us select, for the sake of simplicity, the Landau gauge (3.44) of the magnetic potential with  $x_0 = 0$ , so  $A_x = 0$  and  $A_y = \mathcal{B}x$ . (It is straightforward, though more bulky, to show that the final result for the commutator is the same in any gauge.) Then Eq. (\*\*) is reduced to

$$\hat{v}_x = \frac{\hat{P}_x}{m}, \quad \hat{v}_y = \frac{\hat{P}_y - q\mathcal{B}\hat{x}}{m} \equiv \frac{\hat{P}_y}{m} + \omega_c \hat{x},$$

so the operators corresponding to the variable combinations (\*) are

<sup>126</sup> In contrast to Eq. (3.48) of the lecture notes, giving the cyclotron frequency’s *magnitude*, this expression may have any sign, and describes the correct direction of the particle’s rotation in the  $[x, y]$  plane: say, clockwise ( $\omega_c < 0$ ) if  $q\mathcal{B} > 0$ .

<sup>127</sup> See also the solution of the previous problem.



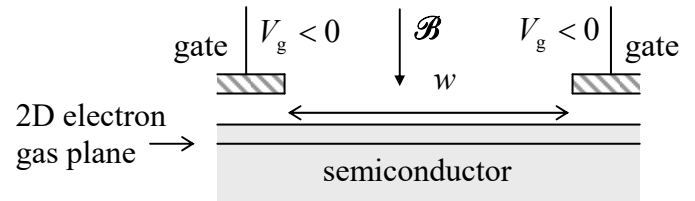
$$\hat{X} \equiv \hat{x} - \frac{1}{\omega_c} \hat{v}_y = \hat{x} - \frac{1}{m\omega_c} (\hat{P}_y + m\omega_c \hat{x}) \equiv -\frac{1}{m\omega_c} \hat{P}_y, \quad \hat{Y} \equiv \hat{y} + \frac{1}{\omega_c} \hat{v}_x \equiv \hat{y} + \frac{1}{m\omega_c} \hat{P}_x.$$

Now it is straightforward to use Eqs. (\*\*\*) to calculate the commutator of these operators:

$$[\hat{X}, \hat{Y}] = \left[ -\frac{\hat{P}_y}{m\omega_c}, \hat{y} + \frac{\hat{P}_x}{m\omega_c} \right] = \frac{i\hbar}{m\omega_c} \equiv \pm i r_L^2,$$

where  $r_L$  is the Landau radius (see Eq. (3.51) of the lecture notes), while the sign is determined by that of the product  $q\mathcal{B}$ . This result shows that in the Landau problem, the observables  $X$  and  $Y$  are not independent and that  $r_L$  gives the spatial scale of their uncertainty.

**Problem 3.4.\*** Analyze how are the Landau levels (3.50) modified by an additional uniform electric field  $\mathcal{E}$  directed along the plane of the particle's motion. Contemplate the physical meaning of your result and its implications for the quantum Hall effect in a gate-defined Hall bar. (The area  $l \times w$  of such a bar is defined by metallic "gate" electrodes parallel to the 2D electron gas plane – see the figure on the right. The negative voltage  $V_g$  applied to the gates squeezes the 2D gas from the area under them into the complementary, Hall-bar part of the plane.)



*Solution:* The constant electric field directed along a certain coordinate axis (say,  $x$ ) creates the additional potential

$$\Delta U = -q\mathcal{E}x.$$

Reviewing the calculations carried out at the beginning of Sec. 3.2 of the lecture notes with the account of this additional potential, we see that Eq. (3.47) is now modified as follows:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} X_k + \frac{q^2}{2m} \mathcal{B}^2 (x - x_0')^2 X_k - q\mathcal{E}x X_k = E X_k,$$

where, as in Sec. 3.2,

$$x_0' \equiv x_0 + \frac{\hbar k}{q\mathcal{B}}.$$

This equation may be rewritten in a form similar to the initial one:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} X_k + \frac{q^2}{2m} \mathcal{B}^2 \tilde{x}^2 X_k = \tilde{E} X_k,$$

but with an additional shift of the reference point:

$$\tilde{x} \equiv x - x_0'', \quad \text{where } x_0'' \equiv x_0' + \frac{m}{q\mathcal{B}^2} \mathcal{E},$$

and, more importantly, with a different constant on the right-hand side:

$$\tilde{E} \equiv E + q\mathcal{E}x_0'' - \frac{m\mathcal{E}^2}{2\mathcal{B}^2}.$$

This means that Eq. (3.50) of the lecture notes is now valid for the parameter  $\tilde{E}$  rather than for the eigenenergy  $E$ , and the genuine energy spectrum now depends on  $x_0''$ , i.e. on the position of the wavefunction's center:

$$E_n = \hbar\omega_c \left( n + \frac{1}{2} \right) - q\mathcal{E}x_0'' + \text{const.}$$

The physical interpretation of this result is straightforward: the whole set of Landau levels moves up or down together with the electrostatic potential energy the particle *would have* if it was classically localized at the center  $\{x_0'', y_0\}$  of its wavefunction:

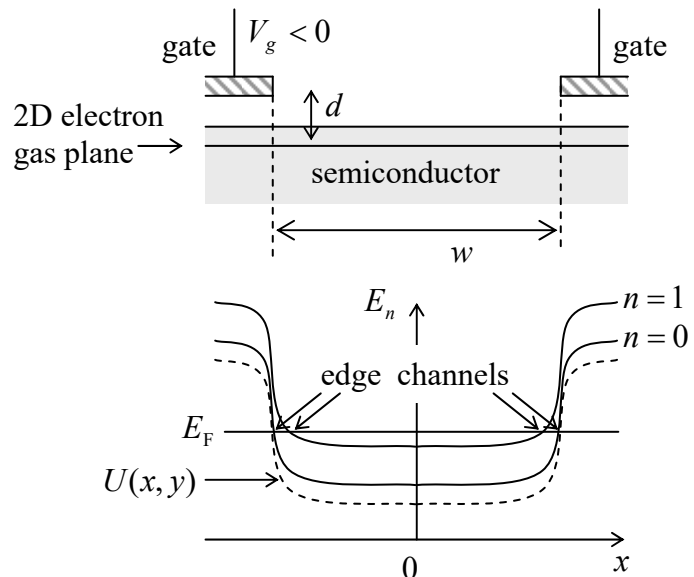
$$E_n = \hbar\omega_c \left( n + \frac{1}{2} \right) + U(x_0'', y_0), \quad (*)$$

where, in our particular case,  $U(x, y) = -q\mathcal{E}x + \text{const.}$  It is virtually evident that Eq. (\*) is valid for any external potential  $U(x, y)$  if it changes in space smoothly enough. Indeed, it may be shown that Eq. (\*) is asymptotically correct if the potential's curvature is sufficiently small; for example, for  $U = U(x)$  and relatively low Landau levels,  $n \sim 1$ , the potential has to satisfy the following condition:<sup>128</sup>

$$\left| \frac{\partial^2 U}{\partial x^2} \right| \ll \frac{1}{r_L} \left| \frac{\partial U}{\partial x} \right|, \quad (**)$$

where  $r_L$  is the Landau radius (3.51):  $r_L \equiv (\hbar/|q\mathcal{B}|)^{1/2}$ . For the usual quantum Hall experiments, with  $|q| \sim e \approx 1.6 \times 10^{-19} \text{C}$  and  $\mathcal{B}$  of a few teslas, the Landau radius is of the order of 10 nm, while the walls of the potential well  $U(x)$  in the gate-defined Hall bar are smeared by a distance of the order of the gate electrode's distance  $d$  from the 2D electron gas plane – typically of the order of a few hundred nm. Hence the condition (\*\*) is reasonably well fulfilled; as a result, one may analyze the quantum Hall effect in such a bar using the picture of *space-dependent Landau levels*  $E_n(x, y)$  repeating the potential well's profile – see the figure on the right.

As was discussed in Sec. 3.2 of the lecture notes, at sufficiently low temperatures, the electron states corresponding to the regions where these levels are submerged below the Fermi energy  $E_F$  are fully occupied, while those above it are empty. As I hope the reader knows from undergraduate physics (and as will be discussed in detail in SM Chapter 6), the electric-field-driven electron transport may take place only at the Fermi surface, because it requires



<sup>128</sup> If this condition is not met, the electric field may also affect the distance between the Landau levels – see, e.g., the next problem.

repeated pick-ups of small portions of energy from the driving field and their consequent drain to electron scattering centers. Hence, at the quantum Hall effect, the transport is only possible in quasi-1D *edge channels* (of a small width  $\sim r_L$ ) formed by each Landau-level surface  $E_n(x, y)$  crossing the Fermi energy plane  $E = E_F = \text{const.}$

Detailed analyses (for whose description I do not have time/space this series) show that electrons traveling along these channels cannot be back-scattered by (unavoidable) small inhomogeneities of the sample. This fact is exactly the origin of the unprecedented accuracy of the Hall resistance  $R_H$  (3.56), which is so unusual for solid-state physics.

**Problem 3.5.** Analyze how are the Landau levels (3.50) modified if a 2D particle is confined in an additional 1D potential well  $U(x) = m\omega_0^2 x^2/2$ .

*Solution:* With this additional potential, the Schrödinger equation (3.41) becomes

$$-\frac{\hbar^2}{2m} \left( \mathbf{n}_x \frac{\partial}{\partial x} + \mathbf{n}_y \frac{\partial}{\partial y} - i \frac{q}{\hbar} \mathbf{A} \right)^2 \psi + \frac{m}{2} \omega_0^2 x^2 \psi = E \psi .$$

With the same choice of the vector-potential as in Eq. (3.44), and the Fourier expansion (3.45), instead of Eq. (3.47) we now get

$$-\frac{\hbar^2}{2m} \frac{d^2}{d\tilde{x}^2} X_k + \left[ \frac{q^2}{2m} \mathcal{B}^2 \tilde{x}^2 + \frac{m}{2} \omega_0^2 x^2 \right] X_k = E X_k, \quad \text{with } \tilde{x} \equiv x - x_0', \quad x_0' \equiv x_0 + \frac{\hbar k}{q\mathcal{B}} .$$

The two terms inside the square brackets (both quadratic-parabolic functions of  $x$ ) may be merged:

$$\frac{q^2}{2m} \mathcal{B}^2 \tilde{x}^2 + \frac{m}{2} \omega_0^2 x^2 = \frac{m}{2} (\omega_c^2 \tilde{x}^2 + \omega_0^2 x^2) \equiv \frac{m}{2} \omega_{\text{ef}}^2 \tilde{x}^2 + \text{const},$$

where  $\omega_{\text{ef}}$  is the effective frequency defined by the following relation:

$$\omega_{\text{ef}}^2 \equiv \omega_c^2 + \omega_0^2, \quad \text{with } \omega_c \equiv \frac{|q\mathcal{B}|}{m}, \quad (*)$$

and  $\tilde{x} \equiv x - x_k$  is the coordinate  $x$  referred to a certain point  $x_k$ , which depends on our arbitrary choice of  $x_0$ , and hence is itself arbitrary. As a result, besides an arbitrary (and inconsequential) choice of the energy and coordinate offsets, the Schrödinger equation is again reduced to that of a 1D harmonic oscillator, and hence has a similar energy spectrum,

$$E_n = \hbar \omega_{\text{ef}} \left( n + \frac{1}{2} \right),$$

but now with the modified (increased) frequency defined by Eq. (\*). Hence the “soft” confinement increases the distance between the Landau levels.

**Problem 3.6.** Find the stationary states of a spinless, charged 3D particle moving in “crossed” (mutually perpendicular) uniform electric and magnetic fields, with  $\mathcal{E} \ll c\mathcal{B}$ . For such states, calculate the expectation values of the particle’s velocity in the direction normal to both fields and compare the result with the solution of the corresponding classical problem.

*Hint:* You may like to generalize Landau's solution for 2D particles, discussed in Sec. 3.2 of the lecture notes, to the 3D case.

*Solution:* Just as was done in Sec. 3.2, let us direct the  $z$ -axis along the magnetic field and the  $x$ -axis along the electric field; then we may use the same choice (3.44) of the vector-potential:

$$A_x = 0, \quad A_y = \mathcal{B}(x - x_0), \quad A_z = 0,$$

and write the electrostatic potential in the form

$$\phi(\mathbf{r}) = -\mathcal{E}x, \quad \text{so } U(\mathbf{r}) = q\phi(\mathbf{r}) = -q\mathcal{E}x.$$

With these choices, the Schrödinger equation (3.27) takes the form

$$-\frac{\hbar^2}{2m} \left\{ \frac{\partial^2}{\partial x^2} + \left[ \frac{\partial}{\partial y} - \frac{iq}{\hbar} \mathcal{B}(x - x_0) \right]^2 + \frac{\partial^2}{\partial z^2} \right\} \psi - q\mathcal{E}x\psi = E\psi.$$

It is evidently satisfied by the following eigenfunction (which is a natural generalization of the function used in Eq. (3.45) of the lecture notes):<sup>129</sup>

$$\psi_k = X_k(x) \exp\{ik_y(y - y_0) + ik_z(z - z_0)\}, \quad (*)$$

where the function  $X_k(x)$  obeys the following 1D equation:

$$-\frac{\hbar^2}{2m} \left\{ \frac{d^2}{dx^2} - \left[ k_y - \frac{q}{\hbar} \mathcal{B}(x - x_0) \right]^2 - k_z^2 \right\} X_k - q\mathcal{E}xX_k = E_k X_k.$$

This equation may be rewritten in the form of Eq. (3.47):

$$-\frac{\hbar^2}{2m} \frac{d^2}{d\tilde{x}^2} X_k + \frac{q^2}{2m} \mathcal{B}^2 \tilde{x}^2 X_k = \tilde{E} X_k, \quad (**)$$

where  $\tilde{x} \equiv x - x_0''$  is the coordinate  $x$  offset by the value (now depending on both applied fields):

$$x_0'' \equiv x_0' + \frac{m\mathcal{E}}{q\mathcal{B}^2} \equiv x_0 + \frac{\hbar k_y}{q\mathcal{B}} + \frac{m\mathcal{E}}{q\mathcal{B}^2}, \quad (***)$$

and  $\tilde{E}_k$  is the eigenenergy  $E_k$ , offset by a constant.<sup>130</sup> As was discussed in Sec. 3.2, Eq. (\*\*) is satisfied by eigenfunctions of a 1D harmonic oscillator with the frequency  $\omega_c$  equal to the cyclotron frequency of the particle's motion in the applied magnetic field – see Eq. (3.48) of the lecture notes.

Now we may combine Eqs. (3.20) and (3.25) of the lecture notes to calculate the operator of the particle's velocity along the  $y$ -axis normal to both applied fields:

$$\hat{v}_y = \frac{1}{m} \left( -i\hbar \frac{\partial}{\partial y} - qA_y \right) = \frac{1}{m} \left[ -i\hbar \frac{\partial}{\partial y} - q\mathcal{B}(x - x_0) \right].$$

<sup>129</sup> Here the index  $k$  symbolizes the set of  $c$ -number parameters  $k_y$ ,  $k_z$ ,  $x_0$ ,  $y_0$ , and  $z_0$ .

<sup>130</sup> Eqs. (\*\*) and (\*\*\*) are a natural 3D generalization of the corresponding formulas derived in the model solution of Problem 4.

By using Eq. (\*\*\*), this result may be represented as

$$\hat{v}_y = \frac{1}{m} \left[ -i\hbar \frac{\partial}{\partial y} - q\mathcal{B} \left( \tilde{x} + \frac{\hbar k_y}{q\mathcal{B}} + \frac{m\mathcal{E}}{q\mathcal{B}^2} \right) \right] \equiv \frac{1}{m} \left( -i\hbar \frac{\partial}{\partial y} - \hbar k_y \right) - \frac{q\mathcal{B}}{m} \tilde{x} - \frac{\mathcal{E}}{\mathcal{B}}.$$

For the properly normalized eigenfunction (\*), the expectation value of the operator  $\partial/\partial y$  is  $ik_y$ , so the expectation value of the expression in the last parentheses vanishes. Also, due to the symmetry of the confining potential of a harmonic oscillator and the resulting symmetry of its eigenfunctions,<sup>131</sup>

$$X_k(-\tilde{x}) = \pm X_k(\tilde{x}), \quad \text{i.e. } |X_k(-\tilde{x})| = |X_k(\tilde{x})|,$$

the expectation value of its coordinate equals zero for any eigenstate:

$$\langle \tilde{x} \rangle \equiv \int_{-\infty}^{+\infty} X_k^*(\tilde{x}) \tilde{x} X_k(\tilde{x}) d\tilde{x} = \int_{-\infty}^{+\infty} |X_k(\tilde{x})|^2 \tilde{x} d\tilde{x} = 0,$$

so we finally get

$$\langle v_y \rangle = -\frac{\mathcal{E}}{\mathcal{B}}, \quad \text{for } \left| \langle v_y \rangle \right| \ll c. \quad (\text{****})$$

(The last strong equality explains the condition  $\mathcal{E} \ll c\mathcal{B}$  in the assignment; if it is not fulfilled, the analysis of this problem requires relativistic quantum mechanics.)

Very counter-intuitively, this simple result is valid for *any* eigenfunction (\*) of the system, i.e. *any* set of parameters  $k_y, k_z, x_0, y_0,$  and  $z_0$ .<sup>132</sup> This fact becomes (slightly :- ) less surprising if we recall the classical solution of this problem:<sup>133</sup> it shows that the trochoid-like trajectory of the particle “drifts”, in the direction normal to both vectors  $\mathcal{E}$  and  $\mathcal{B}$ , exactly with the velocity expressed by Eq. (\*\*\*\*), independently of initial conditions.<sup>134</sup> Of course, the instant velocity  $\mathbf{v}$  of a classical particle, besides the average drift component (\*\*\*\*), generally has other components oscillating with the cyclotron frequency, whose amplitude and phase do depend on the initial conditions. But the same may be true for the expectation value  $\langle \mathbf{v} \rangle$  in quantum mechanics if the initial state of the particle is a superposition of two or more eigenstates (\*) rather than just one of them, as was implied at the calculation of Eq. (\*\*\*\*).

**Problem 3.7.** Use the Born approximation to calculate the angular dependence and the total cross-section of scattering of an incident plane wave propagating along the  $x$ -axis, by the following pair of similar point inhomogeneities:

$$U(\mathbf{r}) = \mathcal{W} \left[ \delta \left( \mathbf{r} - \mathbf{n}_z \frac{a}{2} \right) + \delta \left( \mathbf{r} + \mathbf{n}_z \frac{a}{2} \right) \right].$$

<sup>131</sup> See Eqs. (2.281) and (2.284) and/or Fig. 2.35 of the lecture notes.

<sup>132</sup> In particular, it gives the average velocity of the particle’s motion along the edge channels that were discussed in the solution of Problem 2.

<sup>133</sup> See, e.g., EM Sec. 9.6 (iii), and in particular Eq. (9.168) and Fig. 9.12.

<sup>134</sup> Even the reader unfamiliar with this general classical result should readily recognize its following particular, simple case: a linear, uniform motion of the particle along axis  $y$  is possible only with such velocity  $v_y$  that the electric and magnetic components of the Lorentz force cancel each other, so the total force vanishes:  $\mathbf{F} = q(\mathcal{E} + \mathbf{v} \times \mathcal{B}) \equiv q(\mathcal{E} \mathbf{n}_x + v_y \mathbf{n}_y \times \mathcal{B} \mathbf{n}_z) \equiv \mathbf{n}_x q(\mathcal{E} + v_y \mathcal{B}) = 0$ , giving the result identical to Eq. (\*\*\*\*).

Analyze the results in detail. Derive the condition of the Born approximation's validity for such delta-functional scatterers.

*Solution:* Plugging the given  $U(\mathbf{r})$  into the general Born integral given by Eq. (3.86) of the lecture notes, we get the following scattering function:

$$f(\mathbf{k}, \mathbf{k}_i) = -\frac{m\omega}{2\pi\hbar^2} \left( \exp\left\{-i\mathbf{q} \cdot \mathbf{n}_z \frac{a}{2}\right\} + \exp\left\{i\mathbf{q} \cdot \mathbf{n}_z \frac{a}{2}\right\} \right).$$

Since in this problem (see the figure on the right)

$$\mathbf{q} \cdot \mathbf{n}_z \equiv (\mathbf{k} - \mathbf{k}_i) \cdot \mathbf{n}_z = \mathbf{k} \cdot \mathbf{n}_z = k \cos \Theta,$$

where  $\Theta$  is the angle between the direction of the vector  $\mathbf{k}$  (toward the observer) and the  $z$ -axis,<sup>135</sup> our result may be rewritten as

$$f(\mathbf{k}, \mathbf{k}_i) = -\frac{m\omega}{\pi\hbar^2} \cos\left(\frac{ka}{2} \cos \Theta\right),$$

so, according to Eq. (3.84), the differential cross-section of scattering is

$$\frac{d\sigma}{d\Omega} \equiv |f(\mathbf{k}, \mathbf{k}_i)|^2 = \left(\frac{m\omega}{\pi\hbar^2}\right)^2 \cos^2\left(\frac{ka}{2} \cos \Theta\right) \equiv \frac{1}{2} \left(\frac{m\omega}{\pi\hbar^2}\right)^2 [1 + \cos(ka \cos \Theta)] \quad (*)$$

Now we can calculate the total cross-section, by using spherical coordinates with the  $z$ -axis taken for the polar one:

$$\sigma = 2\pi \int_0^\pi \frac{d\sigma}{d\Omega} \sin \Theta d\Theta = \sigma_1 \int_{-1}^{+1} [1 + \cos(ka\xi)] d\xi = 2\sigma_1 \left(1 + \frac{\sin ka}{ka}\right),$$

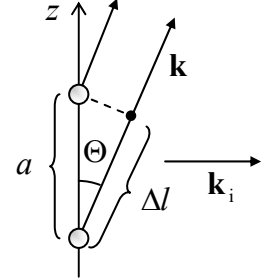
where  $\sigma_1$  is the energy-independent total cross-section of each point scatterer:

$$\sigma_1 \equiv \frac{1}{\pi} \left(\frac{m\omega}{\hbar^2}\right)^2.$$

This situation is of course just a variety of the Young-type experiment (cf. Fig. 3.1 of the lecture notes), and Eq. (\*) is a particular embodiment of Eq. (3.11) with  $|a_1| = |a_2|$  and the alternative path lengths difference  $l_2 - l_1 = \Delta l = a \cos \Theta$  – see the figure above. For this particular geometry, the scattered wave is symmetric about the  $z$ -axis. This is natural, because in the Born approximation, the role of the incident wave, in our case propagating along the  $x$ -axis, is reduced to the excitation of spherical secondary waves  $\psi_s$  from all (in our case, just two) partial scatterers. As a result of the interference of these two spherical waves, the scattered wave's intensity oscillates with the angle  $\Theta$ , reaching its maxima at

$$\cos \Theta_n = \frac{2\pi}{ka} n \equiv \frac{\lambda}{a} n, \quad \text{with } n = 0, 1, 2, \dots,$$

i.e. at the angles at which the path difference  $\Delta l$  between the two waves is a multiple of the de Broglie wavelength  $\lambda = 2\pi/k$ .



<sup>135</sup> Note that  $\Theta$  is different from what is usually called the *scattering angle*  $\theta$  (between the vectors  $\mathbf{k}$  and  $\mathbf{k}_i$ ).

However, at low particle energies ( $ka \ll 1$ , i.e.  $a \ll \lambda$ ), this “constructive interference” condition may be satisfied only for  $n = 0$ , and the scattering is spherically-symmetric and energy-independent:  $\sigma = 4\sigma_1$ , the factor of 4 arising from the *coherent* addition of the two waves in all scattering directions. On the other hand, at high energies ( $ka \gg 1$ ) the intensity of the scattered wave oscillates rapidly with the angle  $\Theta$ , so the total cross-sections of the scatterers add up as if they were incoherent:  $\sigma = 2\sigma_1$ .

In order to estimate the Born approximation’s validity condition, let us replace the delta-functional scatterer with one of a finite (though very small) size  $R \ll a$ ,  $k^{-1}$ , and a potential of such a magnitude  $\sim U_0$  that  $\mathcal{W} \sim U_0 R^3$ . According to Eq. (3.77) of the lecture notes, to have  $|\psi_s| \ll |\psi_i|$  inside the scatterer, we should have

$$U_0 \ll \frac{\hbar^2}{mR^2}, \quad \text{i.e. } \sigma_1^{1/2} \sim \frac{m\mathcal{W}}{\hbar^2} \ll R.$$

For a fixed  $\mathcal{W}$  (and hence  $\sigma_1$ ), this condition is *never fulfilled* at  $R \rightarrow 0$ . This means that we cannot take the above expression for  $\sigma_1$  too literally (unless it is indeed much less than  $R^2$ , where  $R$  is the physical size of the “point” scatterer).

However, the calculated interference pattern as such, i.e. the functional dependence of the intensity on the angle  $\Theta$ , has a much broader validity. Indeed, in order for the Born approximation to be correct on this issue, it is sufficient for the wave scattered by one point not to interfere with the incident wave at the other point. For that, in the integral (3.72) calculated for that location, we can approximately replace  $U d^3r$  with  $\mathcal{W}$ ,  $\psi$  with  $\psi_i$ , and the denominator with  $a$ . Then the generic requirement of the Born approximation,  $|\psi_s| \ll |\psi_i|$  gives a much milder condition,

$$\sigma_1^{1/2} \sim \frac{m\mathcal{W}}{\hbar^2} \ll a,$$

which does not involve the scatterer’s size  $R$ .

**Problem 3.8.** Use the Born approximation to analyze the scattering of particles of energy  $E$  by a very thin, straight, uniform rod of length  $l$ , oriented normally to the incident particle’s velocity. In particular, calculate the differential and total cross-sections of scattering and analyze the results in the low-energy and high-energy limits.

*Solution:* Let us direct the  $z$ -axis along the incident particle’s velocity, and the  $x$ -axis along the scattering rod’s length, with the origin in its middle. Then we can describe the scattering potential as

$$U(\mathbf{r}) = \begin{cases} \mathcal{W}\delta(\mathbf{\rho}), & \text{for } |x| < l/2, \\ 0, & \text{otherwise,} \end{cases}$$

where  $\mathbf{\rho} \equiv \{y, z\}$ . For this potential, Eq. (3.88) of the lecture notes yields

$$\frac{d\sigma}{d\Omega} = \left( \frac{m}{2\pi\hbar^2} \right)^2 \left| \int_{-l/2}^{+l/2} \mathcal{W} e^{-iq_x x} dx \right|^2 = \left( \frac{m}{2\pi\hbar^2} \mathcal{W} l \operatorname{sinc} \frac{kl \cos \Theta}{2} \right)^2, \quad (*)$$

where  $\Theta$  is the angle between the  $x$ -axis and the vector  $\mathbf{k}$  (and hence the direction toward the observer),<sup>136</sup> while

$$\text{sinc } \xi \equiv \frac{\sin \xi}{\xi}$$

is the function frequently met in the theory of diffraction of waves of any physical nature, its square describing, in particular, the famous *Fraunhofer diffraction pattern* – see, e.g., EM Secs. 8.4-8.8.

Eq. (\*) shows that the scattering pattern is axially symmetric, with the axis defined by the rod's orientation ( $x$ ) rather than the initial particle propagation direction ( $z$ ). In particular, at  $kl \ll 1$ , the scattering is completely isotropic, while in the opposite limit  $kl \gg 1$ , the scattered wave is concentrated near the plane normal to the rod's axis, where  $|\Theta - \pi/2| \sim 1/kl \ll 1$ , so

$$\text{sinc } \frac{kl}{2} \cos \Theta \approx \text{sinc} \left[ \frac{kl}{2} \left( \frac{\pi}{2} - \Theta \right) \right].$$

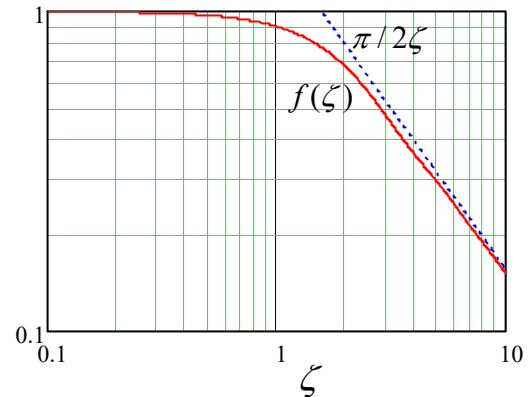
The total cross-section of scattering may be readily obtained by the integration of the right-hand part of Eq. (\*) in spherical coordinates, with the polar axis directed along the  $x$ -axis:

$$\sigma = 2\pi \int_0^\pi \left( \frac{m}{2\pi\hbar^2} \omega l \text{sinc} \frac{kl \cos \Theta}{2} \right)^2 \sin \Theta d\Theta = 4\pi \left( \frac{m}{2\pi\hbar^2} \omega l \right)^2 f \left( \frac{kl}{2} \right),$$

where the dimensionless function

$$f(\zeta) \equiv \frac{1}{\zeta} \int_0^\zeta \text{sinc}^2 \xi d\xi$$

is plotted, together with its asymptote  $f(\zeta) \rightarrow \pi/2\zeta$ ,<sup>137</sup> in the figure on the right. Thus in the low-energy limit  $kl \ll 1$ , the cross-section is energy-independent, while at high particle energies, it decreases with energy as  $\sigma \propto 1/kl \propto E^{-1/2}$ .



**Problem 3.9.** Complete the analysis of the Born scattering by a uniform spherical potential (3.97), started in Sec. 3.3 of the lecture notes, by calculation of its total cross-section. Analyze the result in the limits  $kR \ll 1$  and  $kR \gg 1$ .

**Solution:** The scattering intensity has the axial symmetry about the axis of the incident wave's propagation, so the total cross-section may be calculated as

<sup>136</sup> Again (as in the previous problem), please mind the difference between this angle and the scattering angle, typically denoted as  $\theta$  – the angle between the vectors  $\mathbf{k}$  and  $\mathbf{k}_i$  (the latter one, in our current notation, is directed along the  $z$ -axis). The integration in Eq. (\*) has used the fact that the wave vector  $\mathbf{k}_i$  of the incident wave does not have an  $x$ -component, so  $q_x \equiv (\mathbf{k} - \mathbf{k}_i)_x = k_x = k \cos \Theta$ .

<sup>137</sup> See, e.g., MA Eq. (6.12).



$$\sigma = 2\pi \int_0^\pi \frac{d\sigma}{d\Omega} \sin \theta d\theta, \quad (*)$$

with the differential cross-section given by the last of Eqs. (3.98) of the lecture notes:

$$\frac{d\sigma}{d\Omega} = u_0^2 R^4 \left( \frac{qR \cos qR - \sin qR}{q^3} \right)^2, \quad \text{where } q = 2k \sin \frac{\theta}{2}, \quad u_0 \equiv \frac{U_0}{\hbar^2 / 2mR^2}.$$

(The dimensionless parameter  $u_0$  was already used in Fig. 3.10 of the lecture notes.)

The easiest way to calculate the integral in Eq. (\*) is to notice that since

$$dq = k \cos \frac{\theta}{2} d\theta, \quad \text{and} \quad qdq = 2k^2 \sin \frac{\theta}{2} \cos \frac{\theta}{2} d\theta \equiv k^2 \sin \theta d\theta,$$

the product  $\sin \theta d\theta$  may be replaced with  $q dq / k^2$ , so

$$\sigma = \frac{2\pi}{k^2} u_0^2 R^4 \int_0^{2kR} \frac{(\sin qR - qR \cos qR)^2}{q^6} q dq \equiv \frac{2}{(kR)^2} \sigma_g u_0^2 \int_0^{2kR} \frac{(\sin \xi - \xi \cos \xi)^2}{\xi^5} d\xi,$$

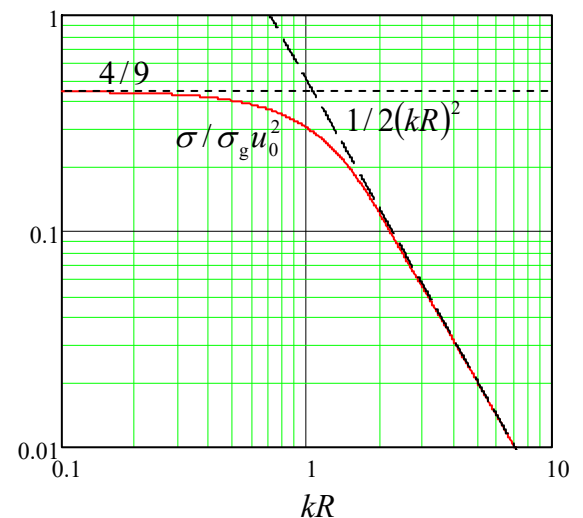
where  $\xi \equiv qR$ , while  $\sigma_g \equiv \pi R^2$  is the largest geometric cross-section of the sphere, i.e. its cross-section “as seen by the incident particles”. This is a table integral,<sup>138</sup> finally giving

$$\frac{\sigma}{u_0^2 \sigma_g} = \frac{2}{(kR)^2} \left[ \frac{2(2kR) \sin(4kR) + \cos(4kR) - 2(2kR)^2 - 1}{8(2kR)^4} + \frac{1}{4} \right]. \quad (**)$$

The figure on the right shows the normalized cross-section given by Eq. (\*\*) as a function of the dimensionless product  $kR$  proportional to  $E^{1/2}$ . In the low-energy limit ( $kR \rightarrow 0$ ), the result tends to the energy-independent value  $4/9$ , which could be readily obtained without the general integration, just by using the fact (discussed in Sec. 3.3 of the lecture notes) that in this limit, the scattering is isotropic, with  $d\sigma/d\Omega = \sigma_0 u_0^2 / 9\pi$ .

$$\sigma|_{kR \ll 1} = 4\pi \left. \frac{d\sigma}{d\Omega} \right|_{kR \ll 1} = \frac{4}{9} u_0^2 \sigma_g.$$

Note also that according to the analysis in the model solution of the previous problem, the Born approximation is only valid if the parameter  $u_0$  is much smaller than 1, i.e. if the calculated total cross-section is much smaller than  $\sigma_g$ .<sup>139</sup>



<sup>138</sup> See, e.g. MA Eq. (6.3b).

<sup>139</sup> As will be discussed in Sec. 3.8 of the lecture notes, the exact (i.e. beyond-Born) theory of scattering by an opaque sphere (which may be described by our current model with  $u_0 \gg 1$ ) gives, in this limit, the total cross-section  $\sigma = 4\sigma_0$ .

In the opposite, high-energy limit  $kR \gg 1$ , the general result (\*\*) is reduced to

$$\sigma|_{kR \gg 1} = \frac{u_0^2}{2(kR)^2} \sigma_g,$$

i.e. the cross-section decreases as  $1/E$ . This happens because, as Fig. 3.10 of the lecture notes shows, substantial diffraction takes place only at  $qR \sim 1$ , i.e. at small scattering angles  $\theta \approx q/k \sim 1/kR$ , and hence within a small solid angle of the order of  $\theta^2 \sim 1/(kR)^2 \ll 1$ .

**Problem 3.10.** Use the Born approximation to calculate the differential cross-section of particle scattering by a very thin spherical shell, whose potential may be approximated as  $U(\mathbf{r}) = \mathcal{W}\delta(r - R)$ . Analyze the results in the limits  $kR \ll 1$  and  $kR \gg 1$ , and compare them with those for a uniform sphere considered in Sec. 3.3 of the lecture notes.

*Solution:* Plugging the given (spherically-symmetric) potential into Eq. (3.90) of the lecture notes, we get

$$f(\mathbf{k}, \mathbf{k}_i) = -\frac{2mR^2\mathcal{W}}{\hbar^2} \frac{\sin qR}{qR} \equiv -\frac{2mR^2\mathcal{W}}{\hbar^2} \text{sinc} qR,$$

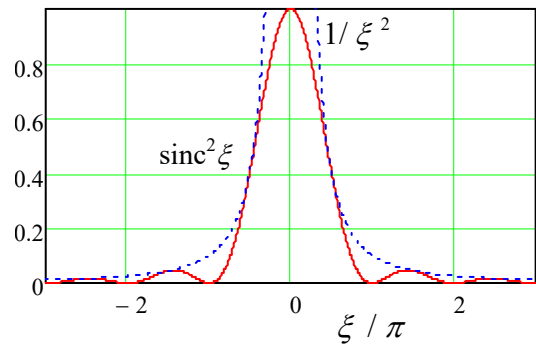
so the differential cross-section (3.84) of the shell is

$$\frac{d\sigma}{d\Omega} \equiv |f(\mathbf{k}, \mathbf{k}_i)|^2 = \left( \frac{2mR^2\mathcal{W}}{\hbar^2} \right)^2 \text{sinc}^2 qR. \quad (*)$$

As was already mentioned in the model solution of Problem 8, the square of the function

$$\text{sinc} \xi \equiv \frac{\sin \xi}{\xi},$$

describes, in particular, the well-known Fraunhofer diffraction pattern – see the solid red line in the figure on the right. (The dashed blue line shows its envelope  $1/\xi^2$ .)



In a qualitative (but not quantitative!) similarity to Eq. (3.98) of the lecture notes, which gives the differential cross-section of a uniform sphere in the same Born approximation, Eq. (\*) also describes an infinite set of zero-scattering points  $q_n = \pi n/R$ , with  $n = \pm 1, \pm 2, \dots$ , now exactly periodic in  $q$ , besides the forward-scattering point  $q \equiv 2k \sin(\theta/2) = 0$ , i.e.  $\theta = 0$ .

However, just as in the case of a uniform sphere, these diffraction minima (which may be observed as “dark” rings with constant values of the diffraction angle  $\theta$ ) are physically implemented only at sufficiently large values of the product  $kR$ : in order to have  $N$  rings,  $kR$  has to be larger than  $\pi N$ . In the opposite case  $kR \ll 1$ , the product  $qR$  is much lower than 1 for any angle  $\theta$ , so  $\text{sinc}(qR) \approx 1$ , and the scattering is virtually isotropic, with the total cross-section

$$\sigma = 4\pi \frac{d\sigma}{d\Omega} = 4\pi \left( \frac{2mR^2\mathcal{W}}{\hbar^2} \right)^2 \equiv 4\sigma_g \beta^2, \quad (**)$$

where  $\sigma_g \equiv \pi R^2$  is the largest geometric cross-section of the sphere, and  $\beta$  is the dimensionless parameter characterizing  $w$  and defined similarly to the one used in Chapter 2 for the discussion of 1D problems – see Eq. (2.197):

$$\beta \equiv \frac{w}{\hbar^2 / 2mR}.$$

With the proper replacements  $a \rightarrow R$ ,  $U_0 \rightarrow wR$ , Eq. (3.75) of the lecture notes shows that Eq. (\*\*\*) is valid only if  $\beta \ll 1$ , i.e. if the total cross-section of scattering is much smaller than its geometric cross-section. Note also that  $d\sigma/d\Omega$  and  $\sigma$  do not depend on the sign of  $w$ ; as will be shown in the exact analysis of scattering by this potential (see the solution of Problem 47), this independence only holds in the Born approximation. The same analysis will show that the Born approximation also misses the spectacular *Ramsauer-Townsend effect* of high- $Q$  resonant scattering due to long-living metastable states of the system at positive and sufficiently high values of the parameter  $\beta$  – see the solution of Problem 46.

**Problem 3.11.** Use the Born approximation to calculate the differential and total cross-sections of electron scattering by a screened Coulomb field of a point charge  $Ze$ , with the electrostatic potential<sup>140</sup>

$$\phi(\mathbf{r}) = \frac{Ze}{4\pi\epsilon_0 r} e^{-\lambda r},$$

neglecting spin interaction effects, and analyze the result's dependence on the screening parameter  $\lambda$ . Compare the results with those given by the classical (“Rutherford”) formula<sup>141</sup> for the unscreened Coulomb potential ( $\lambda \rightarrow 0$ ), and formulate the condition of the Born approximation's validity in this limit.

*Solution:* Applying Eq. (3.90) of the lecture notes to the spherically symmetric scattering potential energy

$$U(r) = -e\phi(\mathbf{r}) = -\frac{C}{r} e^{-\lambda r}, \quad \text{with } C \equiv \frac{Ze^2}{4\pi\epsilon_0},$$

we get

$$f(\mathbf{k}, \mathbf{k}_i) = -\frac{2m}{\hbar^2 q} \int_0^\infty U(r) \sin(qr) r dr = \frac{2mC}{\hbar^2 q} I, \quad \text{with } I \equiv \int_0^\infty e^{-\lambda r} \sin(qr) dr.$$

This integral may be easily worked out by representing  $\sin(qr)$  as  $\text{Im}[\exp\{iqr\}]$ :

$$I = \text{Im} \int_0^\infty e^{(-\lambda+iq)r} dr = \text{Im} \left. \frac{e^{(-\lambda+iq)r}}{-\lambda+iq} \right|_0^\infty = \frac{q}{\lambda^2 + q^2},$$

so Eq. (3.84) yields the following differential cross-section of scattering:

$$\frac{d\sigma}{d\Omega} = \left( \frac{2mC}{\hbar^2 q} \frac{q}{\lambda^2 + q^2} \right)^2 \equiv \frac{\beta^2}{(\lambda^2 + q^2)^2}, \quad \text{where } \beta \equiv \frac{C}{\hbar^2 / 2m}. \quad (*)$$

<sup>140</sup> This *Yukawa potential* was first suggested in 1935 by H. Yukawa as a model for strong interactions.

<sup>141</sup> See, e.g., CM Sec. 3.5, in particular Eq. (3.73).

In order to calculate the total cross-section  $\sigma$  from Eq. (3.85), we can use the geometric relation  $q = 2k\sin(\theta/2)$  (see Fig. 3.9b), and also the trigonometric identity  $\sin^2(\theta/2) = (1 - \cos\theta)/2$ , to get

$$\begin{aligned}\sigma &\equiv \oint \frac{d\sigma}{d\Omega} d\Omega = 2\pi \int_0^\pi \frac{d\sigma}{d\Omega} \sin\theta d\theta = 2\pi\beta^2 \int_{-1}^{+1} \frac{d(\cos\theta)}{[\lambda^2 + 2k^2(1 - \cos\theta)]^2} \\ &\equiv 2\pi\beta^2 \int_{-1}^{+1} \frac{d\xi}{[\lambda^2 + 2k^2(1 - \xi)]^2} = \frac{\pi\beta^2}{k^2} \frac{1}{\lambda^2 + 2k^2(1 - \xi)} \Big|_{\xi = -1}^{\xi = +1} \equiv \frac{4\pi\beta^2}{\lambda^2(\lambda^2 + 4k^2)}.\end{aligned}\quad (**)$$

In the limit of strong screening,  $\lambda \rightarrow \infty$ , there is a growing range of the values of  $k^2$  (and hence of the electron energies  $E$ ), in which we may neglect  $q^2$  in comparison with  $\lambda^2$  in the denominator of Eq. (\*), so the scattering becomes virtually energy- and angle-independent. In this limit, Eq. (\*\*) yields

$$\sigma \approx \frac{4\pi\beta^2}{\lambda^4} = \frac{4\pi}{\lambda^4} \left( \frac{2mC}{\hbar^2} \right)^2,$$

i.e. the total cross-section is also energy-independent and scales as  $a^4 \sim A^2 \propto 1/\lambda^4 \rightarrow 0$ , where  $a \sim 1/\lambda$  is the effective screening radius, i.e.  $A \propto a^2$  is the potential's "physical" cross-section.

In the opposite limit of negligible screening ( $\lambda \rightarrow 0$ ), i.e. of the unscreened Coulomb potential, the total cross-section (\*\*) diverges as  $A \propto a^2 = 1/\lambda^2$ , just as it does in the classical theory.<sup>142</sup> In this limit, Eq. (\*) yields

$$\frac{d\sigma}{d\Omega} = \left( \frac{2mC}{\hbar^2 q^2} \right)^2 = \left[ \frac{mC}{2\hbar^2 k^2 \sin^2(\theta/2)} \right]^2.$$

Noticing that  $(\hbar k)^2/2m$  is just the energy  $E$  of the scattered particles, we see that this result *exactly* coincides with the classical Rutherford formula

$$\frac{d\sigma}{d\Omega} = \left( \frac{C}{4E} \right)^2 \frac{1}{\sin^4(\theta/2)}.$$

This coincidence is quite remarkable in view of the completely different conceptual structures of classical and quantum calculations.

The divergence of the effective screening radius  $a \sim 1/\lambda$  at  $\lambda \rightarrow 0$  also affects the application, in this limit, of Eq. (3.77) of the lecture notes for the Born approximation validity. Indeed, since our potential diverges at  $r \rightarrow 0$ , i.e. does not have an immediately apparent magnitude scale  $U_0$ . We may give a fair estimate of this scale by identifying the magnitude of the integral  $\int U(\mathbf{r}) d^3r$  with  $U_0 a^3$ . For our particular potential,

$$\int U(\mathbf{r}) d^3r = -4\pi C \int_0^\infty \frac{1}{r} e^{-\lambda r} r^2 dr = -\frac{4\pi C}{\lambda^2} \propto C a^2,$$

so  $U_0 \sim C/a$ . With this estimate, Eq. (3.77) yields the following limitation on the constant  $C$ :

<sup>142</sup> As was mentioned in CM Sec. 3.5, this divergence disappears at the account of a nonvanishing spatial density  $n$  of such scattering centers, with the average reciprocal distance  $\lambda_{\text{ave}} = n^{1/3}$  between them playing a role qualitatively similar to that of our parameter  $\lambda$ .

$$C \ll \frac{\hbar^2}{ma} \max[ka, 1].$$

But in the limit  $\lambda \rightarrow 0$ , i.e.  $a \rightarrow \infty$ ,  $ka$  becomes much larger than 1 for virtually any values of  $k$ , so for the unscreened Coulomb potential we may replace  $\max[ka, 1]$  with just  $ka$ , and the validity condition takes the form

$$C \ll \frac{\hbar^2}{ma} ka \equiv \frac{\hbar^2 k}{m}, \quad \text{i.e. } \frac{Ze^2}{4\pi\epsilon_0} \ll \frac{\hbar^2 k}{m} \equiv \frac{\hbar p}{m} \equiv \hbar v,$$

where  $v$  is the scale of velocity of the scattered electron. (With this estimate's accuracy, the difference between the phase and group velocities, given by Eq. (2.33b), is insignificant.) Using the definition of the *fine structure constant* (which will be repeatedly discussed later in this course):

$$\alpha \equiv \frac{e^2}{4\pi\epsilon_0 \hbar c} \approx \frac{1}{137},$$

this condition may be rewritten as

$$Z\alpha \ll \frac{v}{c}. \quad (***)$$

Since all our results so far are only valid for non-relativistic particles, with  $v/c \ll 1$ , the Born approximation is valid only for relatively light atoms;<sup>143</sup> for the important case of a hydrogen atom ( $Z = 1$ ), Eq. (\*\*\*) takes the form

$$\frac{v}{c} \gg \alpha \approx \frac{1}{137}.$$

**Problem 3.12.** A quantum particle with electric charge  $Q$  is scattered by the field of a localized distributed charge with a spherically symmetric density  $\rho(r)$  and zero total charge. Use the Born approximation to calculate the differential cross-section of the *forward scattering* (with the scattering angle  $\theta = 0$ ), and evaluate it for the scattering of electrons by a hydrogen atom in its ground state.

*Solution:* According to classical electrostatics, the potential energy of a point charge  $Q$  in an external electric field is  $U(\mathbf{r}) = Q\phi(\mathbf{r})$ , where  $\phi(\mathbf{r})$  is the electrostatic potential of the field. If the field is created by a static charge distribution  $\rho(\mathbf{r})$ , its potential satisfies the Poisson equation<sup>144</sup>

$$\nabla^2 \phi = -\frac{\rho}{\epsilon_0}. \quad (*)$$

In our current case, the charge distribution is spherically symmetric, and so is the potential distribution:  $\phi(\mathbf{r}) = \phi(r)$ . In this case, the Laplace operator is (relatively :-) simple,

$$\nabla^2 = \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d}{dr} \right),$$

enabling us to write an explicit expression for  $\phi(r)$  as the following double integral:

<sup>143</sup> Note that for heavy atoms, the potential model explored in this problem is very approximate anyway; a better approximation is given by the so-called *Fermi-Thomas model* – see Chapter 8.

<sup>144</sup> See, e.g., EM Eq. (1.41).

$$\phi(r) = -\frac{1}{\varepsilon_0} \int_0^r \frac{dr'}{r'^2} \int_0^{r'} \rho(r'') r''^2 dr'' + \text{const},$$

where the integration constant, for convenience, may be selected from the usual condition  $\phi(\infty) = 0$ . The resulting expression for  $U(r) = Q\phi(r)$  may be plugged into Eq. (3.90) of the lecture notes, written for the forward-scattering limit  $\mathbf{k} \rightarrow \mathbf{k}_i$  (i.e. at  $\mathbf{q} \equiv \mathbf{k} - \mathbf{k}_i \rightarrow 0$ ):

$$f(\mathbf{k}_i, \mathbf{k}_i) = -\frac{2m}{\hbar^2} \int_0^\infty U(r) r^2 dr,$$

and the resulting triple integral may be reduced to a single one via a double integration by parts. (This additional exercise is highly recommended to the reader.)

However, the same final result may be obtained more simply way from Eq. (3.86) by recalling that (as was already noted in that section of the lecture notes) the integral

$$U_{\mathbf{q}} \equiv \int U(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}} d^3r$$

in that expression is just the complex amplitude in the 3D Fourier expansion of the function  $U(\mathbf{r})$  into the Fourier integral over monochromatic plane wavefunctions  $e^{-i\mathbf{q}\cdot\mathbf{r}}$ . The Laplace operator's action on such a function is equivalent to its multiplication by the factor  $(-i\mathbf{q})\cdot(-i\mathbf{q}) \equiv -q^2$ , so Eq. (\*) immediately yields the following simple relation between  $U_{\mathbf{q}}$  and the similarly defined Fourier amplitude  $\rho_{\mathbf{q}}$  of the charge distribution:

$$U_{\mathbf{q}} = Q\phi_{\mathbf{q}} = \frac{Q}{\varepsilon_0 q^2} \rho_{\mathbf{q}},$$

and the Born integral (3.86) takes the form

$$f(\mathbf{k}, \mathbf{k}_i) = -\frac{mQ}{2\pi\hbar^2 \varepsilon_0} U_{\mathbf{q}} = -\frac{mQ}{2\pi\hbar^2 \varepsilon_0} \frac{1}{q^2} \int \rho(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}} d^3r.$$

This expression is valid for an arbitrary localized charge distribution. If it is spherically symmetric, the formula may be readily reduced to a 1D integral, exactly as it was done for an arbitrary potential profile in Eq. (3.90) of the lecture notes:

$$f(\mathbf{k}, \mathbf{k}_i) = -\frac{2mQ}{\hbar^2 \varepsilon_0} \frac{1}{q^3} \int_0^\infty \rho(r) \sin(qr) r dr.$$

At the nearly-forward scattering,  $q \rightarrow 0$ , and the sine function under the integral may be well approximated by just two leading terms of its Taylor series at  $q \approx 0$ :

$$\sin qr \approx qr - \frac{1}{3!} (qr)^3.$$

The integral of the resulting first term,  $q \int \rho(r) r^2 dr$ , is proportional to the net charge of the scattering center and, by the problem's condition, equals zero. This leaves us with the integral of the second term:

$$f(\mathbf{k}, \mathbf{k}_i) = -\frac{2mQ}{\hbar^2 \varepsilon_0} \frac{1}{q^3} \int_0^\infty \rho(r) \left( -\frac{q^3 r^3}{6} \right) r dr \equiv \frac{mQ}{3\hbar^2 \varepsilon_0} \int_0^\infty \rho(r) r^4 dr,$$

which does not depend on  $q$ , and hence is valid for the purely-forward scattering ( $\mathbf{k} = \mathbf{k}_i$ ) as well. The corresponding differential cross-section is given by Eq. (3.84):

$$\frac{d\sigma}{d\Omega}\Big|_{\theta=0} \equiv |f(\mathbf{k}_i, \mathbf{k}_i)|^2 = \left[ \frac{mQ}{3\hbar^2 \epsilon_0} \int_0^\infty \rho(r) r^4 dr \right]^2. \quad (**)$$

For the hydrogen atom, the charge distribution  $\rho(\mathbf{r})$  consists of a proton's contribution, which is well approximated by  $e\delta(\mathbf{r})$ , and hence does not contribute to our integral, and that of the electron:  $\rho(\mathbf{r}) = -e|\psi(\mathbf{r})|^2$ . According to Eq. (3.174), (3.179), and (3.208) of the lecture notes, in the ground state, with the quantum numbers  $n = 1$ ,  $l = 0$ , and  $m = 0$ ,

$$\rho(r) = -e |Y_0^0(\theta, \varphi)|^2 |\mathcal{R}_{1,0}(r)|^2 = -e \frac{1}{4\pi} \frac{4}{r_0^3} e^{-2r/r_0},$$

with  $r_0 = r_B$ , so the required integration is easy:<sup>145</sup>

$$\int_0^\infty \rho(r) r^4 dr = -\frac{e}{\pi r_B^3} \int_0^\infty e^{-2r/r_B} r^4 dr = -\frac{e}{\pi r_B^3} \left(\frac{r_B}{2}\right)^5 \int_0^\infty \xi^4 e^{-\xi} d\xi = -\frac{e}{\pi r_B^3} \left(\frac{r_B}{2}\right)^5 4! \equiv -\frac{3}{4\pi} e r_B^2.$$

Now with Eq. (1.10) for the Bohr radius,

$$r_B = \frac{4\pi\epsilon_0 \hbar^2}{e^2 m_e},$$

Eq. (\*\*), with  $m = m_e$  and  $Q = -e$ , yields a remarkably simple result:

$$\frac{d\sigma}{d\Omega}\Big|_{\theta=0} = r_B^2.$$

**Problem 3.13.** Prove the optical theorem (3.99).

*Hint:* For the general solution (3.64) of the scattering problem, with  $\psi_i$  given by Eq. (3.6) and  $\psi_s$  in the form (3.81), calculate the full probability current  $I$  through a spherical surface of radius  $r \gg k^{-1}$ , and then require that in accordance with the continuity relation (1.48), in this stationary situation,  $I = 0$ .

*Solution:* Following the *Hint*, at large distances ( $r \gg k^{-1}$ ) from the scatterer we may represent the full wavefunction as

$$\psi(\mathbf{r}) = \psi_i(\mathbf{r}) + \psi_s(\mathbf{r}) = |\psi_i| \left[ e^{i\mathbf{k}_i \cdot \mathbf{r}} + \frac{f(\mathbf{k}, \mathbf{k}_i)}{r} e^{ikr} \right].$$

Plugging this sum into the basic Eq. (1.47), in the form

$$\mathbf{j} = \frac{\hbar}{m} \text{Im}(\psi^* \nabla \psi),$$

which is valid for any stationary wavefunction (1.69), we may represent the probability current density as a sum of three terms: the incident wave's current

<sup>145</sup> See, e.g., MA Eq. (6.7d) with  $n = 4$ .

$$\mathbf{j}_i = \frac{\hbar}{m} \text{Im}(\psi_i^* \nabla \psi_i) = \frac{\hbar \mathbf{k}_i}{m} |\psi_i|^2,$$

the scattered wave's current

$$\mathbf{j}_s = \frac{\hbar}{m} \text{Im}(\psi_s^* \nabla \psi_s) = \frac{\hbar}{m} |\psi_i|^2 \text{Im} \left[ \frac{f^*(\mathbf{k}, \mathbf{k}_i) e^{-ikr}}{r} \nabla \frac{f(\mathbf{k}, \mathbf{k}_i) e^{ikr}}{r} \right],$$

and the interference term

$$\mathbf{j}_{\text{int}} = \frac{\hbar}{m} \text{Im}(\psi_i^* \nabla \psi_s + \psi_s^* \nabla \psi_i) = \frac{\hbar}{m} |\psi_i|^2 \text{Im} \left[ e^{-i\mathbf{k}_i \cdot \mathbf{r}} \nabla \frac{f(\mathbf{k}, \mathbf{k}_i) e^{ikr}}{r} + \frac{f^*(\mathbf{k}, \mathbf{k}_i) e^{-ikr}}{r} \nabla e^{i\mathbf{k}_i \cdot \mathbf{r}} \right].$$

The first term, i.e. the uniform current density  $\mathbf{j}_i$  of a plane de Broglie wave, does not contribute to the full probability current

$$I \equiv \int_S \mathbf{j}_n d^2r = r^2 \int_{4\pi} \mathbf{j} \cdot \mathbf{n}_r d\Omega$$

through any spherical surface.<sup>146</sup> Calculating the (only needed) radial components of the two other terms ( $\mathbf{j}_s$  and  $\mathbf{j}_{\text{int}}$ ), we may take into account that due to the strong inequality  $kr \gg 1$ , the corresponding component  $\mathbf{n}_r \cdot \partial / \partial r$  of the gradient is dominated by the fast-changing exponents, while the derivative of the factor  $f/r$  is negligible. Indeed, for the first of these two terms, this fact was already used in Sec. 3.3 of the lecture notes, giving Eq. (3.83):

$$\mathbf{j}_s(\theta) = \frac{\hbar}{m} |\psi_i|^2 \frac{|f(\mathbf{k}, \mathbf{k}_i)|^2}{r^2} \mathbf{k} \equiv \frac{\hbar k}{m} |\psi_i|^2 \frac{|f(\mathbf{k}, \mathbf{k}_i)|^2}{r^2} \mathbf{n}_r,$$

and hence

$$I_s \equiv r^2 \int_{4\pi} \mathbf{j}_s \cdot \mathbf{n}_r d\Omega = \frac{\hbar k}{m} |\psi_i|^2 \int_{4\pi} |f(\mathbf{k}, \mathbf{k}_i)|^2 d\Omega \equiv \frac{\hbar k}{m} |\psi_i|^2 \sigma, \quad (*)$$

where the last step used Eq. (3.85).

What remains is to apply the same “far-zone” approximation to the interference current  $\mathbf{j}_{\text{int}}$ :

$$\begin{aligned} \mathbf{j}_{\text{int}} \cdot \mathbf{n}_r &= \frac{\hbar}{m} |\psi_i|^2 \text{Im} \left[ \frac{f(\mathbf{k}, \mathbf{k}_i)}{r} e^{-i\mathbf{k}_i \cdot \mathbf{r}} \frac{\partial}{\partial r} e^{ikr} + \frac{f^*(\mathbf{k}, \mathbf{k}_i)}{r} e^{-ikr} \frac{\partial}{\partial r} e^{i\mathbf{k}_i \cdot \mathbf{r}} \right] \\ &= \frac{\hbar}{m} |\psi_i|^2 \text{Im} \left[ \frac{f(\mathbf{k}, \mathbf{k}_i)}{r} e^{i(-\mathbf{k}_i \cdot \mathbf{r} + kr)} ik + \frac{f^*(\mathbf{k}, \mathbf{k}_i)}{r} e^{i(-kr + \mathbf{k}_i \cdot \mathbf{r})} i\mathbf{k}_i \cdot \mathbf{n}_r \right] \\ &\equiv \frac{\hbar k}{m} |\psi_i|^2 \text{Re} \left[ \frac{f(\mathbf{k}, \mathbf{k}_i)}{r} e^{ikr} (-\cos\theta + 1) + \cos\theta \frac{f^*(\mathbf{k}, \mathbf{k}_i)}{r} e^{ikr} (-1 + \cos\theta) \right], \end{aligned}$$

where  $\cos\theta \equiv \mathbf{k}_i \cdot \mathbf{r} / kr$  – see also the previous footnote. Now integrating this expression over the solid angle to calculate  $I_{\text{int}}$ , we should note that since  $kr \gg 1$ , both complex exponents in the square brackets oscillate fast at minor changes of  $\theta$ , so their averages over almost all elementary angles  $d\Omega$  vanish. The

<sup>146</sup> If this is not evident, take into account that  $\mathbf{j}_i \cdot \mathbf{n}_r \propto \mathbf{k}_i \cdot \mathbf{n}_r \propto \cos\theta$ , where  $\theta$  is the polar angle in the spherical coordinates with the incident wave direction taken for the  $z$ -axis, and that the integral of  $\cos\theta$  over the whole solid angle vanishes.



only exception is a close vicinity of the positive direction of the  $\mathbf{k}_i$ -axis, where  $\mathbf{k} \approx \mathbf{k}_i$ , i.e.  $|\theta| \ll 1$ , so the function  $(\cos\theta - 1)$  is near its maximum (equal to 0) and hence changes very slowly. In this vicinity, we may expand this function to the Taylor series ( $\cos\theta - 1 = -\theta^2/2 + \dots$ ) and keep only the leading term in this expression, as well as in the pre-exponential factor  $\cos\theta = 1 - \theta^2/2 \dots$  and in the spherical area's polar factor  $\sin\theta = \theta - \theta^3/6 + \dots$ :<sup>147</sup>

$$\begin{aligned} I_{\text{int}} &\equiv r^2 \int_{4\pi} \mathbf{j}_s \cdot \mathbf{n}_r d\Omega \approx 2\pi r^2 \int_{\theta \approx 0} \mathbf{j}_s \cdot \mathbf{n}_r \sin\theta d\theta \approx 2\pi r^2 \int_{\theta \approx 0} \mathbf{j}_s \cdot \mathbf{n}_r \theta d\theta \\ &= 2\pi \frac{\hbar k r}{m} |\psi_i|^2 \int_{\theta \approx 0} \text{Re} \left[ f(\mathbf{k}_i, \mathbf{k}_i) \exp\left\{ ikr \frac{\theta^2}{2} \right\} + f^*(\mathbf{k}_i, \mathbf{k}_i) \exp\left\{ -ikr \frac{\theta^2}{2} \right\} \right] \theta d\theta \\ &\equiv 2\pi \frac{\hbar k r}{m} |\psi_i|^2 \int_{\theta \approx 0} \left[ \text{Re} f(\mathbf{k}_i, \mathbf{k}_i) \cos \frac{kr\theta^2}{2} - \text{Im} f(\mathbf{k}_i, \mathbf{k}_i) \sin \frac{kr\theta^2}{2} \right] d(\theta^2) \end{aligned}$$

Only the second term in the last square brackets, which is an odd function of  $\theta^2$ , gives a nonvanishing contribution to this integral:

$$I_{\text{int}} = -2\pi \frac{\hbar k r}{m} |\psi_i|^2 \text{Im} f(\mathbf{k}_i, \mathbf{k}_i) \int_{\theta \approx 0} \sin \frac{kr\theta^2}{2} d(\theta^2) \equiv -4\pi \frac{\hbar}{m} |\psi_i|^2 \text{Im} f(\mathbf{k}_i, \mathbf{k}_i) \int_0^{\infty} \sin \xi d\xi,$$

where  $\xi \equiv kr\theta^2/2$ . The “infinite” upper limit in this integral should be understood as an average of some values  $\xi_{\text{max}} \gg 1$ . Since the integral, equal to  $(1 - \cos\xi_{\text{max}})$ , is a fast-changing function of  $\xi_{\text{max}}$ , it has to be taken equal to the average value of this function,<sup>148</sup> in our case to 1. Hence,

$$I_{\text{int}} = -4\pi \frac{\hbar}{m} |\psi_i|^2 \text{Im} f(\mathbf{k}_i, \mathbf{k}_i),$$

so that using Eq. (\*), we get

$$I = I_s + I_{\text{int}} = \frac{\hbar}{m} |\psi_i|^2 [k\sigma - 4\pi \text{Im} f(\mathbf{k}_i, \mathbf{k}_i)].$$

Requiring this full probability current to vanish for any  $\psi_i$ , we get the optical theorem (3.99).

Besides proving the theorem, the above calculation yields a very clear physical picture of its physical origin: the incident and scattered waves strongly interfere in the forward direction where  $\mathbf{k} \rightarrow \mathbf{k}_i$ . Depending on the sign of  $\text{Im}f(\mathbf{k}_i, \mathbf{k}_i)$ , this interference may be either constructive or destructive. Now there should be no surprise that the Born approximation fails to satisfy the theorem: in it, the mutual interference between the incident and scattered waves is completely neglected – please revisit Eq. (3.83). As we have just seen, this deficiency most strongly affects the forward scattering's description.

**Problem 3.14.** Reformulate the Born approximation for the 1D case. Use the result to find the scattering and transfer matrices of a “rectangular” (flat-top) scatterer with

<sup>147</sup> We are also assuming that the scattering function  $f(\mathbf{k}, \mathbf{k}_i)$  is sufficiently smooth at  $\mathbf{k} \approx \mathbf{k}_i$ , so within the small polar region where  $kr\theta^2 \sim 1$ , it may be replaced with its forward-scattering value  $f(\mathbf{k}_i, \mathbf{k}_i)$ .

<sup>148</sup> This fact may be proved, for example, using the standard following trick: multiplying the function under the integral by  $\exp\{-\varepsilon\xi\}$  where  $\varepsilon$  is a small positive constant, working out the integral in the limits  $[0, \infty]$ , and then following the limit  $\varepsilon \rightarrow 0$ .

$$U(x) = \begin{cases} U_0, & \text{for } |x| < d/2, \\ 0, & \text{otherwise.} \end{cases}$$

Compare the results with those of the exact calculations carried out in Chapter 2 and analyze how their relationship changes in the eikonal approximation.

*Solution:* Just as in the 3D case discussed in Sec. 3.3 of the lecture notes, the solution of the 1D version of the Born equation (3.66),

$$\left( \frac{d^2}{dx^2} + k^2 \right) \psi_s = \frac{2m}{\hbar^2} U(x) \psi_0,$$

may be expressed as

$$\psi_s(x) = \frac{2m}{\hbar^2} \int U(x') \psi_0(x') G(x, x') dx'$$

via the 1D Green's function that satisfies the following equation:

$$\left( \frac{\partial^2}{\partial x^2} + k^2 \right) G(x, x') = \delta(x - x').$$

At  $x \neq x'$ , the equation is evidently satisfied by the usual monochromatic de Broglie waves propagating from the source, i.e. *from* the point  $x'$ :

$$G(x, x') = \begin{cases} C_+ \exp\{ik(x - x')\}, & \text{for } x > x', \\ C_- \exp\{-ik(x - x')\}, & \text{for } x < x'. \end{cases}$$

(As in the 3D case, the waves converging *upon* the source point  $x'$  are irrelevant.) The coefficients  $C_{\pm}$  in this relation may be found from the boundary conditions at the source point  $x = x'$ . First, the Green's function (as any wavefunction) should be continuous, giving  $C_+ = C_- \equiv C$ , so we may write

$$G(x, x') = C \exp\{ik|x - x'|\}.$$

Second, integrating the above differential equation for  $G$  over a small interval of  $x$  around  $x'$ , just as this was done at the derivation of Eq. (2.75), we get another boundary condition:

$$\frac{\partial G}{\partial x} \Big|_{x=x'+0} - \frac{\partial G}{\partial x} \Big|_{x=x'-0} = 1,$$

giving  $C = 1/2ik$ , so in the 1D Born approximation,

$$G(x, x') = \frac{1}{2ik} \exp\{ik|x - x'|\}, \quad \text{i.e. } \psi_s(x) = \frac{m}{ik\hbar^2} \int U(x') \psi_0(x') \exp\{ik|x - x'|\} dx'.$$

For the “rectangular” scatterer specified in the assignment, and an incident wave of a unit amplitude arriving from the left,  $\psi_0(x) = \exp\{ikx\}$ , this approximation yields

$$\psi_s(x) = \frac{mU_0}{ik\hbar^2} \int_{-d/2}^{+d/2} \begin{cases} \exp\{ikx'\} \exp\{ik(x - x')\}, & \text{for } x \geq +d/2 \\ \exp\{ikx'\} \exp\{ik(x' - x)\}, & \text{for } x \leq -d/2 \end{cases} dx'.$$

(For our current purposes, we do not care too much about the wave inside the scattering region.) Carrying out these elementary integrations, and adding the incident wave to the scattered one, for the total wavefunction outside of the scatterer, we get

$$\psi(x) = e^{ikx} - i\alpha \times \begin{cases} e^{ikx}, & \text{for } x \geq +d/2, \\ \frac{\sin kd}{kd} e^{-ikx}, & \text{for } x \leq -d/2. \end{cases} \quad (*)$$

where I have used the convenient dimensionless parameter:

$$\alpha \equiv \frac{mU_0d}{\hbar^2 k} \equiv \frac{U_0}{E} \frac{kd}{2},$$

which reduces to our old friend (2.78),  $\alpha = m\omega/k\hbar^2$ , for a short scatterer with  $d \ll 1/k$  and  $\omega \equiv U_0d$ . (Please note that according to Eq. (\*), the Born approximation is only valid if  $\alpha \ll \max[1, kd]$ , i.e. only if  $U_0/E \ll \max[1/kd, 1]$ .)

Comparing Eq. (\*) with the definition of the complex amplitudes used in the discussion of the 1D transfer and scattering matrices (see Eq. (2.120) of the lecture notes), with the reference points  $x_1 = -d/2$  and  $x_2 = +d/2$ ,

$$\psi_{1,2}(x) = A_{1,2} \exp\left\{ik\left(x \pm \frac{d}{2}\right)\right\} + B_{1,2} \exp\left\{-ik\left(x \pm \frac{d}{2}\right)\right\},$$

we see that in our case,

$$A_1 = \exp\left\{-ik\frac{d}{2}\right\}, \quad B_1 = -i\alpha \frac{\sin ka}{ka} \exp\left\{ik\frac{d}{2}\right\}, \quad A_2 = (1-i\alpha) \exp\left\{ik\frac{d}{2}\right\}, \quad B_2 = 0.$$

Now here and the definition (2.123) of the scattering matrix components, we obtain

$$S_{11} \equiv \frac{B_1}{A_1} \Big|_{B_2=0} = -i\alpha \frac{\sin kd}{kd} e^{ikd}, \quad S_{21} \equiv \frac{A_2}{A_1} \Big|_{B_2=0} = (1-i\alpha) e^{ikd}.$$

As a sanity check, for a short scatterer ( $kd \ll 1$ ) with  $\alpha \ll 1$ , the above results for  $S_{11}$  and  $S_{21}$  coincide with the results obtained in Sec. 2.5 of the lecture notes – see Eqs. (2.133). The two remaining elements of the scattering matrix,

$$S_{22} = -i\alpha \frac{\sin kd}{kd} e^{ikd}, \quad S_{12} = (1-i\alpha) e^{ikd},$$

may be found by repeating our calculations for a wave incident from the right.<sup>149</sup> Now we can use Eqs. (2.126) to calculate the transfer matrix. Keeping only the main terms proportional to  $\alpha^0 \equiv 1$  and  $\alpha^1 \equiv \alpha$ , we get

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<sup>149</sup> Note that using, for this purpose, the general relations discussed in Sec. 2.5, is dangerous because of the approximate character of the Born approximation. For example, for the transfer matrix obtained by using it, the first two general relations derived in the solution of Problem 2.15 are violated in the second order in  $\alpha$ . This situation is similar to that with the optical theorem (see Sec. 3.3 and Problem 13), which is also violated in the Born approximation.

$$T_{\text{Born}} \approx \begin{pmatrix} (1-i\alpha)e^{ikd} & -i\alpha \frac{\sin kd}{kd} \\ i\alpha \frac{\sin kd}{kd} & (1+i\alpha)e^{-ikd} \end{pmatrix}. \quad (**)$$

On the other hand, the exact transfer matrix for this scatterer, whose derivation was the task of Problem 2.29, is (for the relevant case  $E > U_0$ ):

$$T = \begin{pmatrix} \cos k'd + \frac{i}{2} \left( \frac{k}{k'} + \frac{k'}{k} \right) \sin k'd & -\frac{i}{2} \left( \frac{k}{k'} - \frac{k'}{k} \right) \sin k'd \\ \frac{i}{2} \left( \frac{k}{k'} - \frac{k'}{k} \right) \sin k'd & \cos k'd - \frac{i}{2} \left( \frac{k}{k'} + \frac{k'}{k} \right) \sin k'd \end{pmatrix}.$$

In the limit  $U_0 \rightarrow 0$ , pertinent to the Born approximation, i.e. at

$$\frac{k}{k'} \equiv \left( \frac{E}{E-U_0} \right)^{1/2} \approx 1 + \frac{U_0}{2E} \equiv 1 + \frac{\alpha}{kd}, \quad \text{so } \frac{k}{k'} - \frac{k'}{k} \approx \frac{2\alpha}{kd}, \quad \frac{k}{k'} + \frac{k'}{k} \approx 2,$$

the matrix takes the form

$$T = \begin{pmatrix} \cos k'd + i \sin k'd & -i\alpha \frac{\sin k'd}{kd} \\ i\alpha \frac{\sin k'd}{kd} & \cos k'd - i \sin k'd \end{pmatrix} \equiv \begin{pmatrix} e^{ik'd} & -i\alpha \frac{\sin k'd}{kd} \\ i\alpha \frac{\sin k'd}{kd} & e^{-ik'd} \end{pmatrix}.$$

Comparing the last form of this relation with Eq. (\*\*), we can see that the main deficiency of the Born approximation<sup>150</sup> is that, by construction, it ignores the changes in the propagation speed of the incident and scattered waves, due to the scatterer's potential. (This deficiency disappears only if the difference between  $kd$  and  $k'd$  is much smaller than 1 – which is, for large  $d$ , a very tough call.)

This drawback of the Born approximation is corrected in the eikonal approximation – see Eq. (3.102) of the lecture notes. Indeed, applying that formula to our current problem, we see that it yields a result similar to Eq. (\*\*), but with the replacement

$$kd \rightarrow k''d, \quad \text{where } k'' \equiv k - \frac{mU_0}{\hbar^2 k} \equiv k \left( 1 - \frac{U_0}{2E} \right).$$

At  $U_0/E \rightarrow 0$ , the wave number participating in the exact matrix  $T$ ,

$$k' \equiv \frac{[2m(E-U_0)]^{1/2}}{\hbar} \equiv k \left( 1 - \frac{U_0}{E} \right)^{1/2} \approx k \left( 1 - \frac{U_0}{2E} - \frac{U_0^2}{8E^2} - \dots \right),$$

tends to the so-corrected value  $k''$  much faster than to the uncorrected (free-space) value  $k$ .

<sup>150</sup> In addition, the Born approximation gives, in the diagonal elements of the transfer matrix, a term proportional to  $\alpha$ , which is not apparent in its exact form. It is easy to check, however, that such a term appears in the first order of the Taylor expansion of  $\exp\{k'd\}$  in this small parameter.

**Problem 3.15.** In the tight-binding approximation, find the lowest stationary states of a particle placed into a system of three similar, isotropic, weakly-coupled potential wells located in the vertices of an equilateral triangle.

*Solution:* Since in this system, just like in the 1D chain analyzed in Sec. 2.6 of the lecture notes, each potential well is coupled equally with its two neighbors, we may repeat all arguments that had led us to Eq. (2.206) of the lecture notes, and rewrite that relation as

$$E = E_1 - 2\delta_1 \cos \alpha,$$

where  $\alpha \equiv qa$ , and  $\delta_1$  is given by Eq. (2.204) for the ground state (with  $n = 1$ ). However, in contrast to the infinitely long chain, in our current ring-like, periodic system, the phase shift  $\alpha$  in Eq. (2.205),

$$a_j(t) = a \exp\left\{i\alpha j - i\frac{\epsilon_1}{\hbar}t + \text{const}\right\},$$

cannot take an arbitrary real value. Indeed, a shift by three positions ( $\Delta j = 3$ ) has to lead to a physically indistinguishable probability amplitude  $a_j$ , so  $3\alpha$  should be a multiple of  $2\pi m$ , where  $m$  is any integer. This gives us only three physically distinguishable values of  $\alpha$ , and hence only two possible eigenenergy values:

$$\begin{aligned} \alpha = 0, & \quad \text{with } E = E_g \equiv E_1 - 2\delta_1, \\ \alpha = \pm\frac{2\pi}{3}, & \quad \text{with } E = E_e \equiv E_1 + \delta_1. \end{aligned}$$

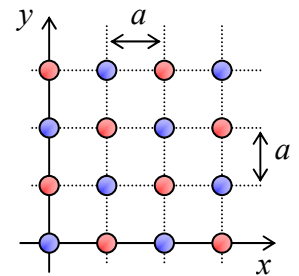
Hence, due to the wells' coupling, the ground-state energy level splits into two sublevels, with the lower (genuine ground-state) one being non-degenerate, and the higher sublevel doubly-degenerate.

Please note a deep analogy between these quantum states and the states (with  $n = 0$  and  $\pm 1$ ) of the particle on a ring, which was analyzed in Sec. 3.5 – see, e.g., the eigenenergy diagram shown in Fig. 3.18, for  $\Phi = 0$ . Similarly to that system, if the particle in our current problem is electrically charged, a magnetic field with a non-zero component normal to the well's common plane lifts the higher level's degeneracy.

**Problem 3.16.** The figure on the right shows a fragment of a periodic 2D lattice, with the red and blue points showing the positions of different local potentials.

- (i) Find the reciprocal lattice and the 1<sup>st</sup> Brillouin zone of the system.
- (ii) Calculate the wave number  $k$  of a monochromatic de Broglie wave incident along the  $x$ -axis, at which the lattice creates the lowest-order diffraction peak within the  $[x, y]$  plane, and the direction toward this peak.

(iii) Semi-quantitatively, describe the evolution of the intensity of the peak when all local potentials become similar.



*Hint:* The *order of diffraction* on a multidimensional Bravais lattice is a somewhat ambiguous notion dependent on the lattice type, but the *lowest-order peak* is always that corresponding to the smallest non-zero magnitude of the vector  $\mathbf{Q}$ .

*Solution:* The unit cell of the lattice evidently has to consist of at least two points – one “red” and one “blue”. A natural (though by no means not unique) selection of the cell and the primitive vectors is shown in the figure on the right:

$$\mathbf{a}_1 = \{2a, 0\}; \quad \mathbf{a}_2 = \{a, a\}.$$

For a 2D lattice, we may define the third primitive vector  $\mathbf{a}_3$  formally, for example as a normalized vector product of  $\mathbf{a}_1$  and  $\mathbf{a}_2$ , in our case getting<sup>151</sup>

$$\mathbf{a}_3 \equiv \frac{\mathbf{a}_1 \times \mathbf{a}_2}{a} = \frac{1}{a} \begin{vmatrix} \mathbf{n}_x & \mathbf{n}_y & \mathbf{n}_z \\ 2a & 0 & 0 \\ a & a & 0 \end{vmatrix} = \{0, 0, 2a\},$$

so the products participating in Eqs. (3.111) are

$$\mathbf{a}_2 \times \mathbf{a}_3 = \begin{vmatrix} \mathbf{n}_x & \mathbf{n}_y & \mathbf{n}_z \\ a & a & 0 \\ 0 & 0 & 2a \end{vmatrix} = \{2a^2, -2a^2, 0\}, \quad \mathbf{a}_3 \times \mathbf{a}_1 = \begin{vmatrix} \mathbf{n}_x & \mathbf{n}_y & \mathbf{n}_z \\ 0 & 0 & 2a \\ 2a & 0 & 0 \end{vmatrix} = \{0, 4a^2, 0\},$$

and  $\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) = 4a^3$ . With these expressions, the first two of Eqs. (3.111) yield the following primitive vectors of the reciprocal lattice:

$$\mathbf{b}_1 = \frac{\pi}{a} \{+1, -1\}, \quad \mathbf{b}_2 = \frac{\pi}{a} \{0, +2\}.$$

This result shows that the reciprocal lattice is also of the square type, but turned by  $\pi/4$  relative to the axes  $\mathbf{n}_x$  and  $\mathbf{n}_y$  – see the figure on the right. Naturally, the 1<sup>st</sup> Brillouin zone of this lattice is also a square – see the dashed lines in that figure.

(ii) Of all the reciprocal lattice vectors (3.109), in our case

$$\mathbf{Q} \equiv l_1 \mathbf{b}_1 + l_2 \mathbf{b}_2 \equiv \frac{\pi}{a} \{l_1, 2l_2 - l_1\},$$

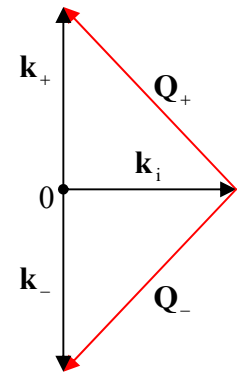
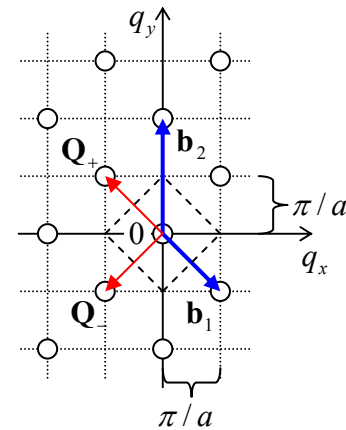
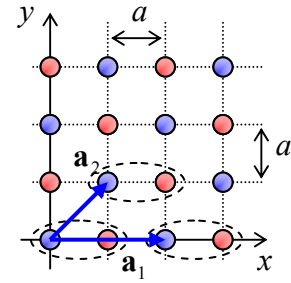
four vectors

$$\mathbf{Q} = \frac{\pi}{a} \{\pm 1, \pm 1\}$$

have the smallest nonvanishing magnitude  $Q = \sqrt{2}\pi/a$ . The red arrows in the figure above show the two of them,

$$\mathbf{Q}_+ = -\mathbf{b}_1 = \frac{\pi}{a} \{-1, +1\}, \quad \text{and} \quad \mathbf{Q}_- = -\mathbf{b}_1 - 2\mathbf{b}_2 = \frac{\pi}{a} \{-1, -1\},$$

that are responsible for the lowest order of diffraction for particles incident from the left, with  $\mathbf{k}_i = \{k, 0\}$ . The figure on the right shows that in this case, the lowest-order



<sup>151</sup> There is no need to be overly concerned by this choice, because for 2D lattices the third primitive vector  $\mathbf{a}_3$  is a formal (mathematical) construct, which enables us to use the 3D relations (3.111) directly, and it is only important to keep it linearly independent of  $\mathbf{a}_1$  and  $\mathbf{a}_2$ .

elastic scattering (with  $|\mathbf{k}_\pm| = |\mathbf{k}_i| \equiv k$ ) is by the angles  $\theta = \pm\pi/2$  and that the resonant value of the incident wave vector, for both peaks, is

$$k = \frac{Q_\pm}{\sqrt{2}} \equiv \frac{\pi}{a}.$$

(iii) According to Eq. (3.84) of the lecture notes, the diffraction intensity (as quantified by the differential cross-section of scattering) in a particular direction scales as the modulus square of the Born integral (3.86). For our particular case ( $\mathbf{q} = \mathbf{Q}_\pm$ ), the function under this integral is

$$U(\mathbf{r}) \exp\{-i\mathbf{Q}_\pm \cdot \mathbf{r}\} = U(\mathbf{r}) \exp\left\{-i\frac{\pi}{a}(-x \pm y)\right\} \equiv U(\mathbf{r}) \exp\left\{i\frac{\pi}{a}x\right\} \exp\left\{\pm i\frac{\pi}{a}y\right\}.$$

The positions of the local potentials, symbolized by the red and blue points in the figure given in the assignment, differ by  $\Delta x = a$ , corresponding to equal and opposite values of the factor  $\exp\{i\pi x/a\}$ , in each unit cell. Hence if these potentials become equal, the Born integral along the  $x$ -axis vanishes for any fixed  $y$ , so the whole integral equals zero, i.e. this particular diffraction peak disappears.

This result is natural, because in this case, the scattering system may be represented with a simple square lattice (the 2D version of the one shown in Fig. 3.11a of the lecture notes), having a single-point unit cell and a different (simpler) set of primitive vectors. The reader is challenged to work out this simpler case, and in particular to calculate the direction toward the lowest-order diffraction peak and the necessary value of  $k$ .

**Problem 3.17.** For the 2D hexagonal lattice (see Fig. 3.12b of the lecture notes):

- (i) find the reciprocal lattice  $\mathbf{Q}$  and the 1<sup>st</sup> Brillouin zone;
- (ii) use the tight-binding-approximation to calculate the dispersion relation  $E(\mathbf{q})$  for a 2D particle moving through a potential profile with such periodicity, with an energy close to the eigenenergy of similar isotropic states quasi-localized at the lattice points;
- (iii) analyze and sketch/plot the resulting dispersion relation  $E(\mathbf{q})$  inside the 1<sup>st</sup> Brillouin zone.

*Solutions:*

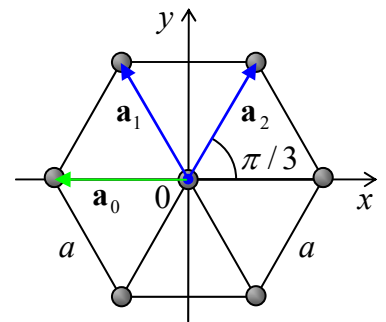
- (i) Let us choose the primitive vectors of the direct Bravais lattice  $\mathbf{R}$  as shown with the blue arrows in the figure on the right:

$$\mathbf{a}_1 = \frac{a}{2}(-\mathbf{n}_x + \sqrt{3}\mathbf{n}_y), \quad \mathbf{a}_2 = \frac{a}{2}(\mathbf{n}_x + \sqrt{3}\mathbf{n}_y),$$

where  $a$  is the so-called *lattice constant* – in this case, the distance between the adjacent points. Making also a natural choice  $\mathbf{a}_3 = a\mathbf{n}_z$  (so that this artificial primitive vector is linearly independent of the substantial two), we get

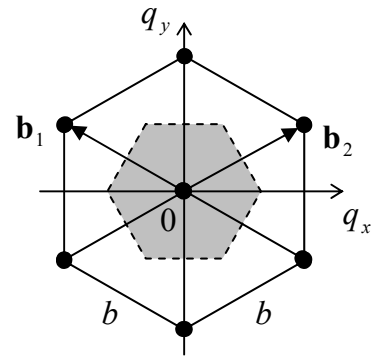
$$\mathbf{a}_2 \times \mathbf{a}_3 = \frac{a^2}{2}(\sqrt{3}\mathbf{n}_x - \mathbf{n}_y), \quad \mathbf{a}_3 \times \mathbf{a}_1 = \frac{a^2}{2}(-\sqrt{3}\mathbf{n}_x - \mathbf{n}_y), \quad \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) = -\frac{\sqrt{3}a^3}{2},$$

so for the primitive vectors of the reciprocal lattice  $\mathbf{Q}$ , Eqs. (3.111) yield



$$\mathbf{b}_1 = 2\pi \frac{1}{\sqrt{3}a} (-\sqrt{3}\mathbf{n}_x + \mathbf{n}_y), \quad \mathbf{b}_2 = 2\pi \frac{1}{\sqrt{3}a} (\sqrt{3}\mathbf{n}_x + \mathbf{n}_y).$$

The vectors  $\mathbf{b}_{1,2}$  have equal lengths,  $b = 4\pi/\sqrt{3}a$ , and the angle between them is a multiple of  $\pi/3$ . Hence the reciprocal lattice  $\mathbf{Q}$  is also hexagonal, with the lattice constant equal to  $b$ , but turned by  $\pi/6$  with respect to the direct lattice – see the figure on the right. Now we can form the 1<sup>st</sup> Brillouin zone by connecting the central point of the lattice ( $q_x = q_y = 0$ ) with its 6 nearest neighbors and drawing the perpendicular to the middle of each segment – see the dashed lines in the figure on the right. We see that the zone (shaded in this figure) is a hexagon whose side's closest approach to the origin is  $q_{\min} = b/2 = 2\pi/\sqrt{3}a$  and the farthest is  $q_{\max} = (2/\sqrt{3})q_{\min} = 4\pi/3a$ .



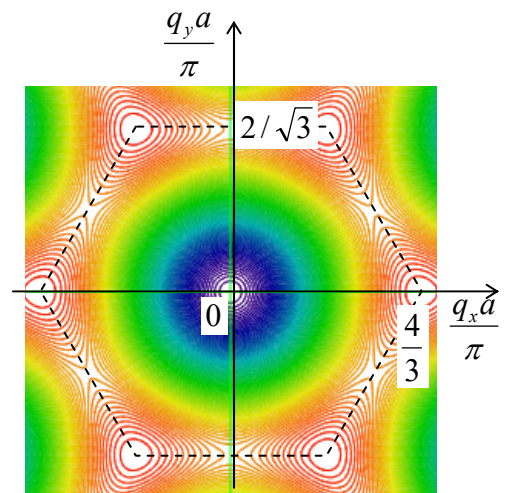
(ii) In the direct hexagonal lattice  $\mathbf{R}$ , each quasi-localized state has 6 closest similar neighbors, at the same distance  $a$ , so the tight-binding approximation should account for 6 corresponding state couplings. For isotropic localized states, all coupling coefficients  $\delta_n$  are equal, so instead of Eq. (3.118) of the lecture notes (derived for a square lattice), we may write

$$E = E_n - \delta_n \sum_{j=\text{nearest neighbors}} e^{i\mathbf{q}\cdot\mathbf{r}_j} = E_n - 2\delta_n [\cos(\mathbf{q}\cdot\mathbf{a}_0) + \cos(\mathbf{q}\cdot\mathbf{a}_1) + \cos(\mathbf{q}\cdot\mathbf{a}_2)],$$

where  $\mathbf{a}_0 \equiv -a\mathbf{n}_x$  (see the green arrow in the first figure above). Plugging into this relation the Cartesian representations of the vectors  $\mathbf{a}_{1,2}$  (spelled out above) and  $\mathbf{q} = q_x\mathbf{n}_x + q_y\mathbf{n}_y$ , we get

$$E - E_n = -2\delta_n \left( \cos q_x a + 2 \cos \frac{q_x a}{2} \cos \frac{\sqrt{3}q_y a}{2} \right).$$

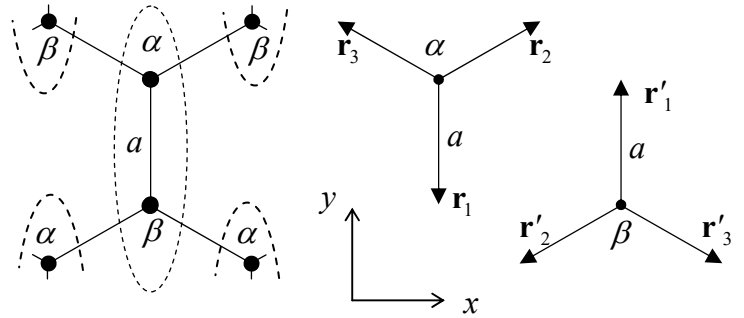
(iii) The energy given by this formula is shown in the figure on the right as a color-coded contour plot, with the dashed line showing the boundary of the hexagonal 1<sup>st</sup> Brillouin zone calculated in Task (i) – cf. the previous figure. We see that the function  $E(\mathbf{q})$  has the periodicity of the honeycomb lattice, with the “summits” and “passes” along that boundary. Note that finding this zone from the plot of  $E(\mathbf{q})$  would be even simpler than that via the reciprocal lattice construction! (Practically, it is prudent to use both ways and compare the results, as a sanity check.)



**Problem 3.18.** Complete the tight-binding calculation of the band structure of the honeycomb lattice, that was started at the end of Sec. 3.4 of the lecture notes. Analyze the results; in particular, prove that the Dirac points  $\mathbf{q}_D$  are located in the corners of the 1<sup>st</sup> Brillouin zone and express the velocity  $v_n$  participating in Eq. (3.122), in terms of the coupling energy  $\delta_n$ . Show that the final results do not change if the quasi-localized wavefunctions are not isotropic but are proportional to  $\exp\{im\varphi\}$ , where  $\varphi$  is the angle in the lattice plane – as they are, with  $m = \pm 1$ , for the  $2p_z$  electrons of carbon atoms in graphene, which are responsible for its transport properties.



*Solution:* Let us select the two-point unit cell of the lattice as shown in Fig. 3.12a of the lecture notes, which is partly reproduced on the left panel of the figure on the right, with the letters  $\alpha$  and  $\beta$  marking the probability amplitudes of the quasi-localized wavefunctions participating in Eqs. (3.119). The right two panels show the vectors  $\mathbf{r}_j$  and  $\mathbf{r}'_j$  participating in Eqs. (3.120)-(3.121), conveniently numbered to have  $\mathbf{r}'_j = -\mathbf{r}_j$ . Due to that symmetry, the double sum in Eq. (3.121) may be simplified as



$$\begin{aligned}\Sigma &= \sum_{j,j'=1}^3 e^{i\mathbf{q}\cdot(\mathbf{r}_j-\mathbf{r}_{j'})} = 3 + 2 \sum_{\substack{j,j'=1 \\ (j'<j)}}^3 \cos[\mathbf{q}\cdot(\mathbf{r}_j-\mathbf{r}_{j'})] \\ &= 3 + 2 \cos[\mathbf{q}\cdot(\mathbf{r}_2-\mathbf{r}_1)] + 2 \cos[\mathbf{q}\cdot(\mathbf{r}_3-\mathbf{r}_1)] + 2 \cos[\mathbf{q}\cdot(\mathbf{r}_3-\mathbf{r}_2)].\end{aligned}$$

Selecting the coordinate axes as shown at the bottom of the same figure above, and taking into account that all the angles between the vectors  $\mathbf{r}_j$  are multiples of  $2\pi/3$ , the vector differences participating in the last expression may be represented in the Cartesian coordinates as

$$\mathbf{r}_2 - \mathbf{r}_1 = \frac{\sqrt{3}}{2}a(\mathbf{n}_x + \sqrt{3}\mathbf{n}_y), \quad \mathbf{r}_3 - \mathbf{r}_1 = \frac{\sqrt{3}}{2}a(-\mathbf{n}_x + \sqrt{3}\mathbf{n}_y), \quad \mathbf{r}_3 - \mathbf{r}_2 = -\sqrt{3}a\mathbf{n}_x,$$

where  $a$  is the distance between adjacent points of the lattice (see the figure above), so Eq. (3.121) yields:<sup>152</sup>

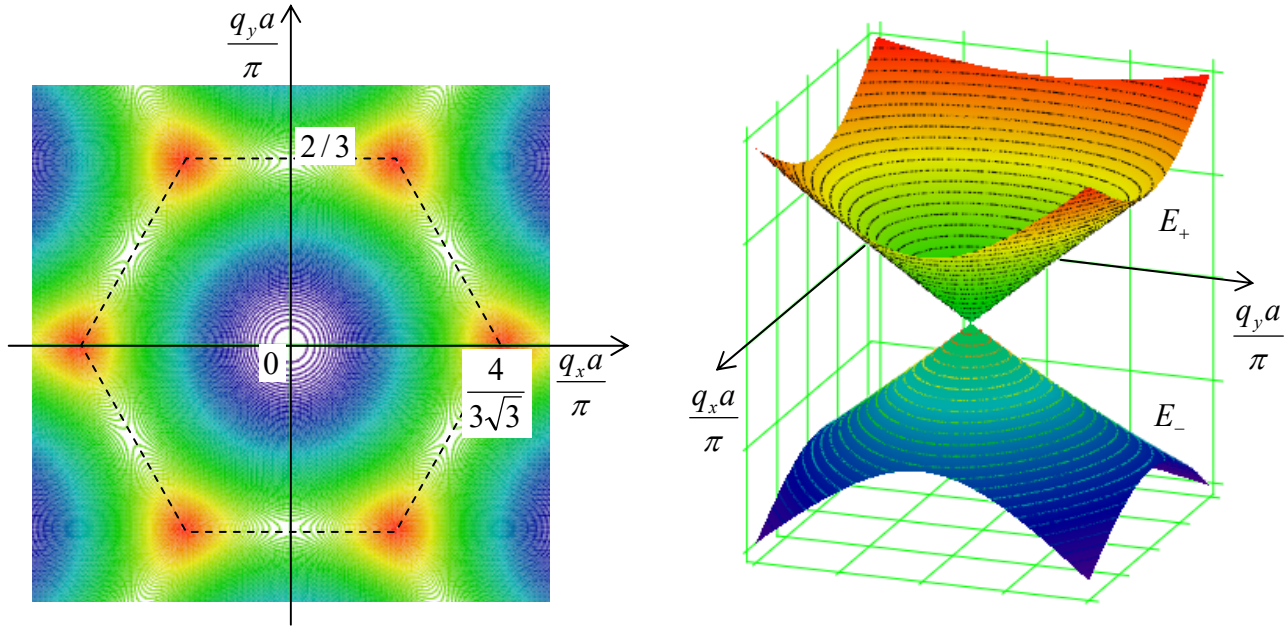
$$\begin{aligned}\frac{E_{\pm} - E_n}{\delta_n} &= \pm\Sigma^{1/2} = \pm \left\{ 3 + 2 \cos\left[\frac{\sqrt{3}}{2}(q_x a + \sqrt{3}q_y a)\right] + 2 \cos\left[\frac{\sqrt{3}}{2}(-q_x a + \sqrt{3}q_y a)\right] + 2 \cos(-\sqrt{3}q_x a) \right\}^{1/2} \\ &\equiv \pm \left[ 3 + 4 \cos\left(\frac{\sqrt{3}}{2}q_x a\right) \cos\left(\frac{3}{2}q_y a\right) + 2 \cos(\sqrt{3}q_x a) \right]^{1/2}.\end{aligned}$$

The left panel of the figure below shows the “global” 2D contour plot of the lower energy sheet, proportional to  $-\Sigma^{1/2}$ , on the  $\mathbf{q}$ -plane, while its right panel is a local 3D plot of both sheets, i.e.  $\pm\Sigma^{1/2}$ , near one of the special “Dirac” points (at that  $\Sigma = 0$ , i.e. the sheets touch), namely the point with

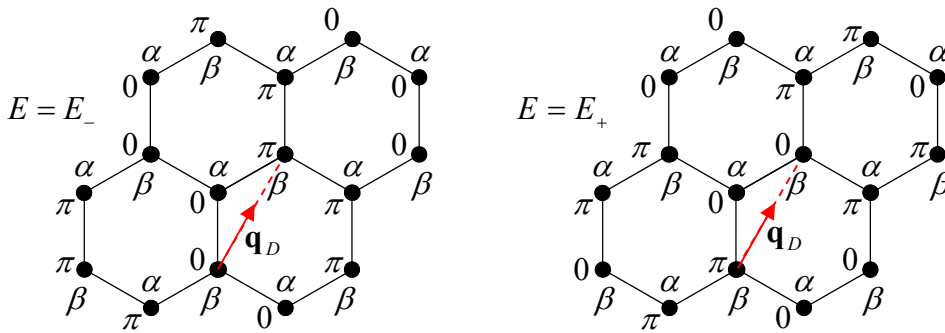
$$q_x|_D = \frac{4\pi}{3\sqrt{3}a}, \quad q_y|_D = 0. \quad (*)$$

(As the global plot shows, there are six such Dirac points at the same distance from the origin, separated by angles  $\pi/3$ , i.e. located in the corners of a honeycomb cell.)

<sup>152</sup> This result was first obtained (as a part of a theoretical analysis of the usual graphite) by P. Wallace in 1947. Note that the shape of each energy sheet is similar to that for the hexagonal lattice, calculated in the previous problem (besides a proportional re-scaling of  $q_x$  and  $q_y$ ); however, the existence of the top sheet is specific for the honeycomb direct lattice, with its two-point unit cell.



The physics of these points is as follows. If the Bloch wave’s quasimomentum is directed along any of the vectors  $\mathbf{q}_D$  (see, for example, the red arrows in the figure below), the wave propagates from a particular point of a unit cell (say, that with the localized wavefunction of amplitude  $\beta$ ) straight to similar points of other unit cells. As we know from 1D band theory, at the 1<sup>st</sup> Brillouin zone boundary, the phase shift between the probability amplitudes of the adjacent points equals  $\pi$  (plus any inconsequential multiple of  $2\pi$ ). Hence both possible phase shifts (either 0 or  $\pi$ ) between the probability amplitudes  $\alpha$  and  $\beta$ , describing the two energy sheets, lead to the phase patterns that differ only by a common rotation by  $\pm\pi/3$  (cf. the panels below) and hence have the same energy:  $E_+(\mathbf{q}_D) = E_-(\mathbf{q}_D)$ .



However, any deviation of the quasimomentum  $\mathbf{q}$  from  $\mathbf{q}_D$  (in either magnitude or direction) immediately breaks this balance. Indeed, expanding the function  $\Sigma(q_x, q_y)$  in the Taylor series near any of the Dirac points, for example, the point described by Eq. (\*), and neglecting all the terms beyond the quadratic ones, we see that the constant and linear terms cancel, giving

$$\Sigma_{\mathbf{q}\approx\mathbf{q}_D} \approx \frac{9}{4}(\tilde{q}_x^2 + \tilde{q}_y^2)a^2, \quad \text{where } \tilde{q}_x \equiv q_x - q_x|_D, \quad \tilde{q}_y \equiv q_y - q_y|_D.$$

This result shows that the dispersion relation  $E_{\pm}(\mathbf{q})$  near that point is indeed linear and isotropic,<sup>153</sup> as Eq. (3.122) of the lecture notes has promised:

$$E_{\pm} \Big|_{\mathbf{q} \approx \mathbf{q}_D} \approx E_n \pm \hbar v_n |\tilde{\mathbf{q}}|,$$

with the dispersion-free velocity

$$v_n = \frac{3}{2} \delta_n \frac{a}{\hbar}.$$

For the  $2p_z$  electrons in graphene ( $a \approx 0.142$  nm),  $\delta_n \approx 2.8$  eV, and this result yields  $v_n \approx 0.9 \times 10^6$  m/s.

The simple theory described above is applicable to these electron states even though their quasi-localized functions  $u_n(\mathbf{r})$  are not isotropic but are proportional to  $\exp\{im\varphi\}$ . Indeed, as Eq. (2.204) implies, to take account of such proportionality, each of the coefficients  $\delta_n$  participating in Eqs. (3.119) has to be multiplied by the factor  $\exp\{im(\varphi - \varphi')\}$ , where  $\varphi$  is the angle of the 2D vector connecting two adjacent lattice points number  $j$  and  $j'$ , and  $\varphi'$  is the angle of the opposite vector. Evidently,  $\varphi - \varphi' = \pi$ , so the additional factor in  $\delta_n$  is just  $\exp\{im\pi\}$ , i.e. either  $+1$  or  $-1$ , depending on whether  $m$  is even (e.g., as  $m = 0$  for axially symmetric states) or odd (e.g., as  $m = \pm 1$  for the  $2p_z$  states of carbon atom electrons in graphene). Since the dispersion relation (3.121) has the sign  $\pm$  before  $\delta_n$  anyway, the sign of  $m$  does not affect it.

**Problem 3.19.** Examine the basic properties of the so-called *Wannier functions*<sup>154</sup> defined as

$$\phi_{\mathbf{R}}(\mathbf{r}) \equiv C \int_{\text{BZ}} \psi_{\mathbf{q}}(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{R}} d^3q,$$

where  $\psi_{\mathbf{q}}(\mathbf{r})$  is the Bloch wavefunction (3.108),  $\mathbf{R}$  is any vector of the Bravais lattice,  $C$  is a normalization constant, and the integration over the quasimomentum  $\mathbf{q}$  is extended over any (e.g., the first) Brillouin zone.

*Solution:* According to the Wannier function's definition, it is just the 3D Fourier image of the Bloch function (i.e. of any extended eigenfunction of the stationary Schrödinger equation for a particle in a periodic potential) considered a function of its quasimomentum  $\mathbf{q}$ . (Notice the index attached to  $\psi(\mathbf{r})$  to emphasize its dependence on  $\mathbf{q}$ ; this index was just implied in Secs. 2.7 and 3.4 of the lecture notes.) Let us plug Eq. (3.108) of the lecture notes (with the same index  $\mathbf{q}$  attached to the periodic functions  $u(\mathbf{r})$  as well) into the Wannier function's definition:

$$\phi_{\mathbf{R}}(\mathbf{r}) = C \int_{\text{BZ}} u_{\mathbf{q}}(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} e^{-i\mathbf{q}\cdot\mathbf{R}} d^3q \equiv C \int_{\text{BZ}} u_{\mathbf{q}}(\mathbf{r}) e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{R})} d^3q.$$

Since the functions  $u_{\mathbf{q}}(\mathbf{r})$  are, by definition, invariant with respect to the translation by any Bravais lattice vector  $\mathbf{R}'$ ,

$$u_{\mathbf{q}}(\mathbf{r} + \mathbf{R}') = u_{\mathbf{q}}(\mathbf{r}),$$

we may calculate

<sup>153</sup> An additional exercise for the reader: describe the motion of electrons with  $E \approx E_n$  in an additional uniform magnetic field  $\mathcal{B} = \mathcal{B}\mathbf{n}_z$ , assuming that it is not too strong ( $\mathcal{B}a^2 \ll \Phi'_0$ ), and using the quasi-classical approximation analogous to Eq. (2.237).

<sup>154</sup> Named after G. Wannier who introduced these functions in 1939.

$$\phi_{\mathbf{R}+\mathbf{R}'}(\mathbf{r}+\mathbf{R}') = C \int_{\text{BZ}} u_{\mathbf{q}}(\mathbf{r}+\mathbf{R}') e^{i\mathbf{q}\cdot(\mathbf{r}+\mathbf{R}'-\mathbf{R}-\mathbf{R}')} d^3q \equiv C \int_{\text{BZ}} u_{\mathbf{q}}(\mathbf{r}) e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{R})} d^3q \equiv \phi_{\mathbf{R}}(\mathbf{r}).$$

This result means that the Wannier function depends only on the difference between  $\mathbf{r}$  and  $\mathbf{R}$ , i.e. is repeated near each point of the Bravais lattice.

Next, the Wannier functions centered at different Bravais lattice points  $\mathbf{R}$  and based on (mutually orthogonal) Bloch functions  $\psi_{\mathbf{q},n}(\mathbf{r})$  of particular energy bands  $n$  form a full orthogonal basis:

$$\begin{aligned} \int_{\text{UC}} \phi_{\mathbf{R},n}^*(\mathbf{r}) \phi_{\mathbf{R}',n'}(\mathbf{r}) d^3r &\propto \int_{\text{UC}} d^3r \int_{\text{BZ}} d^3q \int_{\text{BZ}'} d^3q' \psi_{\mathbf{q},n}^*(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{R}} \psi_{\mathbf{q}',n'}(\mathbf{r}) e^{-i\mathbf{q}'\cdot\mathbf{R}'} \\ &\equiv \int_{\text{BZ}} d^3q \int_{\text{BZ}'} d^3q' e^{i\mathbf{q}\cdot\mathbf{R}} e^{-i\mathbf{q}'\cdot\mathbf{R}'} \int_{\text{UC}} \psi_{\mathbf{q},n}^*(\mathbf{r}) \psi_{\mathbf{q}',n'}(\mathbf{r}) d^3r \\ &= \int_{\text{BZ}} d^3q \int_{\text{BZ}'} d^3q' e^{i\mathbf{q}\cdot\mathbf{R}} e^{-i\mathbf{q}'\cdot\mathbf{R}'} \delta(\mathbf{q}-\mathbf{q}') \delta_{n,n'} \propto \delta_{\mathbf{R},\mathbf{R}'} \delta_{n,n'}, \end{aligned}$$

where the  $\mathbf{r}$ -integration is over the unit cell (UC) of the Bravais lattice. (The set may be readily made orthonormal, with the appropriate choice of the constant  $C$  in the Wannier function definition.)

In order to appreciate the practical value of the Wannier functions, notice that the Bloch functions (as all eigenfunctions of any time-independent Hamiltonian) are only defined to an arbitrary  $\mathbf{r}$ -independent phase coefficients  $\exp\{i\varphi\}$ , where the choice of the real phase  $\varphi$ , for any  $\mathbf{q}$ , is arbitrary. Hence the shape of Wannier functions depends on the choice of the function  $\varphi(\mathbf{q})$ ; in particular, this function may be hand- (or rather computer-<sup>155</sup>) crafted to make  $\phi_{\mathbf{R},n}(\mathbf{r})$  maximally localized near the point  $\mathbf{r} = \mathbf{R}$ . This property of the Wannier functions, together with their evident independence of the quasimomentum  $\mathbf{q}$ , and hence of the eigenenergy  $E_n(\mathbf{q})$ , makes their basis convenient for several applications, for example, for numerical simulations of the electron structure in condensed matter and of the electron transport in nanostructures.<sup>156</sup>

**Problem 3.20.** Evaluate the long-range interaction (the so-called *London dispersion force*) between two similar, electrically neutral atoms or molecules, modeling each of them as an isotropic 3D harmonic oscillator with the electric dipole moment  $\mathbf{d} = q\mathbf{s}$ , where  $\mathbf{s}$  is the oscillator's displacement from its equilibrium position.

*Hint:* You may like to represent the total Hamiltonian of the system as a sum of Hamiltonians of independent 1D harmonic oscillators, and calculate their total ground-state energy as a function of the distance between the dipoles.<sup>157</sup>

*Solution:* According to classical electrostatics, the potential energy of interaction between two electric dipoles is<sup>158</sup>

<sup>155</sup> See, e.g., A. Mostofi *et al.*, *Comput. Phys. Commun.* **178**, 685 (2008).

<sup>156</sup> See, e.g., <http://www.wannier-transport.org/wiki/index.php/>.

<sup>157</sup> This explanation of the interaction between electrically-neutral atoms was put forward in 1930 by F. London, on the background of a prior (1928) work by C. Wang. Note that in some texts this interaction is (rather inappropriately) referred to as the “van der Waals force”, though it is only one (long-range) component of the van der Waals model – see, e.g., SM Sec. 4.1.

<sup>158</sup> See, e.g., EM Eq. (3.16), which uses a different notation ( $\mathbf{p}$ ) for the dipole moments.

$$U_{\text{int}} = \frac{1}{4\pi\epsilon_0 r^3} (d_{1x}d_{2x} + d_{1y}d_{2y} - 2d_{1z}d_{2z}),$$

where the  $z$ -axis is directed along the vector  $\mathbf{r}$  connecting the dipoles with moments  $\mathbf{d}_1$  and  $\mathbf{d}_2$ . In the single-particle model of an electrically-neutral molecule,  $\mathbf{d}_{1,2} = q\mathbf{s}_{1,2}$ , where  $\mathbf{s}_1 = \{x_1, y_1, z_1\}$  and  $\mathbf{s}_2 = \{x_2, y_2, z_2\}$  are the displacements of the effective particles, with electric charges  $q$ , from the oppositely charged immobile centers. In the isotropic 3D oscillator model, the interaction energy  $U_{\text{int}}$  should be added to the sum of the potential energies (3.123) of the two oscillators, so the total potential energy is

$$U = \frac{m\omega_0^2}{2} (x_1^2 + y_1^2 + z_1^2 + x_2^2 + y_2^2 + z_2^2) + \frac{q^2}{4\pi\epsilon_0 r^3} (x_1x_2 + y_1y_2 - 2z_1z_2).$$

Since the dipole approximation is only valid at large distances  $r \gg a \sim x_0 \equiv (\hbar/m\omega_0)^{1/2}$ , i.e. when the second term of this expression is relatively small,  $U$  has a stable minimum (at the point  $\mathbf{s}_1 = \mathbf{s}_2 = 0$ ), which does not depend on  $r$ , so classical electrodynamics cannot describe the London dispersion force. However, such force appears in quantum mechanics (and also in statistical physics at temperature  $T \neq 0$ ), in which Heisenberg's uncertainty relation forbids the oscillators from fully static positions at these potential minima. To quantify this effect, let us notice that in new coordinates defined as

$$\mathbf{s}_{\pm} \equiv \frac{\mathbf{s}_1 \pm \mathbf{s}_2}{\sqrt{2}}, \quad \hat{\mathbf{p}}_{\pm} \equiv \frac{\hat{\mathbf{p}}_1 \pm \hat{\mathbf{p}}_2}{\sqrt{2}}, \quad \text{so that } \mathbf{s}_{1,2} = \frac{\mathbf{s}_{+} \pm \mathbf{s}_{-}}{\sqrt{2}}, \quad \hat{\mathbf{p}}_{1,2} = \frac{\hat{\mathbf{p}}_{+} \pm \hat{\mathbf{p}}_{-}}{\sqrt{2}},$$

the system's potential energy  $U$  and hence its Hamiltonian as a whole fall apart into sums of coordinate and momentum components squared:

$$\begin{aligned} \hat{H} &= \frac{1}{2m} (\hat{p}_{1x}^2 + \hat{p}_{1y}^2 + \hat{p}_{1z}^2 + \hat{p}_{2x}^2 + \hat{p}_{2y}^2 + \hat{p}_{2z}^2) + U \\ &= \frac{1}{2m} (\hat{p}_{+x}^2 + \hat{p}_{+y}^2 + \hat{p}_{+z}^2 + \hat{p}_{-x}^2 + \hat{p}_{-y}^2 + \hat{p}_{-z}^2) \\ &\quad + \frac{m\omega_0^2}{2} (x_+^2 + y_+^2 + z_+^2 + x_-^2 + y_-^2 + z_-^2) + \frac{q^2}{8\pi\epsilon_0 r^3} (x_+^2 - x_-^2 + y_+^2 - y_-^2 - 2z_+^2 + 2z_-^2). \end{aligned}$$

This is just the sum of Hamiltonians of six independent 1D harmonic oscillators with the following frequencies:

$$\text{for } x_+ \text{ and } y_+ : \quad \omega_{t+} = \omega_0(1 + \mu)^{1/2} \approx \omega_0(1 + \mu/2 - \mu^2/8 + \dots),$$

$$\text{for } x_- \text{ and } y_- : \quad \omega_{t-} = \omega_0(1 - \mu)^{1/2} \approx \omega_0(1 - \mu/2 - \mu^2/8 + \dots),$$

$$\text{for } z_+ : \quad \omega_{t+} = \omega_0(1 - 2\mu)^{1/2} \approx \omega_0(1 - \mu - \mu^2/2 + \dots),$$

$$\text{for } z_- : \quad \omega_{t-} = \omega_0(1 + 2\mu)^{1/2} \approx \omega_0(1 + \mu - \mu^2/2 + \dots),$$

$$\text{where } \mu \equiv \frac{q^2}{4\pi\epsilon_0 r^3 m\omega_0^2} \ll 1.$$

Here the Taylor expansions in the small parameter  $\mu$  are extended to the third (quadratic) terms, because in the full Hamiltonian, the sum of the linear terms vanishes, and the first nonvanishing correction to the ground-state energy of the whole system is proportional to  $\mu^2$ :

$$E_g = \sum_{\omega} \frac{\hbar\omega}{2} = \frac{\hbar}{2}(2\omega_{l+} + 2\omega_{l-} + \omega_{l+} + \omega_{l-}) \approx \frac{\hbar\omega_0}{2} \left[ 6 - \mu^2 \left( 4\frac{1}{8} + 2\frac{1}{2} \right) \right] \equiv 3\hbar\omega_0 - \frac{3}{4}\hbar\omega_0\mu^2.$$

The first term of the last expression is evidently the ground-state energy of two fully separated 3D oscillators, while the second term may be interpreted as the effective potential of their interaction:

$$U_{\text{ef}} = -\frac{3}{4}\hbar\omega_0\mu^2 \equiv -\frac{3}{4} \frac{\hbar q^4}{(4\pi\epsilon_0)^2 m^2 \omega_0^3 r^6} \equiv -\frac{3}{4} Z^4 \left( \frac{m_e}{m} \right)^2 \left( \frac{x_0}{r} \right)^6 E_H,$$

where  $E_H$  is the Hartree energy unit (1.13), and  $Z \equiv q/e$ . (The factor  $Z^4(m_e/m)^2$  may be much larger than 1 in large atoms/molecules, where the polarization is due to a simultaneous displacement of  $N \gg 1$  electrons, so  $Z^4 \propto N^4$  while  $(m/m_e)^2 \propto N^2$ .)

Note the following features of the result for  $U_{\text{ef}}$ :

- the interaction is always attractive – for any sign of the charge  $q$ ;
- the interaction potential is proportional to  $1/r^6$ , i.e. drops with the distance much faster than that ( $U \propto 1/r^3$ ) for atoms with permanent (field-independent) dipole moments.
- $U_{\text{ef}}$  is proportional to  $\hbar$ , emphasizing again the quantum nature of the long-range attraction – at least when thermal excitations of the oscillators are negligible.

Later in the course (in Chapters 5 and 6), we will explore a completely different way to derive the same formula and its generalization to an arbitrary single-particle model of the atom. The latter result will show that the listed general features of the London dispersion force are very insensitive to model details. That alternative approach, while being somewhat less concise, will also reveal this force's physics much more explicitly.

**Problem 3.21.** Derive expressions for the stationary functions and the corresponding energies of a 2D particle of mass  $m$ , free to move inside a round disk of radius  $R$ . What is the degeneracy of each energy level? Calculate the five lowest energy levels with an accuracy better than 1%.

*Solution:* We may start the solution of this problem (which is just the 2D version of the problem solved at the end of Sec. 3.6 of the lecture notes) from Eq. (3.147) of the lecture notes, with  $U(\rho) = 0$ ,

$$-\frac{\hbar^2}{2m} \left[ \frac{1}{\rho\mathcal{R}} \frac{d}{d\rho} \left( \rho \frac{d\mathcal{R}}{d\rho} \right) - \frac{m^2}{\rho^2} \right] = E. \quad (*)$$

For our problem, this equation has to be solved with the boundary condition

$$\mathcal{R}(R) = 0, \quad (**)$$

due to the continuity of each partial wavefunction  $\mathcal{R}(\rho)\mathcal{A}(\varphi) \propto \mathcal{R}(\rho)e^{im\varphi}$  on the whole border  $\rho = R$ , i.e. for all values of the angle  $\varphi$  and the integer quantum number  $m$ . After the introduction of the dimensionless argument  $\xi \equiv k\rho$  and with the usual definition of the free particle's wave number  $k$  (as  $\hbar^2 k^2 / 2m \equiv E$ ), Eq. (\*) is reduced to the canonical form of the Bessel equation:<sup>159</sup>

<sup>159</sup> See, e.g. EM Sec. 2.7 of the lecture notes.

$$\frac{d^2\mathcal{R}}{d\xi^2} + \frac{1}{\xi} \frac{d\mathcal{R}}{d\xi} + \left(1 - \frac{m^2}{\xi^2}\right)\mathcal{R} = 0.$$

Its general solution is a linear combination of the Bessel functions of the first and second kind, of the same integer order  $m$ :

$$\mathcal{R}(\xi) = C_1 J_m(\xi) + C_2 Y_m(\xi).$$

However, the functions  $Y_m(\xi)$  diverge at  $\xi \rightarrow 0$ ,<sup>160</sup> while the wavefunction has to stay finite in the center of the disk. Hence, the coefficient  $C_2$  has to equal zero, and Eq. (\*\*\*) is reduced to the following requirement:

$$J_m(kR) = 0.$$

This condition, which plays the role of the characteristic equation, is satisfied if the product  $kR$  is equal to any nontrivial root of the Bessel function,  $\xi_{m,l} \neq 0$ , where the index  $l = 1, 2, 3, \dots$  numbers the roots. As a result, the eigenfunctions are

$$\psi_{m,l} = C_l J_m\left(\frac{\rho}{R} \xi_{m,l}\right) e^{im\varphi},$$

and the energy spectrum is

$$E_{m,l} = E_0 \xi_{m,l}^2, \quad \text{where } E_0 \equiv \frac{\hbar^2}{2mR^2}. \quad (***)$$

Each energy level with  $m \neq 0$  is doubly degenerate, due to two possible signs of  $m$ . Indeed, the Bessel function  $J_{-m}(\xi)$  equals  $(-1)^m J_m(\xi)$ , and hence has the same set of roots  $\xi_{m,l}$  as  $J_m(\xi)$ . So, the eigenenergies of the states with the equal but opposite values of  $m$  are exactly equal, while their eigenfunctions are different, due to different azimuthal factors  $\mathcal{A}(\varphi) = \exp\{im\varphi\}$ .

Per Eq. (\*\*\*), the lowest energy levels correspond to the smallest roots  $\xi_{m,l}$ . Using a table of the roots,<sup>161</sup> we get the following approximate values for the five lowest levels:

$m$	$l$	$\xi_{n,l}$	$E_{m,l}/E_0 = (\xi_{n,l})^2$
0	1	2.405	5.78
1	1	3.832	14.68
2	1	5.136	26.38
0	2	5.520	30.47
3	1	6.380	40.70

Note the sudden “intrusion” of the second root of  $J_0(\xi)$  ( $m = 0, l = 2$ ) into the initially orderly sequence of the first roots of  $J_m(\xi)$ , very similar to that of a similar 3D problem solved at the end of Sec. 3.6 of the lecture notes. The comparison of these two problems also shows that the lowest eigenenergies of this 2D system (a particle inside the disk of radius  $R$ ) are lower than those of a similar 3D system – a particle of the same mass inside a sphere of the same radius. Let me challenge the reader: could you

<sup>160</sup> See, e.g., EM Eq. (2.152) and/or Fig. 2.19.

<sup>161</sup> See, e.g., EM Table 2.1 – or virtually any math handbook listed in MA Sec. 16(ii).

predict this fact before doing calculations? Also, would this relation hold if the 2D disk has a small but non-zero thickness, i.e. is a 3D system?

**Problem 3.22.** Calculate the ground-state energy of a 2D particle of mass  $m$ , localized in a very shallow flat-bottom potential well

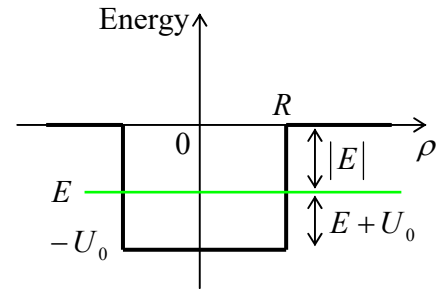
$$U(\rho) = \begin{cases} -U_0, & \text{for } \rho < R, \\ 0, & \text{for } \rho > R, \end{cases} \quad \text{with } 0 < U_0 \ll \frac{\hbar^2}{mR^2}.$$

*Solution:* Starting from the case of an arbitrary (but positive)  $U_0$ , and repeating the arguments made in the model solution of the previous problem (with  $E$  replaced with the difference  $E - (-U_0) \equiv E + U_0$ , i.e. with the wave number  $k$  now defined by the relation

$$\frac{\hbar^2 k^2}{2m} = E + U_0 \geq 0,$$

due to the different position of the well's bottom – see the figure on the right), we get the following radial wavefunctions inside the well:

$$\mathcal{R}(\rho) = C_- J_m(k\rho), \quad \text{for } \rho \leq R. \quad (*)$$



Outside of the well (at  $\rho > R$ ), where  $U(\rho) = 0$ , Eq. (3.147) of the lecture notes may be similarly reduced to the modified Bessel equation,<sup>162</sup>

$$\frac{d^2 \mathcal{R}}{d\xi^2} + \frac{1}{\xi} \frac{d\mathcal{R}}{d\xi} - \left(1 + \frac{m^2}{\xi^2}\right) \mathcal{R} = 0, \quad \text{with } \xi \equiv \kappa\rho, \quad \text{where } \frac{\hbar^2 \kappa^2}{2m} = |E| \geq 0,$$

whose general solution is a linear superposition of the modified Bessel functions  $I_m(\xi)$  and  $K_m(\xi)$ . Since the former functions diverge at  $\xi \rightarrow \infty$  (i.e. at  $\rho \rightarrow \infty$ ),  $\mathcal{R}(\rho)$  has to be proportional to the latter function alone:

$$\mathcal{R}(\rho) = C_+ K_m(\kappa\rho), \quad \text{for } \rho \geq R. \quad (**)$$

At the well's wall (at  $\rho = R$ ), the wavefunction and its radial derivative have to be continuous. Plugging Eqs. (\*) and (\*\*) into these boundary conditions, we get two equations:

$$C_- J_m(kR) = C_+ K_m(\kappa R), \quad C_- k J'_m(kR) = C_+ \kappa K'_m(\kappa R),$$

where each prime sign denotes the corresponding function's derivative over its total argument. The condition of compatibility of these two homogeneous linear equations for two constants  $C_{\pm}$  gives the following characteristic equation for two constants  $k$  and  $\kappa$ , and hence for energy  $E$ :

$$\begin{vmatrix} J_m(kR) & -K_m(\kappa R) \\ kJ'_m(kR) & -\kappa K'_m(\kappa R) \end{vmatrix} = 0, \quad \text{i.e. } \kappa J_m(kR) K'_m(\kappa R) = k K_m(\kappa R) J'_m(kR). \quad (***)$$

<sup>162</sup> See, e.g., EM Eq. (2.155) and its discussion.



Now let us consider the ground state, with the lowest, zero value of the magnetic quantum number  $m$ , in the limit of very low  $U_0$  and hence of very low values of  $|E|$  and  $E + U_0$ , which are both contained between 0 and  $U_0$  (see the figure above):

$$E + U_0, |E| \leq U_0 \ll E_0, \quad \text{where } E_0 \equiv \frac{\hbar^2}{mR^2}.$$

According to the above definitions of the parameters  $k$  and  $\kappa$ , this means that both arguments,  $kR$  and  $\kappa R$ , of the Bessel functions, are much smaller than 1. In this case, these functions may be approximated as<sup>163</sup>

$$J_0(kR) \approx 1 - \left(\frac{kR}{2}\right)^2 \approx 1, \quad K_0(\kappa R) \approx -\left[\ln\left(\frac{\kappa R}{2}\right) + \gamma\right] \equiv \ln \frac{2e^{-\gamma}}{\kappa R},$$

(where  $\gamma \approx 0.5771$  is the Euler constant), so

$$J'_0(kR) \approx -\frac{kR}{2}, \quad K'_0(\kappa R) \approx -\frac{1}{\kappa R},$$

and Eq. (\*\*\*) is reduced to

$$\kappa \frac{1}{\kappa R} = k \ln\left(\frac{2e^{-\gamma}}{\kappa R}\right) \frac{kR}{2}, \quad \text{i.e. } \frac{(E + U_0)}{2E_0} \ln \frac{2e^{-2\gamma} E_0}{|E|} = 1.$$

Since in the limit we are analyzing, the factor before the last logarithm function is much smaller than 1, the function itself has to be large, so its argument has to be extremely large. (Recall that this function grows very slowly at large values of its argument.) Since the sum of  $|E|$  and  $(E + U_0)$  is equal to  $U_0$ , i.e. is fixed (see the figure above), this is only possible if  $|E|$  is much smaller than not only  $E_0$  but than  $(E + U_0)$  as well. Hence, we may neglect  $E$  in the numerator of the pre-logarithm fraction, getting

$$E = -|E| = -2e^{-2\gamma} E_0 \exp\left\{-\frac{2E_0}{U_0}\right\} \approx -0.631 E_0 \exp\left\{-\frac{2E_0}{U_0}\right\}, \quad \text{for } U_0 \ll E_0. \quad \text{****}$$

This formula shows that a bound (localized) state, though with an exponentially small  $|E|$ , exists for any  $U_0$ , however small. Qualitatively, this is also true for a similar 1D system (see the solutions of Problems 2.17 and 2.18), but there, the ground state's energy level is much deeper than the exponentially shallow level (\*\*\*\*):  $|E| \sim U_0^2/E_0 \equiv E_0(U_0/E_0)^2$ .

**Problem 3.23.** Estimate the energy  $E$  of the localized ground state of a 2D particle of mass  $m$ , in an axially-symmetric potential well of a finite radius  $R$ , with an arbitrary but very small potential  $U(\rho)$ . (Quantify this condition.)

*Solution:* Just as in the previous problem, we may argue that the ground state has the “magnetic” quantum number  $m$  equal to 0, so Eq. (3.147) of the lecture notes for the radial factor  $\mathcal{R}(\rho)$  of its wavefunction takes the form

$$-\frac{\hbar^2}{2m} \frac{1}{\rho} \frac{d}{d\rho} \left( \rho \frac{d\mathcal{R}}{d\rho} \right) + U(\rho)\mathcal{R} = E\mathcal{R}, \quad (*)$$

<sup>163</sup> See, e.g., EM Eqs. (2.146) and (2.157).

with a negative  $E$ . Also as in the previous problem, at distances  $\rho > R$  where  $U(\rho) = 0$ , this equation reduces to the modified Bessel equation,

$$\frac{d^2 \mathcal{R}}{d\xi^2} + \frac{1}{\xi} \frac{d\mathcal{R}}{d\xi} - \mathcal{R} = 0, \quad \text{with } \xi \equiv \kappa\rho, \quad \text{where } \frac{\hbar^2 \kappa^2}{2m} = -E \geq 0,$$

and has the same solution  $\mathcal{R} = CK_0(\kappa\rho)$ . From the solution of the previous problem, we may expect that if  $|U(\rho)|$  is sufficiently small, the magnitude  $-E \equiv |E|$  of the ground state energy  $E$  is even much smaller, so  $\kappa R \ll 1$ . Hence, there is a broad range of intermediate distances  $\rho$ , with  $R < \rho \ll 1/\kappa$ , where we may use the same approximation for the function  $K_0$  and hence  $\mathcal{R}$ :

$$\mathcal{R} \approx C \ln \left( \frac{2e^{-\gamma}}{\kappa\rho} \right) \equiv -C \ln \rho + \text{const}, \quad \frac{d\mathcal{R}}{d\rho} \approx -\frac{C}{\rho}, \quad \frac{1}{\mathcal{R}} \frac{d\mathcal{R}}{d\rho} \approx -\frac{1}{\rho} \bigg/ \ln \frac{2e^{-\gamma}}{\kappa\rho}. \quad (**)$$

Because of the same smallness of  $|E|$ , at  $\rho < R$  we may neglect, in Eq. (\*), the full energy in comparison with the potential energy:

$$-\frac{\hbar^2}{2m} \frac{1}{\rho} \frac{d}{d\rho} \left( \rho \frac{d\mathcal{R}}{d\rho} \right) + U(\rho)\mathcal{R} = 0.$$

Let us quantify the smallness of the potential  $U$  by assuming that the scale of its magnitude is much smaller than the kinetic energy scale  $E_0 \equiv \hbar^2/mR^2$  – again just as in the previous problem. Then we may integrate the last equation from  $\rho = 0$  (where  $d\mathcal{R}/d\rho = 0$  because of the axial symmetry of the wavefunction) to the same intermediate value of the 2D radius,  $R < \rho \ll 1/\kappa$ , neglecting the small change of  $\mathcal{R}$  in the second term, i.e. taking it to be equal to the value  $\mathcal{R}(0)$  at the center of the well. An elementary integration yields

$$\frac{d\mathcal{R}}{d\rho} = \mathcal{R}(0) \frac{2m}{\hbar^2 \rho} \int_0^R U(\rho') \rho' d\rho', \quad \text{i.e. } \frac{1}{\mathcal{R}} \frac{d\mathcal{R}}{d\rho} = \frac{2m}{\hbar^2 \rho} \int_0^R U(\rho') \rho' d\rho'.$$

The last expression still differs from the last formula in Eq. (\*\*) by the logarithm, but since it is a very slow function of its argument, we may require these two results to be close to each other at  $\rho \sim R$ , getting the following estimate<sup>164</sup>

$$-\frac{2m}{\hbar^2} \int_0^R U(\rho) \rho d\rho \sim 1 / \ln \frac{1}{\kappa R},$$

finally giving

$$\kappa \sim \frac{1}{R} \exp \left\{ \frac{\hbar^2}{2m} \bigg/ \int_0^R U(\rho) \rho d\rho \right\}, \quad \text{i.e. } -E = \frac{\hbar^2 \kappa^2}{2m} \sim \frac{\hbar^2}{2mR^2} \exp \left\{ \frac{\hbar^2}{m} \bigg/ \int_0^R U(\rho) \rho d\rho \right\}. \quad (***)$$

In order for this estimate to be valid,  $-E$  should be much smaller than the scale of  $U$ , and hence than  $E_0 \equiv \hbar^2/mR^2$ , so the integral in the exponent of Eq. (\*\*\*) has to be negative and small by magnitude:

<sup>164</sup> Taking into account the difference between  $2e^{-\gamma} \approx 1.123$  and 1 would be beyond the accuracy of this estimate.

$$0 < -\int_0^R U(\rho') \rho' d\rho' \ll \frac{\hbar^2}{m} \equiv E_0 R^2,$$

essentially repeating the assumption already made above.

Note that Eq. (\*\*\*) yields the correct exponent (though only a rough estimate of the pre-exponential coefficient) for the particular system considered in the previous problem,  $U(\rho) = U_0 = \text{const}$ , because in this case

$$\int_0^R U(\rho) \rho d\rho = -U_0 \int_0^R \rho d\rho = -U_0 \frac{R^2}{2}, \quad \text{i.e.} \quad \frac{\hbar^2}{m} \int_0^R U(\rho) \rho d\rho = -\frac{\hbar^2}{m} U_0 \frac{R^2}{2} \equiv -\frac{2E_0}{U_0}.$$

**Problem 3.24.** Spell out the spherical harmonics  $Y_4^0(\theta, \varphi)$  and  $Y_4^4(\theta, \varphi)$ .

*Solution:* According to Eqs. (3.165)-(3.171) of the lecture notes, any  $Y_l^m(\theta, \varphi) = C_l^m \sin^l \theta e^{im\varphi}$ , so  $Y_4^4(\theta, \varphi) = C_4^4 \sin^4 \theta e^{4i\varphi}$ . The normalization, by using Eq. (3.173), is straightforward:

$$|C_4^4|^2 = \int_0^{2\pi} d\varphi \int_0^\pi \sin^8 \theta \sin \theta d\theta \equiv 4\pi \int_0^1 (1-\xi^2)^4 d\xi = 4\pi \frac{128}{315},$$

so, finally,

$$Y_4^4(\theta, \varphi) = \frac{3}{16} \left( \frac{35}{2\pi} \right)^{1/2} \sin^4 \theta e^{4i\varphi}.$$

Now proceeding to  $Y_4^0(\theta, \varphi)$ : since  $Y_l^m(\theta, \varphi) \propto e^{im\varphi} \Theta(\theta)$ , for  $m = 0$ , the azimuthal-angle factor of spherical harmonics is just a constant. Hence, we need to calculate only the polar factor  $\Theta(\theta) \propto P_4^0(\cos \theta) \equiv P_4(\cos \theta)$ . From the Rodrigues formula (3.165), leaving the numerical coefficient aside for a while, we have

$$P_4(\xi) \propto \frac{d^4}{d\xi^4} (\xi^2 - 1)^4.$$

The differentiation is not as hard as one could imagine because

$$(\xi^2 - 1)^4 \equiv \xi^8 - 4\xi^6 + 6\xi^4 - 4\xi^2 + 1$$

and the two lowest-power terms are not important, since they gradually disappear at the sequential differentiation:

$$\begin{aligned} \frac{d}{d\xi} (\xi^2 - 1)^4 &= 8\xi^7 - 4 \cdot 6\xi^5 + 6 \cdot 4\xi^3 - 4 \cdot 2\xi, \\ \frac{d^2}{d\xi^2} (\xi^2 - 1)^4 &= 8 \cdot 7\xi^6 - 4 \cdot 6 \cdot 5\xi^4 + 6 \cdot 4 \cdot 3\xi^2 - 4 \cdot 2, \\ \frac{d^3}{d\xi^3} (\xi^2 - 1)^4 &= 8 \cdot 7 \cdot 6\xi^5 - 4 \cdot 6 \cdot 5 \cdot 4\xi^3 + 6 \cdot 4 \cdot 3 \cdot 2\xi, \end{aligned}$$

$$\frac{d^4}{d\xi^4}(\xi^2 - 1)^4 = 8 \cdot 7 \cdot 6 \cdot 5 \xi^4 - 4 \cdot 6 \cdot 5 \cdot 4 \cdot 3 \xi^2 + 6 \cdot 4 \cdot 3 \cdot 2 \equiv 2^4 3 \cdot (35 \xi^4 - 30 \xi^2 + 3),$$

so

$$Y_4^0(\theta, \varphi) = C_4^0 (35 \cos^4 \theta - 30 \cos^2 \theta + 3).$$

The normalization is a bit more tedious but still very much doable:

$$|C_4^0|^{-2} = \int_0^{2\pi} d\varphi \int_0^\pi (35 \cos^4 \theta - 30 \cos^2 \theta + 3)^2 \sin \theta d\theta = 4\pi \int_0^1 (35 \xi^4 - 30 \xi^2 + 3)^2 d\xi = 4\pi \frac{64}{9},$$

so, finally,

$$Y_4^0(\theta, \varphi) = \frac{3}{16\pi^{1/2}} (35 \cos^4 \theta - 30 \cos^2 \theta + 3).$$

**Problem 3.25.** Calculate  $\langle x \rangle$  and  $\langle x^2 \rangle$  in the ground states of the planar and spherical rotors of radius  $R$ . What can you say about  $\langle p_x \rangle$  and  $\langle p_x^2 \rangle$ ?

*Solution:* Since for the *planar* rotor, the 2D radius  $\rho \equiv (x^2 + y^2)^{1/2}$  is fixed at value  $R$ , its square  $\rho^2$  is definitely  $R^2$ , so

$$\langle \rho^2 \rangle = R^2.$$

Due to the axial symmetry of the ground state's wavefunction (corresponding to the azimuthal quantum number  $m$  equal to zero), we may write  $\langle x \rangle = 0$  and  $\langle x^2 \rangle = \langle y^2 \rangle$ , so  $\langle \rho^2 \rangle \equiv \langle x^2 \rangle + \langle y^2 \rangle = 2\langle x^2 \rangle$  and hence,

$$\langle x^2 \rangle = \frac{1}{2} \langle \rho^2 \rangle = \frac{R^2}{2}.$$

For the *spherical* rotor, with fixed  $r^2 \equiv x^2 + y^2 + z^2 = R^2$ ,

$$\langle r^2 \rangle = R^2.$$

Due to the spherical symmetry of the ground state,  $\langle x \rangle = 0$  and  $\langle x^2 \rangle = \langle y^2 \rangle = \langle z^2 \rangle$ , so  $\langle r^2 \rangle \equiv \langle x^2 \rangle + \langle y^2 \rangle + \langle z^2 \rangle = 3\langle x^2 \rangle$ , and

$$\langle x^2 \rangle = \frac{1}{3} \langle r^2 \rangle = \frac{R^2}{3}.$$

Using the same symmetry arguments, we may write  $\langle p_x \rangle = 0$  (for both systems),  $\langle p_x^2 \rangle = \langle p^2 \rangle / 2$  for the planar rotor, and  $\langle p_x^2 \rangle = \langle p^2 \rangle / 3$  for the spherical rotor. However, calculating the  $\langle p^2 \rangle$  participating in these formulas exclusively from the angular motion of a real (3D) particle would be wrong. (Indeed, in the ground,  $s$ -state of both systems, in which  $\psi$  does not have any angular dependence, this would give us  $\langle p^2 \rangle = 0$  and  $\langle p_x^2 \rangle = 0$ , in a clear contradiction with the Heisenberg's uncertainty principle, because  $\langle x^2 \rangle$  is finite.) Actually, the momentum's uncertainty in such systems is dominated by the lateral confinement of the motion<sup>165</sup> and cannot be calculated exactly unless the confinement potential that forces the particle to be a rotor, is specified quantitatively. We can, however, use the uncertainty relation for the following estimate:  $\delta p_x \sim \delta p \sim \hbar / \delta R$ , where  $\delta R$  is the radial width of the potential well providing

<sup>165</sup> If needed, please revisit Sec. 2.1 of the lecture notes and the solution of Problem 2.1.

the radial confinement. Since for the validity of the rotor models, we need  $\delta R \ll R$ ,<sup>166</sup> we may write  $\delta x \delta p_x \sim R\hbar/\delta R \gg \hbar$ .

**Problem 3.26.** A spherical rotor, with  $r = R = \text{const}$  and mass  $m$ , is in a state with the following wavefunction:  $\psi = C(\frac{1}{3} + \sin^2\theta)$ , where  $C$  is a constant. Calculate the energy of its angular motion.

*Solution:* Rewriting the wavefunction as

$$\psi = C\left(\frac{1}{3} + 1 - \cos^2\theta\right) \equiv C\left[1 - \frac{1}{3}(3\cos^2 - 1)\right],$$

and comparing the terms of this linear superposition with Eq. (3.174) and the third line of Eq. (3.176) of the lecture notes, we may write

$$\psi = C\left[(4\pi)^{1/2}Y_0^0 - \frac{1}{3}\left(\frac{16\pi}{3}\right)^{1/2}Y_2^0\right] \equiv (4\pi)^{1/2}C\left[Y_0^0 - \frac{2}{3\sqrt{3}}Y_2^0\right].$$

This expression shows that our state is a linear combination of two eigenfunctions of the rotor, both with the magnetic quantum number  $m$  equal to zero, but with different orbital numbers: one with  $l = 0$ , and another with  $l = 2$ . The ratio of the probabilities  $W_0$  and  $W_2$  of these eigenstates equals that of the squares of the probability amplitude moduli:

$$\frac{W_2}{W_0} = \left(\frac{2}{3\sqrt{3}}\right)^2 \equiv \frac{4}{27}.$$

Requiring the sum of the probabilities to equal 1, we get

$$W_0 = \frac{1}{1 + 4/27} = \frac{27}{31}, \quad W_2 = \frac{4/27}{1 + 4/27} = \frac{4}{31}.$$

From here, and using Eq. (3.163) of the lecture notes for the eigenenergies of the rotor, we get

$$E = W_0E_0 + W_2E_2 = \frac{27}{31} \cdot 0 + \frac{4}{31} \cdot \frac{\hbar^2 \cdot 2(2+1)}{2mR^2} \equiv \frac{12}{31} \frac{\hbar^2}{mR^2}.$$

As a reminder, for a genuinely 3D particle, this energy does not include that of radial confinement. (If necessary, please revisit the beginning of Sec. 2.1 and the previous problem's solution.)

**Problem 3.27.** According to the discussion at the beginning of Sec. 3.5 of the lecture notes, stationary wavefunctions of a 3D isotropic harmonic oscillator may be calculated as products of three similar 1D “Cartesian oscillators” – see, in particular Eq. (3.125), with  $d = 3$ . However, per the discussion in Sec. 3.6, the wavefunctions of the type (3.200), proportional to the spherical harmonics  $Y_l^m$ , also describe stationary states of this spherically symmetric system. Represent the wavefunctions (3.200) of:

- (i) the ground state of the oscillator, and
- (ii) each of its lowest excited states,

<sup>166</sup> This condition ensures, in particular, that the above calculations of  $\langle x^2 \rangle$  are correct.

as linear combinations of products of the 1D oscillator's stationary wavefunctions. Also, calculate the degeneracy of the  $n^{\text{th}}$  energy level of the oscillator.

*Solutions:*

(i) The ground state of a system is always degenerate, and according to (3.125) of the lecture notes (with  $d = 3$ ), for the harmonic oscillator it is merely the product,

$$\psi_0(\mathbf{r}) = \psi_0(x)\psi_0(y)\psi_0(z),$$

of the ground-state wavefunctions  $\psi_0$  of three 1D Cartesian oscillators – see Eq. (2.275):

$$\psi_0(x) = C_0 \exp\left\{-\frac{x^2}{2x_0^2}\right\}, \quad \text{with } C_0 = \frac{1}{\pi^{1/4}x_0^{1/2}}, \quad x_0 \equiv \left(\frac{\hbar}{m\omega_0}\right)^{1/2}, \quad (*)$$

and similarly for the other two coordinates. So, we may rewrite  $\psi_0(\mathbf{r})$  in the form (3.200) with  $l = m = 0$ :

$$\psi_0(\mathbf{r}) = \mathcal{R}_{1,0}(r)Y_0^0(\theta, \varphi), \quad \text{with } Y_0^0 = \text{const}, \quad \text{and } \mathcal{R}_{1,0}(r) \propto \exp\left\{-\frac{m\omega_0 r^2}{2\hbar}\right\},$$

and verify, by the direct differentiation, that this radial function indeed satisfies Eq. (3.181) with  $l = 0$ ,  $U(r) = m\omega_0^2 r^2/2$ , and  $E = \hbar\omega_0/2$ .<sup>167</sup>

(ii) In the 1D oscillator language, the three lowest excited states of the 3D oscillator correspond to three possible combinations of the three indices  $n_j$  (see Eq. (3.124) of the lecture notes with  $d = 3$ ) with the lowest nonvanishing sum  $n \equiv n_x + n_y + n_z = 1$ :

$$\psi_{1x}(\mathbf{r}) \equiv \psi_1(x)\psi_0(y)\psi_0(z), \quad \psi_{1y}(\mathbf{r}) \equiv \psi_0(x)\psi_1(y)\psi_0(z), \quad \text{and } \psi_{1z}(\mathbf{r}) \equiv \psi_0(x)\psi_0(y)\psi_1(z). \quad (**)$$

Here the wavefunction  $\psi_1$  of the first excited state of a 1D oscillator may be calculated, for example, from Eq. (2.284) with  $n = 1$ , and the second of Eqs. (2.282):

$$\psi_1(x) = C_1 x \exp\left\{-\frac{x^2}{2x_0^2}\right\}, \quad \text{with } C_1 = \frac{2^{1/2}}{\pi^{1/4}x_0^{3/2}},$$

and similarly for two other coordinates. Using these relations and then expressing the Cartesian coordinates in the pre-exponential factors via the spherical coordinates, we may write

$$\psi_{1x}(\mathbf{r}) \pm i\psi_{1y}(\mathbf{r}) = C_1 C_0^2 (x \pm iy) \exp\left\{-\frac{m\omega_0 r^2}{2\hbar}\right\} = \text{const} \times \mathcal{R}_{2,1}(r) \sin\theta e^{\pm i\varphi},$$

$$\psi_{1z}(\mathbf{r}) = C_1 C_0^2 z \exp\left\{-\frac{m\omega_0 r^2}{2\hbar}\right\} = \text{const} \times \mathcal{R}_{2,1}(r) \cos\theta, \quad \text{with } \mathcal{R}_{2,1}(r) \propto r \exp\left\{-\frac{m\omega_0 r^2}{2\hbar}\right\}.$$

Comparing these expressions with Eqs. (3.175), we see that their angular parts are proportional, respectively, to the spherical harmonics  $Y_1^{\pm 1}(\theta, \varphi)$  and  $Y_1^0(\theta, \varphi)$ . Finally, it is straightforward to verify,

<sup>167</sup> The apparently unnatural increase of  $n$  by 1 in the first index of the radial functions reflects the difference in the conventions accepted for 1D harmonic oscillators (where the ground state is traditionally denoted with the quantum number  $n = 0$ ) and for the spherical-wavefunctions representation (3.200) – where it is convenient (and hence common) to start counting the principal quantum numbers  $n$  from 1.

by the direct differentiation, that the radial function  $\mathcal{R}_{2,1}(r)$  does satisfy Eq. (3.181), again with  $U(r) = m\omega_0^2 r^2/2$ , but now with  $l = 1$  and  $E = 5\hbar\omega_0/2$ . Thus, the stationary wavefunctions (3.200) with  $n = 2$ ,  $l = 1$ , and all three possible values  $m = \{-1, 0, +1\}$  may be indeed expressed as linear combinations of the Cartesian wavefunction products (\*\*).

Finally, the degeneracy  $g$  of the  $n^{\text{th}}$  energy level of the system, following from Eq. (3.124) of the lecture notes, with  $d = 3$ ,

$$E_n = \hbar\omega_0 \left( \frac{3}{2} + n \right),$$

equals to the number of different sets  $\{n_x, n_y, n_z\}$  of these non-negative quantum numbers, with the fixed sum  $n = n_x + n_y + n_z$ . In the usual combinatorics lingo, this is just the number of different ways to place  $n$  *indistinguishable* balls into three *distinct* boxes. According to MA Eq. (2.4), this number is

$$g = M_n^{(3)} = {}^{n+2}C_2 \equiv \frac{(n+2)!}{2!n!} \equiv \frac{(n+1)(n+2)}{2}.$$

In particular, for the ground state with  $n_x = n_y = n_z = 0$  and hence  $n = 0$ , this formula yields  $g = 1$ , while for the first excited state with  $n = 1$ , it gives  $g = 3$ , reflecting the wavefunctions spelled out above.

Note that this result for  $g$ , even after the necessary increase of  $n$  by 1 to compensate for the notation quantum number difference, differs from Eq. (3.204) of the lecture notes, which would give, in particular,  $g = 4$  for our  $n$  equal to 1. There is no contradiction here: the latter formula was derived and is valid only for the Coulomb potential (3.190), while the radial functions of the 3D harmonic oscillator, with  $n \equiv n_x + n_y + n_z \geq 1$ , have very different properties. For example, in our particular case  $n = 1$ , the radial equation (3.181) with  $U(r) = m\omega_0^2 r^2/2$  does *not* have a solution corresponding to a  $2s$ -state with  $l = 0$  and the same energy  $E = 5\hbar\omega_0/2$ .

**Problem 3.28.** A particle of mass  $m$  is placed into a spherical, flat-bottom potential well

$$U(\mathbf{r}) = \begin{cases} -U_0, & \text{for } r < R, \\ 0, & \text{for } R < r, \end{cases} \quad \text{with } U_0 > 0.$$

- (i) Calculate the smallest  $U_0$  at which the particle has a bound (localized) stationary state.
- (ii) Calculate the energy of this state if  $U_0$  is barely larger than that minimum value.
- (iii) Does such a localized state exist in a very narrow and deep well that may be described as  $U(\mathbf{r}) = -\mathcal{W}\delta(\mathbf{r})$  with a positive and finite  $\mathcal{W}$ ?

*Solution:* As was discussed in Sec. 3.6 of the lecture notes, the lowest eigenenergy (and hence the smallest possible value of  $U_0$ ) corresponds to the  $s$ -state, with  $l = 0$  and hence  $m = 0$ .<sup>168</sup> The functional form of its wavefunction inside the well may be calculated just as in the particle-inside-a-sphere problem discussed at the end of Sec. 3.6 of the lecture notes, besides the proper energy offset:

$$\psi = A \frac{\sin kr}{r}, \quad \text{with } \frac{\hbar^2 k^2}{2m} \equiv E - U(r) \equiv E + U_0, \quad \text{for } r \leq R.$$

<sup>168</sup> A more formal proof of this fact by using the Hellmann-Feynman theorem is one of the tasks of Problem 43.

The corresponding solution outside the well is formally the same (just with  $U(r) = 0$ ), but since the localized state's energy  $E$  cannot be positive, it is more adequately represented as

$$\psi = C \frac{\exp\{-\kappa r\}}{r}, \quad \text{with } \frac{\hbar^2 \kappa^2}{2m} \equiv -E > 0, \quad \text{for } r \geq R. \quad (*)$$

Writing the usual conditions of continuity of the wavefunction and its first derivative (or even easier, of the function  $f \equiv r\psi$ ) at  $r = R$ , we get two equations for the coefficients  $A$  and  $C$ :

$$A \sin kR = C e^{-\kappa R}, \quad Ak \cos kR = -C \kappa e^{-\kappa R}.$$

The equations are compatible if

$$\begin{vmatrix} \sin kR & -e^{-\kappa R} \\ k \cos kR & \kappa e^{-\kappa R} \end{vmatrix} = 0, \quad \text{i.e. if } k \cos kR = -\kappa \sin kR. \quad (**)$$

This characteristic equation contains answers to all the questions posed in the assignment.

(i) As  $U_0$  tends to its minimum value, the external wavefunction tends to become a delocalized one, i.e.  $\kappa \rightarrow 0$ . In this limit, Eq. (\*\*) becomes  $\cos kR = 0$ . The lowest value of  $k > 0$  that satisfies this equation is  $k_{\min} = \pi/2R$ . According to Eq. (\*), at  $U_0 \rightarrow (U_0)_{\min}$ , i.e. at  $\kappa \rightarrow 0$ , the eigenenergy  $E$  tends to zero, so the above definition of  $k$  yields<sup>169</sup>

$$(U_0)_{\min} = \frac{\hbar^2 k_{\min}^2}{2m} = \frac{\pi^2 \hbar^2}{8mR^2}. \quad (***)$$

It is instructive to compare this result for the localization threshold in the 3D case with the solutions of similar problems in 2D (Problem 22) and 1D (Problem 2.21): in contrast with the 3D case, at lower dimensionalities, there is *no* lower bound on  $U_0$  for the localization.<sup>170</sup>

(ii) If  $U_0$  is larger than, but very close to its minimal value,

$$U_0 = (U_0)_{\min} + \Delta U_0, \quad \text{with } 0 < \Delta U_0 \ll (U_0)_{\min},$$

the bound state does exist but its localization energy  $|E| = -E$  is small, and so is the parameter  $\kappa$ . In this limit, the characteristic equation (\*\*) may be solved approximately by taking  $k = k_{\min} + \Delta k$  with  $\Delta kR \ll 1$ , expanding both sides into the Taylor series in this small parameter, and keeping only the terms proportional to  $\Delta k$  and  $\kappa$ :

$$k \cos kR \approx k \left( \frac{\pi}{2} - kR \right) \equiv -k\Delta kR, \quad -\kappa \sin kR \approx -\kappa.$$

<sup>169</sup> A (very simple) additional exercise for the reader: use Eq. (\*\*) to prove that to have  $n$  spherically-symmetric ( $s$ -) states, the well's depth  $U_0$  has to be larger than  $U_n = (U_0)_{\min}(2n-1)^2$ .

<sup>170</sup> Historically, this difference had interesting implications for the development of the theory of superconductivity, where the weak phonon-mediated attraction between electrons (fermions) leads to their binding into Cooper pairs (i.e. effective bosons capable of the Bose-Einstein condensation) only because the Fermi-Dirac statistics confines them to a quasi-2D momentum layer at the Fermi surface – see, e.g., Chapter 3 in M. Tinkham, *Introduction to Superconductivity*, 2<sup>nd</sup> ed., McGraw-Hill, 1996.



The resulting equation is  $k\Delta kR = \kappa$ , i.e.  $(R/2)\Delta(k^2) = \kappa$ . With the above definitions of  $k$  and  $\kappa$ , and per Eq. (\*\*\*) , it gives the following relation between the corresponding energies:

$$\frac{R}{2} \frac{2m}{\hbar^2} \Delta(U_0 - |E|) = \frac{(2m|E|)^{1/2}}{\hbar}, \quad \text{i.e. } \Delta(U_0 - |E|) = \frac{4}{\pi} [(U_0)_{\min} |E|]^{1/2}.$$

At  $|E|/U_0 \rightarrow 0$ , the second term on the left-hand side of the last equation is negligible, so we, finally, get

$$|E| = \frac{\pi^2 (\Delta U_0)^2}{16 (U_0)_{\min}}.$$

(iii) In the delta-functional approximation  $U(\mathbf{r}) = -\mathcal{W}\delta(\mathbf{r})$ , we should take

$$\mathcal{W} = - \int_{r < R} U(r) d^3r = \frac{4\pi}{3} U_0 R^3,$$

so our result for  $(U_0)_{\min}$  may be rewritten as

$$\mathcal{W}_{\min} = \frac{\pi^3 \hbar^2}{6m} R. \quad (****)$$

We see that if  $R \rightarrow 0$ , then  $\mathcal{W}_{\min} \rightarrow 0$ , i.e. despite the limit (\*\*\*) , a well with a sufficiently small  $R$  has a localized state for *any* finite  $\mathcal{W}$ .

In this context: a thoughtful reader might be surprised by the fact that neither at this point nor anywhere else in this course, the localization properties of this 3D delta-functional potential,  $U(\mathbf{r}) = -\mathcal{W}\delta(\mathbf{r})$ , are discussed in more detail. The reason is that most of these properties are not universal: due to the (integrable) divergence of the wavefunctions of the type (\*) at  $r \rightarrow 0$ , its interaction with a short-range potential  $U(\mathbf{r})$  depends on the “internal design” of the potential, not only on its 3D integral,  $-\mathcal{W}$ . (A clear illustration of this fact is given by Eq. (\*\*\*\*): it shows that the state-localization ability of the flat-bottom potential well, even in the limit  $R \rightarrow 0$ , depends not only on  $\mathcal{W}$  but also on another parameter,  $R$ .) This is why properties of short-range interactions are frequently described by less natural but also less ambiguous models, for example

$$U(r) = 0, \quad \text{for } r > 0; \quad \left. \frac{df}{dr} \right|_{r \rightarrow 0} \rightarrow -\kappa_0 f,$$

where, as above,  $f(r) \equiv r\psi(r)$ , while  $\kappa_0$  is a given parameter. The ground ( $s$ -) state of this model is described by Eqs. (\*) with  $\kappa = \kappa_0$ , and hence with  $E = -\hbar^2 \kappa_0^2 / 2m$ .

**Problem 3.29.** A 3D particle of mass  $m$  is placed into a spherically symmetric potential well with  $-\infty < U(r) \leq U(\infty) = 0$ . Relate its ground-state energy to that of a 1D particle of the same mass, moving in the following potential well:

$$U'(x) = \begin{cases} U(x), & \text{for } x \geq 0, \\ +\infty, & \text{for } x \leq 0. \end{cases}$$

Use the found relation to:

(i) discuss the origin of the difference between the solutions of Task (i) of the previous problem and of Problem 2.21, and

(ii) calculate the energy spectrum of an electron moving over an impenetrable plane surface of a perfect conductor.

*Solution:* As was discussed in Sec. 3.6 of the lecture notes (and in the model solutions of several previous problems), the ground state of a spherically symmetric system is always an  $s$ -state, with the wavefunction

$$\psi(\mathbf{r}) = Y_0^0(\theta, \varphi) \mathcal{R}(r) \equiv \frac{1}{(4\pi)^{1/2}} \mathcal{R}(r)$$

corresponding to the orbital quantum numbers  $l = m = 0$ . In this case, Eq. (3.181) for the radial function is reduced to

$$-\frac{\hbar^2}{2mr^2} \frac{d}{dr} \left( r^2 \frac{d\mathcal{R}}{dr} \right) + U(r) \mathcal{R} = E \mathcal{R}. \quad (*)$$

At the beginning of Sec. 3.1, it was shown that in the particular case of a free particle, i.e.  $U(r) = 0$ , a similar equation (3.3) for the radially-symmetric wavefunction  $\psi(r)$  yields a 1D Schrödinger equation (also with  $U(r) = 0$ ) for the function  $f(r) \equiv r\psi(r)$ . Inspired by this fact, let us look for the solution of Eq. (\*) in the similar form

$$\mathcal{R}(r) = \frac{f(r)}{r}. \quad (**)$$

Indeed, this substitution, followed by the cancellation of the common factor  $1/r$ , yields:

$$-\frac{\hbar^2}{2m} \frac{d^2 f}{dr^2} + U(r) f = E f, \quad \text{for } r \geq 0. \quad (***)$$

Due to the condition  $U(r) \leq U(\infty) \equiv 0$ , the ground-state energy  $E$  corresponding to this equation has to be negative, so at large distances from the center, where  $U(r) \rightarrow 0$ , the ground-state wavefunction has to decay exponentially (see, e.g., the solution of the previous problem) and hence we have to require  $f(r) \equiv r\psi(r) \rightarrow 0$  at  $r \rightarrow \infty$ . On the other hand, to keep the wavefunction (\*\*) finite at  $r \rightarrow 0$ ,  $f(0)$  has to equal zero. But Eq. (\*\*\*) with these boundary conditions are exactly those satisfied by the ground-state wavefunction  $\psi(x)$  and the energy  $E$  of the 1D system mentioned in the assignment; hence the values of  $E$  of these 3D and 1D ground states are also equal. Moreover, this mapping may be extended to all antisymmetric eigenfunctions with  $\psi(-x) = -\psi(x)$  of this and other 1D problems, and enables one to reuse the solutions of some key 1D problems for the corresponding 3D spherically-symmetric problems, and vice versa – as an example, see (ii) below.

(i) Note, however, that this 3D  $\leftrightarrow$  1D mapping is valid only if the 1D potential at  $x < 0$  is positively-infinite, thus enforcing the boundary condition  $f(0) = 0$  on the 1D wavefunction. For example, the solutions of the apparently similar Problems 2.21 (1D) and 3.28 (3D), on the particle motion in a flat-bottom potential well of depth  $U_0$ , are radically different. As a reminder, in the 1D case, a localized ground state exists for an arbitrarily small  $U_0$ ,<sup>171</sup> while in the 3D case, there is a minimal value

$$(U_0)_{\min} = \frac{\pi^2 \hbar^2}{8mR^2}$$

<sup>171</sup> See also the solution of Problem 2.18 for a more general potential.

(where  $R$  is the well's radius) necessary for such localization. The reason for this difference is that (as the solution of Problem 2.21 shows) the 1D well's ground state wavefunction is symmetric, with  $f(0) \neq 0$ , and hence does not satisfy the 3D  $\leftrightarrow$  1D mapping condition  $\psi(0) = \lim_{r \rightarrow 0} [f(r)/r] < \infty$ .

(ii) An electron moving over the plane surface  $x = 0$  of a perfect conductor<sup>172</sup> but not penetrating into it, i.e. into the half-space  $x < 0$ , may be described by the following Hamiltonian:

$$\hat{H} \equiv -\frac{\hbar^2}{2m} \nabla^2 \psi - U(x), \quad \text{with } U(x) = \begin{cases} -(e^2 / 4\pi\epsilon_0) / 4x, & \text{for } x > 0, \\ +\infty, & \text{for } x < 0, \end{cases}$$

where the top line describes the Coulomb interaction between the electron and its positive charge image located at  $\mathbf{r}' = \{-x, y, z\}$ , where  $\mathbf{r} = \{x, y, z\}$  is the electron's position.<sup>173</sup> The corresponding stationary Schrödinger equation is satisfied with the product  $\psi(\mathbf{r}) = X(x)Y(y)Z(z)$ , where the components  $Y$  and  $Z$  describe the free motion of the electron along the surface and hence give continuous contributions (2.18) to the electron's energy spectrum:

$$E_y + E_z = \frac{\hbar^2}{2m_e} (k_y^2 + k_z^2)$$

On the other hand, the resulting equation for the function  $X(x)$  is similar to Eq. (\*\*\*) with the potential energy

$$U(r) = -\frac{e^2}{4\pi\epsilon_0(4r)},$$

that differs from that of the hydrogen atom's electron only by the additional factor  $1/4$ . As Eq. (3.192) shows, such an additional factor reduces the energy scale  $E_0$  by a factor of 16, so that we may immediately use Eq. (1.12) to write the following expression for the discrete  $x$ -contribution to the electron's spectrum:

$$E_x = -\frac{E_H}{32n^2}, \quad \text{with } n = 1, 2, 3, \dots$$

(As the analysis of the Coulomb potential problem in Sec. 3.7 has shown, all the radial factors  $\mathcal{R}_{n,l}(r)$  of the 3D wavefunctions in that problem are finite at  $r = 0$ , and hence the corresponding 1D wavefunctions  $X_{n,l}(x) = x\mathcal{R}_{n,l}(x)$  tend to zero at  $x \rightarrow 0$ , i.e. satisfy the boundary condition  $X(0) = 0$ .)

**Problem 3.30.** Calculate the smallest value of the parameter  $U_0$ , for which the following spherically symmetric potential well:

$$U(r) = -U_0 e^{-r/R}, \quad \text{with } U_0, R > 0,$$

has a bound (localized) eigenstate for a particle of mass  $m$ .

*Hint:* You may like to introduce the following new variables:  $f \equiv r\mathcal{R}$  and  $\xi \equiv Ce^{-r/2R}$ , with a proper constant  $C$ .

<sup>172</sup> Here the term "perfect conductor" means, most importantly, a conductor with a sufficiently high plasma frequency  $\omega_p \gg |E|/\hbar$  – see, e.g., the concluding discussion in the model solution of EM Problem 7.19.

<sup>173</sup> See, e.g., EM Sec. 2.9 and in particular Eq. (2.192).

*Solution:* For this potential, Eq. (3.181) of the lecture notes, with  $l=0$  (corresponding to the ground state of the system, which is always an  $s$ -state) and  $E=0$  (corresponding to the particle localization threshold), takes the form

$$-\frac{\hbar^2}{2mr^2} \frac{d}{dr} \left( r^2 \frac{d\mathcal{R}}{dr} \right) + U(r)\mathcal{R} = 0 .$$

Introducing the first replacement suggested in the *Hint*,  $\mathcal{R} \equiv fr$ ,<sup>174</sup> we get

$$-\frac{\hbar^2}{2m} \frac{d^2 f}{dr^2} + U(r)f = 0 . \quad (*)$$

Now using the second of the suggested replacements,  $\xi \equiv Ce^{-r/2R}$ , so  $d\xi = -(Ce^{-r/2R})dr/2R \equiv -\xi dr/2R$ , i.e.  $dr = -2Rd\xi/\xi$ , and our particular function  $U(r) = -U_0 e^{-r/R} \equiv -U_0 \xi^2/C^2$ , we see that if we choose  $C$  as

$$C \equiv \left( \frac{8mR^2 U_0}{\hbar^2} \right)^{1/2} , \quad (**)$$

Eq. (\*) reduces to

$$\frac{d}{d\xi} \left( \xi \frac{df}{d\xi} \right) + \xi f = 0, \quad \text{i.e.} \quad \frac{d^2 f}{d\xi^2} + \frac{1}{\xi} \frac{df}{d\xi} + f = 0 .$$

This is the canonical form of the Bessel equation of order  $\nu=0$ ,<sup>175</sup> and its only solution that is finite at  $\xi=0$  (i.e. at  $r \rightarrow \infty$ ) is the Bessel function  $J_0(\xi)$ , so our radial wavefunction (up to a constant multiplier) is

$$\mathcal{R} \equiv \frac{f}{r} = \frac{1}{r} J_0 \left( C e^{-r/2R} \right).$$

In order for this function to be finite at  $r \rightarrow 0$ , i.e. at  $Ce^{-r/2R} \rightarrow C$ , this constant has to coincide with one of the roots of the function  $J_0(\xi)$ . According to Eq. (\*\*), the smallest possible depth  $U_0$  of the potential well corresponds to the smallest  $C$ , i.e. to the smallest, first root  $\xi_{01} \approx 2.405$ ,<sup>176</sup> so we finally get

$$C_{\min} \equiv \left[ \frac{8mR^2 (U_0)_{\min}}{\hbar^2} \right]^{1/2} = \xi_{01}, \quad \text{i.e.} \quad (U_0)_{\min} = \frac{\xi_{01}^2 \hbar^2}{8mR^2} .$$

Comparing this result with the solutions of the two previous problems, we see that they differ only by the numerical constant:  $\pi^2 \approx 9.87 \leftrightarrow \xi_{01}^2 \approx 5.78$ . Hence in our current case of the exponential confining potential, its minimum depth necessary for particle localization is approximately twice smaller than that in the case of a flat-bottom potential well with the same radius  $R$ . (Of course, for the exponential potential well, the definition of its radius is to a certain extent conditional.)

**Problem 3.31.\*** A particle of mass  $m$  moves in the field of an attractive spherically symmetric potential  $U(r) \leq U(\infty) \equiv 0$ . Find a condition necessary for it to have at least one bound state. Compare the result with those of Problems 28 and 30.

<sup>174</sup> See also Sec. 3.1 of the lecture notes and the solutions of the two previous problems.

<sup>175</sup> See, e.g., EM Sec. 2.7, in particular, Eq. (2.130) with  $\nu=0$ .

<sup>176</sup> See, e.g., the top-left cell of EM Table 2.1.

*Hint:* You may like to use Eqs. (3.67) and (3.71).

*Solution:* Reviewing the calculation that has led to Eq. (3.67a), we may see that it is much more general than the scattering problem it was derived for. In particular, if we take  $\psi_1 = 0$ , this integral form of the Schrödinger equation is valid for any stationary state of a particle in the time-independent potential  $U(\mathbf{r})$ . Eq. (3.71) is also general, so by combining these two formulas we may write

$$\psi(\mathbf{r}) = -\frac{m}{2\pi\hbar^2} \int U(\mathbf{r}') \frac{\psi(\mathbf{r}')}{R} e^{ikR} d^3r', \quad \text{where } \mathbf{R} \equiv \mathbf{r} - \mathbf{r}'.$$

As was discussed in Sec. 3.6 of the lecture notes (and in the model solutions of several previous problems), the lowest-energy eigenstate of any spherically-symmetric system in an  $s$ -state, with

$$\psi(\mathbf{r}) = \psi(r). \quad (*)$$

Since all localized states must have  $E < 0$ , the last bound (localized) state to disappear at a gradual decrease of  $|U(r)|$  is its ground  $s$ -state. So for our task, we may consider only such states. For a spherically-symmetric potential  $U(r) \leq 0$  and the wavefunction (\*), the above equation becomes

$$\psi(r) = \frac{m}{2\pi\hbar^2} \int |U(r')| \frac{\psi(r')}{R} e^{ikR} d^3r'.$$

Let us select the wavefunction's phase so that  $\psi$  is real and positive at all points,<sup>177</sup> and apply this equation to the point  $\mathbf{r} = \mathbf{r}_0$  with the largest value of  $\psi$ :

$$\psi_{\max} \equiv \psi(r_0) = \frac{m}{2\pi\hbar^2} \int |U(r')| \frac{\psi(r')}{R} e^{ikR} d^3r', \quad \text{with } R = |\mathbf{r}_0 - \mathbf{r}'|$$

So far, this is an exact equality. Now let us turn it into an inequality by changing the right-hand part so that it may only increase. For that, first, let us replace  $\psi(r')$  with  $\psi_{\max}$ , and  $e^{ikR}$  with 1:

$$\psi_{\max} \leq \frac{m}{2\pi\hbar^2} \int |U(r')| \frac{\psi_{\max}}{R} d^3r', \quad \text{i.e. } 1 \leq \frac{m}{2\pi\hbar^2} \int |U(r')| \frac{d^3r'}{R} \equiv \frac{m}{2\pi\hbar^2} \int |U(r')| \frac{d^3r'}{|\mathbf{r}_0 - \mathbf{r}'|}. \quad (**)$$

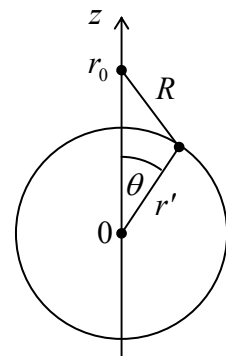
Next, let us spell the last integral:

$$\int |U(r')| \frac{d^3r'}{|\mathbf{r}_0 - \mathbf{r}'|} = \int_0^\infty |U(r')| r'^2 dr' \oint_{4\pi} \frac{d\Omega'}{|\mathbf{r}_0 - \mathbf{r}'|},$$

The internal integral may be directly calculated.<sup>178</sup> Indeed, directing the polar axis toward the point  $\mathbf{r}_0$  (see the figure on the right), we may use the axial symmetry to write

$$I \equiv \oint_{4\pi} \frac{d\Omega'}{|\mathbf{r}_0 - \mathbf{r}'|} = 2\pi \int_0^\pi \frac{\sin\theta d\theta}{(r_0^2 + r'^2 - 2r_0r'\cos\theta)^{1/2}} \equiv 2\pi \int_{-1}^{+1} \frac{d\xi}{(r_0^2 + r'^2 - 2r_0r'\xi)^{1/2}},$$

where  $\xi \equiv \cos\theta$ , and continue as



<sup>177</sup> As was discussed at the end of Sec. 2.9 and also in the model solution of Problem 2.46, the lowest-state 1D wavefunction  $\psi$  cannot have zeros, i.e. change its sign.

<sup>178</sup> This calculation may be used to prove the *mean value theorem* of electrostatics – see, e.g., EM Problem 1.11.

$$\begin{aligned}
 I &= -\frac{2\pi}{r_0 r'} \left( r_0^2 + r'^2 - 2r_0 r' \xi \right)^{1/2} \Big|_{\xi=-1}^{\xi=+1} = \frac{2\pi}{r_0 r'} \left[ \left( r_0^2 + r'^2 + 2r_0 r' \right)^{1/2} - \left( r_0^2 + r'^2 - 2r_0 r' \right)^{1/2} \right] \\
 &= \frac{2\pi}{r_0 r'} \left( r_0 + r' - |r_0 - r'| \right) = \frac{2\pi}{r_0 r'} \times \max[2r_0, 2r'] \equiv 4\pi \times \min \left[ \frac{1}{r_0}, \frac{1}{r'} \right].
 \end{aligned}$$

Hence  $I$  cannot decrease if we replace it with  $4\pi/r'$ . Making this replacement in Eq. (\*\*), we get the desired necessary condition on the confining potential  $U(r)$ :

$$1 \leq \frac{2m}{\hbar^2} \int_0^\infty |U(r')| r' dr', \quad \text{i.e.} \quad \int_0^\infty |U(r)| r dr \geq \frac{\hbar^2}{2m}. \quad (***)$$

For the case considered in Problem 28,

$$U(\mathbf{r}) = \begin{cases} -U_0, & \text{for } r < R, \\ 0, & \text{for } R < r, \end{cases}$$

this condition becomes

$$U_0 \frac{R^2}{2} \geq \frac{\hbar^2}{2m}, \quad \text{i.e.} \quad U_0 \geq \frac{\hbar^2}{mR^2},$$

while, as we have seen, the exact threshold for  $U_0$  is just a factor of  $\pi^2/8 \approx 1.23$  higher. On the other hand, for the case considered in Problem 30,  $U(r) = -U_0 e^{-r/R}$ , Eq. (\*\*\*) gives

$$U_0 R^2 \geq \frac{\hbar^2}{2m}, \quad \text{i.e.} \quad U_0 \geq \frac{\hbar^2}{2mR^2},$$

while the exact bound for  $U_0$  is a factor of  $\xi_{01}^2/4 \approx 1.44$  higher.

The reader should agree that these are very good results for the bound so general.

**Problem 3.32.** A particle of mass  $m$ , moving in a certain central potential  $U(r)$ , has a stationary state with the following wavefunction:

$$\psi = Ar^\alpha e^{-\beta r} \cos \theta,$$

where  $A$ ,  $\alpha$ , and  $\beta > 0$  are constants. Calculate:

- (i) the probabilities of all possible values of the quantum numbers  $l$  and  $m$ , and
- (ii) the confining potential and the state's energy.

*Solutions:*

(i) Comparing the angular part of the given wavefunction,  $\cos \theta$ , with the second line of Eq. (3.175) of the lecture notes, we may see that it coincides (to a constant multiplier) with the spherical harmonic  $Y_1^0$ , indicating that this is the state with  $l = 1$  and  $m = 0$ , so the probability of any other set of  $l$  and  $m$  is zero.

- (ii) Plugging the expression for the radial factor of the wavefunction,<sup>179</sup>

$$\mathcal{R}(r) = r^\alpha e^{-\beta r},$$

<sup>179</sup> Due to the linearity of the Schrödinger equation, the constant multiplier may be dropped for this calculation.

into Eq. (3.181) of the lecture notes, with the above-found value  $l = 1$ , and performing a straightforward differentiation, we get

$$U(r) = E + \frac{\hbar^2}{2m} \left[ \frac{\alpha^2 + \alpha - 2}{r^2} - \frac{2\beta(\alpha + 1)}{r} + \beta^2 \right].$$

Imposing the convenient (and common) condition  $U(\infty) = 0$ , we have to assign the  $r$ -independent term to the state's energy  $E$ , so, finally:

$$E = -\frac{\hbar^2 \beta^2}{2m}, \quad U(r) = \frac{\hbar^2}{2m} \left[ \frac{\alpha^2 + \alpha - 2}{r^2} - \frac{2\beta(\alpha + 1)}{r} \right].$$

As a sanity check, the radial function  $\mathcal{R}_{2,1}(r)$  given by the second of Eqs. (3.209) of the lecture notes, also corresponding to  $l = 1$  (and to  $n = 2$ ), is proportional to our current  $\mathcal{R}(r)$  for the particular value  $\alpha = 1$  (so  $\alpha^2 + \alpha - 2 = 0$ ); in this case, we recover the Coulomb potential (3.190) with  $C = 2\hbar^2\beta/m$ . With this value of  $C$ , the first of Eqs. (3.192) yields  $E_0 = 4\hbar^2\beta^2/m$ , so the above eigenenergy  $E$  is equal to  $-E_0/8$ , as it should be for  $n = 2$ , according to Eq. (3.201).

**Problem 3.33.** For an isotropic 3D harmonic oscillator, calculate:

- (i) the energy spectrum resulting from the Bohr quantization of circular classical orbits, and
- (ii) the energy spectrum of the  $s$ -states in the WKB approximation.

Compare the results with the exact energy spectrum of the oscillator, and comment.

*Solution:* As was discussed in Sec. 3.5 of the lecture notes, such an oscillator may be formed by a particle of mass  $m$ , moving in the spherically-symmetric potential  $U(r) = \kappa r^2/2$ . Its energy spectrum is given by Eq. (3.124) with  $d = 3$ :

$$E = \hbar\omega_0 \left( \frac{3}{2} + n_x + n_y + n_z \right) \quad \text{with } \omega_0 = \left( \frac{\kappa}{m} \right)^{1/2}, \quad n_j = 0, 1, 2, \dots \quad (*)$$

Our task is to compare this exact result with those following from the following two approximations.

- (i) For a circular orbit, The Bohr quantization rule,<sup>180</sup>

$$\oint \mathbf{p} \cdot d\mathbf{r} = 2\pi m\hbar, \quad \text{with } m = 1, 2, 3, \dots,$$

takes the simple form

$$(2\pi r p)_m = 2\pi m\hbar, \quad \text{i.e. } (rp)_m \equiv m(rv)_m = m\hbar.$$

The second relation for  $r$  and  $v$  is given by the 2<sup>nd</sup> Newton law

$$m \frac{v^2}{r} = -F,$$

where  $F = -dU/dr$  is the radial force, for our potential equal to  $-\kappa r$ . From here,

<sup>180</sup> Here the integer number is denoted  $m$  because of its (loose) analogy to the angular quantum number used in the 2D problems (see, e.g., Eq. (3.128) and on) and to distinguish it clearly from the radial quantum number to be used in the next task.

$$mv^2 = \kappa r^2, \quad \text{i.e. } v = \left(\frac{\kappa}{m}\right)^{1/2} r \equiv \omega_0 r, \quad rv = \omega_0 r^2,$$

and the Bohr quantization yields

$$m\omega_0 r_m^2 = m\hbar, \quad \text{i.e. } r_m^2 = \frac{m\hbar}{m\omega_0} \equiv \frac{m\hbar\omega_0}{\kappa},$$

and hence

$$E_m = \left(\frac{mv^2}{2} + \frac{\kappa r^2}{2}\right)_m = \kappa r_m^2 = \hbar\omega_0 m, \quad \text{i.e. } \frac{E_m}{\hbar\omega_0} = 1, 2, 3, \dots$$

(iii) Wavefunctions of the  $s$ -states can depend only on the radial coordinate  $r$ , and hence they obey Eq. (3.181a) with  $l = 0$ :

$$-\frac{\hbar^2}{2mr^2} \frac{d}{dr} \left( r^2 \frac{d\psi}{dr} \right) + U(r)\psi = E\psi.$$

By introducing, as we repeatedly did in this chapter (see especially Problem 29), the function  $f(r) \equiv r\psi(r)$ , we may reduce this equation to the standard 1D Schrödinger form:

$$-\frac{\hbar^2}{2m} \frac{d^2 f}{dr^2} + U(r)f = Ef.$$

For it, the WKB approximation in the classically allowed region with  $E > U(r)$  has the standard form (2.94) with the notation replacements  $\psi \rightarrow f$ ,  $x \rightarrow r$ . Since we are interested only in stationary states, whose wavefunctions may be always represented by real functions, we may rewrite that expression as

$$f_{\text{WKB}}(r) = \frac{c}{k^{1/2}(r)} \sin \left( \int_0^r k(r') dr' + \varphi \right), \quad \text{with } k^2(r) \equiv \frac{2m}{\hbar^2} [E - U(r)] > 0. \quad (**)$$

If the function  $U(r)$  satisfied the validity condition (2.107) of the connection formulas (2.105) at both classical turning points where  $U(r_c) = E$ , we would not even need this expression but could directly use the Wilson-Sommerfeld quantization rule (2.110) – also with the replacement  $x \rightarrow r$ . However, in our 3D case, we have the special point  $r = 0$  where the exact function  $f(r)$  has to turn to zero in order to avoid the divergence of the wavefunction  $\psi = f(r)/r$ . The only way to fit such a function with Eq. (\*\*) valid for  $r > 0$  is to take  $\varphi = 0$ , so at  $r \rightarrow 0$  where  $U \rightarrow 0$  and hence  $k \rightarrow k_0 \equiv (2mE)^{1/2}/\hbar = \text{const}$ , we get  $f_{\text{WKB}} \rightarrow ck_0^{1/2} r \rightarrow 0$ , and  $\psi_{\text{WKB}} \rightarrow ck_0^{1/2} = \text{const}$ .<sup>181</sup> This choice of  $\varphi$  is equivalent to saying that our effective 1D de Broglie wave  $f(r)$  is reflected from the point  $r = 0$  as from a hard infinite potential wall, i.e. to replacing the last term  $\pi/2$  in Eq. (2.109) with 0. With this replacement, we get the following quantization rule:

$$2 \int_0^{r_c} k(r) dr + \frac{\pi}{2} = 2\pi n, \quad \text{with } n = 1, 2, 3, \dots,$$

where  $r_c > 0$  is the regular classical turning point. For our potential  $U(r) = \kappa r^2/2$ , it is  $r_c = (2E/\kappa)^{1/2}$ , and the above integral is the same as was worked out in Sec. 2.4 at a similar calculation for a 1D oscillator – see Eq. (2.113):

<sup>181</sup> Indeed, as Eq. (3.187) and the first of Eqs. (3.186) show, in the case  $U(r) = 0$ , this wavefunction is *exact*.



$$\int_0^{r_c} k(r) dr = \frac{(2mE)^{1/2}}{\hbar} \int_0^{r_c} \left[1 - \frac{U(r)}{E}\right]^{1/2} dr = \frac{(2mE)^{1/2}}{\hbar} \int_0^{r_c} \left(1 - \frac{r^2}{r_c^2}\right)^{1/2} dr = \frac{(2mE)^{1/2}}{\hbar} \frac{\pi}{4} r_c = \frac{\pi}{2} \frac{E}{\hbar\omega_0}.$$

so the quantization rule yields

$$E_n = \hbar\omega_0(2n - 1/2), \quad \text{i.e. } \frac{E_n}{\hbar\omega_0} = \frac{3}{2}, \frac{7}{2}, \frac{11}{2}, \frac{15}{2}, \dots \quad (***)$$

The results of Tasks (i) and (ii) show that in contrast to the 1D harmonic oscillator (see Eq. (2.114) of the lecture notes), the 3D oscillator cannot be exactly and fully described by simple WKB-based approximate methods. In particular, the Bohr quantization of the particle's *angular* motion, while giving the correct energy level interval

$$\Delta E \equiv E_{m+1} - E_m = \hbar\omega_0,$$

fails to describe the genuine ground-state energy  $E_g = (3/2)\hbar\omega_0$ , giving a value 50% lower. In this sense, N. Bohr's success with the quantitative explanation of the hydrogen atom's spectrum by using this approach (see Sec. 1.1(iii) again) was a bit of luck – for him and for physics as a whole.

On the other hand, the WKB approximation applied to the particle's *radial* motion gives the correct ground state energy but cannot describe the full energy spectrum (\*). This is natural because this approximation (in the used form) is only applicable to the spherically symmetric *s*-states, i.e. the states with the angular quantum number  $l = 0$ , while Eq. (\*) describes states with higher values of  $l$  as well – see, e.g., the solution of Problem 27.

In this context, Eq. (\*\*\*) has an aspect that may look, at first glance, puzzling. Namely, while correctly describing the energy of the ground state, whose wavefunction may be represented as the product of symmetric wavefunctions of 1D ground states:<sup>182</sup>

$$\psi_g(\mathbf{r}) = \psi_{000}(\mathbf{r}) \equiv \psi_0(x)\psi_0(y)\psi_0(z), \quad \text{with } \psi_0(-\xi) = \psi_0(\xi),$$

it obviously cannot describe similar products with any one operand being a different 1D eigenfunction, even if this function is symmetric, for example

$$\psi_{200}(\mathbf{r}) \equiv \psi_2(x)\psi_0(y)\psi_0(z),$$

because it would not remain its value at a swap of some coordinates (say, of  $x$  and  $y$ ) – the symmetry requirement necessary for any *s*-state. Hence one might think that the lowest excited *s*-state covered by Eq. (\*\*\*) should be

$$\psi_{222}(\mathbf{r}) \equiv \psi_2(x)\psi_2(y)\psi_2(z),$$

because the function  $\psi_2$  is symmetric just like  $\psi_0$  – see, e.g., Fig. 2.35. According to Eq. (\*), the energy of this state is  $\hbar\omega_0(3/2 + 2 + 2 + 2) \equiv (15/2)\hbar\omega_0$ . This value is indeed listed in Eq. (\*\*\*), but there are two other energies separating it from  $E_g$ ; what are the corresponding *s*-states?

The answer becomes simple if we recall one of the basic principles of wave mechanics (and indeed of quantum mechanics as a whole), the linear superposition principle: if a few functions are eigenfunctions of some eigenproblem, any of their linear superpositions is also its eigenfunction.

<sup>182</sup> See Eq. (3.125) of the lecture notes.

Moreover, if all these eigenfunctions correspond to one energy, their superposition has the same energy. In particular, in our problem, the function

$$\psi = \frac{1}{\sqrt{3}}(\psi_{200} + \psi_{020} + \psi_{002}),$$

is an eigenfunction of the oscillator, and simultaneously is an  $s$ -state, with the eigenenergy equal to  $\hbar\omega_0(3/2 + 2 + 0 + 0) \equiv (7/2)\hbar\omega_0$ , giving the explanation of the second-lowest value in the list (\*\*\*) . Similar state identifications may be performed for all other values of that list – the additional task left for the reader’s exercise.

Hence, for the  $s$ -states of the isotropic 3D oscillator, the radial WKB approximation works as perfectly as for all states of its 1D cousin.

**Problem 3.34.** For a particle of mass  $m$ , moving in the spherically symmetric potential  $U(\mathbf{r}) = ar^4$ :

- (i) use the variational method to estimate the ground-state energy,
- (ii) calculate the energy spectrum resulting from the Bohr quantization of circular orbits, and
- (iii) calculate the energy spectrum of the  $s$ -states in the WKB approximation.

Compare the results and comment.

*Solutions:*

(i) As was discussed in Sec. 3.6 of the lecture notes, for a motion in any spherically symmetric potential, the ground state is always an  $s$ -state, with a spherically symmetric wavefunction  $\psi(r)$ . Since, in addition, our confining potential is continuous everywhere, including the origin  $r = 0$ , the most natural simple trial function is the 3D Gaussian

$$\psi_{\text{trial}} = C \exp\left\{-\frac{\lambda^2}{4}r^2\right\},$$

with some real  $\lambda$ . (Indeed, as was shown in Sec. 2.9 of the lecture notes, such a trial function of  $x$  gives the exact value of the ground state energy  $\hbar\omega_0/2$  of a 1D harmonic oscillator, so the 3D function we are trying now, which is just a product of three similar functions of  $x$ ,  $y$ , and  $z$ , also gives the exact result  $E_g = E_g = (3/2)\hbar\omega_0$  for the isotropic 3D harmonic oscillator explored in the previous problem.) Calculating the constant  $C$  (or rather its modulus) from the normalization requirement,

$$\int \psi_{\text{trial}}^*(r)\psi_{\text{trial}}(r)d^3r = 1,$$

we get

$$\begin{aligned} |C|^{-2} &= \int \exp\left\{-\frac{\lambda^2}{2}r^2\right\}d^3r \equiv \int \exp\left\{-\frac{\lambda^2}{2}(x^2 + y^2 + z^2)\right\}dxdydz = \left(\int_{-\infty}^{+\infty} \exp\left\{-\frac{\lambda^2}{2}x^2\right\}dx\right)^3 \\ &\equiv \left(\frac{2^{1/2}}{\lambda} \int_{-\infty}^{+\infty} \exp\{-\xi^2\}d\xi\right)^3 = \left(\frac{2^{1/2}}{\lambda} \pi^{1/2}\right)^3 \equiv \frac{(2\pi)^{3/2}}{\lambda^3}. \end{aligned}$$

Now we can calculate the expectation value of the system’s Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + U(\mathbf{r}) = -\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d}{dr} \right) + ar^4$$

(in the last expression, the angular part of the Laplace operator is dropped due to the spherical symmetry of the trial state), for our trial function:

$$\begin{aligned} \langle H \rangle_{\text{trial}} &= \int \psi_{\text{trial}}^*(r) \hat{H} \psi_{\text{trial}}(r) d^3r \\ &= 4\pi |C|^2 \int_0^\infty \exp\left\{-\frac{\lambda^2}{4} r^2\right\} \left[ -\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d}{dr} \right) + ar^4 \right] \exp\left\{-\frac{\lambda^2}{4} r^2\right\} r^2 dr \\ &= 4\pi \frac{\lambda^3}{(2\pi)^{3/2}} \int_0^\infty \left[ -\frac{\hbar^2}{2m} \frac{\lambda^2}{2} \left( \frac{\lambda^2 r^2}{2} - 3 \right) + ar^4 \right] \exp\left\{-\frac{\lambda^2}{2} r^2\right\} r^2 dr \\ &\equiv 4\pi \frac{\lambda^3}{(2\pi)^{3/2}} \times \left[ \frac{3\hbar^2 \lambda^2}{4m} \left( \frac{2^{1/2}}{\lambda} \right)^3 \int_0^\infty \xi^2 e^{-\xi^2} d\xi - \frac{\hbar^2 \lambda^4}{8m} \left( \frac{2^{1/2}}{\lambda} \right)^5 \int_0^\infty \xi^4 e^{-\xi^2} d\xi + a \left( \frac{2^{1/2}}{\lambda} \right)^7 \int_0^\infty \xi^6 e^{-\xi^2} d\xi \right]. \end{aligned}$$

All these three integrals belong to the same Gaussian family,<sup>183</sup> and the final result is

$$\begin{aligned} \langle H \rangle_{\text{trial}} &= 4\pi \frac{\lambda^3}{(2\pi)^{3/2}} \left[ \frac{3\hbar^2 \lambda^2}{4m} \left( \frac{2^{1/2}}{\lambda} \right)^3 \frac{\pi^{1/2}}{4} - \frac{\hbar^2 \lambda^4}{8m} \left( \frac{2^{1/2}}{\lambda} \right)^5 \frac{3\pi^{1/2}}{8} + a \left( \frac{2^{1/2}}{\lambda} \right)^7 \frac{15\pi^{1/2}}{16} \right] \\ &\equiv \frac{3\hbar^2}{8m} \lambda^2 + \frac{15a}{\lambda^4}. \end{aligned}$$

This is a smooth function of  $\lambda^2$ , diverging at both very small and very large values of this argument, and hence having just one minimum between them. This minimum may be found from the usual requirement

$$\left. \frac{\partial \langle H \rangle_{\text{trial}}}{\partial (\lambda^2)} \right|_{\lambda=\lambda_{\text{opt}}} \equiv \left( \frac{3\hbar^2}{8m} - \frac{30a}{\lambda^6} \right) \Big|_{\lambda=\lambda_{\text{opt}}} = 0,$$

so we get

$$\lambda_{\text{opt}} = \left( \frac{80ma}{\hbar^2} \right)^{1/6}, \quad E_{\text{var}} \equiv \langle H \rangle_{\text{trial}} \Big|_{\lambda=\lambda_{\text{opt}}} = \frac{9}{8} \left( \frac{10\hbar^4 a}{m^2} \right)^{1/3} \approx 2.424 \left( \frac{\hbar^4 a}{m^2} \right)^{1/3}. \quad (*)$$

The ground state energy, naturally, grows with the potential's magnitude parameter  $a$ , i.e. with the confinement of the wavefunction becoming more tough.

(ii) Performing the same calculation as in Task (i) of the previous problem (for the spherical harmonic oscillator) but now for the potential  $U = ar^4$ , with  $F = -dU/dr = -4ar^3$ , we get,

$$\frac{mv^2}{r} = 4ar^3, \quad \text{i.e. } mrv = 2(ma)^{1/2} r^3,$$

and the Bohr quantization condition  $m(rv)_m = m\hbar$  yields

$$r_m = \left[ \frac{m\hbar}{2(ma)^{1/2}} \right]^{1/3} \quad \text{and} \quad E_m = \left( \frac{mv^2}{2} + ar^4 \right)_m = 3ar_m^4 = 3 \left( \frac{\hbar^4 a}{16m^2} \right)^{1/3} m^{4/3}.$$

<sup>183</sup> See, e.g., MA Eqs. (6.9).

For the ground state with  $m = 1$ , this formula gives the result

$$E_g = 3 \left( \frac{\hbar^4 a}{16 m^2} \right)^{1/3} \approx 1.191 \left( \frac{\hbar^4 a}{m^2} \right)^{1/3}, \quad (**)$$

which is functionally similar but numerically lower than the estimate (\*).

(iii) Since in the limit  $r \rightarrow 0$ , our potential  $U = ar^4$  behaves qualitatively similar to the  $U = \kappa r^2/2$  explored in Task (ii) of the previous problem, in particular giving  $U \rightarrow 0$  and hence  $k \rightarrow k_0 \equiv (2mE)^{1/2}/\hbar = \text{const}$ , we may follow that solution by using the similarly modified quantization rule

$$2 \int_0^{r_c} k(r) dr + \frac{\pi}{2} = 2\pi n, \quad \text{with } n = 1, 2, 3, \dots, \quad (***)$$

where  $r_c > 0$  is the regular classical turning point. For our current potential  $U(r) = ar^4$ , it is  $r_c = (E/a)^{1/4}$ , and the above integral is

$$\int_0^{r_c} k(r) dr = \frac{(2mE)^{1/2}}{\hbar} \int_0^{r_c} \left[ 1 - \frac{U(r)}{E} \right]^{1/2} dr = \frac{(2mE)^{1/2}}{\hbar} \int_0^{r_c} \left( 1 - \frac{r^4}{r_c^4} \right)^{1/2} dr \equiv \frac{(2mE)^{1/2} r_c}{\hbar} I \equiv \frac{(2mE)^{1/2} (E/a)^{1/4}}{\hbar} I,$$

where<sup>184</sup>

$$I \equiv \int_0^1 (1 - \xi^4)^{1/2} d\xi = \frac{\sqrt{2}\pi^{3/2}}{6[\Gamma(3/4)]^2} \approx 0.87402,$$

and Eq. (\*\*\*) becomes

$$I \frac{(2m)^{1/2}}{\hbar a^{1/4}} E_n^{3/4} = \pi(n - 1/4), \quad \text{i.e. } E_n = \left( \frac{\pi}{\sqrt{2}I} \right)^{4/3} \left( \frac{\hbar^4 a}{m^2} \right)^{1/3} (n - 1/4)^{4/3}.$$

For the ground state with  $n = 1$ , this formula yields

$$E_g = \left( \frac{3}{4} \frac{\pi}{\sqrt{2}I} \right)^{4/3} \left( \frac{\hbar^4 a}{m^2} \right)^{1/3} \approx 2.364 \left( \frac{\hbar^4 a}{m^2} \right)^{1/3}. \quad (***)$$

Now let us compare and discuss the results. First of all, all three methods give the same functional dependence of the ground state energy on the problem's parameters  $m$  and  $a$  and the Planck constant  $\hbar$ . This is barely surprising because  $(\hbar^4 a/m^2)^{1/3}$  is the only possible combination of these parameters with the dimensionality of energy. At the same time, all three methods give substantially different results for the numerical constant before this combination. There is not much surprise here because all these methods are approximate.

In particular, the variational method's results depend on the chosen trial functions, and encouragingly, in our case, it gave the highest value of  $E_g$ . (As a reminder, such a value is always higher than the genuine ground state energy.) On the contrary, the Bohr quantization of circular orbits gave the lowest value (\*) of all three, but as we have seen in the previous problem, it underestimates  $E_g$  significantly in the harmonic oscillator as well. Of course, the quantization rules based on the WKB approximation guarantee asymptotically correct results only for high values of the corresponding

<sup>184</sup> Since this integral is just a numerical coefficient, evidently close to 1, let me skip the derivation of its value to avoid unnecessary math distraction.

quantum numbers, but note that the two WKB-based formulas have different numerical factors even in this limit:

$$E_m \rightarrow 3 \left( \frac{\hbar^4 a}{16m^2} \right)^{1/3} m^{4/3} \approx 1.191 \left( \frac{\hbar^4 a}{m^2} \right)^{1/3} m^{4/3}, \quad E_n \rightarrow \left( \frac{\pi}{\sqrt{2}I} \right)^{4/3} \left( \frac{\hbar^4 a}{m^2} \right)^{1/3} n^{4/3} \approx 3.469 \left( \frac{\hbar^4 a}{m^2} \right)^{1/3} n^{4/3}.$$

That is true for the 3D harmonic oscillator as well – see the previous problem’s solution. This is one more reminder of the fact that in an arbitrary spherically symmetric potential, the energy levels may depend differently on the radial and angular quantum numbers, so their high degeneracy in the Coulomb potential case is a rare exception rather than the general rule.

**Problem 3.35.** For a particle of mass  $m$ , moving in the attracting Coulomb potential  $U(r) = -C/r$  (e.g., the electron in a hydrogen atom):

- (i) estimate the ground-state energy by using the trial wavefunction  $\psi_{\text{trial}} = A/(r+a)^b$ , where both  $a > 0$  and  $b > 1$  are fitting parameters, and
- (ii) calculate the energy spectrum of the  $s$ -states in the WKB approximation.

Compare the results with the exact energy spectrum of the atom.

*Solution:*

- (i) Due to the spherical symmetry of the trial wavefunction, in the system’s Hamiltonian,

$$\hat{H} = \frac{\hat{p}^2}{2m} - \frac{C}{r} \equiv -\frac{\hbar^2}{2m} \nabla^2 - \frac{C}{r}, \quad \text{where } C \equiv \frac{e^2}{4\pi\epsilon_0},$$

we may keep only the radial part of the Laplace operator:

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d}{dr} \right) - \frac{C}{r},$$

so the expectation value of energy in the trial state is

$$\begin{aligned} \langle H \rangle_{\text{trial}} &\equiv \int \psi_{\text{trial}}^*(\mathbf{r}) \hat{H} \psi_{\text{trial}}(\mathbf{r}) d^3r = 4\pi |A|^2 \int_0^\infty r^2 dr (r+a)^{-b} \left[ -\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d}{dr} \right) - \frac{C}{r} \right] (r+a)^{-b} \\ &= 4\pi |A|^2 \int_0^\infty \left\{ \frac{\hbar^2 b}{2m} \left[ 2r(r+a)^{-2b-1} - (b+1)r^2(r+a)^{-2b-2} \right] - C(r+a)^{-2b} r \right\} dr \\ &\equiv 4\pi |A|^2 \times \left\{ \begin{aligned} &\frac{\hbar^2 b}{2m} \left[ 2 \left( \int_a^\infty r'^{-2b} dr' - a \int_a^\infty r'^{-2b-1} dr' \right) - (b+1) \left( \int_a^\infty r'^{-2b} dr' - 2a \int_a^\infty r'^{-2b-1} dr' + a^2 \int_a^\infty r'^{-2b-2} dr' \right) \right] \\ &- C \left( \int_a^\infty r'^{-2b+1} dr' - a \int_a^\infty r'^{-2b} dr' \right) \end{aligned} \right\}, \end{aligned}$$

where  $r' \equiv r+a$ , so  $r = r' - a$ . Per the given conditions  $a > 0$  and  $b > 1$ , all these integrals converge at both limits, with zero contributions from the upper of them, giving

$$\begin{aligned} \langle H \rangle_{\text{trial}} &= 4\pi |A|^2 \times \left\{ \frac{\hbar^2 b}{2ma^{2b-1}} \left[ 2 \left( \frac{1}{2b-1} - \frac{1}{2b} \right) - (b+1) \left( \frac{1}{2b-1} - \frac{1}{b} + \frac{1}{2b+1} \right) \right] \right. \\ &\quad \left. - \frac{C}{a^{2b-2}} \left( \frac{1}{2b-2} - \frac{1}{2b-1} \right) \right\} \quad (*) \\ &\equiv 4\pi |A|^2 \left[ \frac{\hbar^2 b}{2ma^{2b-1}(2b-1)(2b+1)} - \frac{C}{2a^{2b-2}(b-1)(2b-1)} \right]. \end{aligned}$$

The calculation of the normalization coefficient  $A$  is similar and less bulky:

$$\begin{aligned} 1 &= \int \psi_{\text{trial}}^*(\mathbf{r}) \psi_{\text{trial}}(\mathbf{r}) d^3 r = 4\pi |A|^2 \int_0^\infty (r+a)^{-2b} r^2 dr = 4\pi |A|^2 \int_a^\infty r'^{-2b} (r'-a)^2 dr' \\ &\equiv 4\pi |A|^2 \left( \int_a^\infty r'^{-2b+2} dr' - 2a \int_a^\infty r'^{-2b+1} dr' + a^2 \int_a^\infty r'^{-2b} dr' \right) = \frac{4\pi |A|^2}{a^{2b-3}(b-1)(2b-1)(2b-3)}. \end{aligned}$$

Plugging the resulting expression for  $|A|^2$  into Eq. (\*), we get

$$\langle H \rangle_{\text{trial}} = \frac{\hbar^2 b(b-1)(2b-3)}{2ma^2(2b+1)} - \frac{C(2b-3)}{2a}.$$

Now let us optimize this expression, starting with the parameter  $a$ . Since for  $b > 1$ , all parentheses in it are positive,  $\langle H \rangle_{\text{trial}}$  this is a smooth function of  $a > 0$ , going from  $+\infty$  at  $a \rightarrow 0$  to  $-\infty$  at  $a \rightarrow \infty$ , and thus having just one (negative) minimum, which may be calculated from the condition

$$\frac{\partial \langle H \rangle_{\text{trial}}}{\partial a} \Big|_{a=a_{\text{opt}}} = 0, \quad \text{i.e.} \quad -\frac{\hbar^2 b(b-1)(2b-3)}{ma_{\text{opt}}^3(2b+1)} + \frac{C(2b-3)}{2a_{\text{opt}}^2} = 0.$$

This simple equation yields

$$a_{\text{opt}} = \frac{2b(b-1)}{2b+1} r_0, \quad \min_a \langle H \rangle_{\text{trial}} = -\frac{(2b-3)(2b+1)}{8b(b-1)} E_0,$$

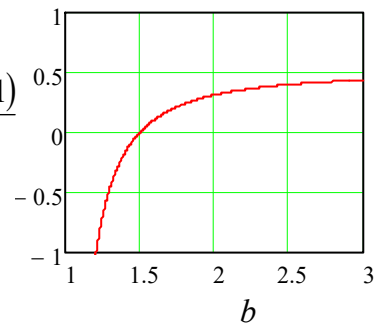
where  $r_0 \equiv \hbar^2/mC$ , and  $E_0 \equiv \hbar^2/mr_0^2 \equiv m(C/\hbar)^2$  – see Eqs. (3.192) of the lecture notes.

For the optimization over  $b$ , we may notice that within the possible range of this parameter,  $1 < b < \infty$ , the fraction in the last displayed expression always grows with  $b$  (see the figure on the right), approaching  $\frac{1}{2}$  asymptotically at  $b \rightarrow \infty$ . In this limit, the expectation value approaches the exact ground state energy:

$$\min_{a,b} \langle H \rangle_{\text{trial}} = -\frac{1}{2} E_0$$

– cf. Eq. (3.201) with  $n = 1$ . (Note that in this limit,  $a_{\text{opt}}/r_0 \rightarrow b \rightarrow \infty$ .)

The fact that a good fitting requires the power in the expression for  $\psi_{\text{trial}}$  to tend to infinity should not be surprising because, in this limit, the trial function tends to the genuine, exponential



ground-state wavefunction – see Eq. (3.208) of the lecture notes.<sup>185</sup> What is indeed counter-intuitive is that the fitting by an apparently different function enables finding the exact value of the ground-state energy. This fact demonstrates the power of the variational method with more than one fitting parameter – at the cost of longer calculations.

(ii) For finding the  $s$ -state spectrum, we may try to follow the approach used in the two previous problems but run into a complication: for the Coulomb potential, at  $r \rightarrow 0$ , the difference  $E - U(r)$  tends to  $C/r \rightarrow \infty$  rather than to a constant, so the effective wave vector  $k(r) \propto [E - U(r)]^{1/2}$  diverges as  $r^{-1/2}$ , and the WKB approximation for the effective 1D wavefunction  $f(r) \equiv r\psi(r)$ ,

$$f_{\text{WKB}}(r) = \frac{C}{k^{1/2}(r)} \sin \left( \int_0^r k(r') dr' + \varphi \right),$$

converges too slowly (even with the best phase choice  $\varphi = 0$ ) to prevent the divergence of the 3D wavefunction itself:

$$f_{\text{WKB}}(r) \rightarrow \text{const} \times \frac{1}{k^{1/2}(r)} \int_0^r k(r') dr' \propto r^{1/4} \int_0^r \frac{dr'}{r'^{1/2}} \propto r^{3/4}, \quad \text{so } \psi_{\text{WKB}}(r) \equiv \frac{f_{\text{WKB}}(r)}{r} \propto r^{-1/4} \rightarrow \infty.$$

As a result, we have to write the quantization condition in a somewhat less certain form

$$2\pi n = \Delta\varphi_{\text{total}} = 2 \int_0^{r_c} k(r) dr + \frac{\pi}{2} + \varphi_0, \quad \text{with } n = 1, 2, 3, \dots, \quad (*)$$

where the classical turning point  $r_c$  is defined by the relation  $E - U(r_c) \equiv E + C/r_c = 0$ , giving  $r_c = -C/E \equiv C/|E|$ , and  $\varphi_0$  is some constant having the sense of the de Broglie wave's phase shift at its reflection from the point  $r_{\text{min}} = 0$ . (From what we know about such reflections from the cases discussed in the lecture notes and the solutions of earlier problems, we may expect  $\varphi_0$  to be negative and to have a magnitude of the order of 1.) Now calculating the involved integral<sup>186</sup>

$$\begin{aligned} \int_0^{r_c} k(r) dr &= \frac{1}{\hbar} \int_0^{r_c} p_r(r) dr = \frac{1}{\hbar} \int_0^{r_c} \left[ 2m \left( E + \frac{C}{r} \right) \right]^{1/2} dr = \frac{(2m|E|)^{1/2}}{\hbar} \int_0^{r_c} \left( \frac{r_{\text{max}}}{r} - 1 \right)^{1/2} dr \\ &\equiv \frac{(2m|E|)^{1/2}}{\hbar} r_c \int_0^1 \left( \frac{1}{\xi} - 1 \right)^{1/2} d\xi = \frac{(2m|E|)^{1/2}}{\hbar} r_c \frac{\pi}{2} \equiv \frac{\pi C}{\hbar} \left( \frac{m}{2|E|} \right)^{1/2} \end{aligned}$$

and dividing all terms of Eq. (\*) by  $2\pi$ , we obtain

$$n - \frac{1}{4} - \frac{\varphi_0}{2\pi} = \frac{C}{\hbar} \left( \frac{m}{2|E|} \right)^{1/2} \equiv \left( \frac{E_0}{2|E|} \right)^{1/2},$$

where  $E_0 \equiv m(C/\hbar)^2$  – see Eq. (3.191). This relation gives us the following energy spectrum of the  $s$ -states:

$$E_n = -|E| = -\frac{E_0}{2(n - 1/4 - \varphi_0/2\pi)^2}. \quad (**)$$

<sup>185</sup> As MA Eq. (1.2a) with  $n = br_0/r$  shows, at  $a = r_0b$  and  $b \rightarrow \infty$ ,  $\psi_{\text{trial}}(r)/\psi_{\text{trial}}(0) = (1 + r/r_0b)^{-b} \rightarrow \exp\{-r/r_0\}$ .

<sup>186</sup> The resulting dimensionless integral may be readily worked out, for example, by the substitution  $\xi \equiv \sin^2\alpha$ .

Regardless of the finite constant  $\varphi_0$ , the values  $E_n$  rapidly approach the exact result (3.201) (valid for all states including the  $s$ - ones) at  $n \gg 1$ , i.e. in the only limit when we may expect the WKB approximation to be quantitatively correct.

Summarizing the results of both tasks, we see that the Coulomb potential is really a lucky one. Indeed, first, its ground state energy may be correctly calculated using even a trial wavefunction that looks different from the genuine one. Second, despite the formal divergence of the radial WKB approximation at  $r \rightarrow 0$ , it still gives the energy spectrum that is asymptotically correct at large values of the principal quantum number  $n$ . Finally, let us not forget that the Bohr quantization rule for circular classical orbits gives an exact result for any  $n$  – see Eqs. (1.9)-(1.12) of the lecture notes; in this unique case, with no difference between the radial and angular quantum numbers.

**Problem 3.36.** Calculate the energy spectrum of a particle moving in a monotonic but otherwise arbitrary spherically symmetric attractive potential  $U(r) < 0$ , in the approximation of very large orbital quantum numbers  $l$ . Formulate the quantitative condition(s) of validity of your theory. Check that for the Coulomb potential  $U(r) = -C/r$ , your result agrees with Eq. (3.201) of the lecture notes.

*Hint:* Try to solve Eq. (3.181) of the lecture notes approximately by introducing the same new function  $f(r) \equiv r\mathcal{R}(r)$  that was already used in Sec. 3.1 of the lecture notes and in the solutions of a few earlier problems.

*Solution:* The suggested substitution,

$$\mathcal{R}(r) \equiv \frac{f(r)}{r},$$

reduces Eq. (3.181) to 1D Schrödinger equation

$$-\frac{\hbar^2}{2m} \frac{d^2 f}{dr^2} + U_{\text{ef}}(r)f = Ef, \quad (*)$$

with the following effective potential energy:

$$U_{\text{ef}}(r) \equiv U(r) + \frac{\hbar^2 l(l+1)}{2mr^2}.$$

This is the same potential that participates in the classical theory of orbital (“planetary”) motion,<sup>187</sup> besides that the square of the angular momentum is replaced with its quantum value (3.178):

$$L^2 = \hbar^2 l(l+1).$$

The classical theory of the orbital motion gives us a hint of how our current problem may be solved. Indeed, if the magnitude of the attractive potential  $U(r) < 0$  does not grow too fast (faster than  $1/r^2$ ) at  $r \rightarrow 0$ , then the effective potential has a minimum at a certain radius  $r_0$ , determined by the condition

$$\left. \frac{dU_{\text{ef}}(r)}{dr} \right|_{r=r_0} \equiv \left. \frac{dU(r)}{dr} \right|_{r=r_0} - \frac{\hbar^2 l(l+1)}{mr_0^3} = 0. \quad (**)$$

<sup>187</sup> See, e.g., CM Secs. 3.4-3.5, in particular Eq. (3.44).



In the classical limit,  $r_0$  is the radius of a circular orbit of the particle, at which the attractive force  $F = -dU/dr$  provides exactly the necessary centripetal acceleration  $\omega^2 r = (L/mr^2)^2 r \equiv (L^2/mr^3)/m$ , so  $r$  does not change in time, i.e. the radial component of its momentum,  $p_r \equiv mv_r = mdr/dt$ , equals zero. On the other hand, in quantum mechanics, according to the Heisenberg principle,  $r$  and  $p_r$  cannot be exactly fixed simultaneously, so the radial motion has to be quantized.

Let us assume that this quantization does not prevent the particle's energy  $E$  from being close to the effective potential energy's minimum,

$$[U_{\text{ef}}(r)]_{\text{min}} = U_{\text{ef}}(r_0) = U(r_0) + \frac{\hbar^2 l(l+1)}{2mr_0^2}.$$

Then the motion takes place at  $r \approx r_0$ , and we may replace the genuine effective potential with its Taylor expansion near the minimum:

$$U_{\text{ef}}(r) \approx U_{\text{ef}}(r_0) + \frac{\kappa}{2}(r - r_0)^2, \quad \text{with } \kappa \equiv \left. \frac{d^2 U_{\text{ef}}(r)}{dr^2} \right|_{r=r_0} = \left. \frac{d^2 U(r)}{dr^2} \right|_{r=r_0} + \frac{3\hbar^2 l(l+1)}{mr_0^4}. \quad (***)$$

In this approximation, Eq. (\*) describes the usual 1D harmonic oscillator with frequency

$$\omega_0 = \left( \frac{\kappa}{m} \right)^{1/2} = \left[ \frac{1}{m} \left. \frac{d^2 U(r)}{dr^2} \right|_{r=r_0} + \frac{3\hbar^2 l(l+1)}{m^2 r_0^4} \right]^{1/2},$$

whose energy spectrum is given by Eq. (2.262),  $E_r = \hbar\omega_0(n_r + 1/2)$ , with  $n_r = 0, 1, 2, \dots$ . As a result, the total energy of the system becomes

$$E = U_{\text{ef}}(r_0) + \hbar\omega_0 \left( n_r + \frac{1}{2} \right) \equiv U(r_0) + \frac{\hbar^2 l(l+1)}{2mr_0^2} + \hbar\omega_0 \left( n_r + \frac{1}{2} \right).$$

The validity of this result is determined by that of the approximation (\*\*\*). If the potential  $U(r)$  is sufficiently smooth, the approximation is valid if the radial spread  $\delta r$  of the wavefunction is much smaller than  $r_0$ . As we know from Sec. 2.9 of the lecture notes, the spread may be estimated as

$$\delta r \sim \left[ \frac{\hbar}{m\omega_0} (2n_r + 1) \right]^{1/2}.$$

Since, according to Eq. (\*\*),  $r_0$  grows with  $l$  faster than  $\delta r \propto \omega_0^{-1/2}$ , this theory works well for large values of  $l$  and not very high values of  $n_r$ , though the exact condition depends on the particular function  $U(r)$ .

For the Coulomb potential,  $U(r) = -C/r$ , the above general relations yield

$$U_{\text{ef}}(r) = -\frac{C}{r} + \frac{\hbar^2 l(l+1)}{2mr^2}, \quad \frac{C}{r_0^2} - \frac{\hbar^2 l(l+1)}{mr_0^3} = 0, \quad \text{i.e. } r_0 = \frac{\hbar^2 l(l+1)}{mC},$$

$$U_{\text{ef}}(r_0) = -\frac{C^2 m}{2\hbar^2 l(l+1)}, \quad \hbar\omega_0 = \hbar \left[ -\frac{2C}{mr_0^3} + \frac{3\hbar^2 l(l+1)}{m^2 r_0^4} \right]^{1/2} = \frac{C^2 m}{\hbar^2 [l(l+1)]^{3/2}},$$

and the calculated energy spectrum is

$$E = -\frac{1}{2} m \left( \frac{C}{\hbar} \right)^2 \left\{ \frac{1}{l(l+1)} - \frac{2n_r + 1}{[l(l+1)]^{3/2}} \right\}.$$

For  $l \gg 1$ , the expression in the figure brackets may be Taylor-expanded in the small parameter  $1/l$ , giving

$$\frac{1}{l(l+1)} - \frac{2n_r + 1}{[l(l+1)]^{3/2}} \equiv \frac{1}{l^2} \frac{(1+1/l)^{1/2} - 2n_r/l - 1/l}{(1+1/l)^{3/2}} \approx \frac{1}{l^2} \left( 1 - \frac{2n_r}{l} - \frac{2}{l} \right).$$

These leading terms of the expansion coincide with the similar expansion of the exact formula for this bracket,  $1/n^2$  (see Eq. (3.201) of the lecture notes), provided that we take

$$n = l + n_r + 1. \quad (****)$$

Indeed, for small  $1/l$  and  $n_r/l$ ,

$$\frac{1}{n^2} \equiv \frac{1}{(l + n_r + 1)^2} \equiv \frac{1}{l^2} \frac{1}{(1 + n_r/l + 1/l)^2} \approx \frac{1}{l^2} \left( 1 - \frac{2n_r}{l} - \frac{2}{l} \right).$$

So, for the Coulomb potential, the approximate theory gives the result coinciding with the exact one at  $l \gg n_r, 1$ . Note also that the above calculation gave us, as a byproduct, a very interesting formula (\*\*\*\*) which sheds a new light on the remarkable  $l$ -degeneracy of the hydrogen atom's energy spectrum. Namely, a decrease of the background energy  $U_{\text{el}}(r_0)$  due to a decrease of the orbital number  $l$  by one is exactly equal and opposite to the addition  $\hbar\omega_0$  to the energy of the radial motion, due to an increase of the radial quantum number  $n_r$  by one, so the total energy  $E$  does not change.<sup>188</sup> The above general expression for  $E$  shows clearly that this exact compensation is a "mathematical accident", and is violated for even a small deviation of the attractive potential  $U(r)$  from the Coulomb law, thus lifting the  $l$ -degeneracy. As was discussed in Sec. 3.7 of the lecture notes, this is exactly what happens in the atoms of heavier elements, due to radius-dependent shielding of the positive potential of their nuclei by the negative electric charge of other electrons.

**Problem 3.37.** Prove Eq. (3.210) and the first two of Eqs. (3.211) of the lecture notes for the ground state of a hydrogen-like atom/ion.

*Solution:* According to Eqs. (3.190), (3.174) and (3.198), the ground state's wavefunction is

$$\psi_{1,0,0} = Y_0^0(\theta, \varphi) \mathcal{R}_{1,0}(r) = \frac{1}{(4\pi)^{1/2}} \frac{2}{r_0^{3/2}} e^{-r/r_0},$$

so the expectation value of observable  $r^k$  (with any integer  $k \geq -2$ ) in this state may be calculated as

$$\langle r^k \rangle \equiv \int \psi_{1,0,0}^* r^k \psi_{1,0,0} d^3r = \int_0^\infty |R_{1,0}(r)|^2 r^{k+2} dr = \frac{4}{r_0^3} \int_0^\infty e^{-2r/r_0} r^{k+2} dr = \frac{4}{r_0^3} \left( \frac{r_0}{2} \right)^{k+3} \int_0^\infty e^{-\xi} \xi^{k+2} d\xi,$$

<sup>188</sup> Graphically, we may consider this compensation as a trade-off of the number of "wiggles" (and hence zeros) of the radial and angular wavefunctions, at the same  $n$ , and hence the same total energy of the system. Rather amazingly, in this form, the exact compensation takes place even at lower values of  $l$ , where the radial functions differ rather substantially from those of the harmonic oscillator – please have one more look at Fig. 3.22 of the lecture notes.

where  $\xi \equiv r/(r_0/2)$ . The last integral is a table one,<sup>189</sup> equal to  $(k+2)!$ , so, finally,

$$\langle r^k \rangle = \frac{(k+2)!}{2} \left( \frac{r_0}{2} \right)^k, \quad \text{for } k \geq -2.$$

For the particular case  $k = 0$ , this general result just confirms that the wavefunction is correctly normalized:

$$\langle r^0 \rangle \equiv \int \psi_{1,0,0}^* r \psi_{1,0,0} d^3r = \frac{(0+2)!}{2} \left( \frac{r_0}{2} \right)^0 = 1,$$

while for  $k = +1$ ,  $k = -1$ , and  $k = -2$  it yields the following formulas:

$$\begin{aligned} \langle r \rangle &\equiv \langle r^1 \rangle = \frac{(1+2)!}{2} \left( \frac{r_0}{2} \right)^1 = \frac{3}{2} r_0, \\ \left\langle \frac{1}{r} \right\rangle &\equiv \langle r^{-1} \rangle = \frac{(-1+2)!}{2} \left( \frac{r_0}{2} \right)^{-1} = \frac{1}{r_0}, \quad \left\langle \frac{1}{r^2} \right\rangle \equiv \langle r^{-2} \rangle = \frac{(-2+2)!}{2} \left( \frac{r_0}{2} \right)^{-2} = \frac{2}{r_0^2}, \end{aligned}$$

which coincide, respectively, with Eq. (3.210) and the first two of Eqs. (3.211) taken for  $n = 1$  and  $l = 0$ .

**Problem 3.38.** For the ground state of a particle in the Coulomb potential (3.190), calculate the probability of finding it farther from the attracting center than the radius the same particle with the same energy would have on a classical circular orbit.

*Solution:* As was discussed in Sec. 3.7 of the lecture notes, the ground state's wavefunction (corresponding to quantum numbers  $n = 1$  and  $l = m = 0$ ) is given by the product of the angular function (3.174) and the radial function (3.208) :

$$Y_0^0(\theta, \varphi) = \frac{1}{(4\pi)^{1/2}}, \quad \mathcal{R}_{1,0}(r) = \frac{2}{r_0^{3/2}} e^{-r/r_0}. \quad (*)$$

Both functions are normalized as defined, respectively, by Eqs. (3.73) and (3.194), so for our problem, which does not involve angular coordinates, the requested probability may be calculated merely as

$$W_{r>r_c} = \int_{r_c}^{\infty} |\mathcal{R}_{1,0}(r)|^2 r^2 dr = \frac{4}{r_0^3} \int_{r_c}^{\infty} e^{-2r/r_0} r^2 dr = 4 \int_{r_c/r_0}^{\infty} e^{-2\xi} \xi^2 d\xi,$$

where  $r_c$  is the radius of the classical orbit. This integral may be readily worked out by parts, giving

$$W_{r>r_c} = \left[ 2 \left( \frac{r_c}{r_0} \right)^2 + 2 \frac{r_c}{r_0} + 1 \right] \exp \left\{ -\frac{2r_c}{r_0} \right\}. \quad (**)$$

What remains is to calculate the ratio  $r_c/r_0$  from the given condition of equal energies of the quantum and classical states. For the quantum state (\*), the energy is given by Eqs. (3.201) with  $n = 1$ :

$$E_q = E_1 = -\frac{m}{2} \left( \frac{C}{\hbar} \right)^2,$$

<sup>189</sup> See, e.g., MA Eq. (6.7d).

where  $C$  is the coefficient in the Coulomb potential (3.190):  $U(r) = -C/r$ . In classical mechanics, this potential energy corresponds to an attractive central force of magnitude  $F = C/r^2$ , so that the 2<sup>nd</sup> Newton law for the circular orbit of radius  $r_c$  is

$$m \frac{v^2}{r_c} = \frac{C}{r_c^2},$$

where  $v$  is the particle's velocity. From here,  $mv^2 = C/r_c$ , so the full classical energy of the particle is

$$E_c = T + U = \frac{mv^2}{2} - \frac{C}{r_c} = \frac{C}{2r_c} - \frac{C}{r_c} \equiv -\frac{C}{2r_c}.$$

Now requiring that  $E_c = E_q$ , we get

$$r_c = \frac{\hbar^2}{mC}.$$

But this is exactly the expression (3.192) for the constant  $r_0$ . Thus, for our problem,  $r_c/r_0 = 1$ , and Eq. (\*\*\*) yields

$$W_{r>r_c} = 5e^{-2} \approx 0.6767.$$

**Problem 3.39.** For the ground state and the lowest excited states of the hydrogen atom:

- (i) calculate the spatial distribution of the electric current flowing around the nucleus,
- (ii) evaluate its highest density, and
- (iii) calculate and evaluate its magnetic field at the position of the nucleus.

*Solutions:*

(i) The density  $\mathbf{j}_e$  of the electric current created by the single electron of the hydrogen atom is  $q\mathbf{j} = -e\mathbf{j}$ , where  $\mathbf{j}$  is its probability current density. According to Eq. (1.49) of the lecture notes, if its state's wavefunction is represented as  $|\psi| \exp\{i\phi\}$ ,<sup>190</sup> then

$$\mathbf{j} = \frac{\hbar}{m_e} |\psi|^2 \nabla \phi, \quad \text{i.e. } \mathbf{j}_e = -\frac{e\hbar}{m_e} |\psi|^2 \nabla \phi. \quad (*)$$

As was discussed in Sec. 3.7 of the lecture notes, the ground state of the hydrogen atom is described by the wavefunction

$$(\psi_{n,l,m})_g = \psi_{1,0,0} = \mathcal{R}_{1,0}(r) Y_0^0(\theta, \varphi),$$

where according to Eqs. (3.147) and (3.208), both operands may be taken in purely real forms. Hence, according to Eq. (\*), in this state,  $\mathbf{j}_e = 0$ . (The fact that any of these functions may be multiplied by  $\exp\{i\phi\}$  with any space-independent real phase  $\phi$ , i.e. with  $\nabla\phi = 0$ , does not affect this conclusion.)

The same result is valid for two of the four lowest excited states: the  $2s$ -state (with  $n = 2$ ,  $l = 0$ , and  $m = 0$ ) and one of the three  $2p$ -states (that with  $n = 2$ ,  $l = 1$ , and  $m = 0$ ), which have the same quantum number  $n = 2$  and hence have the same energy  $E_n = -E_H/8$ .<sup>191</sup> Indeed, their wavefunctions

<sup>190</sup> I am using a different notation than in Eq. (1.49) for the wavefunction's phase  $\phi \equiv \arg \psi$  to distinguish it from the azimuthal angle's notation  $\varphi$  used in Secs. 3.5-3.8.

<sup>191</sup> Actually, besides the very small *fine-structure effects* – see Sec. 6.3 and, in particular, Eq. (6.60) and Fig. 6.4.

$$\psi_{2,0,0} = \mathcal{R}_{2,0}(r)Y_0^0(\theta, \varphi) \quad \text{and} \quad \psi_{2,1,0} = \mathcal{R}_{2,1}(r)Y_1^0(\theta, \varphi)$$

may be also made real – see the same Eq. (3.147), the middle of Eqs. (3.175), and the first of Eqs. (3.209).

However, the other two  $2p$ -states (with  $n = 2$ ,  $l = 1$ , and  $m = \pm 1$ ) do have spatial gradients of their wavefunction phases; according to the top and bottom of Eqs. (3.175) and the second of Eq. (3.209) with  $r_0 = r_B$ :

$$\psi_{2,1,\pm 1} = \mathcal{R}_{2,1}(r)Y_1^{\pm 1}(\theta, \varphi) = \frac{1}{(2r_B)^{3/2}} \frac{r}{3^{1/2}r_B} e^{-r/2r_B} \times \left(\frac{3}{8\pi}\right)^{1/2} \sin\theta e^{\pm i\varphi},$$

i.e. their phases  $\phi$  are equal to  $\pm\varphi$ . As vector calculus shows,<sup>192</sup> the gradients of these functions are  $\pm \mathbf{n}_\varphi / r \sin\theta$ , so for these states, Eq. (\*) gives

$$\mathbf{j}_e = \mp \frac{e\hbar}{m_e} \left[ \frac{1}{(2r_B)^{3/2}} \frac{r}{3^{1/2}r_B} e^{-r/2r_B} \times \left(\frac{3}{8\pi}\right)^{1/2} \sin\theta \right]^2 \frac{\mathbf{n}_\varphi}{r \sin\theta} \equiv \mp \frac{e\hbar}{64\pi m_e r_B^5} r e^{-r/r_B} \sin\theta \mathbf{n}_\varphi.$$

This expression may be rewritten in a more physically transparent form

$$\mathbf{j}_e = \mp \frac{1}{32} \frac{I_0}{r_B^2} \frac{r}{r_B} e^{-r/r_B} \sin\theta \mathbf{n}_\varphi, \quad \text{where} \quad I_0 \equiv \frac{e\hbar}{2\pi m_e r_B^2} \equiv \frac{eE_H}{2\pi\hbar}, \quad (**)$$

where the final step used the last of Eqs. (1.13b). Here  $I_0 \approx 1.054$  mA is the natural scale of the electron current; it may be represented as the current  $I_0 = ef_0$  that would be carried by a classical electron rotating around the nucleus with the cyclic frequency  $f_0 = E_H/2\pi\hbar \approx 6.58 \times 10^{15}$  Hz – which is the natural scale of the frequencies related to interstate quantum transitions in the atom.<sup>193</sup> Note a quite macroscopic value of this current – it is not much lower than the currents driving your earbuds to play some deafening music!

Note that Eq. (\*\*) is only valid for the excited  $2p$ -states represented in their traditional form (3.175). (As will be discussed in Sec. 5.6, in this form, they are also the eigenstates of the operator of the angular momentum component  $L_z$ .) Since these states, in the absence of external fields, have the same energy, we may use the linear superposition principle to claim that the state with any wavefunction of the type

$$\psi_e \equiv c_+ \psi_{2,1,1} + c_0 \psi_{2,1,0} + c_- \psi_{2,1,-1}$$

is also the lowest excited state of the atom. The current density in such a state is given by Eq. (\*\*) multiplied by the additional factor  $(|c_+|^2 - |c_-|^2)$ . In particular, in the frequent case when the atom is excited by an agent not carrying any angular momentum (e.g., a linearly-polarized light), the states with the opposite signs of  $m$  have equal probabilities, and the excited state carries no current.

(ii) The value of the largest current density (reached at  $r = r_B$  and  $\theta = \pi/2$ ) is even more impressive than that of the full current:

<sup>192</sup> See, e.g., MA Eq. (10.8).

<sup>193</sup> Note that a similar expression for  $I_0$ , just with the replacement  $r_B \rightarrow R$ , was already discussed in Sec. 3.5 of the lecture notes in the context of a planar rotor of radius  $R$ .

$$(j_e)_{\max} = \frac{\exp\{-1\} I_0}{32 r_B^2} \approx 4.33 \times 10^{15} \frac{\text{A}}{\text{m}^2};$$

a current with such density, driven through a macroscopic sample of any material, would vaporize it instantly.

(iii) Due to the axial symmetry of the current distribution (\*\*), its magnetic field is directed along the  $z$ -axis, so its magnitude may be calculated as a scalar sum of the contributions from all elementary circular currents  $dI = j_e d^2r = j_e r dr d\theta$ . According to basic magnetostatics,<sup>194</sup> this contribution is

$$d\mathcal{B} = \frac{\mu_0}{2} \frac{\rho^2}{(\rho^2 + z^2)^{3/2}} dI = \frac{\mu_0}{2} \frac{\sin^2 \theta}{r} dI,$$

so that the total field produced by a  $2p$  state with  $m = \pm 1$  is

$$\mathcal{B} = \frac{\mu_0}{2} \int_0^\infty r dr \int_0^\pi d\theta \frac{\sin^2 \theta}{r} j_e = \mp \frac{\mu_0 I_0}{64 r_B} \int_0^\infty \xi e^{-\xi} d\xi \int_0^\pi \sin^3 \theta d\theta = \mp \frac{1}{48} \frac{\mu_0 I_0}{r_B}; \quad |\mathcal{B}| \approx 0.521 \text{ T}.$$

Note that the scale

$$\frac{\mu_0 I_0}{r_B} \equiv \frac{\mu_0}{2\pi} \frac{e\hbar}{m_e r_B^3} \equiv \frac{\mu_0}{2\pi} \frac{e\hbar}{m_e} \left( \frac{e^2 / 4\pi\epsilon_0}{\hbar^2 / m_e} \right)^3$$

of this field is typical for all magnetic fields in atoms and condensed magnetic matter (e.g., permanent magnets), and hence explains why a-few-tesla fields may be readily produced in the lab.<sup>195</sup>

**Problem 3.40.** An electron had been in the ground state of a hydrogen-like atom/ion with nuclear charge  $Ze$  when the charge suddenly changed to  $(Z + 1)e$ .<sup>196</sup> Calculate the probabilities for the electron of the changed system to be:

- (i) in its ground state, and
- (ii) in one of the lowest excited states.

*Solutions:* According to Eqs. (3.174), (3.200), and (3.208) of the lecture notes, the electron's wavefunction before the nuclear change was

$$\psi_g(\mathbf{r}) = \left( \frac{1}{4\pi} \right)^{1/2} \frac{2}{r_0^{3/2}} e^{-r/r_0} = \left( \frac{1}{4\pi} \right)^{1/2} \frac{2Z^{3/2}}{r_B^{3/2}} e^{-Zr/r_B}, \quad (*)$$

where  $r_0$  is given by the second of Eqs. (3.192) with  $m = m_e$  and the Coulomb interaction constant  $C = Ze^2/4\pi\epsilon_0$ :

<sup>194</sup> See, e.g., EM Eq. (5.23) with  $R = \rho = r \sin \theta$  and  $z = r \cos \theta$ .

<sup>195</sup> Electron spin effects yield magnetic fields of the same order of magnitude – see Chapters 4-6 of the lecture notes.

<sup>196</sup> Such a fast change happens, for example, at the beta-decay when one of the nucleus' neutrons spontaneously turns into a proton, emitting a high-energy electron and a neutrino, which leave the system very fast (instantly on the atomic time scale), and do not affect directly the atom transition's dynamics.

$$r_0 = \frac{\hbar^2}{m_e C} = \frac{4\pi\epsilon_0 \hbar^2}{m_e Z e^2} \equiv \frac{r_B}{Z},$$

where  $r_B$  is the Bohr radius – see Eq. (1.10).

(i) The ground state wavefunction  $\psi_g'(\mathbf{r})$  after the change of  $Z$  is given by the same formula (\*), but with the replacement

$$r_0 \rightarrow r_0' \equiv \frac{r_B}{Z+1}. \quad (**)$$

According to Eq. (1.68), the probability  $W_g$  for the electron to be in the ground state of the new ion is determined by the wavefunction overlap integral

$$\begin{aligned} c_g &= \int \psi_g'^*(\mathbf{r}) \psi_g(\mathbf{r}) d^3r = \frac{4Z^{3/2}(Z+1)^{3/2}}{r_B^3} \int_0^\infty \exp\left\{-r\left(\frac{Z}{r_B} + \frac{Z+1}{r_B}\right)\right\} r^2 dr \\ &\equiv \frac{4Z^{3/2}(Z+1)^{3/2}}{(2Z+1)^3} \int_0^\infty \xi^2 e^{-\xi} d\xi, \end{aligned}$$

where  $\xi \equiv (2Z+1)r/r_B$ . This is a well-known integral<sup>197</sup> equal to  $2! \equiv 2$ , so, finally,

$$c_g = \frac{8Z^{3/2}(Z+1)^{3/2}}{(2Z+1)^3}, \quad \text{and} \quad W_g \equiv |c_g|^2 = \frac{2^6 Z^3 (Z+1)^3}{(2Z+1)^6}.$$

(ii) Due to the spherical symmetry of the initial wavefunction (\*), of the four lowest excited states (all with  $n=2$ , but with either  $l=0$  and  $m=0$ , or with  $l=1$  and  $m=0, \pm 1$ ), it has a nonvanishing overlap integral only with the  $s$ -state (with  $l=0$ ). Its wavefunction is given by Eqs. (3.174), (3.200), and the first of Eqs. (3.209) of the lecture notes, again with the replacement (\*\*):

$$\psi_e(\mathbf{r}) = \left(\frac{1}{4\pi}\right)^{1/2} \frac{1}{(2r_0')^{3/2}} \left(2 - \frac{r}{r_0'}\right) e^{-r/2r_0'} = \left(\frac{1}{4\pi}\right)^{1/2} \frac{(Z+1)^{3/2}}{(2r_B)^{3/2}} \left[2 - \frac{(Z+1)r}{r_B}\right] e^{-(Z+1)r/2r_B},$$

so the overlap integral is

$$\begin{aligned} c_e &= \int \psi_g'^*(\mathbf{r}) \psi_e(\mathbf{r}) d^3r = \frac{2Z^{3/2}(Z+1)^{3/2}}{2^{3/2} r_B^3} \int_0^\infty \left[2 - \frac{(Z+1)r}{r_B}\right] \exp\left\{-r\left(\frac{Z}{r_B} + \frac{Z+1}{2r_B}\right)\right\} r^2 dr \\ &\equiv 2^{5/2} \frac{Z^{3/2}(Z+1)^{3/2}}{(3Z+1)^3} \left[2 \int_0^\infty \xi^2 e^{-\xi} d\xi - \frac{2(Z+1)}{3Z+1} \int_0^\infty \xi^3 e^{-\xi} d\xi\right], \end{aligned}$$

where now  $\xi \equiv (3Z+1)r/2r_B$ . The first integral is the same as the one in the first task and equals 2, while the second one is of the same type, but with  $n=3$ , and equals  $3! \equiv 6$ , so

$$c_e = 2^{5/2} \frac{Z^{3/2}(Z+1)^{3/2}}{(3Z+1)^3} \left(2 \cdot 2 - \frac{2(Z+1)}{3Z+1} \cdot 6\right) \equiv -2^{11/2} \frac{Z^{3/2}(Z+1)^{3/2}}{(3Z+1)^4}, \quad W_e \equiv |c_e|^2 = 2^{11} \frac{Z^3(Z+1)^3}{(3Z+1)^8}.$$

<sup>197</sup> See, e.g., MA Eq. (6.7d) with  $n=2$ .

The above results show that if  $Z$  is low, then the probabilities  $W_g$  and  $W_e$  are comparable; for example for  $Z = 1$ ,<sup>198</sup>  $W_g = 2^9/3^6 \approx 0.702$ , while  $W_e = 1/4 = 0.25$ .<sup>199</sup> However, in the limit  $Z \gg 1$ , the probability  $W_g$  of staying in the ground state becomes close to 100%:

$$W_g = \frac{(1+1/Z)^3}{(1+1/2Z)^6} \approx \frac{1+3/Z+3/Z^2}{1+6/2Z+15/2Z^2} \approx 1 - \frac{9}{2Z^2} \equiv 1 - \frac{4.5}{Z^2} \rightarrow 1,$$

while the probability of the atom's excitation is small; in particular, for the lowest excited state

$$W_e = 2^{11} \frac{Z^3(Z+1)^3}{(3Z+1)^8} \approx \frac{2^{11}}{3^8 Z^2} \approx \frac{0.312}{Z^2} \rightarrow 0.$$

This is very natural, because on the scale of  $Z \gg 1$ , the change  $\Delta Z = 1$  is relatively very small.

**Problem 3.41.** Due to a very short pulse of an external force, the nucleus of a hydrogen-like atom/ion, initially at rest in its ground state, starts moving with velocity  $\mathbf{v}$ . Calculate the probability  $W_g$  that the atom remains in its ground state. Evaluate the energy to be given, by the pulse, to a hydrogen atom in order to reduce  $W_g$  to 50%.

*Solution:* Repeating the argumentation used in the model solution of Problem 2.42, we may use the Galilean transform

$$\Psi'(\mathbf{r}', t') = \Psi(\mathbf{r}, t) \exp\left\{-i \frac{m\mathbf{v} \cdot \mathbf{r}}{\hbar} + i \frac{mv^2 t}{2\hbar}\right\},$$

whose proof was the subject of Problem 1.6, to conclude that immediately after the application of the force pulse (say, at  $t = +0$ ), its wavefunction, in the reference frame moving with the atom, is

$$\psi_{+0}(\mathbf{r}) = \psi_{-0}(\mathbf{r}) \exp\left\{-i \frac{m\mathbf{v} \cdot \mathbf{r}}{\hbar}\right\},$$

where  $\psi_{-0}$  is the wavefunction immediately before the pulse, i.e., that of the ground state of the atom. Hence the overlap integral (1.68) for the ground state is

$$c_g = \int \psi_g^*(\mathbf{r}) \psi_{+0}(\mathbf{r}) d^3 r = \int |\psi_g(\mathbf{r})|^2 \exp\left\{-i \frac{m\mathbf{v} \cdot \mathbf{r}}{\hbar}\right\} d^3 r.$$

Now using Eqs. (3.174), (3.200), and (3.208) of the lecture notes, and directing the  $z$ -axis along the vector  $\mathbf{v}$ , so  $\mathbf{v} \cdot \mathbf{r} = vz = vrcos\theta$ , in the corresponding spherical coordinates, we get

$$\begin{aligned} c_g &= \int \frac{1}{4\pi} \frac{4}{r_0^3} \exp\left\{-\frac{2r}{r_0} - i \frac{mvr \cos\theta}{\hbar}\right\} d^3 r = \frac{2}{r_0^3} \int_0^\infty \exp\left\{-\frac{2r}{r_0}\right\} r^2 dr \int_{-1}^{+1} \exp\left\{-i \frac{mvr \cos\theta}{\hbar}\right\} d(\cos\theta) \\ &= \frac{2}{r_0^3} \int_0^\infty \exp\left\{-\frac{2r}{r_0}\right\} r^2 dr \left(\frac{\hbar}{mvr} 2 \sin \frac{mvr}{\hbar}\right) \equiv \frac{4\hbar}{mvr_0^3} \text{Im} \int_0^\infty \exp\left\{-\frac{2r}{r_0} + i \frac{mvr}{\hbar}\right\} r dr \end{aligned}$$

<sup>198</sup> This is, for example, the case of the beta-decay of tritium, with its nucleus consisting of one proton and two neutrons.

<sup>199</sup> The small difference between  $W_g + W_e$  and 1 gives the total probability of excitation of higher  $s$ -states.



$$= \frac{4\hbar}{mvr_0^3} \operatorname{Im} \left[ \left( -\frac{2}{r_0} + i \frac{mv}{\hbar} \right)^{-2} \right] \equiv \left[ 1 + \left( \frac{mvr_0}{2\hbar} \right)^2 \right]^{-2},$$

so the probability of staying in the ground state is

$$W_g = |c_g|^2 = \left[ 1 + \left( \frac{mvr_0}{2\hbar} \right)^2 \right]^{-4} \equiv \frac{1}{(1 + v^2/4v_0^2)^4}, \quad (*)$$

where  $v_0 \equiv \hbar/mr_0$  is the natural scale of the velocity of the electron's motion in the ground state. (Indeed, as the solution of the next problem will show,  $v_0 = \langle p^2 \rangle^{1/2}/m$ .)

For the hydrogen atom (with  $m = m_e \approx 0.91 \times 10^{-30}$  kg and  $r_0 = r_B \approx 0.53 \times 10^{-10}$  m), the velocity is close to  $2.2 \times 10^6$  m/s. According to Eq. (\*), in order to get  $W_g = 1/2$ , the velocity  $v$  should be equal to  $2 \cdot (2^{1/4} - 1)^{1/2} v_0 \approx 1.90 \times 10^6$  m/s, giving the atom (whose mass is dominated by that of its single-proton nucleus,  $m_p \approx 1.67 \times 10^{-30}$  kg) the kinetic energy  $T \approx m_p v^2/2 \approx 3.02 \times 10^{-15}$  J  $\approx 18.9$  keV. (Since this energy is much larger than the change of the electron's energy, which is of the order of the Hartree energy unit  $E_H \approx 27$  eV, the electron cannot affect the last calculation significantly.)

**Problem 3.42.** Calculate  $\langle x^2 \rangle$  and  $\langle p_x^2 \rangle$  in the ground state of a hydrogen-like atom/ion. Compare the results with Heisenberg's uncertainty relation. What do these results tell about the electron's velocity in the system?

*Solution:* The simplest way to solve this problem<sup>200</sup> is to notice that due to the spherical symmetry of the ground state's wavefunction (corresponding to the quantum numbers  $n = 1$ ,  $l = 0$ , and  $m = 0$ ), we can write

$$\langle r^2 \rangle \equiv \langle x^2 \rangle + \langle y^2 \rangle + \langle z^2 \rangle = 3\langle x^2 \rangle.$$

Hence we can calculate the first average as

$$\langle x^2 \rangle = \frac{1}{3} \langle r^2 \rangle = \frac{1}{3} \int \psi^* r^2 \psi d^3r = \frac{1}{3} \int |Y_0^0(\theta, \varphi)|^2 d\Omega \int_0^\infty |\mathcal{R}_{1,0}(r)|^2 r^4 dr.$$

Since the spherical harmonics are normalized, the integral over the solid angle equals 1, while for the radial integral, we may use Eq. (3.208) and a table integral<sup>201</sup> to get a surprisingly simple result:

$$\langle x^2 \rangle = \frac{1}{3} \int_0^\infty |\mathcal{R}_{1,0}(r)|^2 r^4 dr = \frac{4}{3r_0^3} \int_0^\infty \exp\left\{-\frac{2r}{r_0}\right\} r^4 dr = \frac{r_0^2}{24} \int_0^\infty e^{-\xi} \xi^4 d\xi = r_0^2.$$

The second assignment may be addressed similarly, though it requires a bit more caution because of the involved differentiation:

$$\langle p_x^2 \rangle = \frac{1}{3} \langle p^2 \rangle = \frac{1}{3} \int \psi^* \hat{p}^2 \psi d^3r = \frac{1}{3} \int |Y_0^0|^2 d\Omega \int_0^\infty r^2 dr \mathcal{R}_{1,0}^* (-i\hbar\nabla)^2 \mathcal{R}_{1,0}.$$

<sup>200</sup> A more straightforward solution, by using integration in spherical coordinates (with  $x^2$  replaced with  $r^2 \sin^2 \theta \cos^2 \varphi$ , etc.), is also doable, but a bit bulkier.

<sup>201</sup> See, e.g., MA Eq. (6.7d) with  $n = 4$ .

At this point, it is vital to remember that even though  $\mathcal{R}_{1,0}$  (as a radial function) depends on  $r$  only, the operator  $\nabla^2$  is still different from  $d^2/dr^2$  – see MA Eq. (10.9) with  $\partial/\partial\theta = \partial/\partial\varphi = 0$ . As a result, we get

$$\langle p_x^2 \rangle = -\frac{4\hbar^2}{3r_0^3} \int_0^\infty r^2 dr e^{-r/r_0} \left\{ \frac{1}{r^2} \left[ \frac{d}{dr} \left( r^2 \frac{d}{dr} e^{-r/r_0} \right) \right] \right\} = \frac{4\hbar^2}{3r_0^3} \int_0^\infty \left( 2\frac{r}{r_0} - \frac{r^2}{r_0^2} \right) \exp\left\{ -\frac{2r}{r_0} \right\} dr.$$

The last integral falls into a sum of two integrals similar to the one already worked out above, with  $n = 2$  and  $n = 1$ :

$$\langle p_x^2 \rangle = \frac{4\hbar^2}{3r_0^2} \left[ 2 \int_0^\infty \xi e^{-2\xi} d\xi - \int_0^\infty \xi^2 e^{-2\xi} d\xi \right] = \frac{\hbar^2}{3r_0^2}.$$

Thus the product of the r.m.s. uncertainties,

$$\delta x \delta p_x = \frac{\hbar}{\sqrt{3}} \approx 0.577\hbar,$$

is only slightly (by  $\sim 15\%$ ) higher than the minimum  $\hbar/2$  allowed by Heisenberg's uncertainty relation.

Note that due to the spherical symmetry of the system, the r.m.s. value of the total momentum is expressed by a very simple formula,

$$\delta p \equiv \langle p^2 \rangle^{1/2} = \left( 3\langle p_x^2 \rangle \right)^{1/2} = \frac{\hbar}{r_0},$$

and that due to the classical relation  $\mathbf{v} = \mathbf{p}/m$ , the result of the division of this result by the particle's mass  $m$ ,

$$v_0 \equiv \frac{\delta p}{m} = \frac{\hbar}{mr_0},$$

may be interpreted as the r.m.s. velocity of the electron in a hydrogen-like atom. As was estimated in the previous problem, for the hydrogen atom (with  $m = m_e \approx 0.91 \times 10^{-30}$  kg and  $r_0 = r_B \approx 0.53 \times 10^{-10}$  m), this velocity is close to  $2.2 \times 10^6$  m/s. The fact that it is much lower than  $c$  justifies, once again, the non-relativistic analysis that was discussed in Sec. 3.6 of the lecture notes.

**Problem 3.43.** Use the Hellmann-Feynman theorem (see Problem 1.7) to prove:

- (i) the first of Eqs. (3.211) of the lecture notes, and
- (ii) the fact that for a spinless particle in an arbitrary spherically symmetric attractive potential  $U(r)$ , the ground state is always an  $s$ -state (with the orbital quantum number  $l = 0$ ).

*Solutions:*

- (i) Let us notice that Eq. (3.181) for the radial part  $\mathcal{R}_{n,l}$  of the eigenfunction may be considered a 1D Schrödinger equation for the following effective Hamiltonian:

$$\hat{H} = -\frac{\hbar^2}{2mr^2} \frac{d}{dr} \left( r^2 \frac{d}{dr} \right) + \frac{\hbar^2 l(l+1)}{2mr^2} + U(r). \quad (*)$$

Temporarily taking the potential in the more general form  $U(r) = -(C - \lambda)/r$  (so it coincides with the genuine Coulomb potential (3.190) at  $\lambda = \lambda_0 \equiv 0$ ), we get

$$\frac{\partial \hat{H}}{\partial \lambda} = \frac{1}{r},$$

so the Hellmann-Feynman theorem, with the proper index generalization  $n \rightarrow \{n, l\}$ , yields

$$\frac{\partial E_{n,l}}{\partial \lambda} = \left\langle \frac{\partial \hat{H}}{\partial \lambda} \right\rangle_{n,l} = \left\langle \frac{1}{r} \right\rangle_{n,l}. \quad (**)$$

On the other hand, with our temporary replacement  $C \rightarrow C - \lambda$ , Eq. (3.201) reads

$$E_{n,l} = -\frac{m(C - \lambda)^2}{2n^2\hbar^2}, \quad \text{so that } \left. \frac{\partial E_{n,l}}{\partial \lambda} \right|_{\lambda=0} = \frac{mC}{n^2\hbar^2}. \quad (***)$$

Comparing Eqs. (\*\*) and (\*\*\*), we get

$$\left\langle \frac{1}{r} \right\rangle_{n,l} = \frac{1}{n^2} \frac{Cm}{\hbar^2}.$$

But according to the second of Eqs. (3.192), the last fraction is just  $1/r_0$ , thus giving us the first of the results (3.211). The remaining two formulas (3.211) may be proved similarly.<sup>202</sup>

(ii) Now let us temporarily consider, in the same Eq. (3.181), the quantum number  $l$  to be a continuous parameter. Now the Hellmann-Feynman theorem yields

$$\frac{\partial E_{n,l}}{\partial l} = \left\langle \frac{\partial \hat{H}}{\partial l} \right\rangle_{n,l} = \frac{\hbar^2}{2m} \left\langle \frac{1}{r^2} \frac{\partial [l(l+1)]}{\partial l} \right\rangle_{n,l} = \frac{\hbar^2}{2m} \left\langle \frac{2l+1}{r^2} \right\rangle_{n,l}.$$

For all allowed values  $l \geq 0$ , the operator inside the last bracket is a positively defined form, so its expectation value cannot be negative for any quantum state  $\{n, l\}$ , and hence

$$\frac{\partial E_{n,l}}{\partial l} \geq 0, \quad \text{for any } l \geq 0,$$

in particular showing that the ground state (with the lowest  $E_{n,l}$ ) always corresponds to  $l = 0$ .

**Problem 3.44.** For the ground state of a hydrogen atom, calculate:

- (i) the expectation value of  $\mathcal{E}$ , where  $\mathcal{E}$  is the electric field created by the atom as a whole, and
- (ii) the expectation value of  $\mathcal{E}^2$  at distances  $r \gg r_0$  from the nucleus.

Interpret the obtained relation between  $\langle \mathcal{E} \rangle^2$  and  $\langle \mathcal{E}^2 \rangle$  at distant observation points.

*Solutions:*

(i) The net electric field  $\mathcal{E}$  of the atom is the sum of the field  $\mathcal{E}_n$  of its nucleus, with the electric charge  $q = +e$ , and that ( $\mathcal{E}_e$ ) of the electron, with the equal and opposite charge,  $q' = -e$ . At distances  $r$  much larger than the size of the nucleus,  $\mathcal{E}_n$  may be calculated as the radial field of a point charge  $q$ :

<sup>202</sup> See, e.g., pp. 470-471 in R. Shankar, *Quantum Mechanics*, 2<sup>nd</sup> ed., Springer, 1980.

$$\mathcal{E}_n(\mathbf{r}) = \mathbf{n}_r \mathcal{E}_n, \quad \text{with } \mathcal{E}_n = \frac{e}{4\pi\epsilon_0 r^2}.$$

Since, according to Eqs. (3.174), (3.200), and (3.208), the ground-state wavefunction  $\psi = \psi_{1,0,0}$  of the electron is spherically symmetric:

$$\psi(\mathbf{r}) = Y_0^0(\theta, \varphi) \mathcal{R}_{1,0}(r) = \frac{1}{(4\pi)^{1/2}} \frac{2}{r_0^{3/2}} e^{-r/r_0}, \quad (*)$$

so is the expectation value of its electric charge density:

$$\langle \rho \rangle(\mathbf{r}) = -e |\psi(r)|^2 = -\frac{e}{4\pi} \frac{4}{r_0^3} e^{-2r/r_0}.$$

Since the relation between the charge density and the electric field it induces in free space is linear, the expectation value of the electric field created by the electron may be calculated from the static inhomogeneous Maxwell equation,<sup>203</sup> with this averaged charge density as the source:

$$\nabla \cdot \langle \mathcal{E}_e \rangle = \frac{\langle \rho \rangle}{\epsilon_0} \equiv -\frac{e}{4\pi\epsilon_0} \frac{4}{r_0^3} e^{-2r/r_0}.$$

Per basic vector algebra,<sup>204</sup> this average field is also spherically symmetric and radial,  $\langle \mathcal{E}_e(\mathbf{r}) \rangle = \mathbf{n}_r \langle \mathcal{E}_e(r) \rangle$ , with its magnitude obeying the ordinary, first-order differential equation

$$\frac{1}{r^2} \frac{d}{dr} (r^2 \langle \mathcal{E}_e \rangle) = -\frac{e}{4\pi\epsilon_0} \frac{4}{r_0^3} e^{-2r/r_0}.$$

This equation (with the boundary condition  $\langle \mathcal{E}_e(0) \rangle = 0$  imposed by the spherical symmetry of the field) may be readily integrated by parts, giving

$$\begin{aligned} \langle \mathcal{E}_e \rangle(\mathbf{r}) &= -\frac{e}{4\pi\epsilon_0 r^2} \frac{4}{r_0^3} \int_0^r r'^2 e^{-2r'/r_0} dr' = \frac{e}{4\pi\epsilon_0 r^2} \left[ e^{-2r'/r_0} \left( \frac{2r'^2}{r_0^2} + \frac{2r'}{r_0} + 1 \right) \right]_0^r \\ &\equiv \frac{e}{4\pi\epsilon_0 r^2} \left[ e^{-2r/r_0} \left( \frac{2r^2}{r_0^2} + \frac{2r}{r_0} + 1 \right) - 1 \right], \end{aligned}$$

so the net average magnitude of the atom's field,<sup>205</sup>

$$\langle \mathcal{E} \rangle(\mathbf{r}) = \mathcal{E}_n(\mathbf{r}) + \langle \mathcal{E}_e \rangle(\mathbf{r}) = \frac{e}{4\pi\epsilon_0} \left( \frac{2}{r_0^2} + \frac{2}{rr_0} + \frac{1}{r^2} \right) e^{-2r/r_0},$$

and its square,

$$\langle \mathcal{E} \rangle^2(\mathbf{r}) = \left( \frac{e}{4\pi\epsilon_0} \right)^2 \left( \frac{2}{r_0^2} + \frac{2}{rr_0} + \frac{1}{r^2} \right)^2 e^{-4r/r_0} \rightarrow 4 \left( \frac{e}{4\pi\epsilon_0 r_0^2} \right)^2 e^{-4r/r_0}, \quad \text{at } r \gg r_0, \quad (**)$$

exponentially drop at large distances.

<sup>203</sup> See, e.g., EM Eq. (1.27).

<sup>204</sup> See, e.g., MA Eq. (10.10), with  $\partial/\partial\theta = \partial/\partial\varphi = 0$ .

<sup>205</sup> Note that the corresponding average electrostatic potential  $\langle \phi \rangle(\mathbf{r})$  differs from the Yukawa potential whose properties were analyzed in Problem 11, even though it also features a similar exponential factor.

(ii) The calculation of  $\langle \mathcal{E}^2 \rangle$  at arbitrary distances  $r \sim r_0$  is more cumbersome, so let us immediately use the given condition  $r \gg r_0$ . At such distances, in classical electrodynamics,<sup>206</sup> the net electric field of an electrically-neutral system consisting of a point charge  $q = +e$ , located at the origin, and an electron charge  $q' = -e$ , located at point  $\mathbf{r}'$ , with  $r' \sim r_0 \ll r$ , tends to the field

$$\mathcal{E}(\mathbf{r}; \mathbf{r}') = \frac{1}{4\pi\epsilon_0} \frac{3\mathbf{r}(\mathbf{r} \cdot \mathbf{p}) - \mathbf{p}r^2}{r^5} \quad (***)$$

of an electric dipole with moment  $\mathbf{p} = q \cdot 0 + q' \cdot \mathbf{r}' = -e\mathbf{r}'$ , so

$$\mathcal{E}^2(\mathbf{r}; \mathbf{r}') = \left( \frac{e}{4\pi\epsilon_0} \right)^2 \left( \frac{3\mathbf{r}(\mathbf{r} \cdot \mathbf{r}') - \mathbf{r}'r^2}{r^5} \right)^2 = \left( \frac{e}{4\pi\epsilon_0} \right)^2 \frac{3r^2(\mathbf{r} \cdot \mathbf{r}')^2 + r'^2r^4}{r^{10}} = \left( \frac{e}{4\pi\epsilon_0} \right)^2 \frac{r'^2}{r^6} (3\cos^2\theta + 1),$$

where  $\theta$  is the angle between the vectors  $\mathbf{r}'$  and  $\mathbf{r}$ , so  $\mathbf{r}' \cdot \mathbf{r} = r'r\cos\theta$ .

Due to the correspondence principle, at the transfer to quantum mechanics, we still may use the above expression for  $\mathcal{E}^2$  but have to understand it as a linear operator acting on the electron's wavefunction  $\psi(\mathbf{r}')$ , so the expectation value of the corresponding observable may be calculated as

$$\langle \mathcal{E}^2 \rangle(\mathbf{r}) = \int \psi^*(\mathbf{r}') \mathcal{E}^2(\mathbf{r}; \mathbf{r}') \psi(\mathbf{r}') d^3r' = \int \mathcal{E}^2(\mathbf{r}; \mathbf{r}') |\psi(\mathbf{r}')|^2 d^3r'.$$

Taking the direction of the vector  $\mathbf{r}$  for the polar axis, and then using Eq. (\*) for the ground-state wavefunction, we get

$$\begin{aligned} \langle \mathcal{E}^2 \rangle(\mathbf{r}) &= \int_0^{2\pi} d\varphi \int_0^\pi \sin\theta d\theta \int_0^\infty r'^2 dr' |Y_0^0(\theta, \varphi)|^2 |\mathcal{R}_{1,0}(r')|^2 \mathcal{E}^2(\mathbf{r}; \mathbf{r}') \\ &= 2 \left( \frac{e}{4\pi\epsilon_0} \right)^2 \frac{1}{r^6 r_0^3} \int_0^\pi (3\cos^2\theta + 1) \sin\theta d\theta \int_0^\infty r'^4 e^{-2r'/r_0} dr' \\ &\equiv \frac{1}{16} \left( \frac{e}{4\pi\epsilon_0} \right)^2 \frac{r_0^2}{r^6} \int_{-1}^+ (3\xi^2 + 1) d\xi \int_0^\infty \zeta^4 e^{-\zeta} d\zeta, \end{aligned}$$

where  $\xi \equiv \cos\theta$  and  $\zeta \equiv r/(r_0/2)$ . The first integral is elementary and equal to 4, while the second one is a table integral<sup>207</sup> equal to  $4! \equiv 24$ , so finally,

$$\langle \mathcal{E}^2 \rangle(\mathbf{r}) = 6 \left( \frac{e}{4\pi\epsilon_0 r_0^2} \right)^2 \left( \frac{r_0}{r} \right)^6, \quad \text{for } r \gg r_0. \quad (***)$$

Comparison of this result with Eq. (\*\*) shows a rather dramatic difference between the square of the average electric field of the atom, and the average of its square: while the former expectation value drops exponentially with distance  $r$  from the atom, the latter one decreases much slower, as  $1/r^6$ . The interpretation of this difference is offered by the (frequently, very useful) notion of *quantum fluctuations* of the field: since  $|\psi(\mathbf{r}')|^2$  may be interpreted as the density of the probability of finding the electron at point  $\mathbf{r}'$ , we may say that its “random motion” in the  $\mathbf{r}'$  space creates random fluctuations of the dipole field  $\mathcal{E}$ , which, according to Eq. (\*\*\*), decays with distance only as  $1/r^3$ , so its square drops as  $1/r^6$ , as

<sup>206</sup> See, e.g., EM Sec. 3.1, in particular Eq. (3.13).

<sup>207</sup> See, e.g., MA Eq. (6.7d) with  $n = 4$ .

described by Eq. (\*\*\*\*). However, due to the randomness of the spatial orientations of the vector  $\mathbf{r}'$ , and hence of the field vector  $\mathcal{E}$ , the bulk of these fluctuations is averaged out from  $\langle \mathcal{E} \rangle$ , leaving behind only the exponentially small “tail” (\*\*). This behavior, very typical for quantum mechanics, has already been met in the course,<sup>208</sup> and will be met several more times.

Note also that Eq. (\*\*\*\*) is closely related to the attractive London dispersion force with the effective potential  $U_{\text{ef}} \propto 1/r^6$  between two neutral atoms/molecules at large distances – see Problems 20, 5.15, and 6.18.

**Problem 3.45.** Find the condition at which a particle of mass  $m$ , moving in the field of a very thin spherical shell with  $U(\mathbf{r}) = \mathcal{W}\delta(r - R)$  and  $\mathcal{W} < 0$ , has at least one localized (“bound”) stationary state.

*Solution:* Repeating the initial arguments of the model solution of Problem 28, with the only difference that now the product  $r\psi(r)$  is given by a linear combination of two exponential functions similar to Eq. (\*\*) of that solution even at  $r < R$  (this linear combination has to vanish at  $r = 0$  to avoid the divergence of  $\psi$ , i.e. to be proportional to  $\sinh \kappa r$ ), we may look for the ground-state eigenfunction in the form

$$\psi(r) = \frac{1}{r} \times \begin{cases} C_- \sinh \kappa r, & \text{for } r \leq R, \\ C_+ e^{-\kappa r}, & \text{for } r \geq R, \end{cases} \quad \text{with } \frac{\hbar^2 \kappa^2}{2m} \equiv -E > 0.$$

As was discussed in the solution of Problem 29, the relation between the coefficients  $C_{\pm}$  may be found from the boundary conditions at  $r = R$ , using Eqs. (2.75) and (2.76) of the lecture notes, with the proper replacement  $\psi \rightarrow r\psi$ . These conditions yield, correspondingly:

$$\kappa \left( -C_+ e^{-\kappa R} - C_- \cosh \kappa R \right) = \frac{2m}{\hbar^2} \mathcal{W} C_+ e^{-\kappa R}, \quad C_+ e^{-\kappa R} - C_- \sinh \kappa R = 0.$$

The condition of consistency of these two linear, homogeneous equations,

$$\begin{vmatrix} \left( -\kappa - \frac{2m\mathcal{W}}{\hbar^2} \right) e^{-\kappa R} & -\kappa \cosh \kappa R \\ e^{-\kappa R} & -\sinh \kappa R \end{vmatrix} = 0,$$

gives us the following characteristic equation for  $\kappa$ :

$$\kappa R (\coth \kappa R + 1) = -\frac{2m\mathcal{W}R}{\hbar^2}. \quad (*)$$

The product  $\kappa R \coth \kappa R$  equals 1 at  $\kappa R = 0$  and grows with the argument  $\kappa R$  (which should be positive by its definition), and the second term in the parentheses of Eq. (\*) only increases this trend. Hence this equation may have a solution only if the magnitude of its right-hand side is larger than 1, i.e. if<sup>209</sup>

<sup>208</sup> For example, the Gaussian wave packet (2.16) of a free 1D particle, as well as the ground state (2.275) of a 1D harmonic oscillator, have  $\langle x \rangle^2 = 0$ , but  $\langle x^2 \rangle = \delta x^2 > 0$ , so if the particle in these situations is charged, its electric field has properties similar to those of the atom.

<sup>209</sup> At the border of this range, at  $2m\mathcal{W}R = \hbar^2$ , the characteristic equation yields  $\kappa R = 0$ , so the solution becomes unlocalized.

$$|\mathcal{W}| > \frac{\hbar^2}{2mR}, \quad (**)$$

i.e. if the dimensionless parameter  $\beta \equiv \mathcal{W}/(\hbar^2/2mR)$ , already used in the model solution of Problem 10 (and is negative in our current problem), is below  $-1$ .

This is the condition we were seeking for. Note that in the limit  $R \rightarrow 0$ , we may associate this potential with a 3D delta function,  $U(\mathbf{r}) = \mathcal{W}_{3D}\delta(\mathbf{r})$ ,<sup>210</sup> with the parameter  $\mathcal{W}_{3D}$  defined by the following condition:

$$\mathcal{W}_{3D} = \int_0^\infty U(\mathbf{r})d^3r = \int_0^\infty 4\pi r^2 U(r)dr = 4\pi R^2 \mathcal{W}.$$

Plugging this relation into Eq. (\*\*), we get the following condition,

$$|\mathcal{W}_{3D}| > \mathcal{W}_{\min}, \quad \text{with } \mathcal{W}_{\min} = \frac{2\pi\hbar^2 R}{m},$$

which is *always* satisfied at  $R \rightarrow 0$  (of course only if  $\mathcal{W}$  and hence  $\mathcal{W}_{3D}$  are negative). At small but nonvanishing  $R$ , the last expression for  $\mathcal{W}_{\min}$  is qualitatively similar but quantitatively different from Eq. (\*\*\*) in the model solution of Problem 28. This is one more illustration of the statement made at the end of that solution: the particle localization properties of a potential well of a very small size cannot be fully characterized by just the “weight” of the 3D delta function, even if the potential is axially symmetric – as it is in both these problems.

**Problem 3.46.** Calculate the lifetime of the lowest metastable state in the same spherical-shell potential as in the previous problem, but now with  $\mathcal{W} > 0$ , for sufficiently large  $\mathcal{W}$ . (Quantify this condition.)

*Solution:* We may follow the approach used in Sec. 2.5 of the lecture notes to solve a similar 1D problem – see Fig. 2.17 and its discussion. If  $\mathcal{W}$  is large enough, the Schrödinger equation inside the shell may be approximately satisfied with a spherically symmetric standing wave vanishing at  $r = R$ . As was discussed at the end of Sec. 3.6 of the lecture notes, in such cases, the lowest eigenfunction is a product of the spherical harmonic with  $l = 0$  and  $m = 0$  (which is just a constant) by a radial function proportional to the lowest spherical Bessel function of the first kind,  $j_0(kr) = \sin kr / kr$  – see the first of Eqs. (3.186). The boundary condition yields  $k = \pi/R$ , and after an easy normalization, we get

$$\psi|_{r \leq R} = A \frac{\sin kr}{r} \equiv \frac{A}{2r} (e^{ikr} - e^{-ikr}), \quad \text{with } A = \left( \frac{W}{2\pi R} \right)^{1/2},$$

where  $W$  (not to be confused with the 1D delta function’s “weight”  $\mathcal{W}$ ) is the total probability of finding the particle inside the shell.

Outside the sphere, we may take only the first term of the  $s$ -wave solution (3.6),

<sup>210</sup> Of course,  $\mathcal{W}_{3D}$  should not be confused with  $\mathcal{W}$ ; these parameters even have different dimensionalities – respectively,  $\text{J/m}^3$  and  $\text{J/m}$ .

$$\psi|_{r \geq R} = C \frac{\exp\{ikr\}}{r},$$

which describes the outward traveling wave due to the particle's "leakage" from the sphere. The coefficient  $C$  may be found exactly as in the 1D case; since for a spherically-symmetric function,  $\nabla = \mathbf{n}_r \partial / \partial r$ , the calculation is literally the same and gives the same result:

$$C = \frac{A}{2} \frac{1}{1+i\alpha} \approx \frac{A}{2i\alpha}, \quad (*)$$

where  $\alpha$  is the dimensionless coefficient defined by Eq. (2.78):

$$\alpha \equiv \frac{m\omega}{k\hbar^2}.$$

(The second step in Eq. (\*) is legitimate because our calculation is valid only if  $|C| \ll A$ , i.e. when  $\alpha \gg 1$ ; by the way, this is exactly the requested condition of validity of our analysis.)

Now everything is ready to calculate the total probability current outside the sphere:

$$I = 4\pi r^2 j, \quad \text{where } j = \frac{\hbar}{m} \text{Im} \left( \psi^* \frac{d}{dr} \psi \right) = \frac{\hbar}{m} \frac{|C|^2}{r^2} k,$$

which does not depend on the value of the radius  $r > R$  we are calculating it at:

$$I = 4\pi \frac{\hbar k}{m} \frac{1}{4\alpha^2} \frac{W}{2\pi R} \equiv \frac{1}{\tau} W, \quad \text{where } \tau \equiv \alpha^2 \frac{2mR^2}{\hbar k}.$$

(With the last form of the expression for  $I$ , the continuity equation (1.48) takes the form

$$\frac{dW}{dt} = -I = -\frac{W}{\tau},$$

so the  $\tau$  so defined is indeed the required lifetime of the metastable state.) The above result for  $\tau$  may be represented in a more transparent form:

$$\frac{\tau}{\hbar} = \frac{\beta^2}{4\pi} \frac{1}{E} \gg \frac{1}{E},$$

where  $\beta \equiv 2mR\omega/\hbar^2 \gg 1$  is the dimensionless parameter already used in the model solutions of Problem 10 and the previous problem for the similar potential, and  $E = \pi^2 \hbar^2 / 2mR^2$  is the eigenenergy of this (lowest) metastable state.

**Problem 3.47.** A particle of mass  $m$  and energy  $E$  is incident on a very thin spherical shell whose localized states were the subject of two previous problems, with an arbitrary "weight"  $\omega$ .

(i) Derive general expressions for the differential and total cross-sections of scattering.

(ii) Spell out the contribution  $\sigma_0$  to the total cross-section  $\sigma$ , given by the spherically symmetric component of the scattered de Broglie wave.



(iii) Analyze the result for  $\sigma_0$  in the limits of very small and very large magnitudes of  $\mathcal{W}$ , for both signs of this parameter. In particular, in the limit  $\mathcal{W} \rightarrow +\infty$ , relate the result to the metastable state's lifetime  $\tau$  calculated in the previous problem.

*Solutions:*

(i) According to Eqs. (3.222) and (3.224) of the lecture notes, for this axially-symmetric problem, both  $d\sigma/d\Omega$  and  $\sigma$  are fully defined by the set of the complex amplitudes  $A_l$  of the so-called “partial waves”, i.e. the spherical-harmonic components of the scattered de Broglie wave

$$\psi_s = a_i \sum_{l=1}^{\infty} \mathcal{R}_l(r) P_l(\cos \theta), \quad \text{with } \mathcal{R}_l(r) \rightarrow (-i)^{l+1} A_l \frac{e^{ikr}}{kr} \quad \text{for } r \rightarrow \infty, \quad (*)$$

where  $a_i$  is the amplitude of the incident wave, which may be also represented as a sum over the spherical harmonics (reduced to the Legendre polynomials  $P_l$ ), using the expansion (3.225):

$$\psi_i = a_i \sum_{l=0}^{\infty} i^l (2l+1) j_l(kr) P_l(\cos \theta).$$

(Here  $j_l(\xi)$  are the spherical Bessel functions of the first kind – see Eqs. (3.185)-(3.186) of the lecture notes, and  $k = (2mE)^{1/2}/\hbar$  is the wave number of the incident and scattered waves.)

For our particular scatterer, described by the 1D delta-functional potential

$$U(\mathbf{r}) = \mathcal{W} \delta(r - R),$$

which vanishes at all points with  $r \neq R$ , the radial functions obey the simple Eq. (3.183) both at  $r \leq R$  and  $r \geq R$ . As was discussed in Sec. 3.6 and 3.8 of the lecture notes, the appropriate solutions in these regions are

$$\mathcal{R}_l(r) = \begin{cases} C_l j_l(kr), & \text{for } r \leq R, \\ A_l h_l^{(1)}(kr), & \text{for } R \leq r, \end{cases}$$

where the coefficient  $A_l$  is the same as in the asymptote (\*), and  $h_l^{(1)}(\xi) \equiv j_l(\xi) + iy_l(\xi)$  is the spherical Hankel function of the first kind – see the first of Eqs. (3.215). By its construction, the  $l^{\text{th}}$  component of the total wavefunction (including  $\psi_i$  and  $\psi_s$ ) is proportional to

$$a_i \left[ i^l (2l+1) j_l(kr) + \mathcal{R}_l(kr) \right],$$

so it already satisfies the boundary conditions at  $r = 0$  and  $r \rightarrow \infty$ , and we only need to impose on it the conditions at  $r = R$ , due to the delta-functional potential of the spherical shell. We may derive these boundary conditions, for example, by using the fact discussed in the model solution of Problem 29: the product  $f_l(r)$  of the  $l^{\text{th}}$  radial function by  $r$  satisfies a 1D Schrödinger equation with the effective potential

$$U_{\text{ef}}(r) = U(r) + \frac{\hbar^2 l(l+1)}{2mr^2}.$$

The second term on the right-hand side is continuous at  $r = R$ , so it does not affect the boundary conditions at that point, which are therefore the same as in the 1D case – see Eqs. (2.75)-(2.76):<sup>211</sup>

$$f_l(R+0) - f_l(R-0) = 0, \quad \frac{d}{dr} f_l(r) \Big|_{r=R+0} - \frac{d}{dr} f_l(r) \Big|_{r=R-0} = \frac{2m\omega}{\hbar^2} f_l(R).$$

Plugging in the above expressions for the total wavefunction into these boundary conditions, we get, respectively,

$$A_l h_l^{(1)}(kR) - C_l j_l(kR) = 0, \\ A_l \frac{d}{dr} [r h_l^{(1)}(kr)] \Big|_{r=R} - C_l \frac{d}{dr} [r j_l(kr)] \Big|_{r=R} = \frac{2m\omega R}{\hbar^2} [i^l (2l+1) j_l(kR) + A_l h_l^{(1)}(kR)].$$

Solving this simple system of two linear equations for the coefficients  $A_l$  and  $C_l$ , we get, in particular,

$$A_l = \frac{\beta i^l (2l+1) j_l(kR)}{d[\xi h_l^{(1)}(\xi)]/d\xi \Big|_{\xi=kR} - [h_l^{(1)}(kR)/j_l(kR)] d[\xi j_l(\xi)]/d\xi \Big|_{\xi=kR} - \beta h_l^{(1)}(kR)}, \quad (**)$$

where  $\beta$  is the dimensionless real coefficient, characterizing the relative strength of the delta-functional potential, that was defined in the model solution of Problem 10 (see also the solutions of the two previous problems):

$$\beta \equiv \frac{\omega}{\hbar^2 / 2mR}.$$

Eq. (\*\*), together with Eqs. (3.222) and (3.224) of the lecture notes, gives a complete (though not immediately transparent) solution of the scattering problem.

(ii) The spherically symmetric component of the scattered wavefunction (with  $l = 0$ ) is proportional to the coefficient  $A_0$ . From the first column of Eq. (3.186), we get

$$\xi j_0(\xi) = \sin \xi, \quad \frac{d}{d\xi} [\xi j_0(\xi)] = \cos \xi; \quad \xi h_0^{(1)}(\xi) \equiv \xi [j_0(\xi) + iy_0(\xi)] = -ie^{i\xi}, \quad \frac{d}{d\xi} [\xi h_0^{(1)}(\xi)] = e^{i\xi},$$

and Eq. (\*\*) with  $l = 0$  is reduced to

$$A_0 = \frac{\beta \operatorname{sinc} kR}{1 + i(\cot kR + \beta/kR)} e^{-ikR},$$

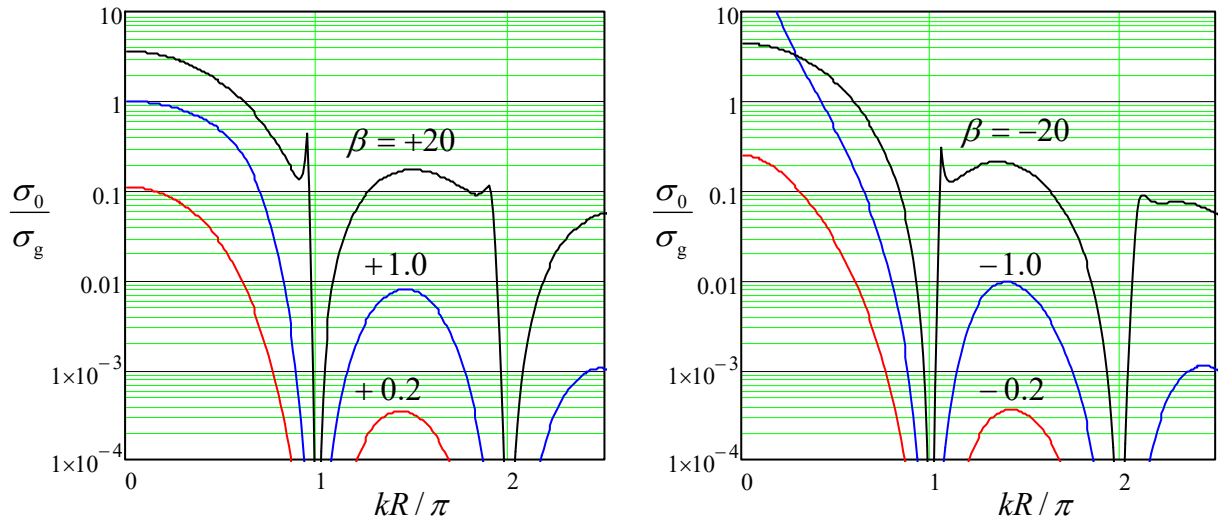
(where  $\operatorname{sinc} \xi \equiv \sin \xi / \xi$ , as in the solution of Problem 10), giving the following contribution to the total cross-section (3.224):

$$\sigma_0 = \frac{4\pi}{k^2} |A_0|^2 = \frac{4\sigma_g}{(kR)^2} \frac{\beta^2 \operatorname{sinc}^2 kR}{1 + (\cot kR + \beta/kR)^2}, \quad (***)$$

where  $\sigma_g \equiv \pi R^2$  is the “geometric” cross-section of the shell.

<sup>211</sup> Note that the model solution of the previous problem used an alternative way to derive the corresponding boundary conditions for  $\psi_l = f_l/r$ .

(iii) Two panels of the figure below show, on the appropriate semi-log scale, the ratio  $\sigma_0/\sigma_g$  as a function of the dimensionless product  $kR \propto E^{1/2}$ , for several representative values and two opposite signs of the parameter  $\beta$  (i.e., of the weight  $w$ ).



In the weak-potential limit  $\beta \rightarrow 0$ , the cross-section does not depend on the sign of this parameter – the usual feature of the Born approximation:

$$\sigma_0 \approx \sigma_g (2\beta)^2 \text{sinc}^4 kR, \quad \text{at } |\beta| \ll 1,$$

In particular, at  $kR \rightarrow 0$ , when scalar scattering by *any* object is spherically symmetric, and hence  $\sigma_0$  dominates the total cross-section  $\sigma$ , this result tends to the value  $\sigma/\sigma_g = 4\beta^2$  that was calculated, in that approximation, in Problem 10. However, as  $|\beta|$  becomes either comparable with or larger than 1, i.e. as we go beyond the Born approximation limit,  $\sigma_0$  does depend on the sign of  $\beta$ , and its dependence on the parameter  $kR$  (i.e. on the particle's energy) shows new effects. Most interestingly, as the figure above shows, at  $|\beta| \gg 1$ , the dependences exhibit sharp resonance peaks<sup>212</sup> at values of  $kR$  close to each  $\pi n$ , with  $n = 1, 2, \dots$

The physics of this effect<sup>213</sup> for the case  $w > 0$  (illustrated by the left panel of the figure) should be clear from the model solution of the previous problem, or rather its straightforward extension to an arbitrary metastable  $s$ -state with  $m = 0$ . Namely, at  $\beta = \infty$ , when the spherical shell is impenetrable, it has localized states; for those with  $l = 0$ ,  $\psi_n \propto \text{sinc} k_n r/r$  and  $k_n = \pi n/R$  – see also Eq. (3.188) of the lecture notes. If  $\beta$  is large but finite, such a state is metastable, i.e. the amplitude of this standing de Broglie wave cannot persist on its own; however, it may be sustained via its weak coupling with a stationary incident wave. As at the resonant tunneling in 1D quantum systems discussed in Chapter 2 of this course (see, e.g., Fig. 2.16 and its discussion), if the energy  $E = \hbar^2 k^2/2m$  of the particle described by this de

<sup>212</sup> As was already mentioned in Sec. 2.5 of the lecture notes, such resonance functions of the incident particle's energy are sometimes called the *Breit-Wigner distributions* (or “cross-sections”, or “functions”).

<sup>213</sup> It belongs to the group of resonant *Ramsauer-Townsend* effects that were discovered (apparently, independently) by C. Ramsauer and J. S. Townsend in the early 1920s at the scattering of low-energy electrons by noble-gas atoms.

Broglie wave approaches that of the metastable state, the amplitude of the induced standing wave strongly increases and so does the scattering intensity, i.e. its cross-section.

The figure on the right shows a zoom-in on the vicinity of the lowest resonance (with  $n = 1$ ); for  $\beta \gg 1$ , its basic features readily follow from Eq. (\*\*\*) . Indeed, the exact resonance is reached at the point  $(kR)_{\text{res}}$  that makes the parentheses in the denominator of that expression vanish:

$$\cot(kR)_{\text{res}} + \frac{\beta}{(kR)_{\text{res}}} = 0;$$

for  $\beta \gg 1$  and  $(kR)_{\text{res}} \approx k_1 R = \pi$ , when  $\cot(kR) \approx -1/(\pi - kR)$ , this equation yields

$$(kR)_{\text{res}} \approx \pi \left( 1 - \frac{1}{\beta} \right).$$

At that point,  $\text{sinc}(kR)_{\text{res}} \approx 1/\beta$ , so the height of the resonance maximum is independent of  $\beta$ :

$$\sigma_{\text{res}} \approx \frac{4\sigma_g}{(kR)_{\text{res}}^2} \frac{\beta^2 \text{sinc}^2(kR)_{\text{res}}}{1+0^2} \approx \frac{4\sigma_g}{\pi^2} \beta^2 \left( \frac{1}{\beta} \right)^2 = \frac{4}{\pi^2} \sigma_g.$$

As the figures above show, these asymptotic analytical expressions for  $(kR)_{\text{res}}$  and  $\sigma_{\text{res}}$  are in good correspondence with the numerical results for  $\beta_{\text{res}} \gg 1$ . Moreover, it is easy to get an expression for the resonance width  $\Delta(kR)$ , just as this was done in Sec. 2.5 for the 1D resonant tunneling – see the derivation of Eq. (2.142). Indeed, Eq. (\*\*\*) shows that  $\sigma_0$  decreases two-fold from its resonance value  $\sigma_{\text{res}}$  when the deviation of the parentheses in its denominator from 0 becomes equal to  $\pm 1$ . Since at  $\beta \gg 1$ , this deviation is dominated by the first term,  $\cot(kR)$ , we should require  $\cot[(kR)_{\text{res}} \pm \Delta(kR)/2]$  to be equal to  $\pm 1$ .<sup>214</sup> With the asymptotic expression  $\cot(kR) \approx -1/(\pi - kR)$  already used above, and the anticipated condition  $|\Delta(kR)| \ll \pi - (kR)_{\text{res}} \approx \pi/\beta \ll 1$ , this requirement readily yields

$$\Delta(kR) \approx \frac{2\pi^2}{\beta^2},$$

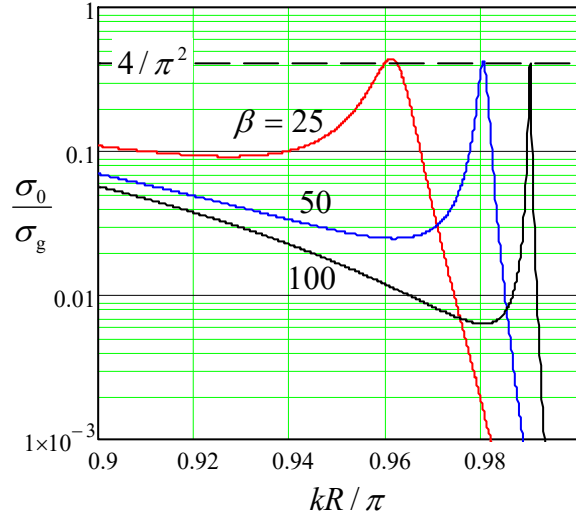
confirming the above assumption, and again in good agreement with the numerical plots. The resulting energy width of the resonance,

$$\Delta E \approx \frac{dE}{dk} \Delta k = \frac{d}{dk} \left( \frac{\hbar^2 k^2}{2m} \right) \Delta k = \frac{\hbar^2 k}{m} \Delta k \equiv 2E \frac{\Delta(kR)}{kR} \approx 2E \frac{2\pi^2 / \beta^2}{\pi} \equiv \frac{4\pi}{\beta^2} E \ll E,$$

is in the same relation with the metastable state's lifetime  $\tau = \hbar\beta^2/4\pi E$  calculated in the previous problem, as for the similar 1D problem:

$$\Delta E \cdot \tau = \hbar,$$

emphasizing again the generality of this relation – with the reservations discussed in Sec. 2.5 of the lecture notes. Note also that all these results for the resonant scattering at  $kR \approx \pi n$  are also valid for the



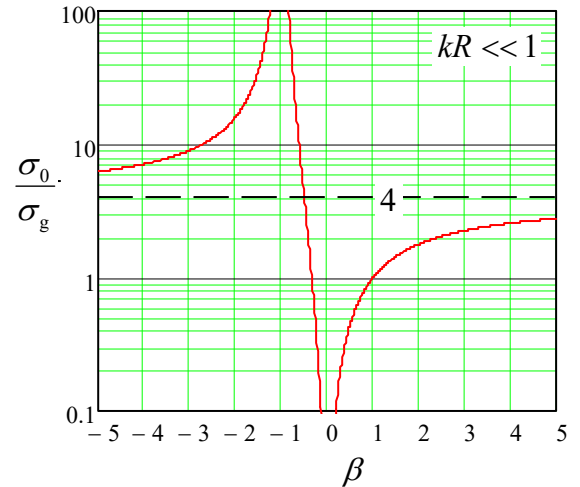
<sup>214</sup> This requirement stems from the usual definition of the “full width (of the resonance curve) at half-maximum” (FWHM) – see Sec. 2.5.

total cross-section  $\sigma$ , because the contributions of the higher components  $\sigma_l$  with  $l > 0$  become comparable with  $\sigma_g$  only near the corresponding non- $s$ -state resonances, i.e. at  $k \approx \xi_{l,n}/R$  with  $l > 0$  – see, e.g., the table following Eq. (3.188) of the lecture notes.

As the right panel of the first figure above shows, at  $\beta < 0$  (i.e. at  $\mathcal{W} < 0$ ), the resonances at  $k \approx n\pi/R$  with  $n = 1, 2, \dots$  are virtually similar to those at  $\beta > 0$ , though they are located on the opposite side of the asymptotic values  $n\pi/R$ . However, the low-energy scattering may be significantly stronger in this case. Indeed, in the limit  $kR \rightarrow 0$ , Eq. (\*\*\*) is reduced to a simple expression,

$$\frac{\sigma_0}{\sigma_g} = \frac{4\beta^2}{(\beta+1)^2}, \quad \text{for } kR \ll 1, |\beta+1|,$$

plotted in the figure on the right. According to this expression (valid also for the total cross-section  $\sigma$ , due to the dominance of the spherically-symmetric scattering in this limit), at  $|\beta| \rightarrow \infty$ , the ratio  $\sigma_0/\sigma_g$  tends to the value 4 (describing the low-energy scattering by an impenetrable sphere, see Sec. 3.8 of the lecture notes, in particular, Fig. 3.25b), independently of the sign of  $\beta$ . However, at finite negative values of  $\beta$ , the scattering is always stronger, with an infinitely high peak at  $\beta = -1$ . The origin of this peak becomes clear if we revisit the solution of Problem 45: as  $\beta$  tends to this value from below, the energy of the localized eigenstate and hence the corresponding eigenvalue of  $k$  tend to zero, enabling effective interaction of the corresponding wide-spread wavefunction with the low- $k$  incident wave.



**Problem 3.48.** Calculate the spherically symmetric contribution  $\sigma_0$  to the total cross-section of particle scattering by a uniform sphere of radius  $R$ , described by the following potential:

$$U(r) = \begin{cases} U_0, & \text{for } r < R, \\ 0, & \text{otherwise,} \end{cases}$$

with an arbitrary  $U_0$ . Analyze the result in detail, and give an interpretation of its most remarkable features.

*Solution:* Let us first assume that  $U_0$  is lower than the particle's energy  $E$ . (Note that in this case,  $U_0$  may be either positive or negative.) Then, according to the discussion in Sec. 3.8 of the lecture notes, we may look for the solution of the scattering problem in the form

$$\psi = a_i \times \begin{cases} \sum_{l=0}^{\infty} [i^l (2l+1) j_l(kr) + A_l h_l^{(1)}(kr)] P_l(\cos \theta), & \text{for } R \leq r, \\ \sum_{l=0}^{\infty} B_l j_l(k'r) P_l(\cos \theta), & \text{for } r \leq R, \end{cases} \quad (*)$$

where  $k$  and  $k'$  are the de Broglie wave numbers, respectively, outside of the sphere and inside it, defined as usual:

$$\frac{\hbar^2 k^2}{2m} \equiv E, \quad \frac{\hbar^2 k'^2}{2m} \equiv E - U_0.$$

Note that in contrast with the solution of the previous problem, the incident wave (represented as a sum over spherical harmonics – see Eq. (3.225) of the lecture notes) is taken into account explicitly only in the upper line of Eq. (\*), i.e. outside the sphere, while inside it, it is included into a single sum with the scattered wave. (The motivation for this approach is that the spherical Bessel functions  $y_l(kr)$ , and hence  $h_l^{(1)}(kr)$ , do not have finite values at  $r \rightarrow 0$ , while the functions  $j_l(kr)$  do.)

The boundary conditions on the sphere's surface (the continuity of the wavefunction and its radial derivative at  $r = R$ ) do not mix different spherical harmonics of the solution, and since we are only interested in the spherically-symmetric contribution  $\sigma_0$  to the total cross-section, proportional to  $|A_0|^2$ , we may limit our analysis to the corresponding components of the wavefunctions (\*):

$$\psi_0 = a_i \times \begin{cases} [j_0(kr) + A_0 h_0^{(1)}(kr)] \equiv (\sin kr - iA_0 e^{ikr})/kr, & \text{for } R \leq r, \\ B_0 j_0(k'r) \equiv B_0 \sin k'r/k'r, & \text{for } r \leq R. \end{cases}$$

For these components, the usual boundary conditions at  $r = R$  yield two linear equations for the coefficients  $A_0$  and  $B_0$ ,

$$(\sin kR - iA_0 e^{ikR})/k = B_0 \sin k'R/k', \quad \cos kR + A_0 e^{ikR} = B_0 \cos k'R,$$

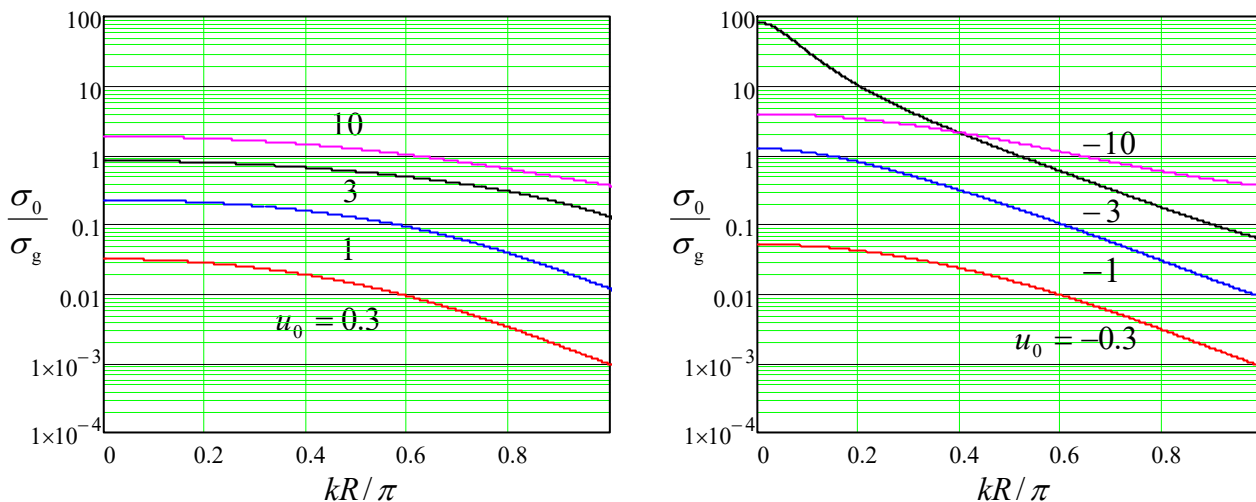
whose solution yields, in particular:

$$A_0 = \frac{k' \sin kR \cos k'R - k \cos kR \sin k'R}{k \sin k'R + ik' \cos k'R} e^{-ikR},$$

so the second of Eqs. (3.231), with  $l = 0$ , gives

$$\sigma_0 = \frac{4\pi}{k^2} |A_0|^2 \equiv \frac{4\sigma_g}{(kR)^2} |A_0|^2 = \frac{4\sigma_g}{(kR)^2} \left| \frac{k' \sin kR \cos k'R - k \cos kR \sin k'R}{k \sin k'R + ik' \cos k'R} \right|^2. \quad (**)$$

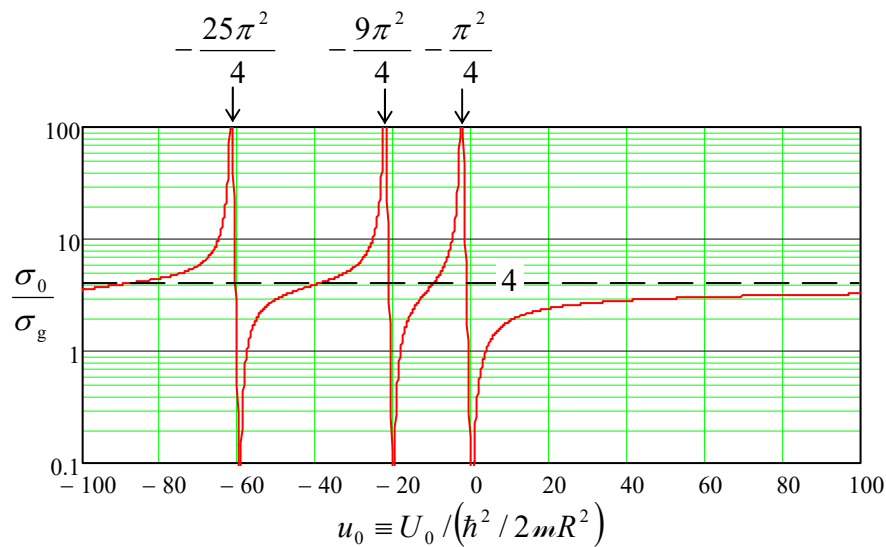
Now reviewing the above calculation, we see that it remains valid in the case  $U_0 > E$  when  $k'$  is imaginary ( $k' = i\kappa$  with real  $\kappa$ , so  $\sin k'r = i \sin \kappa r$ ,  $e^{ikr} = e^{-\kappa r}$ , etc.), so Eq. (\*\*) may be used for any value of  $U_0$ . This result is plotted in the figure below, as a function of the dimensionless product  $kR \propto E^{1/2}$ , for several positive and negative values of the dimensionless parameter  $u_0 \equiv U_0/(\hbar^2/2mR^2)$ .



As the plots show, the energy dependences of  $\sigma_0$  are rather uneventful, showing a fast decrease of this cross-section's component as  $kR$  becomes larger than  $\sim\pi$ . (It does not make much sense to analyze this dependence at higher energies in detail, because here the actual total cross-section  $\sigma$  may be significantly contributed by other spherical-harmonic components  $\sigma_l$  with  $l > 0$  – see, e.g., Fig. 3.25b of the lecture notes.) However, as the plots show, the low-energy scattering (which is dominated by the calculated  $\sigma_0$  for almost all values of  $U_0$ ) has a rather non-trivial dependence on this parameter in the region  $U_0 < 0$ , where  $\sigma \approx \sigma_0$  may be much larger than the “visible” cross-section  $\sigma_g \equiv \pi R^2$  of the sphere. Indeed, in the limit  $kR \rightarrow 0$ , we may readily simplify Eq. (\*\*) to get

$$\frac{\sigma_0}{\sigma_g} \rightarrow 4 \left| 1 - \frac{\tan k'R}{k'R} \right|^2;$$

the figure below shows this result as a function of  $U_0$ , which in this limit equals  $-\hbar^2 k'^2/2m$ .



The plot shows that at  $U_0 > 0$  (i.e. when the spherical scatterer is a flat-top potential “bump”), the cross-section monotonically grows from the Born-approximation value  $(4/9)u_0^2 \sigma_g \ll \sigma_g$  (which was calculated in the solution of Problem 9), to the asymptotic value  $4\sigma_g$  that was calculated and discussed in Sec. 3.8 of the lecture notes – see, e.g., Fig. 3.25b. However, at  $U_0 < 0$ , i.e. when the scatterer is a potential well, the cross-section, on its way to the same asymptotic value  $4\sigma_g$ , exhibits a series of sharp (formally, infinite) resonances at the values  $U_0 = -U_n$ , where

$$U_n \equiv \frac{\pi^2 \hbar^2}{8mR^2} (2n-1)^2, \quad \text{with } n = 1, 2, 3, \dots, \quad \text{i.e. at } k'R = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}, \dots \quad (***)$$

The physics of these resonances (also belonging to the group of Ramsauer-Townsend effects) is that, as was discussed in the model solution of Problem 28, a sufficiently deep potential well, with  $|U_0| < U_n$ , has  $n$  localized  $s$ -states. As  $U_0$  approaches  $-U_n$ , the eigenenergy  $E_n$  of the highest ( $n^{\text{th}}$ ) localized state tends to zero, and the effective radius  $R_{\text{ef}}$  of its eigenfunction tends to infinity. Naturally, such an extended state strongly interacts with the long de Broglie wave of the incident low-energy particle, with the scattering's cross-section  $\sigma \sim R_{\text{ef}}^2 \rightarrow \infty$ .

Note that other contributions  $\sigma_l$  to the cross-section also exhibit similarly sharp resonances at the corresponding values of  $U_0$ ; in close vicinity of such resonance for some  $l > 0$ , the corresponding contribution may become larger than  $\sigma_0$  and dominate the total cross-section  $\sigma$ . The analysis of these resonances by using Eq. (\*) may be carried out absolutely similarly to the above calculation of  $\sigma_0$  but leads to bulkier formulas because it involves the spherical Bessel functions with higher  $l$ .

**Problem 3.49.** Use the finite difference method with the step  $h = a/2$  to calculate as many energy levels as possible, for a particle confined to the interior of:

- (i) a square with sides  $a$ , and
- (ii) a cube with sides  $a$ ,

with hard walls. For the square, repeat the calculations by using the finer step  $h = a/3$ . Compare the results for different values of  $h$  with each other and with the exact formulas.

*Hint:* It is advisable to either first solve (or review the solution of) the similar 1D Problem 1.18, or start from reading about the finite difference method.<sup>215</sup> Also: try to exploit the symmetry of the systems.

*Solutions:*

(i) The simplest 2D finite-difference approximation of  $\nabla^2 \psi(x, y)$  is<sup>216</sup>

$$\frac{\psi(x-h, y) + \psi(x+h, y) + \psi(x, y-h) + \psi(x, y+h) - 4\psi(x, y)}{h^2},$$

where  $h$  is the spatial step (the “mesh size”). For  $h = a/2$ , the only natural choice of the five involved points is shown in the figure on the right. Taking into account that due to the boundary conditions, the values of  $\psi$  at all these points except for the central point A, i.e. on the walls of the confining square, vanish, the finite-difference version of the 2D stationary Schrödinger equation reads

$$-\frac{\hbar^2}{2m} \frac{0 + 0 + 0 + 0 - 4\psi_A}{h^2} = E\psi_A,$$

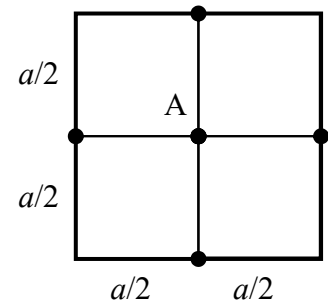
Canceling  $\psi_A \neq 0$  and plugging in  $h = a/2$ , we get

$$E = 8 \frac{\hbar^2}{ma^2}.$$

This value has to be compared with the exact result for the ground state, which follows from the 2D version of Eq. (1.86) with  $n_x = n_y = 1$ :

$$E_{1,1} = \pi^2 \frac{\hbar^2}{2ma^2} (1^2 + 1^2) \equiv \pi^2 \frac{\hbar^2}{ma^2}.$$

We see that the relative error of the numerical method, with this very crude “mesh”, is about 20% ( $8 \leftrightarrow \pi^2 \approx 9.87$ ).



<sup>215</sup> See, e.g., CM Sec. 8.5 or EM Sec. 2.11.

<sup>216</sup> See, e.g., CM Eq. (8.66) or EM Eq. (2.221).



For the finer step  $h = a/3$ , due to the obvious symmetry of the square problem (see the figure on the right), we may distinguish four significantly different (linearly independent) modes:

$$\begin{aligned}(1, 1): \psi_A &= \psi_B = \psi_C = \psi_D, \\(1, 2): \psi_A &= \psi_B = -\psi_C = -\psi_D, \\(2, 1): \psi_A &= -\psi_B = \psi_C = -\psi_D, \\(2, 2): \psi_A &= -\psi_B = -\psi_C = \psi_D.\end{aligned}$$

Here the numbers in the parentheses correspond to the values of quantum numbers  $n_x$  and  $n_y$  in the analytical solution of the problem (see Sec. 1.7 of the lecture notes),

$$\psi(x, y) = \frac{2}{a^2} \sin \frac{\pi n_x x}{a} \sin \frac{\pi n_y y}{a},$$

that have similar wavefunction symmetries.

These relations enable us to solve the problem, for each mode, by writing a finite difference equation for just one internal point, e.g., point A. For example, for the lowest (1, 1) mode, the stationary Schrödinger equation becomes

$$-\frac{\hbar^2}{2m} \left( \frac{0 + \psi_B + \psi_C + 0 - 4\psi_A}{h^2} \right) \equiv -\frac{\hbar^2}{2m} \left( \frac{0 + \psi_A + \psi_A + 0 - 4\psi_A}{h^2} \right) = E_{1,1} \psi_A.$$

From this equation (with  $h = a/3$ ) we get

$$E_{1,1} = 9 \frac{\hbar^2}{ma^2}.$$

This is a substantially better approximation of the exact result than what we had with the initial step  $h = a/2$ , with an error below 10%.

In the same way, for the (1, 2) mode we get

$$-\frac{\hbar^2}{2m} \left( \frac{0 + \psi_B + \psi_C + 0 - 4\psi_A}{h^2} \right) \rightarrow -\frac{\hbar^2}{2m} \left( \frac{0 + \psi_A - \psi_A + 0 - 4\psi_A}{h^2} \right) = E_{1,2} \psi_A,$$

giving the following result:

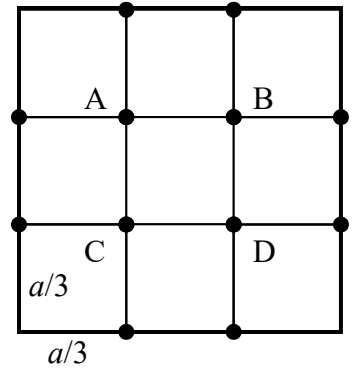
$$E_{1,2} = 18 \frac{\hbar^2}{ma^2}.$$

For the mode (2, 1), we evidently get the same result:  $E_{2,1} = E_{1,2}$ , indicating that this energy level is doubly degenerate – just as it is in the exact theory. However, the above numerical value of the eigenenergy for these excited states is much farther from the exact result,

$$E_{1,2} = \frac{\pi^2 \hbar^2}{2ma^2} (1^2 + 2^2) \approx 24.6 \frac{\hbar^2}{ma^2},$$

than for the ground state: the relative error here is ~35% instead of ~10%.

This trend (at fixed step size) continues as we go to higher energy levels. Indeed, for the highest mode (2, 2) that we can describe with the mesh so coarse, we get



$$-\frac{\hbar^2}{2m} \left( \frac{0 + \psi_B + \psi_C + 0 - 4\psi_A}{h^2} \right) \rightarrow -\frac{\hbar^2}{2m} \left( \frac{0 - \psi_A - \psi_A + 0 - 4\psi_A}{h^2} \right) = E_{2,2} \psi_A,$$

resulting in

$$E_{2,2} = 27 \frac{\hbar^2}{ma^2}$$

– a rather mediocre approximation of the exact result

$$E_{2,2} = \frac{\pi^2 \hbar^2}{2ma^2} (2^2 + 2^2) \approx 39.5 \frac{\hbar^2}{ma^2}.$$

So, we may clearly see the general trend: a finite-difference scheme with  $n$  internal points allows us to find  $n$  eigenstates, with a better accuracy achieved for the states with lower-energy states – because they have more smooth wavefunctions.

(ii) In 3D, the calculation is similar, besides that now the Laplace operator is approximated as<sup>217</sup>

$$\nabla^2 \psi(x, y, z) \approx \frac{1}{h^2} \times \left\{ \begin{array}{l} \psi(x-h, y, z) + \psi(x+h, y, z) + \psi(x, y-h, z) \\ + \psi(x, y+h, z) + \psi(x, y, z-h) + \psi(x, y, z+h) - 6\psi(x, y, z) \end{array} \right\}.$$

The result for the crudest step  $h = a/2$ ,

$$E = 12 \frac{\hbar^2}{ma^2},$$

is ~20% off the exact value given by Eq. (1.86) with  $n_x = n_y = n_z = 1$ :

$$E_{1,1,1} = \pi^2 \frac{\hbar^2}{2ma^2} (1^2 + 1^2 + 1^2) \approx 14.8 \frac{\hbar^2}{ma^2}.$$

<sup>217</sup> See, e.g., EM Eq. (2.222).

## Chapter 4. Bra-ket Formalism

**Problem 4.1.** Prove that if  $\hat{A}$  and  $\hat{B}$  are linear operators, and  $C$  is a  $c$ -number, then:

- (i)  $(\hat{A}^\dagger)^\dagger = \hat{A}$ ;                      (ii)  $(C\hat{A})^\dagger = C^* \hat{A}^\dagger$ ;                      (iii)  $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger \hat{A}^\dagger$ ;  
 (iv) the operators  $\hat{A}\hat{A}^\dagger$  and  $\hat{A}^\dagger \hat{A}$  are Hermitian.

*Solutions:* In order to prove that two operators are equivalent, it is sufficient to prove that all their matrix elements in some full and orthonormal basis  $\{u\}$  are equal. For Task (i), this is very simple to do using Eq. (4.25) of the lecture notes twice (back and forth), and the fact that for any  $c$ -number, in particular any quantum-mechanical bracket,  $(c^*)^* = c$ :

$$\langle u_j | (\hat{A}^\dagger)^\dagger | u_{j'} \rangle = \langle u_{j'} | \hat{A}^\dagger | u_j \rangle^* = \left( \langle u_j | \hat{A} | u_{j'} \rangle^* \right)^* = \langle u_j | \hat{A} | u_{j'} \rangle,$$

thus proving the corresponding operator relation.

For Task (ii), the calculation may be similar, by taking into account that according to Eq. (4.19), any  $c$ -number multipliers may be moved into/out of any bra-ket combination at will, and that for any two  $c$ -numbers,  $(c_1 c_2)^* = c_1^* c_2^*$ :

$$\begin{aligned} \langle u_j | (C\hat{A})^\dagger | u_{j'} \rangle &= \langle u_{j'} | (C\hat{A}) | u_j \rangle^* = \left( C \langle u_{j'} | \hat{A} | u_j \rangle \right)^* = C^* \langle u_{j'} | \hat{A} | u_j \rangle^* \\ &= C^* \langle u_j | \hat{A}^\dagger | u_{j'} \rangle = \langle u_j | (C^* \hat{A}^\dagger) | u_{j'} \rangle. \end{aligned}$$

Note that the proved operator relation may be formulated verbally: for  $c$ -numbers, the Hermitian conjugation is reduced to the complex conjugation.

The proof requested in Task (iii) is also similar but a bit longer, involving the use of the closure relation (4.44) twice – back and forth:

$$\begin{aligned} \langle u_j | (\hat{A}\hat{B})^\dagger | u_{j'} \rangle &= \langle u_{j'} | \hat{A}\hat{B} | u_j \rangle^* = \sum_{j''} \left( \langle u_{j'} | \hat{A} | u_{j''} \rangle \langle u_{j''} | \hat{B} | u_j \rangle \right)^* = \sum_{j''} \langle u_{j'} | \hat{A} | u_{j''} \rangle^* \langle u_{j''} | \hat{B} | u_j \rangle^* \\ &= \sum_{j''} \langle u_{j''} | \hat{B} | u_j \rangle^* \langle u_{j'} | \hat{A} | u_{j''} \rangle^* = \sum_{j''} \langle u_j | \hat{B}^\dagger | u_{j''} \rangle \langle u_{j''} | \hat{A}^\dagger | u_{j'} \rangle = \langle u_j | \hat{B}^\dagger \hat{A}^\dagger | u_{j'} \rangle. \end{aligned}$$

Finally, for Task (iv), we may simply use the relations proved in Tasks (ii) and (iii) to show that both operator products in question do satisfy the Hermitian operator's definition (4.22):

$$(\hat{A}\hat{A}^\dagger)^\dagger = (\hat{A}^\dagger)^\dagger \hat{A}^\dagger = \hat{A}\hat{A}^\dagger, \quad (\hat{A}^\dagger \hat{A})^\dagger = \hat{A}^\dagger (\hat{A}^\dagger)^\dagger = \hat{A}^\dagger \hat{A}.$$

**Problem 4.2.** Prove that for any linear operators  $\hat{A}, \hat{B}, \hat{C}$ , and  $\hat{D}$ ,

$$[\hat{A}\hat{B}, \hat{C}\hat{D}] = \hat{A}\{\hat{B}, \hat{C}\}\hat{D} - \hat{A}\hat{C}\{\hat{B}, \hat{D}\} + \{\hat{A}, \hat{C}\}\hat{D}\hat{B} - \hat{C}\{\hat{A}, \hat{D}\}\hat{B}.$$

*Solution:* By using the associative law of multiplication, i.e. the legitimate ability to remove parentheses just as in the usual scalar products, we may represent the left-hand side of the equality in question as

$$(\hat{A}\hat{B})(\hat{C}\hat{D}) - (\hat{C}\hat{D})(\hat{A}\hat{B}) = \hat{A}\hat{B}\hat{C}\hat{D} - \hat{C}\hat{D}\hat{A}\hat{B},$$

and its right-hand side as

$$\begin{aligned} & \hat{A}(\hat{B}\hat{C} + \hat{C}\hat{B})\hat{D} - \hat{A}\hat{C}(\hat{B}\hat{D} + \hat{D}\hat{B}) + (\hat{A}\hat{C} + \hat{C}\hat{A})\hat{D}\hat{B} - \hat{C}(\hat{A}\hat{D} + \hat{D}\hat{A})\hat{B} \\ & = \hat{A}\hat{B}\hat{C}\hat{D} + \hat{A}\hat{C}\hat{B}\hat{D} - \hat{A}\hat{C}\hat{B}\hat{D} - \hat{A}\hat{C}\hat{D}\hat{B} + \hat{A}\hat{C}\hat{D}\hat{B} + \hat{C}\hat{A}\hat{D}\hat{B} - \hat{C}\hat{A}\hat{D}\hat{B} - \hat{C}\hat{D}\hat{A}\hat{B}. \end{aligned}$$

All adjacent terms of the last form, besides the first one and the last one, mutually cancel and we arrive at the same expression as for the left-hand side.

**Problem 4.3.** Calculate all possible binary products  $\sigma_j\sigma_{j'}$  ( $j, j' = x, y, z$ ) of the Pauli matrices defined by Eqs. (4.105) of the lecture notes:

$$\sigma_x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

and their commutators and anticommutators (defined similarly to those of the corresponding operators). Summarize the results by using the Kronecker delta and Levi-Civita permutation symbols.<sup>218</sup>

*Solution:* A straightforward multiplication of the matrices, by using the basic rule (4.52), yields

$$\begin{aligned} \sigma_x\sigma_y &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} \equiv i\sigma_z, & \sigma_y\sigma_x &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} \equiv -i\sigma_z, \\ \sigma_x^2 &\equiv \sigma_x\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \equiv \mathbf{I}. \end{aligned}$$

Acting absolutely similarly, for other pairs of indices we get

$$\sigma_y\sigma_z = i\sigma_x, \quad \sigma_z\sigma_y = -i\sigma_x, \quad \sigma_z\sigma_x = i\sigma_y, \quad \sigma_x\sigma_z = -i\sigma_y, \quad \sigma_y^2 = \sigma_z^2 = \mathbf{I}.$$

From here, the commutator of  $\sigma_x$  and  $\sigma_y$  is

$$[\sigma_x, \sigma_y] \equiv \sigma_x\sigma_y - \sigma_y\sigma_x = 2i\sigma_z;$$

similarly, we get

$$[\sigma_y, \sigma_z] = 2i\sigma_x, \quad [\sigma_z, \sigma_x] = 2i\sigma_y.$$

So, the index swap on the left-hand side of any of these relations changes the sign of its right-hand side; also, the self-commutators  $[\sigma_j, \sigma_j]$  are equal to zero by definition. All these results may be conveniently summarized using the Levi-Civita and the Kronecker delta symbols:

$$\sigma_j\sigma_{j'} = i \sum_{j''=1}^3 \sigma_{j''} \varepsilon_{jjj''} + \mathbf{I} \delta_{jj'}, \quad [\sigma_j, \sigma_{j'}] = 2i \sum_{j''=1}^3 \sigma_{j''} \varepsilon_{jjj''}, \quad (*)$$

<sup>218</sup> See, e.g., MA Eqs. (13.1) and (13.2).

where the indices  $j$  and  $j'$  may take any values of the set  $\{1, 2, 3\}$ .

The same matrix products may be readily used to calculate their anticommutators:

$$\{\sigma_j, \sigma_{j'}\} \equiv \sigma_j \sigma_{j'} + \sigma_{j'} \sigma_j = 2I \delta_{jj'}.$$

**Problem 4.4.** Calculate the following expressions,

(i)  $(\mathbf{c} \cdot \boldsymbol{\sigma})^n$ , and then

(ii)  $(bI + \mathbf{c} \cdot \boldsymbol{\sigma})^n$ ,

for the scalar product  $\mathbf{c} \cdot \boldsymbol{\sigma}$  of the Pauli vector's matrix  $\boldsymbol{\sigma} \equiv \mathbf{n}_x \sigma_x + \mathbf{n}_y \sigma_y + \mathbf{n}_z \sigma_z$  by an arbitrary  $c$ -number geometric vector  $\mathbf{c}$ , where  $n$  is a non-negative integer  $c$ -number and  $b$  is an arbitrary scalar  $c$ -number.

*Hint:* For Task (ii), you may like to use the binomial theorem<sup>219</sup> and then transform the result to a form enabling you to use the same theorem backward.

*Solutions:*

(i) First, let us calculate

$$\begin{aligned} (\mathbf{c} \cdot \boldsymbol{\sigma})^2 &\equiv (c_x \sigma_x + c_y \sigma_y + c_z \sigma_z)(c_x \sigma_x + c_y \sigma_y + c_z \sigma_z) \\ &= c_x^2 \sigma_x^2 + c_y^2 \sigma_y^2 + c_z^2 \sigma_z^2 + c_x c_y \{\sigma_x, \sigma_y\} + c_y c_z \{\sigma_y, \sigma_z\} + c_z c_x \{\sigma_z, \sigma_x\}. \end{aligned}$$

From the results of the previous problem, this expression is just

$$c_x^2 I + c_y^2 I + c_z^2 I \equiv c^2 I,$$

where  $c$  is the modulus of the vector  $\mathbf{c}$ . Now we can use this result to calculate the expression (i):

$$(\mathbf{c} \cdot \boldsymbol{\sigma})^n = \begin{cases} [(\mathbf{c} \cdot \boldsymbol{\sigma})^2]^{n/2} = (c^2 I)^{n/2} = c^n I, & \text{for even } n, \\ (\mathbf{c} \cdot \boldsymbol{\sigma})^{n-1} \mathbf{c} \cdot \boldsymbol{\sigma} = (c^{n-1} I) \mathbf{c} \cdot \boldsymbol{\sigma} = c^n \frac{\mathbf{c} \cdot \boldsymbol{\sigma}}{c}, & \text{for odd } n. \end{cases}$$

(ii) Here we can first use the binomial theorem and then the above result of Task (i):

$$(bI + \mathbf{c} \cdot \boldsymbol{\sigma})^n = \sum_{k=0}^n {}^n C_k (bI)^{n-k} (\mathbf{c} \cdot \boldsymbol{\sigma})^k = \sum_{k=0}^n {}^n C_k b^{n-k} \times \begin{cases} c^k I, & \text{for even } k, \\ c^k \frac{\mathbf{c} \cdot \boldsymbol{\sigma}}{c}, & \text{for odd } k. \end{cases}$$

This is already the answer, but we may use the sign-alternating property of the factor  $(-1)^k$  to represent it in a more regular form:

$$\sum_{k=0}^n {}^n C_k b^{n-k} c^k \left[ \frac{I + \mathbf{c} \cdot \boldsymbol{\sigma} / c}{2} + (-1)^k \frac{I - \mathbf{c} \cdot \boldsymbol{\sigma} / c}{2} \right] \equiv \frac{I + \mathbf{c} \cdot \boldsymbol{\sigma} / c}{2} \sum_{k=0}^n {}^n C_k b^{n-k} c^k + \frac{I - \mathbf{c} \cdot \boldsymbol{\sigma} / c}{2} \sum_{k=0}^n {}^n C_k b^{n-k} (-c)^k.$$

This transform enables us to apply the binomial theorem again, now backward, to each of the two sums on the right-hand side of the last expression, and get the final result in a more compact form:

<sup>219</sup> See, e.g. MA Eq. (2.9).

$$(b\mathbf{I} + \mathbf{c} \cdot \boldsymbol{\sigma})^n = \frac{\mathbf{I} + \mathbf{c} \cdot \boldsymbol{\sigma} / c}{2} (b+c)^n + \frac{\mathbf{I} - \mathbf{c} \cdot \boldsymbol{\sigma} / c}{2} (b-c)^n = \frac{(b+c)^n + (b-c)^n}{2} \mathbf{I} + \frac{(b+c)^n - (b-c)^n}{2} \frac{\mathbf{c} \cdot \boldsymbol{\sigma}}{c}.$$

Note that this result is very general (and hence very important) because *any*  $2 \times 2$  matrix may be represented in the form  $(b\mathbf{I} + \mathbf{c} \cdot \boldsymbol{\sigma})$  – see Eq. (4.106) of the lecture notes.

**Problem 4.5.** Use the solution of the previous problem to derive Eqs. (2.191) of the lecture notes for the transparency  $\mathcal{T}$  of the Dirac comb – a system of  $N$  similar, equidistant, delta-functional potential barriers.

*Solution:* As was discussed in Sec. 2.7 of the lecture notes, the transparency may be found as  $|T_{11}|^{-2}$ , where  $T$  is the transfer matrix (2.190) of the system:

$$T = \underbrace{T_a T_a T_a \dots T_a}_{N+(N-1) \text{ operands}}, \quad \text{with } T_a = \begin{pmatrix} 1 - i\alpha & -i\alpha \\ i\alpha & 1 + i\alpha \end{pmatrix}, \quad \text{and } T_a = \begin{pmatrix} e^{ika} & 0 \\ 0 & e^{-ika} \end{pmatrix}.$$

First of all, let us notice that an addition of one more operand  $T_a$  to the front of this product, turning it into a pure power of the product  $T_a T_a$ , adds only a phase multiplier to the only matrix element we need:

$$T_{11}^+ \equiv \left\{ (T_a T_a)^N \right\}_{11} = (T_a T_a)_{11} = \left\{ \begin{pmatrix} e^{ika} & 0 \\ 0 & e^{-ika} \end{pmatrix} \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \right\}_{11} = \begin{pmatrix} T_{11} e^{ika} & T_{12} e^{ika} \\ T_{21} e^{-ika} & T_{22} e^{-ika} \end{pmatrix}_{11} = T_{11} e^{ika},$$

while not changing the modulus of this element, and hence the resulting expression for transparency. Thus, it is sufficient for us to calculate the matrix  $T^+ \equiv (T_a T_a)^N$ .

Now let us spell out the elementary product of this expression:

$$T_a T_a = \begin{pmatrix} e^{ika} & 0 \\ 0 & e^{-ika} \end{pmatrix} \begin{pmatrix} 1 - i\alpha & -i\alpha \\ i\alpha & 1 + i\alpha \end{pmatrix} \equiv \begin{pmatrix} (1 - i\alpha)e^{ika} & -i\alpha e^{ika} \\ i\alpha e^{-ika} & (1 + i\alpha)e^{-ika} \end{pmatrix}.$$

As any  $2 \times 2$  matrix, this one may be represented as a linear combination of the three Pauli matrices and the identity matrix, with certain  $c$ -number coefficients:

$$T_a T_a = b\mathbf{I} + \mathbf{c} \cdot \boldsymbol{\sigma} \equiv \begin{pmatrix} b + c_z & c_x - ic_y \\ c_x + ic_y & b - c_z \end{pmatrix}.$$

In our case, a comparison of the two last-displayed equalities yields

$$b = \cos ka + \alpha \sin ka, \quad c_x = \alpha \sin ka, \quad c_y = \alpha \cos ka, \quad c_z = i(\sin ka - \alpha \cos ka).$$

Next, by using the natural notation  $c$  for the modulus of the  $c$ -number vector  $\mathbf{c}$ , we may readily calculate

$$b^2 - c^2 \equiv b^2 - (c_x^2 + c_y^2 + c_z^2) = (\cos ka + \alpha \sin ka)^2 - [(\alpha \sin ka)^2 + (\alpha \cos ka)^2 - (\sin ka - \alpha \cos ka)^2] \equiv 1.$$

Hence, if we consider Eq. (2.191b) of the lecture notes,

$$\cos qa = \cos ka + \alpha \sin ka, \quad (*)$$

the definition of  $q$ , then  $b = \cos qa$ , and

$$c^2 = b^2 - 1 = \cos^2 qa - 1 = (\pm i \sin qa)^2.$$

Hence we may take  $c = \pm i \sin qa$  with either sign, so

$$b + c = e^{\pm iqa}, \quad b - c = e^{\mp iqa}.$$

Now we may use the result obtained in Task (ii) of the previous problem, with the notation replacement  $n \rightarrow N$ :

$$T^+ = (bI + \mathbf{c} \cdot \boldsymbol{\sigma})^N = \frac{(b+c)^N + (b-c)^N}{2} I + \frac{(b+c)^N - (b-c)^N}{2} \frac{\mathbf{c} \cdot \boldsymbol{\sigma}}{c} = I \cos Nqa \pm i \frac{\mathbf{c} \cdot \boldsymbol{\sigma}}{c} \sin Nqa.$$

From here, for the only (top left) matrix element we are interested in, we get:

$$\begin{aligned} T_{11}^+ &= \cos Nqa \pm i \frac{(\mathbf{c} \cdot \boldsymbol{\sigma})_{11}}{c} \sin Nqa = \cos Nqa \pm i \frac{c_x (\sigma_x)_{11} + c_y (\sigma_y)_{11} + c_z (\sigma_z)_{11}}{c} \sin Nqa \\ &= \cos Nqa \pm i \frac{c_z}{c} \sin Nqa = \cos Nqa + i \frac{\sin ka - \alpha \sin ka}{\sin qa} \sin Nqa. \end{aligned}$$

Since, per Eq. (\*),  $q$  is always either purely real or purely imaginary, the first term of the last sum is always purely real while the second one is purely imaginary. (As soon as  $\sin Nqa$  becomes imaginary, so does  $\sin qa$ .) Thus we may write

$$\mathcal{F} = |T_{11}|^{-2} = |T_{11}^+|^{-2} = \left[ (\cos Nqa)^2 + \left( \frac{\sin ka - \alpha \sin ka}{\sin qa} \sin Nqa \right)^2 \right]^{-1},$$

thus proving Eq. (2.191a). As we have seen in Sec. 2.7, this expression is very convenient for exploring the basic features of resonant tunneling and the 1D band theory.

**Problem 4.6.** Use the solution of Problem 4(i) to spell out the following matrix:  $\exp\{i\theta \mathbf{n} \cdot \boldsymbol{\sigma}\}$ , where  $\boldsymbol{\sigma}$  is the 3D vector (4.117) of the Pauli matrices,  $\mathbf{n}$  is a  $c$ -number geometric vector of unit length, and  $\theta$  is a  $c$ -number scalar.

*Solution:* As was discussed in Sec. 4.6 of the lecture notes, operator functions and hence matrix functions (such as the exponential function in this problem) are defined by their Taylor expansions. In our current case,

$$\exp\{i\theta \mathbf{n} \cdot \boldsymbol{\sigma}\} \equiv \sum_{k=0}^{\infty} \frac{1}{k!} (i\theta \mathbf{n} \cdot \boldsymbol{\sigma})^k = \sum_{\substack{k=0 \\ (k \text{ even})}}^{\infty} \frac{1}{k!} (i\theta)^k (\mathbf{n} \cdot \boldsymbol{\sigma})^k + i\theta \mathbf{n} \cdot \boldsymbol{\sigma} \sum_{\substack{k=1 \\ (k \text{ odd})}}^{\infty} \frac{1}{k!} (i\theta)^{k-1} (\mathbf{n} \cdot \boldsymbol{\sigma})^{k-1}.$$

All powers of the product  $\mathbf{n} \cdot \boldsymbol{\sigma}$  in both these sums are even, and hence, according to the solution of Problem 4(i), are equal to the identity matrix  $I$ . Thus the above expression is reduced to

$$I \sum_{\substack{k=0 \\ (k \text{ even})}}^{\infty} \frac{1}{k!} (i\theta)^k + i\theta \mathbf{n} \cdot \boldsymbol{\sigma} \sum_{\substack{k=1 \\ (k \text{ odd})}}^{\infty} \frac{1}{k!} (i\theta)^{k-1} \equiv I \sum_{\substack{k=0 \\ (k \text{ even})}}^{\infty} \frac{(-1)^{k/2}}{k!} \theta^k + i\theta \mathbf{n} \cdot \boldsymbol{\sigma} \sum_{\substack{k=1 \\ (k \text{ odd})}}^{\infty} \frac{(-1)^{(k-1)/2}}{k!} \theta^{k-1}.$$

But the last two sums are the Taylor expansions, at the point  $\theta = 0$ , of the functions  $\cos\theta$  and  $\sin\theta$ , respectively, so, finally,

$$\exp\{i\theta \mathbf{n} \cdot \boldsymbol{\sigma}\} = I \cos\theta + i\mathbf{n} \cdot \boldsymbol{\sigma} \sin\theta.$$

Of course, we could expect in advance that the matrix in question might be represented by a linear combination of  $I$  and  $\mathbf{n} \cdot \boldsymbol{\sigma}$ ; however, it is remarkable how simple the coefficients in this combination are.

**Problem 4.7.** Use the solution of Problem 4(ii) to calculate  $\exp\{A\}$ , where  $A$  is an arbitrary  $2 \times 2$  matrix.

*Solution:* As was discussed in Sec. 4.6 of the lecture notes, analytical functions of the linear operators (and hence of their matrices, in any basis) are defined by their Taylor expansions, with coefficients similar to those of  $c$ -number functions. In particular,

$$\exp\{A\} \equiv \sum_{n=0}^{\infty} \frac{1}{n!} A^n.$$

As was discussed in Sec. 4.4 of the lecture notes, any  $2 \times 2$  matrix may be represented in the form  $(bI + \mathbf{c} \cdot \boldsymbol{\sigma})$ , where  $b$  is a scalar  $c$ -number, and  $\mathbf{c}$  is a geometric vector with three  $c$ -number Cartesian components. Using such representation for the matrix  $A$ , we get

$$\exp\{A\} = \sum_{n=0}^{\infty} \frac{1}{n!} (bI + \mathbf{c} \cdot \boldsymbol{\sigma})^n.$$

Now using the result of Problem 4(ii), we may write

$$\begin{aligned} \exp\{A\} &= \sum_{n=0}^{\infty} \frac{1}{n!} \left[ \frac{(b+c)^n + (b-c)^n}{2} I + \frac{(b+c)^n - (b-c)^n}{2} \frac{\mathbf{c} \cdot \boldsymbol{\sigma}}{c} \right] \\ &\equiv \frac{I}{2} \left[ \sum_{n=0}^{\infty} \frac{1}{n!} (b+c)^n + \sum_{n=0}^{\infty} \frac{1}{n!} (b-c)^n \right] + \frac{\mathbf{c} \cdot \boldsymbol{\sigma}}{2c} \left[ \sum_{n=0}^{\infty} \frac{1}{n!} (b+c)^n - \sum_{n=0}^{\infty} \frac{1}{n!} (b-c)^n \right], \end{aligned}$$

where  $c \equiv (c_x^2 + c_y^2 + c_z^2)^{1/2}$ . The sums in the last expression are just the “usual” ( $c$ -number) exponents of  $(b \pm c)$ , so we finally get

$$\begin{aligned} \exp\{A\} &= \frac{I}{2} (\exp\{b+c\} + \exp\{b-c\}) + \frac{\mathbf{c} \cdot \boldsymbol{\sigma}}{2c} (\exp\{b+c\} - \exp\{b-c\}) \equiv e^b \left( I \cosh c + \frac{\mathbf{c} \cdot \boldsymbol{\sigma}}{c} \sinh c \right) \\ &\equiv e^b \begin{pmatrix} \cosh c + \frac{c_z}{c} \sinh c & \frac{c_x - ic_y}{c} \sinh c \\ \frac{c_x + ic_y}{c} \sinh c & \cosh c - \frac{c_z}{c} \sinh c \end{pmatrix}. \end{aligned}$$

As a sanity check, in the particular case when  $A = i\theta \mathbf{n} \cdot \boldsymbol{\sigma}$ , i.e. if  $b = 0$  and  $\mathbf{c} = i\theta \mathbf{n}$  (i. e.  $c = i\theta$ ,  $c_x/c = \mathbf{n}_x$ , etc.), the last expression reduces to



$$e^0 \begin{pmatrix} \cosh(i\theta) + \mathbf{n}_z \sinh(i\theta) & (\mathbf{n}_x - i\mathbf{n}_y) \sinh(i\theta) \\ (\mathbf{n}_x + i\mathbf{n}_y) \sinh(i\theta) & \cosh(i\theta) - \mathbf{n}_z \sinh(i\theta) \end{pmatrix} \equiv \mathbf{I} \cosh(i\theta) + \mathbf{n} \cdot \boldsymbol{\sigma} \sinh(i\theta) \equiv \mathbf{I} \cos \theta + i\mathbf{n} \cdot \boldsymbol{\sigma} \sin \theta,$$

i.e. to the result that was already obtained in the solution of the previous problem.

**Problem 4.8.** Express all elements of the matrix  $B \equiv \exp\{A\}$  explicitly via those of the  $2 \times 2$  matrix  $A$ . Spell out your result for the following matrices:

$$A = \begin{pmatrix} a & a \\ a & a \end{pmatrix}, \quad A' = \begin{pmatrix} i\varphi & i\varphi \\ i\varphi & i\varphi \end{pmatrix},$$

with real  $a$  and  $\varphi$ .

*Solution:* According to the solution of the previous problem, the elements of the matrix  $B$  are

$$\begin{aligned} B_{11} &= e^b \left( \cosh c + \frac{c_z}{c} \sinh c \right), & B_{12} &= e^b \frac{c_x - ic_y}{c} \sinh c, \\ B_{21} &= e^b \frac{c_x + ic_y}{c} \sinh c, & B_{22} &= e^b \left( \cosh c - \frac{c_z}{c} \sinh c \right). \end{aligned} \quad (*)$$

In that problem, the argument matrix  $A$  was taken in the form

$$A = b\mathbf{I} + \mathbf{c} \cdot \boldsymbol{\sigma} \equiv b \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + c_x \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + c_y \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + c_z \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \equiv \begin{pmatrix} b + c_z & c_x - ic_y \\ c_x + ic_y & b - c_z \end{pmatrix}.$$

Comparing each matrix element of the last form with its explicit notation,

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix},$$

and solving the resulting simple system of four linear equations, we get

$$b = \frac{A_{11} + A_{22}}{2}, \quad c_x = \frac{A_{12} + A_{21}}{2}, \quad c_y = i \frac{A_{12} - A_{21}}{2}, \quad c_z = \frac{A_{11} - A_{22}}{2}, \quad (**)$$

so the combinations participating in Eq. (\*) are as follows:

$$c_x + ic_y = A_{21}, \quad c_x - ic_y = A_{12},$$

$$c \equiv (c_x^2 + c_y^2 + c_z^2)^{1/2} = \frac{1}{2} \left[ (A_{12} + A_{21})^2 - (A_{12} - A_{21})^2 + (A_{11} - A_{22})^2 \right]^{1/2} \equiv \frac{1}{2} \left[ 4A_{12}A_{21} + (A_{11} - A_{22})^2 \right]^{1/2}.$$

For the first particular matrix given in the problem's assignment (with all  $A_{jj} = a$ ), these relations give

$$b = c_x = a, \quad c_y = c_z = 0, \quad c = a,$$

so Eqs. (\*) yield

$$B_{11} = B_{22} = e^a \cosh a \equiv \frac{e^{2a} + 1}{2}, \quad B_{12} = B_{21} = e^a \sinh a \equiv \frac{e^{2a} - 1}{2}.$$

Note that the off-diagonal elements are “boosted” by the exponential operation less than the diagonal ones.

For the second particular matrix (with all  $A'_{jj'} = i\varphi$ ), the general relations (\*\*\*) give

$$b' = c'_x = i\varphi, \quad c'_y = c'_z = 0, \quad c' = i\varphi,$$

so in this case, Eqs. (\*) yield

$$B'_{11} = B'_{22} = e^{i\varphi} \cos \varphi \equiv \frac{e^{2i\varphi} + 1}{2}, \quad B'_{12} = B'_{21} = ie^{i\varphi} \sin \varphi \equiv \frac{e^{2i\varphi} - 1}{2}.$$

**Problem 4.9.** Prove that for arbitrary square matrices A and B,

$$\text{Tr}(AB) = \text{Tr}(BA).$$

Is each diagonal element  $(AB)_{jj}$  necessarily equal to  $(BA)_{jj}$ ?

*Solution:* Using the definition (4.96), and then Eq. (4.52) of the lecture notes, we get

$$\text{Tr}(AB) \equiv \sum_j (AB)_{jj} = \sum_{j,j'} A_{jj'} B_{j'j}.$$

This sum evidently does not depend on the operand order, i.e. does not change if we swap A and B.

However, single diagonal elements of the two products,

$$(AB)_{jj} = \sum_{j'} A_{jj'} B_{j'j} \quad \text{and} \quad (BA)_{jj} = \sum_{j'} B_{jj'} A_{j'j},$$

are not necessarily equal. For example, looking at the Pauli matrix products calculated in Problem 4.3, we see that

$$(\sigma_x \sigma_y)_{11} = i, \quad \text{but} \quad (\sigma_y \sigma_x)_{11} = -i, \text{ etc.}$$

**Problem 4.10.** Calculate the trace of the following  $2 \times 2$  matrix:

$$A \equiv (\mathbf{a} \cdot \boldsymbol{\sigma})(\mathbf{b} \cdot \boldsymbol{\sigma})(\mathbf{c} \cdot \boldsymbol{\sigma}),$$

where  $\boldsymbol{\sigma}$  is the Pauli vector's matrix, while  $\mathbf{a}$ ,  $\mathbf{b}$ , and  $\mathbf{c}$  are arbitrary  $c$ -number geometric vectors.

*Solution:* From the definition of the Pauli matrices (see, e.g., Eq. (4.105) of the lecture notes), we get

$$\mathbf{a} \cdot \boldsymbol{\sigma} = a_x \sigma_x + a_y \sigma_y + a_z \sigma_z = \begin{pmatrix} a_z & a_x - ia_y \\ a_x + ia_y & -a_z \end{pmatrix} \quad (*)$$

and similar expressions for two other operands. A straightforward multiplication of the last two operands yields

$$\begin{aligned}
(\mathbf{b} \cdot \boldsymbol{\sigma})(\mathbf{c} \cdot \boldsymbol{\sigma}) &= \begin{pmatrix} b_z & b_x - ib_y \\ b_x + ib_y & -b_z \end{pmatrix} \cdot \begin{pmatrix} c_z & c_x - ic_y \\ c_x + ic_y & -c_z \end{pmatrix} \\
&= \begin{pmatrix} b_z c_z + (b_x - ib_y)(c_x + ic_y) & b_z(c_x - ic_y) - (b_x - ib_y)c_z \\ (b_x + ib_y)c_z - b_z(c_x + ic_y) & (b_x + ib_y)(c_x - ic_y) + b_z c_z \end{pmatrix}.
\end{aligned} \tag{**}$$

For the calculation of  $\text{Tr}(A) \equiv A_{11} + A_{22}$ , we need only the diagonal terms of the product of matrix (\*) by matrix (\*\*); the multiplication yields

$$\begin{aligned}
A_{11} &= a_z [b_z c_z + (b_x - ib_y)(c_x + ic_y)] + (a_x - ia_y) [(b_x + ib_y)c_z - b_z(c_x + ic_y)], \\
A_{22} &= (a_x + ia_y) [b_z(c_x - ic_y) - (b_x - ib_y)c_z] - a_z [(b_x + ib_y)(c_x - ic_y) + b_z c_z].
\end{aligned}$$

Now summing these two elements, opening all parentheses, canceling the similar but opposite terms, and grouping the remaining ones, we finally get

$$\text{Tr}(A) = 2i \left[ a_x (b_y c_z - b_z c_y) + a_y (b_z c_x - b_x c_z) + a_z (b_x c_y - b_y c_x) \right] \equiv 2i \begin{vmatrix} a_x & a_y & a_z \\ b_x & b_y & b_z \\ c_x & c_y & c_z \end{vmatrix}. \tag{***}$$

A good sanity check is the invariance of the result with respect to the loop replacement of the operand vectors:  $\mathbf{a} \rightarrow \mathbf{b} \rightarrow \mathbf{c} \rightarrow \mathbf{a}$ , etc.; indeed, this feature might be predicted in advance by applying to this trace the property  $\text{Tr}(AB) = \text{Tr}(BA)$  whose proof was the subject of the previous problem:

$$\text{Tr}[(\mathbf{a} \cdot \boldsymbol{\sigma})(\mathbf{b} \cdot \boldsymbol{\sigma})(\mathbf{c} \cdot \boldsymbol{\sigma})] = \text{Tr}[(\mathbf{c} \cdot \boldsymbol{\sigma})(\mathbf{a} \cdot \boldsymbol{\sigma})(\mathbf{b} \cdot \boldsymbol{\sigma})] = \text{Tr}[(\mathbf{b} \cdot \boldsymbol{\sigma})(\mathbf{c} \cdot \boldsymbol{\sigma})(\mathbf{a} \cdot \boldsymbol{\sigma})].$$

Note also that according to Eq. (\*\*\*) , the trace vanishes if any two of the three vectors  $\mathbf{a}$ ,  $\mathbf{b}$ , and  $\mathbf{c}$  are parallel to each other.

**Problem 4.11.** Prove that the matrix trace of an arbitrary operator does not change at its unitary transformation.

*Solution:* Using the notation of Sec. 4.4 of the lecture notes for the “old” basis  $\{u\}$  and “new” basis  $\{v\}$ , for the trace in the new basis we have, by definition,

$$\text{Tr} \hat{A} \Big|_{\text{in } v} \equiv \text{Tr} A \Big|_{\text{in } v} \equiv \sum_j A_{jj} \Big|_{\text{in } v}.$$

Now we can use the general law (4.92) of the unitary transformation, and then change the summation order to get

$$\sum_j A_{jj} \Big|_{\text{in } v} = \sum_{j,k,k'} U_{jk}^\dagger A_{kk'} \Big|_{\text{in } u} U_{kj} \equiv \sum_{k,k'} A_{kk'} \Big|_{\text{in } u} \sum_j U_{jk}^\dagger U_{kj}. \tag{*}$$

In the last sum we can use the explicit expressions (4.82)-(4.84) for the unitary matrix elements (valid in any basis):

$$\sum_j U_{jk}^\dagger U_{kj} = \sum_j \langle v_j | u_k \rangle \langle u_{k'} | v_j \rangle.$$

This expression may be readily simplified by inverting both short brackets per Eq. (4.15) and then employing the completeness relation (4.44) for the identity operator:

$$\sum_j \langle v_j | u_k \rangle \langle u_{k'} | v_j \rangle = \left( \sum_j \langle u_k | v_j \rangle \langle v_j | u_{k'} \rangle \right)^* \equiv \left( \langle u_k | \sum_j | v_j \rangle \langle v_j | | u_{k'} \rangle \right)^* = \langle u_k | u_{k'} \rangle^* = \delta_{kk'}.$$

As a result, Eq. (\*) yields

$$\sum_j A_{jj} | \text{in } v \rangle = \sum_{k,k'} A_{kk'} | \text{in } u \rangle \delta_{kk'} = \sum_k A_{kk} | \text{in } u \rangle,$$

which is just the trace in the “old” basis  $u_j$ . This is why the frequently used notion of “the trace of an operator” (without specifying the basis) is quite meaningful.

**Problem 4.12.** Prove that for any two full and orthonormal bases  $\{u\}$ ,  $\{v\}$  of the same Hilbert space,

$$\text{Tr}(|u_j\rangle\langle v_{j'}|) = \langle v_{j'} | u_j \rangle.$$

*Solution:* By the definition of the trace,

$$\text{Tr}(|u_j\rangle\langle v_{j'}|) \equiv \sum_{j''} (|u_j\rangle\langle v_{j'}|)_{j''j''}.$$

Since the trace of any operator is basis-independent (see the previous problem), we may use the matrix element definition (4.47) to calculate them in any basis, for example, in  $\{u\}$ :

$$\sum_{j''} (|u_j\rangle\langle v_{j'}|)_{j''j''} = \sum_{j''} \langle u_{j''} | (|u_j\rangle\langle v_{j'}|) | u_{j''} \rangle \equiv \sum_{j''} \langle u_{j''} | u_j \rangle \langle v_{j'} | u_{j''} \rangle = \sum_{j''} \delta_{j''j} \langle v_{j'} | u_{j''} \rangle = \langle v_{j'} | u_j \rangle,$$

q.e.d.<sup>220</sup>

**Problem 4.13.** Is the 1D scattering matrix  $S$ , defined by Eq. (2.124) of the lecture notes, unitary? What about the 1D transfer matrix  $T$  defined by Eqs. (2.125)?

*Solution:* It is convenient to use Eq. (2.127a) of the lecture notes (whose proof was the subject of problem 2.11),

$$S = e^{i\theta} \begin{pmatrix} r e^{i\varphi} & t \\ t & -r e^{-i\varphi} \end{pmatrix},$$

which expresses the matrix element symmetry. From here:

$$SS^\dagger = e^{i\theta} \begin{pmatrix} r e^{i\varphi} & t \\ t & -r e^{-i\varphi} \end{pmatrix} e^{-i\theta} \begin{pmatrix} r e^{-i\varphi} & t \\ t & -r e^{i\varphi} \end{pmatrix} = \begin{pmatrix} r^2 + t^2 & 0 \\ 0 & r^2 + t^2 \end{pmatrix}.$$

<sup>220</sup> Just in case the reader has not run yet into this famous acronym: q.e.d. = *quod erat demonstrandum*, Latin for “what had to be demonstrated”.

But according to Eq. (2.127b),  $r^2 + t^2 = 1$ , so this product is just the identity matrix I, i.e. the scattering matrix is unitary – reflecting the so-called *reciprocity principle*.

For the transfer matrix T, we may use the similarly structured expression obtained in the model solution of Problem 2.15:

$$T = \frac{1}{t} \begin{pmatrix} e^{i\theta} & -re^{-i\varphi} \\ -re^{i\varphi} & e^{-i\theta} \end{pmatrix},$$

with the same relation between the real coefficients  $r$  and  $t$ . From here,

$$TT^\dagger = \frac{1}{t} \begin{pmatrix} e^{i\theta} & -re^{-i\varphi} \\ -re^{i\varphi} & e^{-i\theta} \end{pmatrix} \frac{1}{t} \begin{pmatrix} e^{-i\theta} & -re^{-i\varphi} \\ -re^{i\varphi} & e^{i\theta} \end{pmatrix} = \frac{1}{t^2} \begin{pmatrix} 1+r^2 & -2re^{i(\theta-\varphi)} \\ -2re^{-i(\theta-\varphi)} & r^2+1 \end{pmatrix}.$$

Besides the trivial case  $r = 0$  (and hence  $t = 1$ ), this product is different from I, so the matrix T is *not* unitary. Note, however, that

$$T\sigma_z T^\dagger = \frac{1}{t} \begin{pmatrix} e^{i\theta} & -re^{-i\varphi} \\ -re^{i\varphi} & e^{-i\theta} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \frac{1}{t} \begin{pmatrix} e^{-i\theta} & -re^{-i\varphi} \\ -re^{i\varphi} & e^{i\theta} \end{pmatrix} = \frac{1}{t^2} \begin{pmatrix} 1-r^2 & 0 \\ 0 & r^2-1 \end{pmatrix} = \sigma_z;$$

the matrices that obey this relation (including T) are called *anti-unitary*.

**Problem 4.14.** Calculate the trace of the following matrix:

$$\exp\{i\mathbf{a} \cdot \boldsymbol{\sigma}\} \exp\{i\mathbf{b} \cdot \boldsymbol{\sigma}\},$$

where  $\boldsymbol{\sigma}$  is the Pauli vector's matrix, while  $\mathbf{a}$  and  $\mathbf{b}$  are  $c$ -number geometric vectors.

*Solution:* Since we may always take  $\mathbf{a} = a\mathbf{n}$ , where  $\mathbf{n}$  is the unit vector in the same direction, the solution of Problem 6 (with the notation change  $\theta \rightarrow a$ ) may be rewritten as

$$\exp\{i\mathbf{a} \cdot \boldsymbol{\sigma}\} = I \cos a + i \frac{\mathbf{a} \cdot \boldsymbol{\sigma}}{a} \sin a.$$

With a similar expression for the exponent including  $\mathbf{b}$ , we get

$$\begin{aligned} \exp\{i\mathbf{a} \cdot \boldsymbol{\sigma}\} \exp\{i\mathbf{b} \cdot \boldsymbol{\sigma}\} &= \left( I \cos a + i \frac{\mathbf{a} \cdot \boldsymbol{\sigma}}{a} \sin a \right) \left( I \cos b + i \frac{\mathbf{b} \cdot \boldsymbol{\sigma}}{b} \sin b \right) \\ &\equiv I \cos a \cos b + i \left( \frac{\mathbf{a} \cdot \boldsymbol{\sigma}}{a} \sin a \cos b + \frac{\mathbf{b} \cdot \boldsymbol{\sigma}}{b} \cos a \sin b \right) - \frac{(\mathbf{a} \cdot \boldsymbol{\sigma})(\mathbf{b} \cdot \boldsymbol{\sigma})}{ab} \sin a \sin b. \end{aligned} \quad (*)$$

The first term in the last expression is a diagonal matrix, so its trace equals  $2\cos a \cos b$ . Next, since by the definition (4.105) of the Pauli matrices,

$$\mathbf{a} \cdot \boldsymbol{\sigma} = \begin{pmatrix} a_z & a_x - ia_y \\ a_x + ia_y & -a_z \end{pmatrix}, \quad \text{and} \quad \mathbf{b} \cdot \boldsymbol{\sigma} = \begin{pmatrix} b_z & b_x - ib_y \\ b_x + ib_y & -b_z \end{pmatrix}, \quad (**)$$

the traces of these matrices, and hence that of the whole second term of Eq. (\*), equal zero. Finally, the trace of the matrix product in the last term of Eq. (\*) may be readily calculated, for example, directly from Eq. (\*\*):

$$\begin{aligned} \text{Tr}[(\mathbf{a} \cdot \boldsymbol{\sigma})(\mathbf{b} \cdot \boldsymbol{\sigma})] &= \text{Tr} \begin{pmatrix} a_z b_z + (a_x - ia_y)(b_x + ib_y) & \dots \\ \dots & (a_x + ia_y)(b_x - ib_y) + a_z b_z \end{pmatrix} \\ &= 2(a_x b_x + a_y b_y + a_z b_z) \equiv 2\mathbf{a} \cdot \mathbf{b}, \end{aligned}$$

so, finally,

$$\text{Tr}(\exp\{i\mathbf{a} \cdot \boldsymbol{\sigma}\} \exp\{i\mathbf{b} \cdot \boldsymbol{\sigma}\}) = 2 \left( \cos a \cos b - \frac{\mathbf{a} \cdot \mathbf{b}}{ab} \sin a \sin b \right).$$

**Problem 4.15.** Prove the following vector-operator identity:

$$(\boldsymbol{\sigma} \cdot \hat{\mathbf{r}})(\boldsymbol{\sigma} \cdot \hat{\mathbf{p}}) = \mathbf{I} \hat{\mathbf{r}} \cdot \hat{\mathbf{p}} + i\boldsymbol{\sigma} \cdot (\hat{\mathbf{r}} \times \hat{\mathbf{p}}),$$

where  $\boldsymbol{\sigma}$  is the Pauli vector's matrix, and  $\mathbf{I}$  is the  $2 \times 2$  identity matrix.

*Hint:* Take into account that the vector operators  $\hat{\mathbf{r}}$  and  $\hat{\mathbf{p}}$  are defined in the orbital-motion Hilbert space, different from that of the Pauli vector  $\hat{\boldsymbol{\sigma}}$ , and hence commute with it – even though they do not commute with each other.

*Solution:* Perhaps the simplest way to prove this identity is first to use the definitions of the scalar and vector products to express each side via the Cartesian components of the matrices and operators. In particular, the left-hand side is

$$(\boldsymbol{\sigma} \cdot \hat{\mathbf{r}})(\boldsymbol{\sigma} \cdot \hat{\mathbf{p}}) = \sum_{j'} \sigma_{j'} \hat{r}_{j'} \sum_{j''} \sigma_{j''} \hat{p}_{j''} \equiv \sum_{j', j''} \sigma_{j'} \hat{r}_{j'} \sigma_{j''} \hat{p}_{j''}.$$

where all the sums (and all those below in this solution) run from 1 to 3. Since the Pauli matrices commute with the coordinate and momentum operators, we may swap them and continue as

$$(\boldsymbol{\sigma} \cdot \hat{\mathbf{r}})(\boldsymbol{\sigma} \cdot \hat{\mathbf{p}}) = \sum_{j', j''} (\sigma_{j'} \sigma_{j''}) \hat{r}_{j'} \hat{p}_{j''}.$$

Now using the first of Eqs. (\*) of the model solution of Problem 3, we get

$$(\boldsymbol{\sigma} \cdot \hat{\mathbf{r}})(\boldsymbol{\sigma} \cdot \hat{\mathbf{p}}) = \sum_{j, j', j''} (i\sigma_j \varepsilon_{jj''} + \mathbf{I} \delta_{jj''}) \hat{r}_{j'} \hat{p}_{j''} \equiv i \sum_{j, j', j''} \sigma_j \hat{r}_{j'} \hat{p}_{j''} \varepsilon_{jj''} + \mathbf{I} \sum_{j'} \hat{r}_{j'} \hat{p}_{j'}.$$

But this expression exactly coincides with the right-hand side of the identity in question, similarly spelled out via its Cartesian components:<sup>221</sup>

$$\mathbf{I} \hat{\mathbf{r}} \cdot \hat{\mathbf{p}} + i\boldsymbol{\sigma} \cdot (\hat{\mathbf{r}} \times \hat{\mathbf{p}}) = \mathbf{I} \sum_j \hat{r}_j \hat{p}_j + i \sum_j \sigma_j (\hat{\mathbf{r}} \times \hat{\mathbf{p}})_j = \mathbf{I} \sum_j \hat{r}_j \hat{p}_j + i \sum_{jj''} \sigma_j \hat{r}_{j'} \hat{p}_{j''} \varepsilon_{jj''},$$

so the identity is indeed valid.

Finally, notice that the proof did not use the commutation relation between  $\hat{\mathbf{r}}$  and  $\hat{\mathbf{p}}$ , so that actually, a similar identity is valid for *any* two operators that commute with  $\hat{\boldsymbol{\sigma}}$ .

<sup>221</sup> See also Eq. (5.18) of the lecture notes.

**Problem 4.16.** Let  $A_j$  be the eigenvalues of some operator  $\hat{A}$ . Express the following two sums,

$$\Sigma_1 \equiv \sum_j A_j \quad \text{and} \quad \Sigma_2 \equiv \sum_j A_j^2,$$

via the matrix elements  $A_{jj'}$  of this operator in an arbitrary basis.

*Solution:* According to Eq. (4.98) of the lecture notes, in the basis in which the operator's matrix is diagonal, the first sum is just the trace of the matrix:

$$\Sigma_1 = \sum_j A_{jj} = \text{Tr}(\mathbf{A}). \quad (*)$$

But according to the statement whose proof was the subject of Problem 11, an operator's trace does not depend on the choice of the basis, so Eq. (\*) is valid in an arbitrary basis as well, and we may write

$$\Sigma_1 = \text{Tr}(\hat{A}).$$

For the calculation of the sum  $\Sigma_2$ , we may notice that since the operators  $\hat{A}$  and  $\hat{A}^2$  commute, they share their eigenstates  $\alpha_j$ , so we may write

$$\hat{A}^2 |\alpha_j\rangle \equiv \hat{A}\hat{A} |\alpha_j\rangle = \hat{A}A_j |\alpha_j\rangle = A_j \hat{A} |\alpha_j\rangle = A_j^2 |\alpha_j\rangle.$$

This means that the eigenvalues of  $\hat{A}^2$ , corresponding to these states, are just  $A_j^2$ , so  $\Sigma_2$  is the just trace of the operator  $\hat{A}^2$ , and hence may be calculated, in an arbitrary basis, as

$$\Sigma_2 = \text{Tr}(\hat{A}^2) \equiv \sum_j (\mathbf{A}^2)_{jj} = \sum_{j,j'} A_{jj'} A_{j'j}.$$

Note also that if the operator  $\hat{A}$  is Hermitian, then  $A_{jj} = A_{jj'}^*$ , and the last expression may be further simplified:

$$\Sigma_2 = \sum_{j,j'} A_{jj'} A_{j'j}^* = \sum_{j,j'} |A_{jj'}|^2.$$

**Problem 4.17.** Calculate  $\langle \sigma_z \rangle$  of a spin- $1/2$  in the quantum state with the following ket-vector:

$$|\alpha\rangle = \text{const} \times (|\uparrow\rangle + |\downarrow\rangle + |\rightarrow\rangle + |\leftarrow\rangle),$$

where  $(\uparrow, \downarrow)$  and  $(\rightarrow, \leftarrow)$  are the eigenstates of the Pauli matrices  $\sigma_z$  and  $\sigma_x$ , respectively.

*Hint:* Double-check whether your solution is general.

*Solution:* A superficial solution to this problem stems from Eqs. (4.122) of the lecture notes, which yield in particular

$$|\rightarrow\rangle + |\leftarrow\rangle = \sqrt{2} |\uparrow\rangle,$$

so

$$|\alpha\rangle = \text{const} \times [(1 + \sqrt{2})|\uparrow\rangle + |\downarrow\rangle],$$

and after the probability normalization,

$$W_{\uparrow} = \frac{(1+\sqrt{2})^2}{(1+\sqrt{2})^2 + 1^2} \equiv \frac{3+2\sqrt{2}}{4+2\sqrt{2}}, \quad W_{\downarrow} = 1 - W_{\uparrow} = \frac{1}{4+2\sqrt{2}}.$$

we get

$$\langle \sigma_z \rangle = (+1)W_{\uparrow} + (-1)W_{\downarrow} \equiv W_{\uparrow} - W_{\downarrow} = \frac{1}{\sqrt{2}} \approx 0.707. \quad (*)$$

However, this is *not* the general solution of the problem. Indeed, during the discussion of the diagonalization of matrix  $\sigma_x$  in Sec. 4.4, it was emphasized that the coefficients  $U_{11}$  and  $U_{21}$  may be multiplied by the same phase factor  $\exp\{i\varphi_+\}$ , with an arbitrary (real)  $\varphi_+$ . The same is evidently true for the second pair of coefficients,  $U_{22}$  and  $U_{12}$ , whose phase  $\varphi_-$  may be independent of  $\varphi_+$ . As a result, the most general form of that unitary matrix is

$$U_x = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\varphi_+} & e^{i\varphi_-} \\ e^{i\varphi_+} & -e^{i\varphi_-} \end{pmatrix}.$$

From this, Eqs. (4.122) have to be generalized as

$$|\rightarrow\rangle = \frac{\exp\{i\varphi_+\}}{\sqrt{2}} (|\uparrow\rangle + |\downarrow\rangle), \quad |\leftarrow\rangle = \frac{\exp\{i\varphi_-\}}{\sqrt{2}} (|\uparrow\rangle - |\downarrow\rangle).$$

These expressions show that physically,  $\varphi_{\pm}$  are just the (arbitrary) phases of the states  $\rightarrow$  and  $\leftarrow$ , with the phases of the states  $\uparrow$  and  $\downarrow$  taken for the references.

It is easy to verify that these phases do not affect not only the probabilities of these states but also the discussion of all Stern-Gerlach experiments in Sec. 4.4 of the lecture notes, so there we could use the particular values  $\varphi_+ = \varphi_- = 0$  quite legitimately. However, the state  $\alpha$  being discussed in the current problem is affected by these phases:

$$|\alpha\rangle = C \left[ \left( 1 + \frac{e^{i\varphi_+}}{\sqrt{2}} + \frac{e^{i\varphi_-}}{\sqrt{2}} \right) |\uparrow\rangle + \left( 1 + \frac{e^{i\varphi_+}}{\sqrt{2}} - \frac{e^{i\varphi_-}}{\sqrt{2}} \right) |\downarrow\rangle \right],$$

because it is a coherent (pure) state superposition. In particular, its normalization yields

$$|C|^{-2} = \left| 1 + \frac{e^{i\varphi_+}}{\sqrt{2}} + \frac{e^{i\varphi_-}}{\sqrt{2}} \right|^2 + \left| 1 + \frac{e^{i\varphi_+}}{\sqrt{2}} - \frac{e^{i\varphi_-}}{\sqrt{2}} \right|^2 \equiv 4 + 2\sqrt{2} \cos \varphi_+,$$

so finally,

$$\langle \sigma_z \rangle = W_{\uparrow} - W_{\downarrow} = |C|^2 \left[ \left| 1 + \frac{e^{i\varphi_+}}{\sqrt{2}} + \frac{e^{i\varphi_-}}{\sqrt{2}} \right|^2 - \left| 1 + \frac{e^{i\varphi_+}}{\sqrt{2}} - \frac{e^{i\varphi_-}}{\sqrt{2}} \right|^2 \right] = \frac{\cos(\varphi_+ - \varphi_-) + \sqrt{2} \cos \varphi_-}{2 + \sqrt{2} \cos \varphi_+}.$$

For  $\varphi_+ = \varphi_- = 0$ , this expression is reduced to Eq. (\*) but generally, depending on the choice of the phases  $\varphi_+$  and  $\varphi_-$ , the calculated average  $\langle \sigma_z \rangle$  may range all the way from (+1) to (-1).



**Problem 4.18.** A spin- $\frac{1}{2}$  is fully polarized in the positive  $z$ -direction. Calculate the probabilities of the alternative outcomes of a perfect Stern-Gerlach experiment with the magnetic field oriented in an arbitrarily different direction.

*Solution:* As was discussed in Sec. 4.1 of the lecture notes, the Stern-Gerlach experiment measures the probabilities  $W_{\pm}$  of the particle's magnetic moment  $\mathbf{m}$  being oriented in the direction  $\mathbf{n}$  of the magnetic field of the SG apparatus and opposite to it. Hence  $W_{\pm}$  may be calculated using Eq. (4.120) of the lecture notes,

$$W_{\pm} = |\langle \alpha | m_{\pm} \rangle|^2, \quad (*)$$

where  $m_{\pm}$  are normalized eigenstates of the corresponding scalar operator  $\hat{m}_n \equiv \mathbf{n} \cdot \hat{\mathbf{m}}$ , and  $\alpha$  is the given state of the system – in our case, the up-polarized spin state  $\uparrow$ . As Eqs. (4.115)-(4.117) show, in the usual  $z$ -basis, the matrix of the operator  $\hat{m}_n$  is proportional to (and hence has the same eigenstates as) the matrix  $P_n \equiv \mathbf{n} \cdot \boldsymbol{\sigma}$ , where  $\boldsymbol{\sigma}$  is the Pauli vector with the Cartesian components given by Eq. (4.105):

$$\sigma_x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Taking the Cartesian components of the orientation vector  $\mathbf{n}$  in the usual polar-coordinate form,

$$n_x = \sin \theta \cos \varphi, \quad n_y = \sin \theta \sin \varphi, \quad n_z = \cos \theta,$$

where  $\theta$  and  $\varphi$  are the polar angles of the vector, we get

$$\begin{aligned} P_n \equiv \mathbf{n} \cdot \boldsymbol{\sigma} &\equiv n_x \sigma_x + n_y \sigma_y + n_z \sigma_z = \sin \theta \cos \varphi \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \sin \theta \sin \varphi \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \cos \theta \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ &\equiv \begin{pmatrix} \cos \theta & \sin \theta e^{-i\varphi} \\ \sin \theta e^{i\varphi} & -\cos \theta \end{pmatrix}. \end{aligned}$$

Now we may use the procedure discussed in Sec. 4.4 to find the eigenstates  $P_{\pm}$  of this matrix, more specifically, the coefficients  $\langle \uparrow | P_{\pm} \rangle$  and  $\langle \downarrow | P_{\pm} \rangle$  of their expansion over the  $z$ -basis states  $\uparrow$  and  $\downarrow$ . For that, first, we may use the characteristic equation (4.103), in our case taking the form

$$\begin{vmatrix} \cos \theta - P_{\pm} & \sin \theta e^{-i\varphi} \\ \sin \theta e^{i\varphi} & -\cos \theta - P_{\pm} \end{vmatrix} = 0, \quad (**)$$

to calculate the eigenvalues of the matrix:  $P_{\pm} = \pm 1$ .<sup>222</sup> Now plugging these values, one by one, into any of Eqs. (4.101), in our particular case having the form

$$\begin{aligned} (\cos \theta - P_{\pm}) \langle \uparrow | P_{\pm} \rangle + \sin \theta e^{-i\varphi} \langle \downarrow | P_{\pm} \rangle &= 0, \\ \sin \theta e^{i\varphi} \langle \uparrow | P_{\pm} \rangle + (-\cos \theta - P_{\pm}) \langle \downarrow | P_{\pm} \rangle &= 0, \end{aligned}$$

<sup>222</sup> This result could be anticipated, because as we know from Sec. 4.4 of the lecture notes, all Pauli matrices have the same eigenvalues, and they should not be affected by any rotation of the coordinate axes.

we get

$$\begin{aligned}\langle \uparrow | P_+ \rangle &= \langle \downarrow | P_+ \rangle \frac{\sin \theta}{1 - \cos \theta} e^{-i\varphi} \equiv \langle \downarrow | P_+ \rangle \frac{\cos(\theta/2)}{\sin(\theta/2)} e^{-i\varphi}, \\ \langle \uparrow | P_- \rangle &= \langle \downarrow | P_- \rangle \frac{\cos \theta - 1}{\sin \theta} e^{-i\varphi} \equiv -\langle \downarrow | P_- \rangle \frac{\sin(\theta/2)}{\cos(\theta/2)} e^{-i\varphi}.\end{aligned}$$

Now performing the normalization, i.e. requiring  $|\langle \uparrow | P_{\pm} \rangle|^2 + |\langle \downarrow | P_{\pm} \rangle|^2$  to equal 1, we get a very simple result:

$$\begin{aligned}|\langle \uparrow | P_+ \rangle| &= \cos \frac{\theta}{2}, & |\langle \downarrow | P_+ \rangle| &= \sin \frac{\theta}{2}, \\ |\langle \uparrow | P_- \rangle| &= \sin \frac{\theta}{2}, & |\langle \downarrow | P_- \rangle| &= \cos \frac{\theta}{2}.\end{aligned}$$

But according to Eq. (\*), with  $\alpha$  being the state  $\uparrow$ , the squares of the two left expressions give us the required probabilities:

$$W_+ = \cos^2 \frac{\theta}{2}, \quad W_- = \sin^2 \frac{\theta}{2}. \quad (***)$$

This is a very nontrivial<sup>223</sup> and important result (which will be used, in particular, for the discussion of the Bell inequalities in the concluding Chapter 10 of the course), so it makes sense to pass it through the most evident sanity checks. The first (the most elementary) check is that  $W_+ + W_- = 1$ , as it has to be with the sum of all possible experimental outcome probabilities.

Next, let us examine the most important particular cases. If  $\theta = 0$  (i.e. if we measure the spin along the axis of its prior polarization), then  $W_+ = 1$  and  $W_- = 0$  – quite naturally; while if  $\theta = \pi/2$  (the magnetic field is oriented along the axis  $x$ ), we get  $W_+ = W_- = 1/2$ , i.e. the result which was already obtained in the lecture notes – see the first of Eqs. (4.123) and its discussion.

Finally, we may use Eqs. (\*\*\*) and the calculated eigenvalues  $P_{\pm} = \pm 1$  to find the expectation value of the observable  $P_n \propto m_n$  from the general Eq. (1.37):

$$\langle P_n \rangle = P_+ W_+ + P_- W_- = \cos^2 \frac{\theta}{2} - \sin^2 \frac{\theta}{2} \equiv \cos \theta.$$

But the same expectation value may be found simpler, from Eq. (4.125), with the long bracket calculated directly in the  $z$ -basis:

$$\langle P_n \rangle = \langle \uparrow | \hat{P} | \uparrow \rangle = (1, 0) \begin{pmatrix} \cos \theta & \sin \theta e^{-i\varphi} \\ \sin \theta e^{i\varphi} & -\cos \theta \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \cos \theta.$$

So, Eq. (\*\*\*) yields sensible results. A forthcoming discussion in Sec. 5.1 of the lecture notes will enable us to re-derive this formula in a much simpler way – see Problem 5.1.

<sup>223</sup> Naively, one might expect the probability  $W_+$  to be equal to the square of the  $z$ -component  $n_z$  of the vector  $\mathbf{n}$ , i.e. to  $\cos^2 \theta$ . The result given by Eqs. (\*\*\*) is, of course, very much different.

Problem 4.19. In a certain basis, the Hamiltonian of a two-level system is described by the matrix

$$H = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix}, \quad \text{with } E_1 \neq E_2,$$

while the operator of some observable  $A$  of this system, by the following matrix:

$$A = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}.$$

Calculate possible results of measurements of the observable  $A$ , and also the probabilities of the corresponding measurement outcomes for the system's state with the energy definitely equal to  $E_1$ .

*Solution:* Let us calculate the eigenvalues of the operator of the observable  $A$  and also its eigenvectors and in the given basis. For this observable, the system of equations (4.101)-(4.102) becomes

$$\begin{aligned} (1 - A_j)U_{1j} + U_{2j} &= 0, \\ U_{1j} + (1 - A_j)U_{2j} &= 0, \end{aligned} \quad (*)$$

so the characteristic equation (4.103) of their consistency is

$$\begin{vmatrix} 1 - A_j & 1 \\ 1 & 1 - A_j \end{vmatrix} \equiv (1 - A_j)^2 - 1 = 0.$$

Its (very easy :- ) solution yields two roots  $A_j$ :  $A_1 = 0$  and  $A_2 = 2$ ; these are the possible results of measurements of the observable  $A$ .

Now plugging these eigenvalues, one by one, into any equation of the system (\*), for the unitary matrix elements we get

$$U_{11} = -U_{21}, \quad U_{12} = U_{22},$$

so after the proper normalization (4.104), and setting the inconsequential phases to zero, we get<sup>224</sup>

$$U_{11} = -U_{21} = \frac{1}{\sqrt{2}}, \quad U_{12} = U_{22} = \frac{1}{\sqrt{2}}. \quad (**)$$

According to Eqs. (4.82)-(4.83), the obtained unitary transfer matrix elements  $U_{kj}$  (with the indices  $k$  and  $j$  taking, in our case, values 1 and 2) are just the short brackets  $\langle u_k | a_j \rangle$  participating in the expansion,

$$| a_j \rangle = \sum_k \langle u_k | a_j \rangle | u_j \rangle,$$

of the eigenstates of the operator  $\hat{A}$  over the states  $u_1$  and  $u_2$  of the given basis. Hence Eq. (\*\*) means that

<sup>224</sup> You may have noticed that these results coincide with those obtained in Sec. 4.4 of the lecture notes for the Pauli matrix  $\sigma_x$  in the usual  $z$ -basis. This is not surprising, because the given matrix  $A$  is proportional to the sum of  $\sigma_x$  and the identity matrix  $I$  – which is diagonal in any basis and thus cannot affect diagonalization results.

$$|a_1\rangle = \frac{1}{\sqrt{2}}(|u_1\rangle - |u_2\rangle), \quad |a_2\rangle = \frac{1}{\sqrt{2}}(|u_1\rangle + |u_2\rangle),$$

with the reciprocal transform

$$|u_1\rangle = \frac{1}{\sqrt{2}}(|a_1\rangle + |a_2\rangle), \quad |u_2\rangle = \frac{1}{\sqrt{2}}(-|a_1\rangle + |a_2\rangle). \quad (***)$$

Now, since the matrix  $H$  is diagonal in the given basis, and the system's energy  $E$  equals one of its eigenvalues (namely,  $E_1$ ), the system is definitely in the corresponding eigenstate,  $u_1$ . As the first of Eqs. (\*\*\*) shows, in this state, the probability of measuring each eigenvalue of  $A$  is 50%.

**Problem 4.20.** Three states  $u_{1,2,3}$  form a full and orthonormal basis of a system with the following Hamiltonian:

$$\hat{H} = -\delta (|u_1\rangle\langle u_2| + |u_2\rangle\langle u_3| + |u_3\rangle\langle u_1|) + \text{h.c.},$$

where  $\delta$  is a real constant, while h.c. means the Hermitian conjugate of the previous expression. Calculate its stationary states and energy levels. Can you relate this system to any other(s) discussed earlier in the course?

*Solution:* According to Eq. (4.159) of the lecture notes, the stationary states  $a_{1,2,3}$  and the energy levels  $E_{1,2,3}$  of the system are just the eigenstates and eigenvalues of the system's Hamiltonian, so the problem is reduced to the diagonalization of the Hamiltonian matrix  $H$ . According to the assignment, and Eq. (4.59), in the  $u_{1,2,3}$  basis, the matrix has the form

$$H = -\delta \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix},$$

so its characteristic equation (4.103) is

$$\begin{vmatrix} -\varepsilon & -1 & -1 \\ -1 & -\varepsilon & -1 \\ -1 & -1 & -\varepsilon \end{vmatrix} = 0, \quad \text{where } \varepsilon \equiv \frac{E}{\delta}.$$

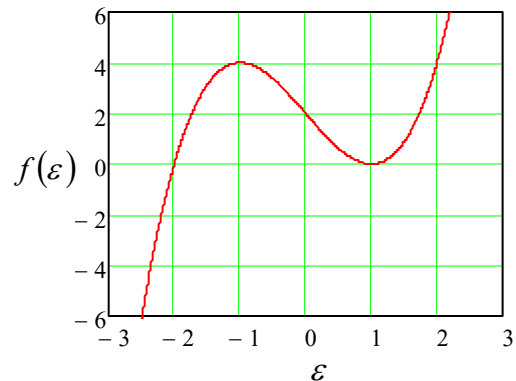
This equality gives a cubic equation for  $\varepsilon$ :

$$f(\varepsilon) \equiv \varepsilon^3 - 3\varepsilon + 2 = 0;$$

fortunately, the equation is so simple that its roots may be readily guessed (and then verified by their substitution into the equation) just by looking either at the equation itself or at the plot of the function on its left-hand side – see the figure on the right:

$$\varepsilon_1 = -2, \quad \varepsilon_{2,3} = +1.$$

In order to calculate the corresponding eigenstates  $a_{1,2,3}$  of the Hamiltonian, i.e. the coefficients in the expansions of its ket-vectors in the basis  $u_{1,2,3}$ :



$$\begin{aligned}
|a_1\rangle &= U_{11}|u_1\rangle + U_{21}|u_2\rangle + U_{31}|u_3\rangle, \\
|a_2\rangle &= U_{12}|u_1\rangle + U_{22}|u_2\rangle + U_{32}|u_3\rangle, \\
|a_3\rangle &= U_{13}|u_1\rangle + U_{23}|u_2\rangle + U_{33}|u_3\rangle,
\end{aligned}
\tag{*}$$

we need to plug in the calculated values  $\varepsilon_{1,2,3}$ , one by one, into the system of equations (4.101) for our matrix H. For the first root,  $\varepsilon_1 = -2$ , the system is

$$\begin{aligned}
+2U_{11} - U_{21} - U_{31} &= 0, \\
-U_{11} + 2U_{22} - U_{31} &= 0, \\
-U_{11} - U_{22} + 2U_{31} &= 0.
\end{aligned}$$

It is evidently satisfied with any set of equal coefficients,  $U_{11} = U_{21} = U_{31}$ . Thus, requiring the set to be normalized in accordance with Eq. (4.104), we may spell out the first of Eqs. (\*) as follows:<sup>225</sup>

$$|a_1\rangle = \frac{1}{\sqrt{3}}(|u_1\rangle + |u_2\rangle + |u_3\rangle). \tag{**}$$

For the (equal) 2<sup>nd</sup> and 3<sup>rd</sup> roots,  $\varepsilon_{2,3} = +1$ , all equations of the system (\*) looks similarly:

$$-U_{1j} - U_{2j} - U_{3j} = 0, \quad \text{with } j = 2, 3. \tag{***}$$

Due to the symmetry of these equations with respect to the rotation of the first indices of the coefficients  $U_{kj}$ , it is natural to assume that the solutions differ only by a constant phase multiplier, i.e. to look for the solutions in the form

$$U_{kj} = U_0 \exp\{ik\alpha\}. \tag{****}$$

Evidently, the change of  $k$  by 3 has to give the initial value  $U_{kj}$ , perhaps besides an inconsequential phase multiplier  $\exp\{i2\pi n\}$ , with any integer  $n$ . This requirement immediately yields just three physically distinguishable values of  $\alpha$  on the  $[-\pi, +\pi]$  segment: 0 and  $\pm 2\pi/3$ . The first of them does not satisfy Eq. (\*\*\*),<sup>226</sup> but two others do, because

$$U_{1j} + U_{2j} + U_{3j} = U_0 \exp\left\{\pm i \frac{2\pi}{3}\right\} + U_0 \exp\left\{\pm i 2 \frac{2\pi}{3}\right\} + U_0 \exp\left\{\pm i 3 \frac{2\pi}{3}\right\} \equiv 0,$$

for any  $U_0$  and any sign of the arguments. This means that the two eigenstates corresponding to the degenerate eigenvalue  $\varepsilon_{2,3} = 1$ , may be taken, for example, in the form<sup>227</sup>

<sup>225</sup> As a reminder: according to Eq. (4.104), all coefficients of the string  $U_{12}, U_{21}, U_{31}$ , and hence the ket-vector  $|a_1\rangle$  as the whole, may be multiplied by coefficients  $\exp\{i\varphi_1\}$ , with an arbitrary real phase shift  $\varphi_1$ . The same is true for each of the two other eigenkets; for each of them, the phase shift may be individual.

<sup>226</sup> Note, however, that the solution (\*\*\*\*) with this  $\alpha = 0$  does describe our first eigenstate (\*\*).

<sup>227</sup> Since these stationary states correspond to the same eigenenergy  $E = 2\delta$ , any of their linear combinations is also a stationary state. Remember, however, that for applications, it is important to keep such linear combinations orthogonal, i.e. their inner product (4.11) equal to zero. (It is straightforward to verify that the above states  $a_{1,2,3}$  do satisfy this requirement.)

$$|a_2\rangle = \frac{1}{\sqrt{3}} \left( |u_1\rangle + \exp\left\{i\frac{2\pi}{3}\right\} |u_2\rangle + \exp\left\{-i\frac{2\pi}{3}\right\} |u_3\rangle \right) \equiv \frac{1}{\sqrt{3}} \left( |u_1\rangle + \frac{-1+i\sqrt{3}}{2} |u_2\rangle + \frac{-1-i\sqrt{3}}{2} |u_3\rangle \right),$$

$$|a_3\rangle = \frac{1}{\sqrt{3}} \left( |u_1\rangle + \exp\left\{-i\frac{2\pi}{3}\right\} |u_2\rangle + \exp\left\{i\frac{2\pi}{3}\right\} |u_3\rangle \right) \equiv \frac{1}{\sqrt{3}} \left( |u_1\rangle + \frac{-1-i\sqrt{3}}{2} |u_2\rangle + \frac{-1+i\sqrt{3}}{2} |u_3\rangle \right).$$

To summarize, all three eigenenergies of this system

$$E_1 = -2\delta, \quad E_{2,3} = +\delta,$$

correspond to the states of the type (\*\*\*) , with different phase shifts  $\alpha$ :  $\alpha_1 = 0$  and  $\alpha_{2,3} = \pm 2\pi/3$ . But this is exactly the result that was obtained in Problem 3.15 for three similar and similarly coupled potential wells (say, located in the vertices of an equilateral triangle) within the tight-binding limit. In this particular physical implementation of our Hamiltonian,  $u_{1,2,3}$  have the physical sense of the particle's localized states inside the corresponding wells.

**Problem 4.21.** Guided by Eq. (2.203) of the lecture notes, and by the solutions of the previous problem and also of Problem 3.15, suggest a Hamiltonian describing particle's dynamics in an infinite 1D chain of similar potential wells within the tight-binding approximation, in the bra-ket formalism. Verify that its eigenstates and eigenvalues correspond to those discussed in Sec. 2.7.

*Solution:* Inspired by the identity of solutions of the previous problem and Problem 3.15, which gave similar sets of eigenstates and eigenvalues, we may readily guess the effective Hamiltonian describing the system in the vicinity of the  $n^{\text{th}}$  localized level:

$$\hat{H}_n = E_n \sum_k |u_k\rangle \langle u_k| - \delta_n \left( \sum_k |u_k\rangle \langle u_{k+1}| + \text{h.c.} \right),$$

where the state  $u_k$  describes the particle's position in the  $k^{\text{th}}$  well. Indeed, in the basis of these states, the (formally, infinite) matrix of this Hamiltonian is *tri-diagonal*:

$$H = \begin{pmatrix} \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & E_n & -\delta_n & 0 & 0 & 0 & \dots \\ \dots & -\delta_n & E_n & -\delta_n & 0 & 0 & \dots \\ \dots & 0 & -\delta_n & E_n & -\delta_n & 0 & \dots \\ \dots & 0 & 0 & -\delta_n & E_n & -\delta_n & \dots \\ \dots & 0 & 0 & 0 & -\delta_n & E_n & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix},$$

so for its eigenstates  $a_j$  (i.e. the coefficients  $U_{kj}$  of their expansion in the series

$$|a_j\rangle = \sum_k \langle u_k | a_j \rangle |u_k\rangle \equiv \sum_k U_{kj} |u_k\rangle$$

over the basis states  $u_k$ ) and eigenvalues  $E_j$ , Eqs. (4.101)-(4.102) of the lecture notes give the following infinite system of equations,

$$-\delta_n U_{(k-1)j} + (E_n - E_j)U_{kj} - \delta_n U_{(k+1)j} = 0. \quad (*)$$

Looking for the solution of this system in the Bloch-wave form,<sup>228</sup>

$$U_{kj} = U_0 \exp\{ik\Delta\varphi_j\},$$

we immediately get the dispersion relation (2.206):

$$E_j = E_n - 2\delta_n \cos \Delta\varphi_j.$$

In this infinite system, the phase shift (i.e. the dimensionless quasimomentum)  $\Delta\varphi_j$  may take any real values.<sup>229</sup>

**Problem 4.22.** In a certain full and orthonormal basis of three states  $u_{1,2,3}$ , operators  $\hat{A}$  and  $\hat{B}$  are defined by the following equalities:

$$\hat{A}|u_1\rangle = |u_3\rangle, \quad \hat{A}|u_2\rangle = |u_2\rangle, \quad \hat{A}|u_3\rangle = |u_1\rangle; \quad \hat{B}|u_1\rangle = |u_1\rangle, \quad \hat{B}|u_2\rangle = 0, \quad \hat{B}|u_3\rangle = -|u_3\rangle.$$

(i) Prove that the operators  $\hat{A}^2$  and  $\hat{B}$  commute and form an orthonormal basis of their common eigenstates.

(ii) Give the most general expression for the matrix (in the  $u$ -basis) of an operator that would commute with  $\hat{B}$ .

*Solutions:*

(i) Per the assignment, the matrices of operators  $\hat{A}$  and  $\hat{B}$  in the  $u$ -basis are as follows:

$$A = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

From here, we may readily calculate the matrix of the operator  $\hat{A}^2$ :

$$A^2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \equiv I.$$

Hence,  $\hat{A}^2$  is just the identity operator and as such, it commutes with any other operator, including  $\hat{B}$ .

This also means that to complete Task (i), it is sufficient to calculate the eigenstates of the operator  $\hat{B}$  alone. But the matrix of this operator in the  $u$ -basis is already diagonal, so the states  $u_{1,2,3}$  of this basis are its eigenstates (with the eigenvalues, respectively, 1, 0, and  $-1$ ), and, per the assignment, these states are already orthonormal.

<sup>228</sup> If necessary, please revisit Eq. (2.193) of the lecture notes and its discussion in Sec. 2.7.

<sup>229</sup> Note, however, that for any such chain of a finite length, the spectrum of possible values of the shift is discrete (and equidistant) – see, e.g., CM Section 6.4.

(ii) Let us consider the most general (in the given three-functional  $u$ -basis) matrix  $M$ :

$$M = \begin{pmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{pmatrix},$$

and calculate its commutator with the given matrix  $B$ :

$$\begin{aligned} [M, B] &\equiv MB - BM = \begin{pmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} - \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{pmatrix} \\ &= \begin{pmatrix} M_{11} & 0 & -M_{13} \\ M_{21} & 0 & -M_{23} \\ M_{31} & 0 & -M_{33} \end{pmatrix} - \begin{pmatrix} M_{11} & M_{12} & M_{13} \\ 0 & 0 & 0 \\ -M_{31} & -M_{32} & -M_{33} \end{pmatrix} = \begin{pmatrix} 0 & -M_{12} & 0 \\ M_{21} & 0 & -M_{23} \\ 0 & M_{32} & 0 \end{pmatrix}. \end{aligned}$$

In order for  $M$  and  $B$  to commute, all elements of the last matrix have to vanish, so the most general form of the qualifying matrix  $M$  is

$$M = \begin{pmatrix} M_{11} & 0 & M_{13} \\ 0 & M_{22} & 0 \\ M_{31} & 0 & M_{33} \end{pmatrix}.$$

**Problem 4.23.** Calculate the eigenvectors and the eigenvalues of the following matrices:

$$A = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$

*Solutions:* Solving the characteristic equation (Eq. (4.103) of the lecture notes) for matrix  $A$ ,

$$\begin{vmatrix} -A & 1 & 0 \\ 1 & -A & 1 \\ 0 & 1 & -A \end{vmatrix} = 0, \quad \text{giving } A^3 - 2A = 0,$$

we are getting three roots (the matrix eigenvalues)  $A_j$ :  $A_1 = 0$  and  $A_{2,3} = \pm\sqrt{2}$ . Now we should plug these values, one by one, into the system of equations (4.101) for the elements  $U_{kj} \equiv \langle u_k | a_j \rangle$  of the unitary matrix  $U$  performing the transformation from the states  $u_{1,2,3}$  of the initial basis (in that the matrix  $A$  has the given form) to the eigenstates (with number  $j$ ):

$$|a_j\rangle = U_{1j}|u_1\rangle + U_{2j}|u_2\rangle + U_{3j}|u_3\rangle.$$

For our matrix  $A$ , the system is



$$\begin{aligned}
-A_j U_{1j} + U_{2j} &= 0, \\
U_{1j} - A_j U_{2j} + U_{3j} &= 0, \\
U_{2j} - A_j U_{3j} &= 0.
\end{aligned}
\tag{*}$$

For the first eigenvalue,  $A_j = A_1 = 0$ , the top and the bottom equations immediately yield  $U_{21} = 0$ , so the middle one yields  $U_{11} = -U_{31}$ . The requirement for the vector  $U_{k1}$  to be normalized (see Eq. (4.104) of the lecture notes), may be satisfied by setting  $U_{11} = 1/\sqrt{2}$ ,  $U_{31} = -1/\sqrt{2}$ .

For the second and third eigenvalues,  $A_{2,3} = \pm\sqrt{2}$ , which differ only by the sign, Eqs. (\*) are reduced to two very similar systems of equations:

$$\begin{aligned}
-\sqrt{2}U_{12} + U_{22} &= 0, & \sqrt{2}U_{13} + U_{23} &= 0, \\
U_{12} - \sqrt{2}U_{22} + U_{32} &= 0, & U_{13} + \sqrt{2}U_{23} + U_{33} &= 0, \\
-U_{22} - \sqrt{2}U_{32} &= 0, & -U_{23} + \sqrt{2}U_{33} &= 0,
\end{aligned}$$

The top and the bottom equations of these systems immediately yield  $U_{12} = -U_{32} = U_{22}/\sqrt{2}$  and  $U_{33} = -U_{13} = U_{23}/\sqrt{2}$ , so the normalization conditions for these two vectors may be satisfied by taking  $U_{22} = U_{23} = 1/\sqrt{2}$ ,  $U_{12} = U_{33} = 1/2$ , and  $U_{32} = U_{13} = -1/2$ . So, the eigenvectors of the matrix are:

$$|a_1\rangle = \frac{1}{\sqrt{2}}(|u_1\rangle - |u_2\rangle), \quad |a_2\rangle = \frac{1}{2}(|u_1\rangle + \sqrt{2}|u_2\rangle - |u_3\rangle), \quad |a_3\rangle = \frac{1}{2}(-|u_1\rangle + \sqrt{2}|u_2\rangle + |u_3\rangle).$$

For matrix B, the characteristic equation is

$$\begin{vmatrix} -B & 0 & 0 & 1 \\ 0 & -B & 1 & 0 \\ 0 & 1 & -B & 0 \\ 1 & 0 & 0 & -B \end{vmatrix} = 0, \quad \text{giving } B^4 - 2B^2 + 1 = 0.
\tag{**}$$

This is just a quadratic equation for  $B^2$ , with two equal roots  $B^2 = 1$ , so the four eigenvalues  $B_j$  of the matrix are

$$B_{1,2} = +1, \quad B_{3,4} = -1.$$

The system of equations (4.101), corresponding to matrix B, is

$$\begin{aligned}
-BU_{1j} + U_{4j} &= 0, \\
-BU_{2j} + U_{3j} &= 0, \\
U_{2j} - BU_{3j} &= 0, \\
U_{1j} - BU_{4j} &= 0,
\end{aligned}
\tag{***}$$

where  $U_{kj} \equiv \langle u_k | a_j \rangle$ , with the indices  $k$  and  $j$  taking values from 1 to 4, are the elements of the unitary matrix performing the transformation from the states  $u_k$  of the initial basis to the eigenvector corresponding to the eigenvalue  $B_j$ :

$$|b_j\rangle = U_{1j}|u_1\rangle + U_{2j}|u_2\rangle + U_{3j}|u_3\rangle + U_{4j}|u_4\rangle.$$

Plugging the first value,  $B = B_1 = 1$ , into Eq. (\*\*), we get  $U_{11} = U_{41}$  and  $U_{21} = U_{31}$ . The result for the equal eigenvalue  $B_2$  is of course similar:  $U_{12} = U_{42}$  and  $U_{22} = U_{32}$ , so the first two linearly independent eigenkets may be constructed, for example, by taking  $U_{21} = U_{31} = 0$  and  $U_{12} = U_{42} = 0$ , giving (after the elementary normalization),

$$|b_1\rangle = \frac{1}{\sqrt{2}}(|u_1\rangle + |u_4\rangle), \quad |b_2\rangle = \frac{1}{\sqrt{2}}(|u_2\rangle + |u_3\rangle).$$

Due to the degeneracy of the corresponding eigenvalues  $B_1 = B_2 = 1$ , not only these kets (multiplied by arbitrary phase factors) but also any pair of their linearly-independent superpositions is also a legitimate eigenvector.

For the two remaining eigenvalues  $B_{3,4} = -1$ , the possible eigenstates are similar, with just the opposite signs in the relations between nonvanishing matrix elements, so we may take

$$|b_3\rangle = \frac{1}{\sqrt{2}}(|u_1\rangle - |u_4\rangle), \quad |b_4\rangle = \frac{1}{\sqrt{2}}(|u_2\rangle - |u_3\rangle),$$

with similar alternative options.

Note that the initial states participate in the final expressions for  $|b_j\rangle$  only as couples  $\{u_1, u_4\}$  and  $\{u_2, u_3\}$ ; this becomes natural from a fresh look at the matrix B: it describes non-zero coupling only between the states within each of these groups.

**Problem 4.24.** A certain state  $\gamma$  is an eigenstate of each of two operators  $\hat{A}$  and  $\hat{B}$ . What can be said about the corresponding eigenvalues  $a$  and  $b$ , if the operators anticommute?

*Solution:* Let us use the definition (4.34) of the anticommutator to write

$$\{\hat{A}, \hat{B}\}|\gamma\rangle \equiv \hat{A}\hat{B}|\gamma\rangle + \hat{B}\hat{A}|\gamma\rangle.$$

Since  $\gamma$  is an eigenstate of each of the operators, we may use Eqs. (4.68) and then (4.19) to proceed as follows:

$$\{\hat{A}, \hat{B}\}|\gamma\rangle = \hat{A}b|\gamma\rangle + \hat{B}a|\gamma\rangle = b\hat{A}|\gamma\rangle + a\hat{B}|\gamma\rangle = ba|\gamma\rangle + ab|\gamma\rangle = 2ab|\gamma\rangle. \quad (*)$$

But the anticommutation of operators  $\hat{A}$  and  $\hat{B}$  means that

$$\{\hat{A}, \hat{B}\} = \hat{0},$$

where  $\hat{0}$  is the null operator defined by Eq. (4.35). It turns each state it acts upon into the null state; in particular,

$$\{\hat{A}, \hat{B}\}|\gamma\rangle = |0\rangle. \quad (**)$$

Since the assignment implies that  $\gamma$  is a really existing (not a null-) state, Eqs. (\*) and (\*\*) may be reconciled only if

$$ab = 0,$$

i.e. if at least one of these eigenvalues equals zero.

**Problem 4.25.** An operator  $\hat{A}$  commutes with each of two other operators  $\hat{B}$  and  $\hat{C}$ , but these two operators do not commute:  $[\hat{B}, \hat{C}] \neq 0$ . Prove that the full set of eigenvalues of the operator  $\hat{A}$  includes some degenerate ones.

*Solution:* Let us consider an arbitrary eigenstate  $a_j$  of the operator  $\hat{A}$ . By its definition given by Eq. (4.68) of the lecture notes,

$$\hat{A}|a_j\rangle = A_j|a_j\rangle, \quad (*)$$

where  $A_j$  is the corresponding eigenvalue. Let us apply the operator  $[\hat{A}, \hat{B}]$  to this state, and then transform the second term by using Eq. (\*):

$$[\hat{A}, \hat{B}]|a_j\rangle \equiv \hat{A}\hat{B}|a_j\rangle - \hat{B}\hat{A}|a_j\rangle = \hat{A}(\hat{B}|a_j\rangle) - A_j(\hat{B}|a_j\rangle) \equiv \hat{A}|b_j\rangle - A_j|b_j\rangle, \quad \text{where } |b_j\rangle \equiv \hat{B}|a_j\rangle.$$

Per the problem's conditions, this commutator equals zero, so the above expression equals zero as well:

$$\hat{A}|b_j\rangle - A_j|b_j\rangle = 0, \quad \text{i.e. } \hat{A}|b_j\rangle = A_j|b_j\rangle.$$

This relation means that the so-formed state  $b_j$  is also an eigenstate of the operator  $\hat{A}$ , with the same eigenvalue  $A_j$ .

Now let us suppose that this  $A_j$  is a non-degenerate eigenvalue of  $\hat{A}$ . Then  $b_j$  has to coincide with  $a_j$  – perhaps besides a different  $c$ -number multiplier before its ket:

$$|b_j\rangle = B_j|a_j\rangle, \quad \text{so } \hat{B}|b_j\rangle = B_j\hat{B}|a_j\rangle = B_j|b_j\rangle,$$

i.e.  $b_j$  is an eigenstate of the operator  $\hat{B}$  as well, with some eigenvalue  $B_j$ . Acting absolutely similarly, we may also conclude that in this case, due to the condition  $[\hat{A}, \hat{C}] = 0$ , the state  $c_j$  with the ket-vector

$$|c_j\rangle \equiv \hat{C}|a_j\rangle$$

is an eigenstate of the operator  $\hat{C}$ , with a certain eigenvalue  $C_j$ . Now let us use these facts while considering the commutator of the operators  $\hat{B}$  and  $\hat{C}$ , applied to the same state  $a_j$

$$[\hat{B}, \hat{C}]|a_j\rangle \equiv \hat{B}\hat{C}|a_j\rangle - \hat{C}\hat{B}|a_j\rangle = B_jC_j|a_j\rangle - C_jB_j|a_j\rangle \equiv 0.$$

But if *all* eigenvalues of  $A_j$  were non-degenerate, such equalities would be valid for all its eigenstates  $a_j$ . Since, per the assignment, such states form a full set, an arbitrary state  $\gamma$  of this Hilbert space may be represented as their linear combination:

$$|\gamma\rangle \equiv \sum_j \gamma_j |a_j\rangle,$$

in that case, we would be able to write

$$[\hat{B}, \hat{C}]|\gamma\rangle = \sum_j \gamma_j [\hat{B}, \hat{C}]|a_j\rangle = 0, \quad \text{i.e. } [\hat{B}, \hat{C}] = 0,$$

contradicting the problem's conditions. Hence, at the given commutation relations, our assumption was wrong: at least some eigenvalues  $A_j$  have to be degenerate. Later in the course (Sec. 5.7), we will see

that this is exactly the situation existing, for example, between the operators of the Cartesian components of the angular momentum  $\mathbf{L}$ , and of its square  $L^2$ .

**Problem 4.26.** Derive the differential equation for the time evolution of the expectation value of an observable, by using (i) the Schrödinger picture and (ii) the Heisenberg picture of quantum dynamics.

*Solution:* Let us differentiate the basic Eq. (4.125) of the lecture notes over time, restoring, for clarity, the time arguments of the participating states and operators:

$$\begin{aligned} \frac{d}{dt} \langle A \rangle_{\alpha}(t) &= \left\langle \frac{\partial \alpha(t)}{\partial t} \middle| \hat{A}(t) \alpha(t) \right\rangle + \langle \alpha(t) \middle| \frac{\partial \hat{A}(t)}{\partial t} \alpha(t) \rangle + \langle \alpha(t) \middle| \hat{A}(t) \frac{\partial \alpha(t)}{\partial t} \rangle \\ &= \left\langle \frac{\partial A}{\partial t} \right\rangle_{\alpha}(t) + \left[ \frac{\partial}{\partial t} \langle \alpha(t) \middle| \hat{A}(t) \alpha(t) \rangle + \langle \alpha(t) \middle| \hat{A}(t) \left[ \frac{\partial}{\partial t} \alpha(t) \right] \right], \end{aligned}$$

where the partial time derivative of  $A$  is over the explicit time dependence of its operator. (This derivative vanishes for such time-independent operators as, for example,  $\hat{\mathbf{p}} = -i\hbar\nabla$ ,  $\nabla^2$ ,  $U(\mathbf{r})$ , etc., even if the observables they describe do evolve in time.) Now we are ready to use the two different pictures of the time evolution.

(i) In the *Schrödinger picture*, the time evolution of the bra- and ket vectors of the state is described by Eq. (4.158) and its Hermitian conjugate (with  $\hat{H}^{\dagger} = \hat{H}$ ),

$$-i\hbar \frac{\partial}{\partial t} \langle \alpha(t) | = \langle \alpha(t) | \hat{H}(t),$$

so we get

$$i\hbar \frac{d}{dt} \langle A \rangle_{\alpha}(t) - i\hbar \left\langle \frac{\partial A}{\partial t} \right\rangle_{\alpha}(t) = -\langle \alpha(t) | \hat{H}(t) \hat{A}(t) \alpha(t) \rangle + \langle \alpha(t) | \hat{A}(t) \hat{H}(t) \alpha(t) \rangle \equiv \langle \alpha(t) | [\hat{A}(t), \hat{H}(t)] \alpha(t) \rangle.$$

Since this result does not include the initial time  $t_0$ , it is usually represented in a shorter form, with not only the state of the system but also the time argument  $t$  just implied:

$$i\hbar \frac{d}{dt} \langle A \rangle = i\hbar \left\langle \frac{\partial A}{\partial t} \right\rangle + \langle [\hat{A}, \hat{H}] \rangle. \quad (*)$$

(ii) In the *Heisenberg picture*, the derivation of the same result is even simpler: it is sufficient to average both sides of Eq. (4.199) – as usual in this picture, over the statistical ensemble of initial states of the system.

In the particular but very common case when the operator  $\hat{A}$  does not depend on time explicitly, the first term on the right-hand side of Eq. (\*) vanishes. If, in addition, the commutator of this observable commutes with the Hamiltonian (at the same time instant), then  $\langle A \rangle$  remains constant in time. This is the quantum-mechanical analog of a classical integral of motion, with the commutator playing the role of the Poisson brackets.<sup>230</sup>

<sup>230</sup> See either Eqs. (4.203)-(4.205) of this course or the discussion at the end of CM Sec. 10.1.

**Problem 4.27.** At  $t = 0$ , a spin- $1/2$  whose interaction with an external field is described by the Hamiltonian

$$\hat{H} = \mathbf{c} \cdot \hat{\boldsymbol{\sigma}} \equiv c_x \hat{\sigma}_x + c_y \hat{\sigma}_y + c_z \hat{\sigma}_z$$

(where  $c_{x,y,z}$  are real  $c$ -number constants, and  $\hat{\sigma}_{x,y,z}$  are the Pauli operators) was in the state  $\uparrow$ , one of the two eigenstates of  $\hat{\sigma}_z$ . In the Schrödinger picture, calculate the time evolution of:

- (i) the ket-vector  $|\alpha\rangle$  of the spin (in any time-independent basis you like),
- (ii) the probabilities to find the spin in the states  $\uparrow$  and  $\downarrow$ , and
- (iii) the expectation values of all three Cartesian components of the spin vector.

Analyze and interpret the results for the particular case  $c_y = c_z = 0$ .

*Hint:* Think about the best basis to use for the solution.

*Solutions:*

The problem is similar to the spin precession problem that was solved in Sec. 4.6 of the lecture notes as an illustration but is a bit more complex because the  $z$ -basis is not the eigenbasis for our present Hamiltonian (unless  $c_x = c_y = 0$ , returning us to the simple spin precession problem). This is why in the general case, we cannot directly use Eqs. (4.161), at least in the  $z$ -basis. There are two simple approaches to the problem, or rather to its Task(i); their comparison is rather instructive.

Approach 1 is to stay in the  $z$ -basis (of the  $\uparrow$  and  $\downarrow$  states) and use the fact that in this basis, the Hamiltonian operator is represented by a very simple matrix:

$$H = c_x \sigma_x + c_y \sigma_y + c_z \sigma_z \equiv \begin{pmatrix} c_z & c_- \\ c_+ & -c_z \end{pmatrix}, \quad \text{where } c_{\pm} \equiv c_x \pm ic_y, \text{ so } c_{\pm} = (c_{\mp})^*, \quad c_+ c_- = c_x^2 + c_y^2.$$

Let us start with the calculation of the time-evolution operator  $\hat{u}$  of the system. In the  $z$ -basis, Eq. (4.157b) becomes the following matrix equation:

$$i\hbar \frac{d}{dt} \begin{pmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{pmatrix} = \begin{pmatrix} c_z & c_- \\ c_+ & -c_z \end{pmatrix} \begin{pmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{pmatrix} \equiv \begin{pmatrix} c_z u_{11} + c_- u_{21} & c_z u_{12} + c_- u_{22} \\ c_+ u_{11} - c_z u_{21} & c_+ u_{12} - c_z u_{22} \end{pmatrix}.$$

This system of four linear ordinary differential equations is actually a set of two independent (and similar) systems of two equations each: one for  $u_{11}$  and  $u_{21}$ , and another one for  $u_{12}$  and  $u_{22}$ . Their general solution is straightforward but a bit bulky. However, due to the initial conditions (4.178):  $u_{11} = u_{22} = 1$  and  $u_{12} = u_{21} = 0$  at  $t = t_0 \equiv 0$ , the solution simplifies to

$$\mathbf{u}(t,0) = \begin{pmatrix} \cos \frac{ct}{\hbar} - i \frac{c_z}{c} \sin \frac{ct}{\hbar} & -i \frac{c_-}{c} \sin \frac{ct}{\hbar} \\ -i \frac{c_+}{c} \sin \frac{ct}{\hbar} & \cos \frac{ct}{\hbar} + i \frac{c_z}{c} \sin \frac{ct}{\hbar} \end{pmatrix}, \quad (*)$$

where the scalar  $c$  is the length of the geometric vector  $\mathbf{c} \equiv \{c_x, c_y, c_z\}$ :

$$c^2 \equiv c_x^2 + c_y^2 + c_z^2 \equiv c_+ c_- + c_z^2.$$

(By the way, by noticing that the matrix (\*) may be represented in the form

$$\mathbf{u}(t,0) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \cos \frac{ct}{\hbar} - \frac{i}{c} \begin{pmatrix} c_z & c_- \\ c_+ & -c_z \end{pmatrix} \sin \frac{ct}{\hbar} \equiv I \cos \frac{ct}{\hbar} - \frac{i}{c} \mathbf{c} \cdot \boldsymbol{\sigma} \sin \frac{ct}{\hbar} \equiv I \cos \frac{ct}{\hbar} - \frac{i}{c} H \sin \frac{ct}{\hbar},$$

we can guess that the same equality would be also valid for the corresponding operators:

$$\hat{u}(t,0) = \hat{I} \cos \frac{ct}{\hbar} - \frac{i}{c} \hat{H} \sin \frac{ct}{\hbar},$$

regardless of the basis. This fact (which is not used in this solution, but may be useful in other cases, including the next problem) may be indeed proved in two ways: either by the direct substitution of the last relation into Eq. (4.157b), for our particular Hamiltonian, or by the Taylor expansion of its solution (4.175), with  $t_0 = 0$ . My strong recommendation to the reader is to work out both proofs, as an additional exercise.)

Now the remaining calculations are easy, using the fact that in the  $z$ -basis we are using, the initial state is represented by a simple row/column matrix of the elements 1 and 0.

(i) According to Eq. (4.157a), the ket-vector of the system evolves as

$$|\alpha(t)\rangle = \hat{u}(t,0)|\alpha(0)\rangle,$$

where in our case  $|\alpha(0)\rangle = |\uparrow\rangle$ , so in the  $z$ -basis,

$$\begin{pmatrix} \alpha_{\uparrow}(t) \\ \alpha_{\downarrow}(t) \end{pmatrix} = \mathbf{u}(t,0) \begin{pmatrix} \alpha_{\uparrow}(0) \\ \alpha_{\downarrow}(0) \end{pmatrix} = \begin{pmatrix} \cos \frac{ct}{\hbar} - i \frac{c_z}{c} \sin \frac{ct}{\hbar} & -i \frac{c_-}{c} \sin \frac{ct}{\hbar} \\ -i \frac{c_+}{c} \sin \frac{ct}{\hbar} & \cos \frac{ct}{\hbar} + i \frac{c_z}{c} \sin \frac{ct}{\hbar} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos \frac{ct}{\hbar} - i \frac{c_z}{c} \sin \frac{ct}{\hbar} \\ -i \frac{c_+}{c} \sin \frac{ct}{\hbar} \end{pmatrix}.$$

(ii) According to Eq. (4.120), the probabilities to find the spin in  $\uparrow$  and  $\downarrow$  states are, respectively,

$$W_{\uparrow} = |\alpha_{\uparrow}(t)|^2 = \cos^2 \frac{ct}{\hbar} + \frac{c_z^2}{c^2} \sin^2 \frac{ct}{\hbar}, \quad W_{\downarrow} = |\alpha_{\downarrow}(t)|^2 = \frac{c_x^2 + c_y^2}{c^2} \sin^2 \frac{ct}{\hbar},$$

withstanding the simplest sanity check:  $W_{\uparrow}(t) + W_{\downarrow}(t) = 1$ . Notice that the matrix elements, and hence the state vectors, oscillate with the frequency  $c/\hbar$  that is twice lower than the classical precession frequency  $\Omega \equiv 2c/\hbar$ , while all the observables oscillate with the full frequency  $\Omega$ .

(iii) Since the operator  $\hat{S}_z$  is diagonal in the  $z$ -basis, we can readily find its expectation value using the first form of Eq. (4.124):

$$\langle S_z \rangle = \left( +\frac{\hbar}{2} \right) W_{\uparrow} + \left( -\frac{\hbar}{2} \right) W_{\downarrow} = \frac{\hbar}{2} \left( \cos^2 \frac{ct}{\hbar} + \frac{c_z^2 - c_x^2 - c_y^2}{c^2} \sin^2 \frac{ct}{\hbar} \right) \equiv \frac{\hbar}{2} \left( 1 - \frac{2c_+ c_-}{c^2} \sin^2 \frac{ct}{\hbar} \right).$$

However, for other spin components, we better use the general rule (4.125). Actually, for  $S_x$ , a part of the calculation was already done in Sec. 4.6 of the lecture notes – see the first form of Eq. (4.171):

$$\langle S_x \rangle = \frac{\hbar}{2} \left[ \alpha_{\uparrow}(t) \alpha_{\downarrow}^*(t) + \alpha_{\downarrow}(t) \alpha_{\uparrow}^*(t) \right] = \hbar \left( \frac{c_y}{c} \cos \frac{ct}{\hbar} + \frac{c_x c_z}{c^2} \sin \frac{ct}{\hbar} \right) \sin \frac{ct}{\hbar}.$$

Carrying out a similar calculation for  $S_y$ , we get

$$\begin{aligned}\langle S_y \rangle &= \langle \alpha(t) | \hat{S}_y | \alpha(t) \rangle = \frac{\hbar}{2} \begin{pmatrix} \alpha_\uparrow^* & \alpha_\downarrow^* \\ \alpha_\uparrow & \alpha_\downarrow \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} \alpha_\uparrow \\ \alpha_\downarrow \end{pmatrix} \\ &= \frac{\hbar}{2} i \left[ \alpha_\uparrow(t) \alpha_\downarrow^*(t) - \alpha_\downarrow(t) \alpha_\uparrow^*(t) \right] = \hbar \left( -\frac{c_x}{c} \cos \frac{ct}{\hbar} + \frac{c_y c_z}{c^2} \sin \frac{ct}{\hbar} \right) \sin \frac{ct}{\hbar}.\end{aligned}$$

For the particular case specified at the end of the assignment,  $c_y = c_z = 0$  (so that  $c_\pm = c_x = \pm c$ ), the precession's half-frequency is determined by the only nonvanishing Cartesian component of the field:  $\Omega/2 = c_x/\hbar$ , and the above results acquire a very simple form:

$$u(t,0) = \begin{pmatrix} \cos \frac{\Omega t}{2} & -i \sin \frac{\Omega t}{2} \\ -i \sin \frac{\Omega t}{2} & \cos \frac{\Omega t}{2} \end{pmatrix}; \quad \langle S_x \rangle = 0, \quad \langle S_y \rangle = -\frac{\hbar}{2} \sin \Omega t, \quad \langle S_z \rangle = \frac{\hbar}{2} \cos \Omega t.$$

Comparing these formulas with Eqs. (4.173)-(4.174) of the lecture notes, we see that our results describe another particular case of the same spin precession about the direction of the field vector  $\mathbf{c} = \{c_x, c_y, c_z\}$  – now oriented along the  $x$ -axis rather than the  $z$ -axis. (A simple generalization of this geometric picture to an arbitrary direction of the field vector  $\mathbf{c}$  will be discussed in Sec. 5.1.)

Approach 2 is to use the relations discussed in Sec. 4.4 of the lecture notes to perform the unitary transform<sup>231</sup> from the  $z$ -basis to the eigenbasis of the Hamiltonian, then use the fact of the very simple time evolution (4.161) of the system in that “new” basis, and finally perform the reciprocal transformation (at arbitrary  $t \geq 0$ ). Though such a program may look rather involved, the calculations are in fact simpler than those in Approach 1.

Indeed, let us call the Hamiltonian's eigenstates  $+$  and  $-$ , while keeping our usual notation ( $\uparrow$  and  $\downarrow$ ) for the states of the “old”  $z$ -basis, and find the eigenstates of the spin- $1/2$  in the field, i.e. calculate the coefficients of their expansion in the  $z$ -basis states:<sup>232</sup>

$$|+\rangle = \langle \uparrow | + \rangle | \uparrow \rangle + \langle \downarrow | + \rangle | \downarrow \rangle, \quad |-\rangle = \langle \uparrow | - \rangle | \uparrow \rangle + \langle \downarrow | - \rangle | \downarrow \rangle. \quad (**)$$

For this, we need to solve the linear system of equations (4.101) (with  $A_{kk'}$  replaced with  $H_{kk'}$ , and the “old” basis  $\{u\}$  now consisting of just two states  $\uparrow$  and  $\downarrow$ ), for each of two energy eigenvalues  $E_j$ :  $E_+ = +c$  and  $E_- = -c$ . For the first of them (in the notation of Sec. 4.4,  $j = 1$ ), the system is

$$\begin{aligned}(c_z - c) \langle \uparrow | + \rangle + c_- \langle \downarrow | + \rangle &= 0, \\ c_+ \langle \uparrow | + \rangle + (-c_z - c) \langle \downarrow | + \rangle &= 0.\end{aligned}$$

Since  $c$  is an eigenvalue of this system, these two equations are compatible and we may use any of them, for example, the second one, giving

<sup>231</sup> The time-independent unitary matrix  $U$  of this transform should not be confused with the time-dependent unitary matrix  $u(t, 0)$  of the time-evolution operator.

<sup>232</sup> Here, “for variety” (actually, for training the reader to use this popular alternative notation), I use short brackets to denote the elements of the unitary transform matrix  $U$  – see Eqs. (4.82)-(4.83) of the lecture notes.

$$\langle \downarrow | + \rangle = \frac{c_+}{c + c_z} \langle \uparrow | + \rangle.$$

Besides this linear relation, these two coefficients (which are just two of four elements of the unitary matrix of the transform between the two bases we are considering – see Eqs. (4.82)-(4.84) of the lecture notes), have to satisfy the normalization relation (4.104):

$$|\langle \uparrow | + \rangle|^2 + |\langle \downarrow | + \rangle|^2 = 1.$$

Solving these two equations together, selecting the arbitrary phase factor in the simplest way, and taking into account that  $|c_{\pm}|^2 = c_+c_- = c_x^2 + c_y^2 = c^2 - c_z^2$ , and  $c \geq c_z$ , so

$$|c_{\pm}|^2 + |c \pm c_z|^2 = (c_x^2 + c_y^2) + (c^2 \pm 2cc_z + c_z^2) = 2c^2 \pm 2cc_z \equiv 2c(c \pm c_z),$$

we readily get

$$\langle \uparrow | + \rangle = \frac{c + c_z}{[2c(c + c_z)]^{1/2}}, \quad \langle \downarrow | + \rangle = \frac{c_+}{[2c(c + c_z)]^{1/2}}.$$

Performing an absolutely similar calculation for  $E_- = -c$ , we get a very similar result for the two remaining coefficients of the unitary transform matrix:

$$\langle \uparrow | - \rangle = -\frac{c_-}{[2c(c + c_z)]^{1/2}}, \quad \langle \downarrow | - \rangle = \frac{c + c_z}{[2c(c + c_z)]^{1/2}}.$$

The first good sanity check is that in the  $z$ -oriented “field”  $\mathbf{c}$  (with  $c_x = c_y = 0$ , and  $c_z = \pm c$ ), the unitary matrix becomes diagonal, so each of the eigenstates  $a_{1,2}$  coincides with one of the  $z$ -states, either  $\uparrow$  or  $\downarrow$ , depending on the sign of  $c_z$ , i.e. on the field direction. Second, in a “horizontal” field (with, say,  $c_y = c_z = 0$ , i.e.  $c = c + c_z = c_x$ ), all the unitary matrix elements are equal to  $\pm 1/\sqrt{2}$ , in agreement with Eq. (4.113).

Now we can use Eqs. (\*\*) to calculate the initial state of the system (at  $t = 0$ ) in the basis of the eigenstates  $\pm$ . Since the system was initially entirely in the spin-up state ( $\uparrow$ ), we get

$$\langle + | \alpha(0) \rangle = \langle + | \uparrow \rangle = \langle \uparrow | + \rangle^* = \frac{c + c_z}{[2c(c + c_z)]^{1/2}}, \quad \langle - | \alpha(0) \rangle = \langle - | \uparrow \rangle = \langle \uparrow | - \rangle^* = -\frac{c_+}{[2c(c + c_z)]^{1/2}}.$$

According to Eq. (4.161), the time evolution of these matrix elements is reduced to their multiplication by the simple phase factors  $\exp\{-iE_j t/\hbar\} = \exp\{\mp i c t/\hbar\}$ :

$$\langle + | \alpha(t) \rangle \equiv \alpha_+(t) = \frac{c + c_z}{[2c(c + c_z)]^{1/2}} \exp\left\{-i \frac{c t}{\hbar}\right\}, \quad \langle - | \alpha(t) \rangle \equiv \alpha_-(t) = -\frac{c_+}{[2c(c + c_z)]^{1/2}} \exp\left\{i \frac{c t}{\hbar}\right\}.$$

Now we may return to the  $z$ -basis, using the unitary transform reciprocal to Eqs. (\*\*):

$$\begin{aligned} \alpha_{\uparrow}(t) &\equiv \langle \uparrow | \alpha(t) \rangle = \langle \uparrow | + \rangle \langle + | \alpha(t) \rangle + \langle \uparrow | - \rangle \langle - | \alpha(t) \rangle \\ &= \frac{(c + c_z)^2}{2c(c + c_z)} \exp\left\{-i \frac{c t}{\hbar}\right\} + \frac{c_+ c_-}{2c(c + c_z)} \exp\left\{i \frac{c t}{\hbar}\right\} \equiv \cos \frac{c t}{\hbar} - i \frac{c_z}{c} \sin \frac{c t}{\hbar}, \end{aligned}$$



$$\begin{aligned}\alpha_{\downarrow}(t) &\equiv \langle \downarrow | \alpha(t) \rangle = \langle \downarrow | + \rangle \langle + | \alpha(t) \rangle + \langle \downarrow | - \rangle \langle - | \alpha(t) \rangle \\ &= \frac{c_+}{[2c(c+c_z)]^{1/2}} \frac{c+c_z}{[2c(c+c_z)]^{1/2}} \exp\left\{-i\frac{ct}{\hbar}\right\} - \frac{c+c_z}{[2c(c+c_z)]^{1/2}} \frac{c_+}{[2c(c+c_z)]^{1/2}} \exp\left\{i\frac{ct}{\hbar}\right\} \equiv -i\frac{c_+}{c} \sin \frac{ct}{\hbar}.\end{aligned}$$

This is the same result as has been obtained using Approach 1. Now we can perform Tasks (ii) and (iii) exactly as it was done in that approach.

**Problem 4.28.** For the same system as in the previous problem, use the Heisenberg picture to calculate the time evolution of:

- (i) all three Cartesian components of the Heisenberg spin operator  $\hat{\mathbf{S}}_H(t)$ , and
- (ii) the expectation values of the spin components.

Compare the latter results with those of the previous problem.

*Solutions:*

(i) With the solutions of the previous problem on hand, one way to proceed is to use the result for the time evolution matrix in the  $z$ -basis:

$$u(t,0) = \begin{pmatrix} \cos \frac{ct}{\hbar} - i \frac{c_z}{c} \sin \frac{ct}{\hbar} & -i \frac{c_-}{c} \sin \frac{ct}{\hbar} \\ -i \frac{c_+}{c} \sin \frac{ct}{\hbar} & \cos \frac{ct}{\hbar} + i \frac{c_z}{c} \sin \frac{ct}{\hbar} \end{pmatrix},$$

where

$$c_{\pm} \equiv c_x \pm ic_y, \quad c \equiv (c_x^2 + c_y^2 + c_z^2)^{1/2},$$

to spell out Eqs. (4.190) of the lecture notes, to write:

$$\begin{aligned}\mathbf{S}_H(t) &= u^\dagger(t,0) \mathbf{S}_S u(t,0) \equiv u^\dagger(t,0) \mathbf{S}_H(0) u(t,0) \\ &= \begin{pmatrix} \cos \frac{ct}{\hbar} + i \frac{c_z}{c} \sin \frac{ct}{\hbar} & i \frac{c_-}{c} \sin \frac{ct}{\hbar} \\ i \frac{c_+}{c} \sin \frac{ct}{\hbar} & \cos \frac{ct}{\hbar} - i \frac{c_z}{c} \sin \frac{ct}{\hbar} \end{pmatrix} \frac{\hbar}{2} \boldsymbol{\sigma} \begin{pmatrix} \cos \frac{ct}{\hbar} - i \frac{c_z}{c} \sin \frac{ct}{\hbar} & -i \frac{c_-}{c} \sin \frac{ct}{\hbar} \\ -i \frac{c_+}{c} \sin \frac{ct}{\hbar} & \cos \frac{ct}{\hbar} + i \frac{c_z}{c} \sin \frac{ct}{\hbar} \end{pmatrix},\end{aligned}$$

where  $\boldsymbol{\sigma}$  is the Pauli vector's matrix – see Eq. (4.117). Now a straightforward multiplication yields, in particular,

$$\begin{aligned}(S_x)_{11} &= \frac{\hbar}{2} \sin \frac{ct}{\hbar} \left( \frac{2c_x c_z}{c^2} \sin \frac{ct}{\hbar} + \frac{2c_y}{c} \cos \frac{ct}{\hbar} \right), \\ (S_y)_{11} &= \frac{\hbar}{2} \sin \frac{ct}{\hbar} \left( \frac{2c_y c_z}{c^2} \sin \frac{ct}{\hbar} - \frac{2c_x}{c} \cos \frac{ct}{\hbar} \right), \\ (S_z)_{11} &= \frac{\hbar}{2} \left( 1 - \frac{2c_+ c_-}{c^2} \sin^2 \frac{ct}{\hbar} \right),\end{aligned} \tag{***}$$

with similar expressions for other 6 matrix elements.

Alternatively, we could use the fact (see the remark in the model solution of the previous problem) that the evolution matrix in these problems may be represented as

$$u(t,0) = I \cos \frac{ct}{\hbar} - i \frac{\mathbf{c} \cdot \boldsymbol{\sigma}}{c} \sin \frac{ct}{\hbar},$$

and make the whole calculation in the vector form, using the multiplication and commutation rules for the Pauli matrices, which we already know from the solution of Problem 3.

One more option to derive the same result is by solving the differential equation (4.199) for the time evolution of the spin- $\frac{1}{2}$  operator, just as it was done in the lecture notes for the simple particular case  $c_x = c_y = 0$  – see Eqs. (4.200)-(4.202).

(ii) Since the initial state of the system was  $\uparrow$ , according to Eq. (4.191) the expectation value of the spin vector is

$$\langle \mathbf{S} \rangle(t) = (1, 0) \begin{pmatrix} \mathbf{S}_{11}(t) & \mathbf{S}_{12}(t) \\ \mathbf{S}_{21}(t) & \mathbf{S}_{22}(t) \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \equiv \mathbf{S}_{11}(t).$$

As a result, by using Eq. (\*\*\*), we get:

$$\begin{aligned} \langle \mathbf{S} \rangle &= \frac{\hbar}{2} \left[ \mathbf{n}_x (S_x)_{11} + \mathbf{n}_y (S_y)_{11} + \mathbf{n}_z (S_z)_{11} \right] \\ &= \frac{\hbar}{2} \left[ \mathbf{n}_x 2 \sin \frac{ct}{\hbar} \left( \frac{c_z c_x}{c^2} \sin \frac{ct}{\hbar} + \frac{c_y}{c} \cos \frac{ct}{\hbar} \right) + \mathbf{n}_y 2 \sin \frac{ct}{\hbar} \left( \frac{c_y c_z}{c^2} \sin \frac{ct}{\hbar} - \frac{c_x}{c} \cos \frac{ct}{\hbar} \right) + \mathbf{n}_z \left( 1 - \frac{2c_+ c_-}{c^2} \sin^2 \frac{ct}{\hbar} \right) \right], \end{aligned}$$

i.e. (very fortunately :-)) the same result as from the Schrödinger picture – see the solution of the previous problem.

**Problem 4.29.** For the same system as in the two previous problems, calculate the matrix elements of the operator  $\hat{\sigma}_z$  in the basis of the stationary states of the system.

*Solution:* The calculation is most straightforward in the  $z$ -basis  $\{\uparrow, \downarrow\}$ , in which the operator  $\hat{\sigma}_z$  has the simplest form – see the last of Eqs. (4.105) of the lecture notes:

$$(\sigma_z)_{++} \equiv \langle + | \hat{\sigma}_z | + \rangle = \left( \langle \uparrow | + \rangle^*, \langle \downarrow | + \rangle^* \right) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \langle \uparrow | + \rangle \\ \langle \downarrow | + \rangle \end{pmatrix} = |\langle \uparrow | + \rangle|^2 - |\langle \downarrow | + \rangle|^2.$$

According to Eqs. (4.82)-(4.84), the short brackets participating in this expression are just the elements of the unitary matrix of transfer between the stationary-state basis  $\{+, -\}$  and the  $z$ -basis, and had already been calculated in Approach 2 in the model solution of Problem 27. Plugging them in, we get a very simple expression:

$$(\sigma_z)_{++} = \left| \frac{c + c_z}{[2c(c + c_z)]^{1/2}} \right|^2 - \left| \frac{c_+}{[2c(c + c_z)]^{1/2}} \right|^2 \equiv \frac{(c + c_z)^2}{2c(c + c_z)} - \frac{c_+ c_-}{2c(c + c_z)} \equiv \frac{c_z}{c},$$

where, as in the two previous problems,  $c \equiv (c_x^2 + c_y^2 + c_z^2)^{1/2}$  and  $c_{\pm} \equiv c_x \pm ic_y$ , so  $|c_+|^2 = c_+ c_- = c_x^2 + c_y^2 = c^2 - c_z^2 = (c + c_z)(c - c_z)$ .

This result readily passes two key sanity checks. First, if  $c_z = \pm c$  (i.e.  $c_x = c_y = 0$ ), then  $(\sigma_z)_{++} = \pm 1$ , as it should be, because in this case, the basis  $\{+, -\}$  coincides either with the  $z$ -basis  $\{\uparrow, \downarrow\}$ , so the answer is given by one of the diagonal elements of familiar matrix  $\sigma_z$  in the  $z$ -basis. Second, if only  $c_x$  is different from zero, i.e.  $c_z = 0$ , our result yields  $(\sigma_z)_{++} = 0$ . This is also what we should have because the stationary states  $\{+, -\}$  in such a “horizontal field”  $\mathbf{c}$  are the eigenstates of the corresponding “horizontal operator”  $\hat{\sigma}_x$  with the eigenstates described by Eqs. (4.122). In their basis,  $(\sigma_z)_{++}$  has to vanish.

Absolutely similar calculations of other matrix elements yield

$$\begin{aligned}
 (\sigma_z)_{--} &\equiv \langle - | \sigma_z | - \rangle = \left( \langle \uparrow | - \rangle^*, \langle \downarrow | - \rangle^* \right) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \langle \uparrow | - \rangle \\ \langle \downarrow | - \rangle \end{pmatrix} = |\langle \uparrow | - \rangle|^2 - |\langle \downarrow | - \rangle|^2 = -\frac{c_z}{c}, \\
 (\sigma_z)_{+-} &\equiv \langle + | \sigma_z | - \rangle = \left( \langle \uparrow | + \rangle^*, \langle \downarrow | + \rangle^* \right) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \langle \uparrow | - \rangle \\ \langle \downarrow | - \rangle \end{pmatrix} = \langle \uparrow | + \rangle^* \langle \uparrow | - \rangle - \langle \downarrow | + \rangle^* \langle \downarrow | - \rangle \\
 &= -\frac{c + c_z}{[2c(c + c_z)]^{1/2}} \frac{c_-}{[2c(c + c_z)]^{1/2}} - \frac{c_-}{[2c(c + c_z)]^{1/2}} \frac{c + c_z}{[2c(c + c_z)]^{1/2}} \equiv -\frac{c_-}{c}, \\
 (\sigma_z)_{-+} &= (\sigma_z)_{+-}^* = -\frac{c_+}{c}.
 \end{aligned}$$

(The last calculation has used Eq. (4.66), which is valid for  $\hat{\sigma}_z$  as a Hermitian operator.)

Note that in contrast to the two previous problems, the results of this solution do not depend on the initial state of the system.

**Problem 4.30.** In the Schrödinger picture of quantum dynamics, certain three operators satisfy the following commutation relation:

$$[\hat{A}, \hat{B}] = \hat{C}.$$

What is their relation in the Heisenberg picture, at a certain time instant  $t$ ?

*Solution:* By using the definition of the commutator, then Eq. (4.190) of the lecture notes, and, finally, the unitary property (4.76) of the time-evolution operator, for the Heisenberg-picture operators (in this solution, indicated just by their displayed dependence on time), we may write

$$\begin{aligned}
 [\hat{A}(t), \hat{B}(t)] &\equiv \hat{A}(t)\hat{B}(t) - \hat{B}(t)\hat{A}(t) \\
 &= \hat{u}^\dagger(t, t_0)\hat{A}(t_0)\hat{u}(t, t_0)\hat{u}^\dagger(t, t_0)\hat{B}(t_0)\hat{u}(t, t_0) - \hat{u}^\dagger(t, t_0)\hat{B}(t_0)\hat{u}(t, t_0)\hat{u}^\dagger(t, t_0)\hat{A}(t_0)\hat{u}(t, t_0) \\
 &= \hat{u}^\dagger(t, t_0)\hat{A}(t_0)\hat{B}(t_0)\hat{u}(t, t_0) - \hat{u}^\dagger(t, t_0)\hat{B}(t_0)\hat{A}(t_0)\hat{u}(t, t_0) \equiv \hat{u}^\dagger(t, t_0)[\hat{A}(t_0), \hat{B}(t_0)]\hat{u}(t, t_0).
 \end{aligned}$$

But by the same definition (4.190) of the Heisenberg operators, at  $t = t_0$ , they are just the Schrödinger-picture operators, so

$$[\hat{A}(t), \hat{B}(t)] = \hat{u}^\dagger(t, t_0)[\hat{A}, \hat{B}]\hat{u}(t, t_0) = \hat{u}^\dagger(t, t_0)\hat{C}\hat{u}(t, t_0) \equiv \hat{u}^\dagger(t, t_0)\hat{C}(t_0)\hat{u}(t, t_0) \equiv \hat{C}(t).$$

Hence, this commutation relation does not depend on the picture they are all considered in. (This conclusion is valid for the interaction picture as well.) Note, however, that this is true only if the time arguments of the operators coincide – for a counter-example, see, e.g., a footnote in Sec. 4.6 of the lecture notes.

**Problem 4.31.** Prove the Bloch theorem given by either Eq. (3.107) or Eq. (3.108), where  $\mathbf{R}$  is an arbitrary vector of the Bravais lattice (3.106).

*Hint:* Analyze the commutation properties of the so-called *translation operator*  $\hat{\tau}_{\mathbf{R}}$ , defined by the following result of its action on an arbitrary function  $f(\mathbf{r})$ :

$$\hat{\tau}_{\mathbf{R}} f(\mathbf{r}) = f(\mathbf{r} + \mathbf{R}),$$

and apply them to an eigenfunction  $\psi(\mathbf{r})$  of the stationary Schrödinger equation for a particle moving in the periodic potential described by Eq. (3.105).

*Solution:* Let us act by the translation operator on the function  $\hat{H}(\mathbf{r})f(\mathbf{r})$ , where the Hamiltonian is  $\mathbf{R}$ -periodic in the sense of Eq. (3.105), and the function  $f(\mathbf{r})$  is so far arbitrary, i.e. may or may not be periodic. The result is

$$\hat{\tau}_{\mathbf{R}} \hat{H}(\mathbf{r})f(\mathbf{r}) = \hat{\tau}_{\mathbf{R}} [\hat{H}(\mathbf{r})f(\mathbf{r})] = \hat{H}(\mathbf{r} + \mathbf{R})f(\mathbf{r} + \mathbf{R}) = \hat{H}(\mathbf{r})f(\mathbf{r} + \mathbf{R}) = \hat{H}(\mathbf{r})\hat{\tau}_{\mathbf{R}} f(\mathbf{r}).$$

Since  $f(\mathbf{r})$  is arbitrary, the comparison of the first and the last forms of this transformation chain shows that the operators  $\hat{\tau}_{\mathbf{R}}$  and  $\hat{H}$  commute. Hence, according to the discussion in Sec. 4.5 of the lecture notes, they share their eigenfunctions  $\psi(\mathbf{r})$ :

$$\hat{H}\psi = E\psi, \quad \hat{\tau}_{\mathbf{R}}\psi = \tau(\mathbf{R})\psi,$$

where  $E$  and  $\tau(\mathbf{R})$  are the corresponding eigenvalues. Without any restrictions, the  $c$ -number function  $\tau(\mathbf{R})$  may be taken in the form

$$\tau(\mathbf{R}) = e^{iF(\mathbf{R})}$$

(where  $F(\mathbf{R})$  may be a complex function), so

$$\hat{\tau}_{\mathbf{R}}\psi = e^{iF(\mathbf{R})}\psi, \quad (*)$$

On the other hand, a successive action of two translation operators on any function evidently results in the net shift of its argument:

$$\hat{\tau}_{\mathbf{R}} \hat{\tau}_{\mathbf{R}'} f(\mathbf{r}) = \hat{\tau}_{\mathbf{R}'} \hat{\tau}_{\mathbf{R}} f(\mathbf{r}) = \hat{\tau}_{\mathbf{R}+\mathbf{R}'} f(\mathbf{r}). \quad (**)$$

Hence, by applying Eqs. (\*) and (\*\*) to a joint eigenfunction  $\psi(\mathbf{r})$  of the operators  $\hat{\tau}_{\mathbf{R}}$  and  $\hat{H}$ , we may get any of the following two expressions:

$$\hat{\tau}_{\mathbf{R}+\mathbf{R}'}\psi(\mathbf{r}) = \begin{cases} \hat{\tau}_{\mathbf{R}} \hat{\tau}_{\mathbf{R}'}\psi(\mathbf{r}) = \hat{\tau}_{\mathbf{R}} e^{iF(\mathbf{R}')} \psi(\mathbf{r}) = e^{iF(\mathbf{R}')} \hat{\tau}_{\mathbf{R}} \psi(\mathbf{r}) = e^{iF(\mathbf{R}')} e^{iF(\mathbf{R})} \psi(\mathbf{r}), \\ e^{iF(\mathbf{R}'+\mathbf{R})} \psi(\mathbf{r}). \end{cases}$$

Hence the function  $F(\mathbf{R})$  has to satisfy the following relation:

$$e^{iF(\mathbf{R}')} e^{iF(\mathbf{R})} = e^{iF(\mathbf{R}'+\mathbf{R})},$$

for an arbitrary choice of  $\mathbf{R}$  and  $\mathbf{R}'$  (from the Bravais lattice set). This is only possible if it is a linear function of each Cartesian component of the vector  $\mathbf{R}$ , with certain coefficients  $q_j$ :

$$F(\mathbf{R}) = q_x X + q_y Y + q_z Z = \mathbf{q} \cdot \mathbf{R}, \quad \text{i.e. if } \hat{\mathcal{T}}_{\mathbf{R}} \psi(\mathbf{r}) \equiv \psi(\mathbf{r} + \mathbf{R}) = \psi(\mathbf{r}) e^{i\mathbf{q} \cdot \mathbf{R}}.$$

This is the Bloch theorem in the form (3.107). The only detail to add is that if the particle's probability density  $\psi(\mathbf{r})\psi^*(\mathbf{r})$  is periodic in the sense of Eq. (3.105), as it is inside each allowed energy band, then the vector  $\mathbf{q}$  should satisfy the following requirement:

$$\psi(\mathbf{r} + \mathbf{R})\psi^*(\mathbf{r} + \mathbf{R}) \equiv \psi(\mathbf{r})e^{i\mathbf{q} \cdot \mathbf{R}}\psi^*(\mathbf{r})e^{-i\mathbf{q} \cdot \mathbf{R}} = \psi(\mathbf{r})\psi^*(\mathbf{r}).$$

This condition gives the following equality:  $\exp\{i(\mathbf{q} - \mathbf{q}^*) \cdot \mathbf{R}\} = 1$ , which may be satisfied (for arbitrary  $\mathbf{R}$ ) only if the quasimomentum is real:  $\mathbf{q}^* = \mathbf{q}$ .

Problem 4.32. A constant force  $F$  is applied to an (otherwise free) 1D particle of mass  $m$ . Calculate the stationary wavefunctions of the particle in:

- (i) the coordinate representation, and
- (ii) the momentum representation.

Discuss the relation between the results.

*Solutions:*

- (i) In the *coordinate* representation, the Hamiltonian of the particle,

$$\hat{H} = \frac{\hat{p}^2}{2m} - F\hat{x}, \quad (*)$$

may be rewritten as

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} - Fx.$$

so the corresponding stationary Schrödinger equation is

$$\left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} - Fx \right) \psi = E\psi.$$

This is the Airy equation, which was discussed in Sec. 2.4 of the lecture notes and may be reduced to its canonical form (2.101),

$$\frac{d^2\psi}{d\zeta^2} - \zeta\psi = 0,$$

by defining the following dimensionless argument:<sup>233</sup>

<sup>233</sup> Cf. Eq. (2.100) of the lecture notes, which differs only by the sign of  $dU/dx = -F$  and hence by the opposite sign of  $x$ , selected to keep the expression under the cubic root positive.

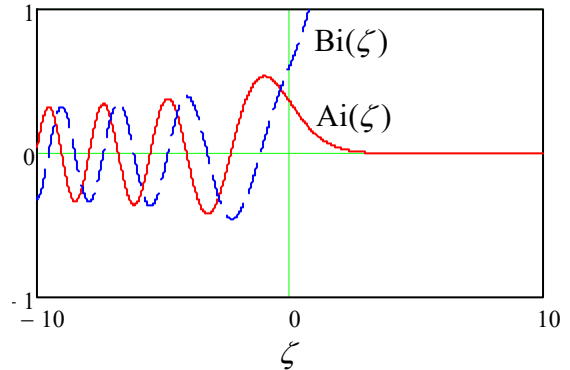
$$\zeta \equiv -\left(\frac{2mF}{\hbar^2}\right)^{1/3} \left(x + \frac{E}{F}\right). \quad (**)$$

As was discussed in Sec. 2.4, the fundamental solutions of this linear differential equation are the Airy functions  $\text{Ai}(\zeta)$  and  $\text{Bi}(\zeta)$  – see Fig. 2.9a, reproduced on the right. Of them, only  $\text{Ai}(\zeta)$  is finite at all  $\zeta$ , so if Eq. (\*) is valid on the whole axis  $-\infty < x < +\infty$ , its solution has to be proportional to this function alone:

$$\psi(\zeta) = C_x \text{Ai}(\zeta),$$

i.e.

$$\psi(x) = C_x \text{Ai} \left[ \left( \frac{2m}{\hbar^2 F^2} \right)^{1/3} (E + Fx) \right], \quad (***)$$



where  $C_x$  is a normalization constant.

(ii) In the *momentum* representation, we may use the first of Eqs. (4.269) to rewrite Eq. (\*) as

$$\hat{H} = \frac{p^2}{2m} - i\hbar F \frac{\partial}{\partial p}.$$

The corresponding stationary Schrödinger equation for the wavefunction  $\varphi(p)$  is

$$\left( \frac{p^2}{2m} - i\hbar F \frac{d}{dp} \right) \varphi = E \varphi.$$

Rewriting this linear ordinary differential equation in the variable-separated form,

$$i\hbar F \frac{d\varphi}{\varphi} = \left( \frac{p^2}{2m} - E \right) dp,$$

we see that it may be readily integrated, giving

$$i\hbar F \ln \varphi = \int \left( \frac{p^2}{2m} - E \right) dp \equiv \left( \frac{p^3}{6m} - Ep \right) + \text{const}, \quad \text{so } \varphi(p) = C_p \exp \left\{ -\frac{i}{\hbar F} \left( \frac{p^3}{6m} - Ep \right) \right\}. \quad (***)$$

Now let us verify that the functions (\*\*\*) and (\*\*\*) are indeed related by the Fourier transform – see Eq. (4.264) of the lecture notes:

$$\psi(x) = \frac{1}{(2\pi\hbar)^{1/2}} \int_{-\infty}^{+\infty} \varphi(p) \exp \left\{ i \frac{px}{\hbar} \right\} dp.$$

For that, by plugging the last of Eqs. (\*\*\*) into this integral, and then introducing the dimensionless integration variable  $\xi \equiv (2m\hbar F)^{-1/3} p$ , we get

$$\psi(x) = \frac{C_p}{(2\pi\hbar)^{1/2}} \int_{-\infty}^{+\infty} \exp \left\{ i \left[ \frac{px}{\hbar} - \frac{1}{\hbar F} \left( \frac{p^3}{6m} - Ep \right) \right] \right\} dp \equiv \frac{C_p (2m\hbar F)^{1/3}}{(2\pi\hbar)^{1/2}} 2\pi \left[ \frac{1}{\pi} \int_0^{+\infty} \cos \left( \frac{\xi^3}{3} + \zeta \xi \right) d\xi \right]$$

where  $\xi \equiv -p/(2m\hbar F)^{1/3}$ , and  $\zeta$  is defined by Eq. (\*\*). But as was mentioned in Sec. 2.4 of the lecture notes, the expression in the last square brackets is just the integral form of the function  $\text{Ai}(\zeta)$ , so this function  $\psi(x)$  is indeed proportional to the one given by Eq. (\*\*\*) . Hence, at the proper relation between their normalization coefficients  $C_x$  and  $C_p$ , the functions  $\psi(x)$  and  $\varphi(p)$  are indeed just the spatial Fourier images of each other.

**Problem 4.33.** Use the momentum representation to re-solve the problem discussed at the beginning of Sec. 2.6 of the lecture notes, i.e. calculate the eigenenergy of a 1D particle of mass  $m$ , localized in a very short potential well with “weight”  $w$ .

*Solution:* The Hamiltonian of the system is

$$\hat{H} = \frac{\hat{p}^2}{2m} + U(\hat{x}), \quad \text{where } U(x) = -w\delta(x), \quad \text{with } w > 0. \quad (*)$$

As was discussed in Sec. 4.7 of the lecture notes, the momentum representation of its first term is just the multiplier  $p^2/2m$ , but in contrast to the previous problem, the direct use of Eq. (4.269) to find the corresponding representation of the second term is problematic due to the ultimately localized character of the delta function, making its Taylor expansion non-trivial. This is why it is more prudent to start at square one, namely from the general form of the eigenproblem:

$$\hat{H}|\alpha\rangle = E|\alpha\rangle.$$

Proceeding just like was done in Sec. 4.7 for the coordinate representation, i.e. inner-multiplying both parts of this equation by  $\langle p|$ , and then using the closure relation analogous to Eq. (4.252),

$$\int dp' |p'\rangle \langle p'| = \hat{I},$$

we get

$$\langle p|\hat{H}|\alpha\rangle \equiv \int dp' \langle p|\hat{H}|p'\rangle \langle p'|\alpha\rangle = E\langle p|\alpha\rangle, \quad \text{i.e. } \int dp' \langle p|\hat{H}|p'\rangle \varphi(p') = E\varphi(p),$$

where  $\varphi(p) \equiv \langle p|\alpha\rangle$  is the eigenfunction in the momentum representation. Now by using, for our particular potential, the general Eq. (4.272) for the above long bracket, we get

$$\frac{1}{2\pi\hbar} \int dp' \int dx \exp\left\{-i\frac{px}{\hbar}\right\} \left[ \frac{\hat{p}^2}{2m} - w\delta(x) \right] \exp\left\{i\frac{p'x}{\hbar}\right\} \varphi(p') = E\varphi(p). \quad (**)$$

The integral of the first term in the square brackets gives just  $(p^2/2m)\varphi(p)$ , as it should:

$$\begin{aligned} \frac{1}{2\pi\hbar} \int dp' \int dx \exp\left\{-i\frac{px}{\hbar}\right\} \frac{\hat{p}^2}{2m} \exp\left\{i\frac{p'x}{\hbar}\right\} \varphi(p') &\equiv \frac{1}{2\pi\hbar} \int dp' \frac{p'^2}{2m} \varphi(p') \int dx \exp\left\{i\frac{(p'-p)x}{\hbar}\right\} \\ &\equiv \int dp' \frac{p'^2}{2m} \varphi(p') \delta(p'-p) = \frac{p^2}{2m} \varphi(p), \end{aligned}$$

while that of the second one is

$$-\frac{w}{2\pi\hbar} \int dp' \int dx \exp\left\{-i\frac{px}{\hbar}\right\} \delta(x) \exp\left\{i\frac{p'x}{\hbar}\right\} \varphi(p') \equiv -\frac{w}{2\pi\hbar} \int \varphi(p') dp',$$

i.e. a  $p$ -independent constant. Hence Eq. (\*\*) is reduced to

$$\frac{p^2}{2m}\varphi(p) - \frac{\omega}{2\pi\hbar} \int \varphi(p') dp' = E\varphi(p),$$

immediately giving the following implicit solution (actually, a homogeneous integral equation):

$$\varphi(p) = \frac{\omega/2\pi\hbar}{p^2/2m - E} \int \varphi(p') dp'.$$

Integrating both sides of this equation over  $p$  in the same (infinite) limits, we get<sup>234</sup>

$$\int \varphi(p) dp = \int \varphi(p') dp' \int \frac{\omega/2\pi\hbar}{p^2/2m - E} dp \equiv \int \varphi(p') dp' \frac{\omega}{2\pi\hbar} \left(\frac{2m}{-E}\right)^{1/2} \int_{-\infty}^{+\infty} \frac{d\xi}{1+\xi^2} \equiv \int \varphi(p') dp' \frac{\omega}{\hbar} \left(\frac{m}{-2E}\right)^{1/2}.$$

Requiring the integrals on both sides of this equality to be equal, we get exactly the same eigenenergy,

$$E = -\frac{m\omega^2}{2\hbar^2},$$

as was obtained in Sec. 2.6 using wave mechanics, i.e. the coordinate representation. (Evidently, using that representation is simpler for this problem – as for most problems with localized potentials.)

**Problem 4.34.** The momentum representation of a certain operator of orbital 1D motion is  $p^{-1}$ . Use two different approaches to find its coordinate representation.

*Solution:* Let us call the operator in question  $\hat{\lambda}$ , then, according to the assignment, if

$$\hat{\lambda}|\alpha\rangle = |\alpha_\lambda\rangle$$

where  $\alpha$  is an arbitrary 1D orbital state of a particle, then

$$\frac{1}{p}\varphi(p) = \varphi_\lambda(p), \quad (*)$$

where  $\varphi(p)$  and  $\varphi_\lambda(p)$  are the momentum representations of the states  $\alpha$  and  $\alpha_\lambda$ , respectively. Hence,

$$\varphi(p) = p\varphi_\lambda(p). \quad (**)$$

Now we may proceed by using either of the following alternative approaches.

**Approach 1.** Let us consider the following ket-vector

$$|\alpha'\rangle \equiv \hat{p}|\alpha_\lambda\rangle.$$

In the momentum representation, this relation takes the form

$$\varphi'(p) = p\varphi_\lambda(p),$$

<sup>234</sup> As was discussed in Sec. 2.6, the eigenenergy  $E$  of the localized state has to be negative, so the denominator of the fraction under the integral is positive for all  $p$ , and we may use for it the standard table integral – see, e.g., MA Eq. (6.5a).



where  $\varphi'(p)$  is the momentum representation of the state  $\alpha'$ . The comparison of this expression with Eq. (\*\*\*) shows that  $\varphi'(p) = \varphi(p)$  for any state  $\alpha$ , i.e. this state and  $\alpha'$  have identical momentum representations. Since the set of the momentum basis states  $p$ , defined by Eq. (4.257) of the lecture notes, is full, this may be only if the states  $\alpha$  and  $\alpha'$  are identical, i.e.

$$|\alpha'\rangle = |\alpha\rangle, \quad \text{so } \hat{p}|\alpha_\lambda\rangle \equiv \hat{p}\hat{\lambda}|\alpha\rangle = |\alpha\rangle,$$

for any state  $\alpha$ . This means that (as we could expect from the very beginning),

$$\hat{p}\hat{\lambda} = \hat{I}.$$

(A similar calculation in the opposite order shows that  $\hat{\lambda}\hat{p} = \hat{I}$  as well, so the operators  $\hat{p}$  and  $\hat{\lambda}$  commute.)<sup>235</sup> Hence the action of this operator product on an arbitrary coordinate-representation wavefunction cannot change it:

$$\hat{p}\hat{\lambda}\psi(x) = \hat{I}\psi(x) = \psi(x).$$

In the coordinate representation, this relation is

$$-i\hbar \frac{\partial}{\partial x} \left[ \left( \hat{\lambda} \right)_{\text{in } x} \psi(x) \right] = \psi(x).$$

Integrating both sides of this relation, after replacing  $x$  with  $x'$ , over the interval  $[-\infty, x]$ , and multiplying them by  $i/\hbar$ , we get:

$$\hat{\lambda} \Big|_{\text{in } x} \psi(x) = \frac{i}{\hbar} \int_{-\infty}^x \psi(x') dx'. \quad (***)$$

This equality,<sup>236</sup> valid for any function  $\psi(x)$ , is the required coordinate representation of the operator  $\hat{\lambda}$ .

Approach 2. Let us use Eq. (4.264), then Eq. (\*), and, finally, Eq. (4.265), to calculate the coordinate-representation wavefunction corresponding to the state  $\alpha_\lambda$ :

$$\begin{aligned} \psi_\lambda(x) &= \frac{1}{(2\pi\hbar)^{1/2}} \int_{-\infty}^{+\infty} \varphi_\lambda(p) \exp\left\{i \frac{px}{\hbar}\right\} dp \equiv \frac{1}{(2\pi\hbar)^{1/2}} \int_{-\infty}^{+\infty} \varphi(p) \exp\left\{i \frac{px}{\hbar}\right\} \frac{dp}{p} \\ &= \frac{1}{(2\pi\hbar)^{1/2}} \int_{-\infty}^{+\infty} \left[ \frac{1}{(2\pi\hbar)^{1/2}} \int_{-\infty}^{+\infty} \psi(x') \exp\left\{-i \frac{px'}{\hbar}\right\} dx' \right] \exp\left\{i \frac{px}{\hbar}\right\} \frac{dp}{p} \\ &\equiv \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} \psi(x') dx' I_p, \quad \text{where } I_p \equiv \int_{-\infty}^{+\infty} \exp\left\{i \frac{p(x-x')}{\hbar}\right\} \frac{dp}{p}. \end{aligned} \quad (***)$$

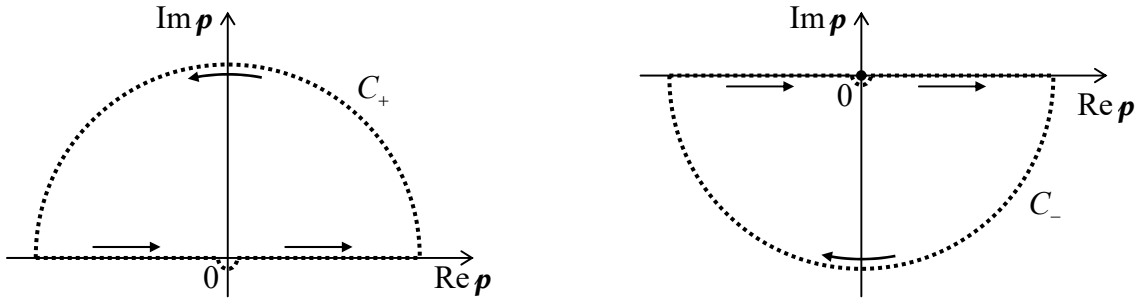
The inner integral  $I_p$  may be readily worked out by comparing it with similar integrals over closed contours on the plane of the complex variable  $\mathbf{p} \equiv \text{Re}\mathbf{p} + i\text{Im}\mathbf{p}$ , where  $\text{Re}\mathbf{p} \equiv p$ . Indeed, the exponential function under such an integral,

<sup>235</sup> Such operators are frequently called the *inverse* of each other, and one may run into symbolic equalities like  $\hat{\lambda} = \hat{p}^{-1}$ . However, such expressions should be treated with utmost mathematical care; in this course, they are avoided.

<sup>236</sup> Actually, as it follows from our derivation, the lower limit of this integral may be an arbitrary constant.

$$\exp\left\{i\frac{\mathbf{p}(x-x')}{\hbar}\right\} \equiv \exp\left\{i\frac{(\text{Re } \mathbf{p} + i \text{Im } \mathbf{p})(x-x')}{\hbar}\right\} \equiv \exp\left\{i\frac{\text{Re } \mathbf{p}(x-x')}{\hbar}\right\} \exp\left\{-\frac{\text{Im } \mathbf{p}(x-x')}{\hbar}\right\},$$

is analytic for any  $\mathbf{p}$ . If  $x - x' > 0$ , it tends to zero exponentially fast at  $\text{Im } \mathbf{p} \rightarrow +\infty$ . Hence  $I_p$  may be replaced with the integral over the contour  $C_+$  shown on the left panel of the figure below, which bypasses the pole point  $\mathbf{p} = 0$  via an infinitesimal semicircle, and returns to the initial point  $p = -\infty$  along another semi-circle, this one with an infinite radius, in the upper half-plane.



Applying the Cauchy integral formula to the exponential function alone,<sup>237</sup> we get

$$I_p = \oint_{C_+} \exp\left\{i\frac{\mathbf{p}(x-x')}{\hbar}\right\} \frac{d\mathbf{p}}{\mathbf{p}} = 2\pi i, \quad \text{for } x - x' > 0.$$

On the other hand, if  $x - x' < 0$ , the exponential function tends to zero at  $\text{Im } \mathbf{p} \rightarrow -\infty$ . In this case,  $I_p$  may be replaced with the integral over the contour  $C_-$  shown on the right panel of the figure above, inside which the whole function under the integral, including the  $1/\mathbf{p}$  factor, is analytic. Here the Cauchy integral theorem, applied to this composite function,<sup>238</sup> yields

$$I_p = \oint_{C_-} \exp\left\{i\frac{\mathbf{p}(x-x')}{\hbar}\right\} \frac{d\mathbf{p}}{\mathbf{p}} = 0, \quad \text{for } x - x' < 0.$$

Plugging these results into Eq. (\*\*\*\*), we get

$$\psi_\lambda(x) \equiv [\hat{\lambda}]_{\text{in } x} \psi(x) = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} \psi(x') dx' \times \begin{cases} 2\pi i, & \text{for } x' < x \\ 0, & \text{for } x' > x \end{cases} \equiv \frac{i}{\hbar} \int_{-\infty}^x \psi(x') dx',$$

i.e. arrive at Eq. (\*\*\*) again.

Finally, note that acting absolutely similarly, for another operator (say,  $\hat{\Lambda}$ ), defined by its coordinate representation as

$$\hat{\Lambda}|_{\text{in } x} = \frac{1}{x},$$

we may readily get the following momentum representation:

<sup>237</sup> See, e.g., MA Eq. (15.2) with  $z = \mathbf{p}$ ,  $z' = \mathbf{p}' = 0$ , and  $f(z) = \exp\{i\mathbf{p}(x-x')/\hbar\}$ , so  $f(z') = 1$ .

<sup>238</sup> See, e.g., MA Eq. (15.1) with  $z = \mathbf{p}$  and  $f(z) = \exp\{i\mathbf{p}(x-x')/\hbar\}/\mathbf{p}$ . Note that, generally, the contour integral taken in this negative (clockwise) direction has to be taken with the negative sign, but in our current case  $I_p = 0$ , so the sign does not matter.

$$\hat{\Lambda} \Big|_{in\ p} \varphi(p) = -\frac{i}{\hbar} \int_{-\infty}^p \varphi(p') dp'.$$

This relation is similar to Eq. (\*\*), besides its opposite sign – the change that might be expected from the comparison of Eqs. (4.264) and (4.265) of the lecture notes.

**Problem 4.35.**\* For a particle moving in a 3D periodic potential, develop the bra-ket formalism for the  $\mathbf{q}$ -representation, in which a complex amplitude similar to  $a_q$  in Eq. (2.234) of the lecture notes (but generalized to 3D and all energy bands) plays the role of the wavefunction. In particular, calculate the operators  $\mathbf{r}$  and  $\mathbf{v}$  in this representation, and use the result to prove Eq. (2.237) for the 1D case in the low-field limit.

*Solution:* Let us consider 3D orbital motion of a particle in a periodic potential  $U(\mathbf{r})$  described by the Hamiltonian

$$\hat{H}_0 \equiv \frac{\hat{p}^2}{2m} + U(\hat{\mathbf{r}}), \quad \text{with } U(\mathbf{r} + \mathbf{R}) = U(\mathbf{R}), \quad (*)$$

where  $\mathbf{R}$  is an arbitrary vector of the Bravais lattice – see Sec. 3.4. According to the Bloch theorem (3.108), in the coordinate representation, the wavefunction of an arbitrary orbital state of the particle may be expressed as an expansion over the eigenfunctions of the Hamiltonian (\*):

$$\psi(\mathbf{r}) = \sum_n \int a_{n,\mathbf{q}} u_{n,\mathbf{q}}(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} d^3q, \quad \text{with } u_{n,\mathbf{q}}(\mathbf{r} + \mathbf{R}) = u_{n,\mathbf{q}}(\mathbf{r}),$$

which is a natural generalization of Eq. (2.234) to the 3D case and an arbitrary number of energy bands (numbered here with the integer index  $n$ ).

The radius-vector's operator acts on this wavefunction as follows:

$$\hat{\mathbf{r}}\psi(\mathbf{r}) = \sum_n \int a_{n,\mathbf{q}} \mathbf{r} u_{n,\mathbf{q}}(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} d^3q. \quad (**)$$

Let us calculate the gradient of the last product under the integral, multiplied by  $(-i)$ , in the reciprocal  $\mathbf{q}$ -space of the quasimomentum:<sup>239</sup>

$$\nabla_q \left( -i u_{n,\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} \right) = \mathbf{r} u_{n,\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} - i e^{i\mathbf{q}\cdot\mathbf{r}} \nabla_q u_{n,\mathbf{q}}.$$

Expressing from this relation the first term on its right-hand side, and plugging it into Eq. (\*\*), we get

$$\hat{\mathbf{r}}\psi = -i \sum_n \int a_{n,\mathbf{q}} \nabla_q \left( u_{n,\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} \right) d^3q + i \sum_n \int a_{n,\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} \nabla_q u_{n,\mathbf{q}} d^3q.$$

Now let us take the integral in first term on the right-hand side by parts over a volume so large that on its surface, we may take  $\psi = 0$ , while in the second term, expand the  $\mathbf{q}$ -gradient of the function  $u_{n,\mathbf{q}}$  into a series over the full set of these (mutually orthogonal) functions in all energy bands:

<sup>239</sup> I am taking the liberty to use this convenient term for  $\mathbf{q}$ , despite the fact (discussed in Sec. 2.7-2.8 and 3.4 of the lecture notes), that the genuine quasimomentum equals  $\hbar\mathbf{q}$ .

$$\nabla_q u_{n,\mathbf{q}} = -i \sum_{n'} \langle n, \mathbf{q} | \hat{\Omega} | n', \mathbf{q} \rangle u_{n',\mathbf{q}}.$$

Here  $|n, \mathbf{q}\rangle$  are the eigenvectors of the Hamiltonian (\*), so the Bloch wavefunctions

$$\psi_{n,\mathbf{q}}(\mathbf{r}) = \langle \mathbf{r} | n, \mathbf{q} \rangle = u_{n,\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}},$$

while the vector operator  $\hat{\Omega}$  is, at this stage, defined just by its matrix elements (geometric vectors!) participating in the above expansion. Then the result of the integration by parts is

$$\hat{\mathbf{r}}\psi = i \sum_n \int u_{n,\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} \nabla_q a_{n,\mathbf{q}} d^3q + \sum_{n,n'} \langle n, \mathbf{q} | \hat{\Omega} | n', \mathbf{q} \rangle a_{n,\mathbf{q}} u_{n',\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} d^3q.$$

Swapping the indices  $n$  and  $n'$  in the last term, we may rewrite our result as

$$\hat{\mathbf{r}}\psi = \sum_n \int \left[ i \nabla_q a_{n,\mathbf{q}} + \sum_{n'} \langle n', \mathbf{q} | \hat{\Omega} | n, \mathbf{q} \rangle a_{n',\mathbf{q}} \right] u_{n,\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} d^3q. \quad (***)$$

On the other hand, in the  $\mathbf{q}$ -representation, the amplitude function  $a_{n,\mathbf{q}}$  plays the role of the wavefunction – just as in the usual momentum representation, which was discussed in detail in Sec. 4.7 for the 1D case, the state with the Schrödinger wavefunction (4.264) is described by the function  $\varphi(p)$ . In this representation, any operator should be described by its action on that wavefunction. This is why in the  $\mathbf{q}$ -representation, Eq. (\*\*\*) may be re-written as

$$\hat{\mathbf{r}} = i \nabla_q + \hat{\Omega}. \quad (****)$$

In the basis of the  $\{n, \mathbf{q}\}$  eigenstates, the matrix of the first term of this sum is diagonal in  $n$ . On the other hand, the matrix of the second operator is, by its definition, diagonal in the  $\mathbf{q}$ -subspace, and hence commutes with the Hamiltonian (\*). Let us use this fact and Eq. (4.199) to calculate the velocity operator in the Heisenberg picture:

$$\hat{\mathbf{v}} \equiv \dot{\hat{\mathbf{r}}} = \frac{1}{i\hbar} [\hat{\mathbf{r}}, \hat{H}_0] = \frac{1}{i\hbar} [i \nabla_q, \hat{H}_0] + \dot{\hat{\Omega}} \equiv \hat{\mathbf{v}}_q + \dot{\hat{\Omega}}.$$

As we know from the band theory, the Hamiltonian (\*) is diagonalized by the kets  $|n, \mathbf{q}\rangle$ , with

$$\langle n, \mathbf{q} | \hat{H}_0 | n, \mathbf{q} \rangle = E_n(\mathbf{q}),$$

so the first contribution ( $\hat{\mathbf{v}}_q$ ) to the velocity operator is diagonal in both the  $n$ - and  $\mathbf{q}$ -spaces, with the diagonal elements that act on the  $\mathbf{q}$ -wavefunction  $a_{n,\mathbf{q}}$  as

$$\hat{\mathbf{v}}_q a_{n,\mathbf{q}} = \frac{1}{i\hbar} [i \nabla_q, E_n(\mathbf{q})] a_{n,\mathbf{q}} \equiv \frac{1}{\hbar} [\nabla_q E_n(\mathbf{q}) a_{n,\mathbf{q}} - E_n(\mathbf{q}) \nabla_q a_{n,\mathbf{q}}] \equiv a_{n,\mathbf{q}} \nabla_q \frac{E_n(\mathbf{q})}{\hbar}.$$

For a wave packet localized in just one energy band  $n$ , with a narrow quasimomentum distribution about some central value  $q_0$ , the action of this operator is reduced to the multiplication by the expression

$$\mathbf{v}_{\text{gr}} = \nabla_q \frac{E_n(\mathbf{q})}{\hbar} \equiv \nabla_q \omega_n(\mathbf{q}),$$

in which we may immediately recognize the natural 3D generalization of Eq. (2.235) for the group velocity of the particle. Hence we may expect that at least in this case, only the first term in Eq. (\*\*\*\*) is important.

To confirm this guess, let us discuss the second component,  $\hat{\Omega}$ , of the velocity operator  $\hat{v}$ . Its matrix is diagonal in the  $\mathbf{q}$ -space, and we may use the same Heisenberg equation Eq. (4.199) to describe the dynamics of its nonvanishing elements:

$$\langle n, \mathbf{q} | \dot{\hat{\Omega}} | n', \mathbf{q} \rangle = \langle n, \mathbf{q} | \frac{1}{i\hbar} [\hat{\Omega}, \hat{H}_0] | n', \mathbf{q} \rangle = \langle n, \mathbf{q} | \frac{1}{i\hbar} (\hat{\Omega} \hat{H}_0 - \hat{H}_0 \hat{\Omega}) | n', \mathbf{q} \rangle = \frac{E_{n'}(\mathbf{q}) - E_n(\mathbf{q})}{\hbar} \langle n, \mathbf{q} | \hat{\Omega} | n', \mathbf{q} \rangle.$$

Due to the definition of the matrix elements  $\langle n, \mathbf{q} | \hat{\Omega} | n', \mathbf{q} \rangle$ , it is clear that they should be finite (because for any finite  $U(\mathbf{r})$ , the functions  $u_{n,\mathbf{q}}(\mathbf{r})$  should be finite and continuous).<sup>240</sup> Hence the second contribution to the velocity operator vanishes for  $n = n'$ , so the operator  $\hat{\Omega}$  is indeed important “only”<sup>241</sup> for interband transitions, and in the absence of such transitions, does not affect the dynamics of a wave packet limited to just one energy band.<sup>242</sup>

In order to analyze such dynamics in the presence of an external classical force  $\mathbf{F}(t)$ , we should add, to the periodic potential energy  $U(\mathbf{q})$ , an additional term with the spatial gradient equal to  $-\mathbf{F}(t)$ . For the simplest 1D case, the total Hamiltonian becomes

$$\hat{H} = \hat{H}_0 - F(t)\hat{x}.$$

If the scale  $F$  of the force magnitude is small in the sense of Eq. (2.236),  $Fa \ll \Delta E_n, \Delta_n$ , it cannot cause interband transitions, so if the system was initially localized in one energy band, we may ignore the second term in Eq. (\*\*\*\*). The remaining first term of that relation obeys the commutation relations similar to the Heisenberg commutator (2.14); in the 1D case its only nonvanishing component is

$$[\hat{x}, \hat{q}_x] = \left[ i \frac{\partial}{\partial q_x}, q_x \right] = i\hat{1}.$$

On the other hand, since the Hamiltonian (\*) is diagonal in the  $q$ -representation, it commutes with the operator of the quasimomentum  $q_x$ . Now we may use these commutation relations to spell out the Heisenberg equation of motion (4.199) for that operator:

$$\dot{\hat{q}}_x = \frac{1}{i\hbar} [\hat{q}_x, \hat{H}] = \frac{1}{i\hbar} \left[ q_x, \hat{H}_0 - iF(t) \frac{\partial}{\partial q_x} \right] \equiv \frac{1}{\hbar} F(t).$$

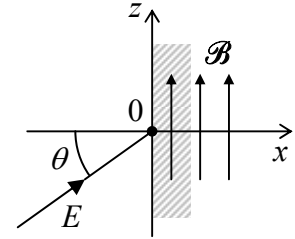
<sup>240</sup> A good additional exercise for the interested reader: calculate these matrix elements explicitly for a 1D periodic potential  $U(x)$ , both in the tight-binding limit and the weak-potential approximation.

<sup>241</sup> Actually, this operator plays a key role in the description of interband transitions in semiconductors, with such important applications as semiconductor lasers, photovoltaic cells, and detectors of radiation. For the reader interested in a detailed discussion of such transitions, I can recommend, for example, the monograph by B. Ridley, *Quantum Processes in Semiconductors*, 4<sup>th</sup> ed., Oxford U. Press, 2000. (See also Sec. 7.6 of this course.)

<sup>242</sup> This fact is the mathematical expression of the vague statement “the quasimomentum is the average momentum” made in Sec. 2.8. Indeed, an elementary 3D generalization of the first of Eqs. (4.269) shows that in the actual-momentum ( $\mathbf{p}$ -) representation,  $\hat{\mathbf{r}} = i\nabla_{\mathbf{k}}$  (where  $\mathbf{k} \equiv \mathbf{p}/\hbar$ ), i.e. coincides with the first component,  $i\nabla_q$ , of that operator in the  $\mathbf{q}$ -representation.

For a narrow wave packet  $a_{s,q}$ , with the center at point  $q_0$ , this equation is equivalent to the quasi-classical equation (2.237), thus (finally!) justifying its applications discussed in Sec. 2.8 of the lecture notes.

**Problem 4.36.** A uniform, time-independent magnetic field  $\mathcal{B} = \mathbf{n}_z \mathcal{B}$  is induced in one semi-space, while the other semi-space is field-free, with a sharp plane boundary  $x = 0$  between these two regions – see the figure on the right. A monochromatic beam of non-relativistic, electrically-neutral spin- $\frac{1}{2}$  particles with a gyromagnetic ratio  $\gamma \neq 0$ ,<sup>243</sup> in a certain spin state and with a kinetic energy  $E$ , propagating within the  $[x, z]$  plane, is incident on this boundary from the field-free side, under angle  $\theta$ . Calculate the coefficient of particle reflection from the boundary.



**Solution:** We may represent the spin ket-vector of the incident particles as a linear superposition of  $z$ -polarized states:

$$|\alpha\rangle = c_{\uparrow} |\uparrow\rangle + c_{\downarrow} |\downarrow\rangle,$$

where the  $z$ -axis is directed along the magnetic field – see the figure above. (The expression “certain spin state” in the problem’s assignment means that the coefficients  $c_{\uparrow}$  and  $c_{\downarrow}$  are known – perhaps up to a common phase factor.) Since the states  $\uparrow$  and  $\downarrow$  are the eigenstates of the Pauli Hamiltonian (4.163), in the field region (in the figure above, at  $x > 0$ ), this operator may be replaced with its eigenvalues in this state basis:  $E_{\uparrow} = -\gamma\mathcal{B}\hbar/2$  and  $E_{\downarrow} = +\gamma\mathcal{B}\hbar/2$ , respectively. Hence we may describe the orbital motion of the beam by a linear superposition of two wavefunctions,<sup>244</sup>  $\psi_{\uparrow}(\mathbf{r})$  and  $\psi_{\downarrow}(\mathbf{r})$ , which obey different Schrödinger equations:

$$\begin{aligned} -\frac{\hbar^2}{2m} \nabla^2 \psi_{\uparrow} + U_{\uparrow}(\mathbf{r}) \psi_{\uparrow} &= E \psi_{\uparrow}, & \text{with } U_{\uparrow}(\mathbf{r}) &= \begin{cases} 0, & \text{for } x < 0, \\ E_{\uparrow}, & \text{for } 0 < x. \end{cases} \\ -\frac{\hbar^2}{2m} \nabla^2 \psi_{\downarrow} + U_{\downarrow}(\mathbf{r}) \psi_{\downarrow} &= E \psi_{\downarrow}, & \text{with } U_{\downarrow}(\mathbf{r}) &= \begin{cases} 0, & \text{for } x < 0, \\ E_{\downarrow}, & \text{for } 0 < x. \end{cases} \end{aligned}$$

But each of these independent<sup>245</sup> boundary problems is exactly similar to that of a spinless particle’s reflection from a potential step – see Problem 3.1. According to its solution, with the replacement of the parameter  $U_0$  with either  $E_{\uparrow}$  or  $E_{\downarrow}$ , respectively, the reflection coefficients  $\mathcal{R}$  of these two waves, referred to the initial intensity of the whole beam, are as follows (provided that  $\gamma\mathcal{B} > 0$ ):

<sup>243</sup> The fact that  $\gamma$  may be different from zero even for electrically-neutral particles such as neutrons, is explained by the Standard Model of elementary particles, in which a neutron “consists” (in a broad sense of this word) of three electrically-charged quarks with a zero net charge.

<sup>244</sup> As will be discussed later in the course, such a set of two wavefunctions is frequently called a *spinor*.

<sup>245</sup> Still note that for the nearly monochromatic incident particles, and in the absence of dephasing (see Chapter 7 of the lecture notes for its discussion), the de Broglie waves  $\psi_{\uparrow}$  and  $\psi_{\downarrow}$  remain coherent, and if their beams are eventually recombined, the particles may exhibit quantum interference phenomena – see, e.g., Sec. 3.1 of the lecture notes.

$$\mathcal{R}_\uparrow = |c_\uparrow|^2 \times \left| \frac{\cos \theta - (\cos^2 \theta + \gamma \mathcal{B} \hbar / 2E)^{1/2}}{\cos \theta + (\cos^2 \theta + \gamma \mathcal{B} \hbar / 2E)^{1/2}} \right|^2,$$

$$\mathcal{R}_\downarrow = |c_\downarrow|^2 \times \begin{cases} \left[ \frac{\cos \theta - (\cos^2 \theta - \gamma \mathcal{B} \hbar / 2E)^{1/2}}{\cos \theta + (\cos^2 \theta - \gamma \mathcal{B} \hbar / 2E)^{1/2}} \right]^2, & \text{for } \frac{\gamma \mathcal{B} \hbar}{2E} < \cos^2 \theta, \\ 1, & \text{for } \cos^2 \theta < \frac{\gamma \mathcal{B} \hbar}{2E}. \end{cases}$$

(For  $\gamma \mathcal{B} < 0$ , these expressions should be interchanged.)

In particular, if the spin polarization energy  $|\gamma \mathcal{B}| \hbar / 2$  is larger than the incident particle energy  $E$ , the reflection of one de Broglie wave (for  $\gamma \mathcal{B} > 0$ ,  $\psi_\downarrow$ ) is total for any incidence angle  $\theta$ , so only the other wave ( $\psi_\uparrow$ ) propagates into the field region  $x > 0$ . Hence such a setup may be used for getting a beam of spin-polarized particles from an incident beam of unpolarized ones.

## Chapter 5. Some Exactly Solvable Problems

**Problem 5.1.** Use the discussion in Sec. 5.1 of the lecture notes to find an alternative solution of Problem 4.18.

*Solution:* According to the discussion in Sec. 5.1, the expectation value of the  $z$ -component of spin- $\frac{1}{2}$ , in the state fully polarized in the direction  $\mathbf{n} = \mathbf{n}_x \sin \theta \cos \varphi + \mathbf{n}_y \sin \theta \sin \varphi + \mathbf{n}_z \cos \theta$ , is given by the last of Eqs. (5.12):

$$\langle S_z \rangle \equiv \frac{\hbar}{2} \langle \sigma_z \rangle = \frac{\hbar}{2} \cos \theta \equiv \frac{\hbar}{2} \left( 2 \cos^2 \frac{\theta}{2} - 1 \right). \quad (*)$$

But according to Eq. (1.37) and the fact that in the  $z$ -basis, the operator  $\hat{S}_z$  has just two eigenstates,  $\uparrow$  and  $\downarrow$ , with the eigenvalues  $\pm \hbar/2$ , this expectation value may be also represented as

$$\langle S_z \rangle = \left( +\frac{\hbar}{2} \right) W_\uparrow + \left( -\frac{\hbar}{2} \right) W_\downarrow \equiv \frac{\hbar}{2} (W_\uparrow - W_\downarrow). \quad (**)$$

where  $W_\uparrow$  and  $W_\downarrow$  are the probabilities of the corresponding states. Since the sum of these two probabilities has to equal 1, i.e.  $W_\downarrow = 1 - W_\uparrow$ , Eq. (\*\*) may be rewritten as

$$\langle S_z \rangle = \frac{\hbar}{2} [W_\uparrow - (1 - W_\uparrow)] \equiv \frac{\hbar}{2} (2W_\uparrow - 1).$$

By requiring this expression to give the same result as Eq. (\*), we get

$$W_\uparrow = \cos^2 \frac{\theta}{2}, \quad \text{and hence } W_\downarrow = 1 - W_\uparrow = 1 - \cos^2 \frac{\theta}{2} \equiv \sin^2 \frac{\theta}{2}.$$

Now we may argue that due to the isotropy of free space, this result has to be independent of the absolute directions of the two axes (those of the initial polarization of the spin and the direction of the magnetic field in the Stern-Gerlach apparatus), and may depend only on the angle  $\theta$  between these axes. Thus we have re-derived the solution of Problem 4.18 – in a much simpler way.

**Problem 5.2.** A spin- $\frac{1}{2}$  with a gyromagnetic ratio  $\gamma$  is placed into an external magnetic field, with a time-independent orientation, its magnitude  $\mathcal{B}(t)$  being an arbitrary function of time. Find explicit expressions for the Heisenberg operators and the expectation values of all three Cartesian components of the spin as functions of time, in a coordinate system of your choice.

*Solution:* In the coordinate system with the  $z$ -axis directed along the applied magnetic field (evidently, the easiest choice), the Hamiltonian of our system is given by Eq. (4.163) of the lecture notes:

$$\hat{H} = -\gamma \mathcal{B}(t) \hat{S}_z \equiv -\gamma \mathcal{B}(t) \frac{\hbar}{2} \hat{\sigma}_z.$$

In the  $z$ -basis, its matrix is



$$H = -\gamma\mathcal{B}(t)\frac{\hbar}{2}\sigma_z \equiv -\gamma\mathcal{B}(t)\frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

This expression coincides with Eq. (5.3) of the lecture notes,<sup>1</sup> with  $b = 0$  and

$$\mathbf{c} = -\gamma\mathcal{B}(t)\frac{\hbar}{2}\mathbf{n}_z.$$

Hence we may use Eq. (5.19) rewritten for the spin operator  $\hat{\mathbf{S}} \equiv (\hbar/2)\hat{\boldsymbol{\sigma}}$ :

$$\dot{\hat{\mathbf{S}}} = \boldsymbol{\Omega}(t) \times \hat{\mathbf{S}}, \quad \text{with } \boldsymbol{\Omega}(t) \equiv \frac{2}{\hbar}\mathbf{c}(t) = -\gamma\mathcal{B}(t)\mathbf{n}_z,$$

so in the Cartesian components,

$$\dot{\hat{S}}_x = -\Omega(t)\hat{S}_y, \quad \dot{\hat{S}}_y = \Omega(t)\hat{S}_x, \quad \dot{\hat{S}}_z = 0. \quad (*)$$

The last equation obviously yields

$$\hat{S}_z(t) = \hat{S}_z(0) = \text{const},$$

while the easiest way to solve the system of the first two equations (\*) is to introduce (just as it was done for the orbital momentum in Sec. 5.6 of the lecture notes), the *spin-ladder operators*<sup>2</sup>

$$\hat{S}_{\pm} \equiv \hat{S}_x \pm i\hat{S}_y,$$

with the reciprocal relations

$$\hat{S}_x = \frac{\hat{S}_+ + \hat{S}_-}{2}, \quad \hat{S}_y(t) = \frac{\hat{S}_+ - \hat{S}_-}{2i}. \quad (**)$$

By using these formulas and Eqs. (\*) to calculate the time derivatives of the ladder operators, we get two simple independent equations

$$\dot{\hat{S}}_{\pm} = \pm i\Omega(t)\hat{S}_{\pm},$$

which are easy to solve:

$$\hat{S}_{\pm}(t) = \hat{S}_{\pm}(0)\exp\{\pm i\varphi(t)\} \equiv [\hat{S}_x(0) \pm i\hat{S}_y(0)]\exp\{\pm i\varphi(t)\}, \quad \text{where } \varphi(t) \equiv \int_0^t \Omega(t')dt'. \quad (***)$$

Now using Eqs. (\*\*) to return the real Cartesian coordinates of the spin operator, we finally get

$$\hat{S}_x(t) = \hat{S}_x(0)\cos\varphi(t) - \hat{S}_y(0)\sin\varphi(t), \quad \hat{S}_y(t) = \hat{S}_y(0)\cos\varphi(t) + \hat{S}_x(0)\sin\varphi(t).$$

In the particular case of a time-independent field, the argument (\*\*\*) of the trigonometric functions in these expressions is just  $\Omega t$ , so our results are reduced to Eq. (4.194)-(4.195) of the lecture notes (written there for the  $z$ -basis matrices, but actually valid, as operator relations, in any basis).

Finally, since in the Heisenberg formalism, according to Eq. (4.191), the expectation value of any observable is calculated with time-independent bra- and ket-vectors, the relations between the

<sup>1</sup> See also Eq. (5.13) with  $\mathcal{B} = \mathcal{B}(t)\mathbf{n}_z$ .

<sup>2</sup> Implicitly, these operators (or rather their expectation values) have already been used in the lecture notes – see Eqs. (4.172)-(4.173).

expectation values of the spin components exactly replicate the above operator relations. Again, for the case of a constant magnetic field, they coincide with Eqs. (4.170), (4.173)-(4.174).

**Problem 5.3.** A two-level system is in the quantum state  $\alpha$  described by the ket-vector  $|\alpha\rangle = \alpha_\uparrow|\uparrow\rangle + \alpha_\downarrow|\downarrow\rangle$ , with given (generally, complex)  $c$ -number coefficients  $\alpha_{\uparrow\downarrow}$ . Prove that we can always select such a geometric  $c$ -number vector  $\mathbf{c} = \{c_x, c_y, c_z\}$  that  $\alpha$  would be an eigenstate of  $\mathbf{c} \cdot \hat{\boldsymbol{\sigma}}$ , where  $\hat{\boldsymbol{\sigma}}$  is the Pauli vector operator. Find all possible values of  $\mathbf{c}$  satisfying this condition, and the second eigenstate (orthogonal to  $\alpha$ ) of the operator  $\mathbf{c} \cdot \hat{\boldsymbol{\sigma}}$ . Give a Bloch-sphere interpretation of your result.

*Solution:* In the  $z$ -basis, the operator  $\mathbf{c} \cdot \hat{\boldsymbol{\sigma}}$  has the following matrix:

$$\mathbf{c} \cdot \hat{\boldsymbol{\sigma}} = c_x \hat{\sigma}_x + c_y \hat{\sigma}_y + c_z \hat{\sigma}_z = c_x \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + c_y \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + c_z \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \equiv \begin{pmatrix} c_z & c_- \\ c_+ & -c_z \end{pmatrix}, \quad \text{where } c_{\pm} \equiv c_x \pm ic_y,$$

so the system of equations (4.102) for its eigenstates and eigenvalues has the form

$$\begin{pmatrix} c_z - \lambda_j & c_- \\ c_+ & -c_z - \lambda_j \end{pmatrix} \begin{pmatrix} \alpha_\uparrow \\ \alpha_\downarrow \end{pmatrix} = 0. \quad (*)$$

The condition of compatibility of these equations, the characteristic equation

$$\begin{vmatrix} c_z - \lambda_j & c_- \\ c_+ & -c_z - \lambda_j \end{vmatrix} = 0,$$

has two roots  $\lambda_{\pm} = \pm c$ , where

$$c \equiv (c_z^2 + c_+ c_-)^{1/2} \equiv (c_x^2 + c_y^2 + c_z^2)^{1/2} \equiv |\mathbf{c}|.$$

Plugging these roots back into the initial system of equations (\*), we get

$$c_- \frac{\alpha_\downarrow}{\alpha_\uparrow} = \pm c - c_z, \quad c_+ \frac{\alpha_\uparrow}{\alpha_\downarrow} = \pm c + c_z.$$

With the characteristic equation satisfied, any one of these relations contains the same information. Moreover, up to this point, this solution repeats Approach 2 in the model solution of Problem 4.27. However, since  $c_-^* = c_+$ , while  $c$  and  $c_z$  are real, for our current purposes, it is convenient to use the second equation together with the complex conjugate of the first equation,

$$c_+ \frac{\alpha_\downarrow^*}{\alpha_\uparrow^*} = \pm c - c_z.$$

Indeed, by adding both sides of these two equations, we may eliminate  $c$  (which is an inconvenient, nonlinear combination of the  $c$ -vector components):

$$c_+ \left( \frac{\alpha_\uparrow}{\alpha_\downarrow} - \frac{\alpha_\downarrow^*}{\alpha_\uparrow^*} \right) = 2c_z. \quad (**)$$

This is the *only* equation we need to satisfy in order to make the given quantum state the eigenstate of our Hamiltonian. Formally solving it for  $c_+$ ,

$$c_+ = 2c_z \left( \frac{\alpha_\uparrow}{\alpha_\downarrow} - \frac{\alpha_\downarrow^*}{\alpha_\uparrow^*} \right)^{-1} \equiv 2c_z \frac{\alpha_\downarrow \alpha_\uparrow^*}{|\alpha_\uparrow|^2 - |\alpha_\downarrow|^2},$$

then finding  $c_-$  as the complex conjugate of  $c_+$ :

$$c_- = 2c_z \frac{\alpha_\uparrow \alpha_\downarrow^*}{|\alpha_\uparrow|^2 - |\alpha_\downarrow|^2},$$

we may return to  $c_x$  and  $c_y$ :

$$c_x = \frac{c_+ + c_-}{2} = c_z \frac{\alpha_\downarrow \alpha_\uparrow^* + \alpha_\uparrow \alpha_\downarrow^*}{|\alpha_\uparrow|^2 - |\alpha_\downarrow|^2}, \quad c_y = \frac{c_+ - c_-}{2i} = c_z \frac{1}{i} \frac{\alpha_\downarrow \alpha_\uparrow^* - \alpha_\uparrow \alpha_\downarrow^*}{|\alpha_\uparrow|^2 - |\alpha_\downarrow|^2}.$$

Now let us assume that the given ket vector  $|\alpha\rangle$  is normalized:  $(|\alpha_\uparrow|^2 + |\alpha_\downarrow|^2)^{1/2} = 1$ , and their (inconsequential) common phase is set so that the coefficient  $\alpha_\uparrow$  is real. Then in the Bloch-sphere representation given by Eq. (5.11) of the lecture notes, the above result takes a much simpler form:

$$c_\pm = c \sin \theta e^{\pm i\varphi} \quad (\text{i.e., } c_x = c \sin \theta \cos \varphi, \quad c_y = c \sin \theta \sin \varphi), \quad c_z = c \cos \theta,$$

where  $c$  may be arbitrary, while  $\theta$  and  $\varphi$  are just the spherical angles of the state-representing point:

$$\theta = 2 \cos^{-1} \alpha_\uparrow, \quad \varphi = \arg \alpha_\downarrow.$$

This result has a very simple interpretation: in order for a state  $\alpha$ , represented by a certain point on the Bloch sphere, to be an eigenstate of the operator  $\mathbf{c} \cdot \hat{\mathbf{c}}$ , it is sufficient to have the “field” vector  $\mathbf{c}$  directed from the origin to this point. This is just an alignment of the (average) spin’s direction with the field; the degree of freedom we still have in the solution corresponds to the arbitrary field’s strength  $c$ .

The Bloch sphere graphics also give a simple way to find the eigenstate  $\alpha'$  orthogonal to the given one ( $\alpha$ ): their representing points should be diametrically opposite. Hence, to find the coefficients  $\alpha'_\uparrow$  and  $\alpha'_\downarrow$  for this second eigenstate, it is sufficient to make the following replacements:  $\theta \rightarrow \pi - \theta$  and  $\varphi \rightarrow \pi + \varphi$  in Eqs. (5.11), getting

$$\alpha'_\uparrow = \sin \frac{\theta}{2} = \alpha_\downarrow \exp\{-i \arg \alpha_\downarrow\}, \quad \alpha'_\downarrow = -\cos \frac{\theta}{2} e^{i\varphi} = -\alpha_\uparrow \exp\{i \arg \alpha_\downarrow\}.$$

(Generally, both coefficients may be multiplied by the common phase factor  $\exp\{i\gamma'\}$  with an arbitrary real  $\gamma'$ , just as it is done in Eq. (5.10) for the initial state.) It is also straightforward to verify that the simultaneous replacement  $\alpha_{\uparrow\downarrow} \rightarrow \alpha'_{\uparrow\downarrow}$  changes the signs of the eigenvalues  $\lambda$ : from  $+c$  to  $-c$  and vice versa.

**Problem 5.4.** Rewrite the key formulas of the solutions of Problems 4.27-4.29 in terms of the Bloch sphere angles, and verify at least one of them using the general relations of Sec. 5.1 of the lecture notes.

*Solution:* In those solutions, the  $c$ -number “field vector”  $\mathbf{c}$  that participates in the problems’ Hamiltonian

$$\hat{H} = \mathbf{c} \cdot \hat{\mathbf{c}}, \quad (*)$$

(where  $\hat{\mathbf{c}}$  is the Pauli matrix operator) was represented by its Cartesian coordinates  $c_x$ ,  $c_y$ , and  $c_z$  in the usual  $z$ -basis, with the convenient complex-number notation  $c_{\pm} \equiv c_x \pm ic_y$ , so that  $c_x^2 + c_y^2 = c_+c_-$ . Here, let us use the standard spherical-coordinate representation of this vector instead:

$$\mathbf{c} = c\{\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta\}, \quad \text{so } \frac{c_{\pm}}{c} = \sin\theta e^{\pm i\varphi}, \quad \frac{c_z}{c} = \cos\theta.$$

It is imperative to distinguish these spherical angles  $\theta$  and  $\varphi$ , describing the direction of the given vector  $\mathbf{c}$ , from the Bloch-sphere angles of an arbitrary state of the two-level system, which were used in most formulas of Sec. 5.1 of the lecture notes; as was shown in the solution of the previous problem, these notions coincide only for the eigenstates of the Hamiltonian (\*).

In this angular notation, Eq. (\*) of the model solution of Problem 4.27 becomes<sup>3</sup>

$$\mathbf{u}(t,0) = \begin{pmatrix} \cos\frac{\Omega t}{2} - i\cos\theta\sin\frac{\Omega t}{2} & -i\sin\theta e^{-i\varphi}\sin\frac{\Omega t}{2} \\ -i\sin\theta e^{i\varphi}\sin\frac{\Omega t}{2} & \cos\frac{\Omega t}{2} - i\cos\theta\sin\frac{\Omega t}{2} \end{pmatrix},$$

where  $\Omega \equiv 2c/\hbar$  is the same quantum oscillation frequency as in Eq. (5.14).<sup>4</sup> For the particular case of the initial state  $\uparrow$ , which was the subject of that problem, the other major results of its solution acquire the following forms:

$$\begin{pmatrix} \alpha_{\uparrow}(t) \\ \alpha_{\downarrow}(t) \end{pmatrix} \equiv \begin{pmatrix} \langle \uparrow | \alpha(t) \rangle \\ \langle \downarrow | \alpha(t) \rangle \end{pmatrix} = \begin{pmatrix} \cos\frac{\Omega t}{2} - i\cos\theta\sin\frac{\Omega t}{2} \\ -i\sin\theta e^{i\varphi}\sin\Omega t \end{pmatrix},$$

$$W_{\uparrow} = \cos^2\frac{\Omega t}{2} + \cos^2\theta\sin^2\frac{\Omega t}{2} \equiv 1 - \sin^2\theta\sin^2\frac{\Omega t}{2}, \quad W_{\downarrow} = \sin^2\theta\sin^2\frac{\Omega t}{2} \equiv 1 - W_{\uparrow},$$

$$\langle S_x \rangle = \hbar\sin\theta \left( \sin\varphi\cos\frac{\Omega t}{2} + \cos\theta\cos\varphi\sin\frac{\Omega t}{2} \right) \sin\frac{\Omega t}{2},$$

$$\langle S_y \rangle = \hbar\sin\theta \left( -\cos\varphi\cos\frac{\Omega t}{2} + \cos\theta\sin\varphi\sin\frac{\Omega t}{2} \right) \sin\frac{\Omega t}{2},$$

$$\langle S_z \rangle = \frac{\hbar}{2} \left( 1 - 2\sin^2\theta\sin^2\frac{\Omega t}{2} \right). \quad (**)$$

As a sanity check, let us re-derive the last expression from the last of Eqs. (5.12) of the lecture notes:

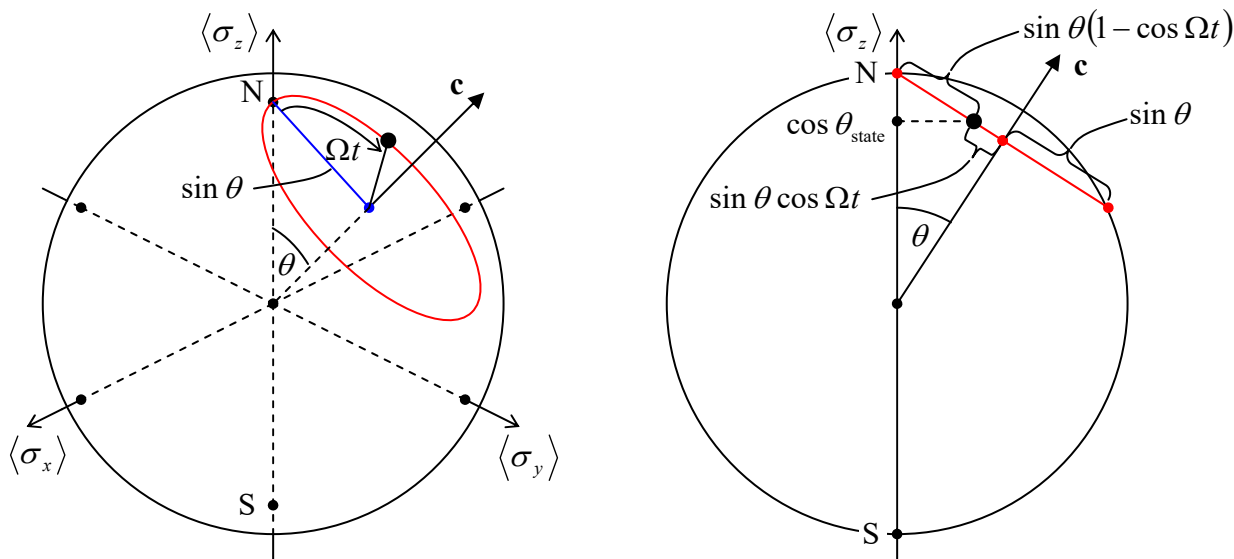
$$\langle \sigma_z \rangle = \cos\theta_{\text{state}}, \quad \text{i.e. } \langle S_z \rangle = \frac{\hbar}{2} \cos\theta_{\text{state}},$$

where the subscript is added to distinguish the polar angle of the Bloch-sphere point representing the quantum state from the tilt  $\theta$  of the  $c$ -number vector  $\mathbf{c}$ . According to Eq. (5.21), in our current case of a time-independent vector  $\mathbf{\Omega} \equiv 2\mathbf{c}/\hbar$ , the state-representing point moves, with a constant angular velocity

<sup>3</sup> In the particular case of a  $z$ -oriented field ( $\theta=0$ ), this expression reduces to Eq. (4.193) of the lecture notes.

<sup>4</sup> In the particular case of the spin- $1/2$  precession in a magnetic field  $\mathcal{B}$  when, according to Eq. (5.163),  $\mathbf{c} = -(\hbar/2)\gamma\mathcal{B}$ , this frequency is reduced to Eq. (4.164):  $\Omega = -\gamma\mathcal{B}$ .

$\Omega$ , along a circle whose symmetry axis is directed along the vector  $\mathbf{c}$ . If the initial state of the system is  $\uparrow$  (as it is in Problems 4.27-29), this circle has to pass through the Bloch sphere's North Pole – see the left figure below, where the circle is shown in red.



The balance of the calculation becomes more clear from the right figure above, which shows the projection of the same geometry on the common plane of the vertical axis and the vector  $\mathbf{c}$ . Since the Bloch sphere has a unit radius, the radius of the circular trajectory of the state point (see also the blue segment in the left figure) is  $\sin \theta$ . The projection of the state point on this plane is offset from the circle's center by the distance  $\sin \theta \cos \Omega t$ , and hence its distance from the North Pole of the sphere is  $\sin \theta - \sin \theta \cos \Omega t \equiv \sin \theta (1 - \cos \Omega t)$ . The projection of this segment on the vertical axis is  $\sin \theta [\sin \theta (1 - \cos \Omega t)] \equiv \sin^2 \theta (1 - \cos \Omega t)$ , so, finally,

$$\langle \sigma_z \rangle = \cos \theta_{\text{state}} = 1 - \sin^2 \theta (1 - \cos \Omega t) \equiv 1 - 2 \sin^2 \theta \sin^2 \frac{\Omega t}{2}, \quad \text{i.e. } \langle S_z \rangle = \frac{\hbar}{2} \left( 1 - 2 \sin^2 \theta \sin^2 \frac{\Omega t}{2} \right),$$

thus confirming Eq. (\*\*). (The above expressions for  $\langle S_x \rangle$  and  $\langle S_y \rangle$  may be verified by using the same sketch and a bit more involved trigonometry.)

Besides that, while developing Approach 2 to the solution of Problem 4.27, we have derived the following relations between the eigenstates  $\pm$  of the Hamiltonian (\*) and the  $z$ -basis states  $\uparrow$  and  $\downarrow$ :

$$\langle \uparrow | + \rangle = \langle \downarrow | - \rangle = \frac{c + c_z}{[2c(c + c_z)]^{1/2}}, \quad \langle \downarrow | + \rangle = \frac{c_+}{[2c(c + c_z)]^{1/2}}, \quad \langle \uparrow | - \rangle = -\frac{c_-}{[2c(c + c_z)]^{1/2}}.$$

In the spherical-coordinate representation of the vector  $\mathbf{c}$ , these relations become

$$\langle \uparrow | + \rangle = \langle \downarrow | - \rangle = \frac{1 + \cos \theta}{[2(1 + \cos \theta)]^{1/2}} \equiv \left( \frac{1 + \cos \theta}{2} \right)^{1/2} \equiv \cos \frac{\theta}{2},$$

$$\langle \downarrow | + \rangle = \frac{\sin \theta}{[2(1 + \cos \theta)]^{1/2}} e^{i\varphi} \equiv \sin \frac{\theta}{2} e^{i\varphi}, \quad \langle \uparrow | - \rangle = -\frac{\sin \theta}{[2(1 + \cos \theta)]^{1/2}} e^{-i\varphi} \equiv -\sin \frac{\theta}{2} e^{-i\varphi}.$$

Since in the notation (5.1) of the lecture notes,  $\langle \uparrow | + \rangle$  is just  $\alpha_\uparrow$ , while  $\langle \downarrow | + \rangle$  is  $\alpha_\downarrow$ , there is no surprise that the expressions for these two short brackets are in agreement with Eqs. (5.11) of the lecture notes, because the points representing the eigenstates  $\pm$  on the Bloch sphere are located where the vector  $\mathbf{c}$  pierces it. (Cf. the solution of the previous problem.)

So, we see that the bulkiness of some formulas in the solution of Problem 4.27 was not due to the complexity of the quantum oscillations at such but rather due to the awkwardness of the Cartesian-component representation of the circular motion of the state point on the Bloch sphere.

Next, the objective of Problem 4.28 was to obtain essentially the same results using the Heisenberg picture, but that of Problem 4.29 was different: to calculate the matrix elements of the operator  $\hat{\sigma}_z$  in the basis of the states  $\pm$ . The result, in the matrix form, was

$$\sigma_z |_{\text{in}\pm} \equiv \frac{1}{c} \begin{pmatrix} c_z & -c_- \\ -c_+ & -c_z \end{pmatrix}.$$

In the angular representation of the vector  $\mathbf{c}$ , this formula reads

$$\sigma_z |_{\text{in}\pm} \equiv \begin{pmatrix} \cos\theta & -\sin\theta e^{-i\varphi} \\ -\sin\theta e^{i\varphi} & -\cos\theta \end{pmatrix}.$$

For the “field vector”  $\mathbf{c}$  aligned with the  $z$ -axis ( $\theta = 0$ ), this result is reduced to the canonical form of the Pauli matrix  $\sigma_z$ , regardless of the azimuthal angle  $\varphi$ . On the other hand, for a field normal to this axis ( $\theta = \pi/2$ ), the result is a function of the azimuthal angle:

$$\sigma_z |_{\text{in}a} \equiv \begin{pmatrix} 0 & -e^{-i\varphi} \\ -e^{i\varphi} & 0 \end{pmatrix},$$

turning into the canonical forms of the Pauli matrices  $\sigma_x$  at  $\varphi = \pm\pi$ , and  $\sigma_y$  at  $\varphi = -\pi/2$ .

**Problem 5.5.** A spin- $1/2$  with a gyromagnetic ratio  $\gamma > 0$  was placed into a time-independent magnetic field  $\mathcal{B}_0 = \mathcal{B}_0 \mathbf{n}_z$  and let relax into the lowest-energy state. At  $t = 0$ , an additional field  $\mathcal{B}_1(t)$  is turned on; its vector has a constant magnitude but rotates within the  $[x, y]$ -plane with an angular velocity  $\omega$ . Calculate the expectation values of all Cartesian components of the spin at  $t \geq 0$ , and discuss the representation of its dynamics on the Bloch sphere.

*Solution:* Let us take the direction of the vector  $\mathcal{B}_1$  at  $t = 0$  for the  $x$ -axis; then the total field at  $t \geq 0$  is<sup>5</sup>

$$\mathcal{B} = \mathcal{B}_1 (\mathbf{n}_x \cos \omega t + \mathbf{n}_y \sin \omega t) + \mathcal{B}_0 \mathbf{n}_z,$$

so the Pauli Hamiltonian (4.163a) becomes

<sup>5</sup> This choice of the sign before  $\mathbf{n}_y$  corresponds to the positive (counterclockwise) rotation of the vector  $\mathcal{B}_1$  within the  $[x, y]$  plane. To describe the opposite rotation, it is sufficient to change the sign before  $\omega$  in all the formulas below.

$$\hat{H} = -\gamma \frac{\hbar}{2} \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{\mathcal{B}} = -\gamma \frac{\hbar}{2} \left[ \mathcal{B}_1 (\hat{\sigma}_x \cos \omega t + \hat{\sigma}_y \sin \omega t) + \mathcal{B}_0 \hat{\sigma}_z \right] \equiv \frac{\hbar}{2} \left[ \Omega_1 (\hat{\sigma}_x \cos \omega t + \hat{\sigma}_y \sin \omega t) + \Omega_0 \hat{\sigma}_z \right]$$

where (as in Sec. 4.6 of the lecture notes),  $\Omega_0 \equiv -\gamma \mathcal{B}_0$  and  $\Omega_1 \equiv -\gamma \mathcal{B}_1$ . In the usual  $z$ -basis, the matrix of this Hamiltonian is

$$H = \frac{\hbar}{2} \left[ \Omega_1 (\sigma_x \cos \omega t + \sigma_y \sin \omega t) + \Omega_0 \sigma_z \right] = \frac{\hbar}{2} \begin{pmatrix} \Omega_0 & \Omega_1 e^{-i\omega t} \\ \Omega_1 e^{+i\omega t} & -\Omega_0 \end{pmatrix}.$$

Let us take the spin's ket-vector in the form (5.1):

$$|\alpha(t)\rangle = \alpha_{\uparrow}(t) |\uparrow\rangle + \alpha_{\downarrow}(t) |\downarrow\rangle, \quad \text{where } \alpha_{\uparrow\downarrow} = \langle \uparrow\downarrow | \alpha \rangle,$$

then the Schrödinger equation (4.158) yields

$$\begin{aligned} \dot{\alpha}_{\uparrow} &= \frac{1}{i\hbar} \langle \uparrow | \hat{H} | \alpha \rangle = \frac{1}{i\hbar} (1, 0) H \begin{pmatrix} \alpha_{\uparrow} \\ \alpha_{\downarrow} \end{pmatrix} = -\frac{i}{2} (\Omega_0 \alpha_{\uparrow} + \Omega_1 e^{-i\omega t} \alpha_{\downarrow}), \\ \dot{\alpha}_{\downarrow} &= \frac{1}{i\hbar} \langle \downarrow | \hat{H} | \alpha \rangle = \frac{1}{i\hbar} (0, 1) H \begin{pmatrix} \alpha_{\uparrow} \\ \alpha_{\downarrow} \end{pmatrix} = -\frac{i}{2} (\Omega_1 e^{+i\omega t} \alpha_{\uparrow} - \Omega_0 \alpha_{\downarrow}). \end{aligned} \quad (*)$$

This is a system of two ordinary linear differential equations with time-dependent coefficients. There are no regular methods for analytical solutions of general equations of this type; however, in our particular case, the functions of time are very simple and may be eliminated by the following trick.<sup>6</sup> Let us define two functions of time, which differ from  $\alpha_{\uparrow\downarrow}(t)$  only by simple phase factors:

$$\beta_{\uparrow} \equiv \alpha_{\uparrow} \exp\left\{ +\frac{i\omega t}{2} \right\}, \quad \beta_{\downarrow} \equiv \alpha_{\downarrow} \exp\left\{ -\frac{i\omega t}{2} \right\}.$$

For these new variables, Eqs. (\*) yield a system of equations with constant coefficients:

$$\dot{\beta}_{\uparrow} = \frac{i}{2} (\xi \beta_{\uparrow} - \Omega_1 \beta_{\downarrow}), \quad \dot{\beta}_{\downarrow} = -\frac{i}{2} (\Omega_1 \beta_{\uparrow} + \xi \beta_{\downarrow}), \quad (**)$$

where  $\xi \equiv \omega - \Omega_0$  is “detuning” – the difference between the frequencies of the ac field  $\mathcal{B}_1(t)$  and of the spin precession in the dc field  $\mathcal{B}_0$ .

The general solution of this system of linear equations may be expressed as

$$\beta_{\uparrow}(t) = b_{\uparrow+} \exp\left\{ i \frac{\Omega_+ t}{2} \right\} + b_{\uparrow-} \exp\left\{ i \frac{\Omega_- t}{2} \right\}, \quad \beta_{\downarrow}(t) = b_{\downarrow+} \exp\left\{ i \frac{\Omega_+ t}{2} \right\} + b_{\downarrow-} \exp\left\{ i \frac{\Omega_- t}{2} \right\}, \quad (***)$$

where the frequencies  $\Omega_{\pm}$  are the roots of the characteristic equation that results from the substitution of any of these exponents into Eq. (\*\*):

$$\begin{vmatrix} \xi - \Omega_{\pm} & -\Omega_1 \\ -\Omega_1 & -\xi - \Omega_{\pm} \end{vmatrix} = 0, \quad \text{giving } \Omega_{\pm} = \pm \Omega, \quad \text{where } \Omega \equiv (\xi^2 + \Omega_1^2)^{1/2} \equiv [(\omega - \Omega_0)^2 + \Omega_1^2]^{1/2}.$$

<sup>6</sup> It will be also used in Sec. 6.5 of the lecture notes for the solution of a very similar problem.

This  $\Omega$  is called the *Rabi oscillation frequency*.<sup>7</sup> In order to find the constant coefficients  $b$ , we may plug each exponent participating in the solution (\*\*\*), one by one, back into Eqs. (\*\*) and solve any of the resulting linear homogeneous algebraic equations for the ratios of these coefficients. The result is<sup>8</sup>

$$\frac{b_{\downarrow+}}{b_{\uparrow+}} = -\frac{\Omega - \xi}{\Omega_1}, \quad \frac{b_{\uparrow-}}{b_{\downarrow-}} = \frac{\Omega - \xi}{\Omega_1} \equiv \frac{\Omega_1}{\Omega + \xi},$$

so Eqs. (\*\*\*) are reduced to

$$\beta_{\uparrow}(t) = b_+ \exp\left\{+i\frac{\Omega t}{2}\right\} + b_- \frac{\Omega - \xi}{\Omega_1} \exp\left\{-i\frac{\Omega t}{2}\right\}, \quad \beta_{\downarrow}(t) = -b_+ \frac{\Omega - \xi}{\Omega_1} \exp\left\{+i\frac{\Omega t}{2}\right\} + b_- \exp\left\{-i\frac{\Omega t}{2}\right\},$$

where  $b_+ \equiv b_{\uparrow+}$  and  $b_- \equiv b_{\downarrow-}$ . These two remaining coefficients are determined by the initial conditions. In our particular case, in the absence of the field  $\mathcal{B}_1$ , i.e. at  $t \leq 0$ , the system's Hamiltonian was simply

$$H = \frac{\hbar}{2} \begin{pmatrix} \Omega_0 & 0 \\ 0 & -\Omega_0 \end{pmatrix} \equiv -\frac{\hbar}{2} \gamma \mathcal{B}_0 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

so at  $\gamma \mathcal{B}_0 > 0$ , the state  $\uparrow$  had the lowest energy and hence is the initial state of our system for its evolution at  $t \geq 0$ . Hence, the initial conditions for the system's evolution at  $t \geq 0$  are as follows:

$$\beta_{\uparrow}(0) \equiv \alpha_{\uparrow}(0) = 1, \quad \beta_{\downarrow}(0) \equiv \alpha_{\downarrow}(0) = 0.$$

For the coefficients  $b_{\uparrow}$  and  $b_{\downarrow}$ , these conditions give a simple system of two linear equations,

$$b_+ + \frac{\Omega - \xi}{\Omega_1} b_- = 1, \quad -\frac{\Omega - \xi}{\Omega_1} b_+ + b_- = 0,$$

with the solution

$$b_+ = \frac{\Omega + \xi}{2\Omega}, \quad b_- = \frac{\Omega_1}{2\Omega},$$

so Eqs. (\*\*\*) become

$$\beta_{\uparrow}(t) = \frac{\Omega + \xi}{2\Omega} \exp\left\{+i\frac{\Omega t}{2}\right\} + \frac{\Omega - \xi}{2\Omega} \exp\left\{-i\frac{\Omega t}{2}\right\} \equiv \cos\frac{\Omega t}{2} + i\frac{\xi}{\Omega} \sin\frac{\Omega t}{2},$$

$$\beta_{\downarrow}(t) = \frac{\Omega_1}{2\Omega} \exp\left\{-i\frac{\Omega t}{2}\right\} - \frac{\Omega_1}{2\Omega} \exp\left\{+i\frac{\Omega t}{2}\right\} \equiv -i\frac{\Omega_1}{\Omega} \sin\frac{\Omega t}{2},$$

and for our original expansion coefficients, we get

$$\alpha_{\uparrow}(t) = \left( \cos\frac{\Omega t}{2} + i\frac{\xi}{\Omega} \sin\frac{\Omega t}{2} \right) \exp\left\{-i\frac{\omega t}{2}\right\}, \quad \alpha_{\downarrow}(t) = -i\frac{\Omega_1}{\Omega} \sin\frac{\Omega t}{2} \exp\left\{i\frac{\omega t}{2}\right\}.$$

Now plugging this solution into Eqs. (4.130) and (4.132)-(4.133) of the lecture notes, we finally get

<sup>7</sup> Indeed, the process considered in this problem is a particular case of the general effect of *Rabi oscillations*, which is ubiquitous in quantum systems driven by periodic external fields – see Sec. 6.5 of the lecture notes.

<sup>8</sup> Note that the above expression for  $\Omega$  implies that  $(\Omega - \xi)/\Omega_1 = \Omega_1/(\Omega + \xi)$ .



$$\begin{aligned}\langle S_x \rangle &= \hbar \frac{\Omega_1}{\Omega} \left( \cos \frac{\Omega t}{2} \sin \omega t - \frac{\xi}{\Omega} \sin \frac{\Omega t}{2} \cos \omega t \right) \sin \frac{\Omega t}{2}, \\ \langle S_y \rangle &= \hbar \frac{\Omega_1}{\Omega} \left( -\cos \frac{\Omega t}{2} \cos \omega t - \frac{\xi}{\Omega} \sin \frac{\Omega t}{2} \sin \omega t \right) \sin \frac{\Omega t}{2}, \\ \langle S_z \rangle &= \frac{\hbar}{2} \left( 1 - 2 \frac{\Omega_1^2}{\Omega^2} \sin^2 \frac{\Omega t}{2} \right).\end{aligned}\tag{****}$$

Let us discuss these results, starting with the last one. It shows that the spin's component aligned with the dc field (or rather its expectation value) oscillates with the Rabi frequency  $\Omega$ . (Note that this law may be also calculated from the probability to find the spin in its initial state ( $\uparrow$ ) as

$$W_{\uparrow}(t) = |\alpha_{\uparrow}|^2 = |\beta_{\uparrow}|^2 = \left| \cos \frac{\Omega t}{2} + i \frac{\xi}{\Omega} \sin \frac{\Omega t}{2} \right|^2 \equiv \cos^2 \frac{\Omega t}{2} + \left( \frac{\Omega_1}{\Omega} \right)^2 \sin^2 \frac{\Omega t}{2} \equiv 1 - \frac{\Omega_1^2}{\Omega^2} \sin^2 \frac{\Omega t}{2}.$$

Just as a sanity check, we may also calculate

$$W_{\downarrow}(t) = |\alpha_{\downarrow}|^2 = |\beta_{\downarrow}|^2 = \left( \frac{\Omega_1}{\Omega} \right)^2 \sin^2 \frac{\Omega t}{2},$$

so  $W_{\uparrow} + W_{\downarrow} = 1$  at all times, as it should be. This is sufficient to calculate  $\langle S_z \rangle$ :

$$\langle S_z \rangle = +\frac{\hbar}{2} W_{\uparrow}(t) - \frac{\hbar}{2} W_{\downarrow}(t),$$

getting the same result as in Eq. (\*\*\*\*).) If the ac field's amplitude is so small that  $\Omega_1 \ll \omega, \Omega_0$ , while  $\omega$  is very close to  $\Omega_0$ , then the Rabi frequency is much lower than both  $\omega$  and  $\Omega_0$ .<sup>9</sup> In this case, the oscillation swing,

$$\langle S_z \rangle_{\max} - \langle S_z \rangle_{\min} = \hbar \frac{\Omega_1^2}{\Omega^2} \equiv \hbar \frac{\Omega_1^2}{\xi^2 + \Omega_1^2} \equiv \hbar \frac{\Omega_1^2}{(\omega - \Omega_0)^2 + \Omega_1^2},$$

is much smaller than  $\hbar$  (and is proportional to  $\mathcal{B}_1^2$ ) at most frequencies  $\omega$ , but shows a sharp resonant maximum at  $\omega$  very close to  $\Omega_0$ , reaching its maximum value of  $\hbar$  at the exact resonance  $\omega = \Omega_0$ .<sup>10</sup> At this *magnetic resonance*, the spin completely reverses its direction each half-period of the Rabi frequency  $\Omega$ .

On the Bloch sphere (see Fig. 5.3 of the lecture notes), this result means that the state-representing point travels periodically from the North Pole to the South Pole and back. However, its trajectory is not circular, i.e. does not follow one of the sphere's meridians, as it would if the field  $\mathcal{B}_1$  applied within the  $[x, y]$ -plane was time-independent. Rather, as the first two of Eqs. (\*\*\*\*) show, the meridional motion of the point is accompanied by its azimuthal rotation about the  $z$ -axis. The difference between these two motion components is especially spectacular at the magnetic resonance in a low ac

<sup>9</sup> Note that this is possible only at similar signs of  $\Omega_0$  and  $\omega$ , i.e. only at a certain direction of the ac-field's rotation.

<sup>10</sup> This resonance condition may be interpreted as the equality of the gap  $\Delta E = \hbar \Omega_0 \equiv \hbar \gamma B_0$  between the spin's energy levels in the dc magnetic field  $\mathcal{B}_0$  and the energy quantum  $\hbar \omega$  of the external ac field, leading to periodic absorption and emission of such quanta by the spin. This general phenomenon and the effect of energy dissipation on it will be discussed in Chapters 6 and 7.

field: in this case, the azimuthal rotation's frequency is close to  $\Omega_0$ , while the Rabi frequency  $\Omega$  of the meridional oscillations is much lower, of the order of  $\Omega_1$ , so that the point's trajectory is a dense spiral winding about the dc field's direction – see the figure on the right, which shows the trajectory during the first half-period of the frequency  $\Omega$ .

Note, however, that if we view this evolution from the reference frame rotating together with the field  $\mathcal{B}_1$ , i.e. measure the linear combinations

$$\langle S_x' \rangle = \langle S_x \rangle \cos \omega t + \langle S_y \rangle \sin \omega t,$$

$$\langle S_y' \rangle = -\langle S_x \rangle \sin \omega t + \langle S_y \rangle \cos \omega t$$

then the fast evolution with the frequency  $\omega$  disappears:

$$\langle S_x' \rangle = -\frac{\hbar}{2} \frac{\Omega_1 \xi}{\Omega^2} (1 - \cos \Omega t), \quad \langle S_y' \rangle = -\frac{\hbar}{2} \frac{\Omega_1}{\Omega} \sin \Omega t.$$

On the Bloch sphere, these formulas (together with Eq. (\*\*\*) for  $\langle S_z \rangle$ , which does not change at this transform) describe the rotation, with the frequency  $\Omega$ , along a circle with the radius  $(\hbar/2) \cos \alpha = (\hbar/2) \Omega_1 / \Omega$ , passing through the initial point  $\langle \mathbf{S} \rangle(0) = (\hbar/2) \mathbf{n}_z$ , with its plane normal to the vector  $\mathbf{\Omega} = \mathbf{n}_x \Omega_1 - \mathbf{n}_z \xi$ . (Figure on the right shows its side view, for the case  $\xi < 0$ , i.e.  $\Omega_0 > \omega$ .) The physics behind this result is that according to basic kinematics,<sup>11</sup> from the point of view of an observer rotating with the angular velocity  $\boldsymbol{\omega} = \mathbf{n}_z \omega$ , the spin's average magnetic moment  $\mathbf{m} = \gamma \langle \mathbf{S} \rangle$  follows not the basic Bloch equation (5.22),

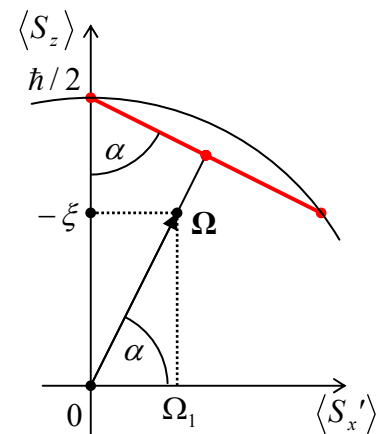
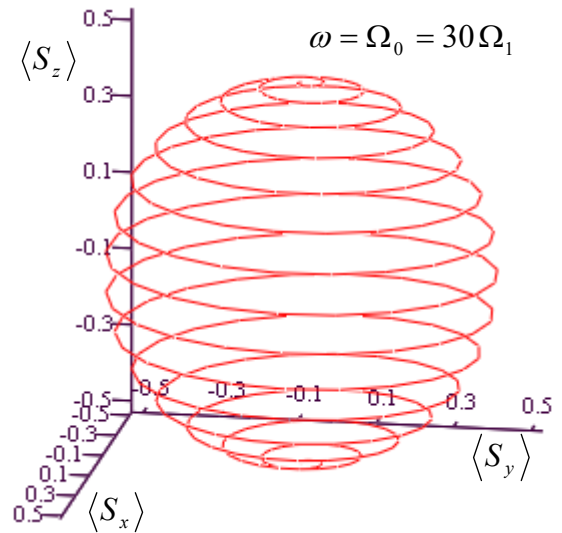
$$\frac{d\mathbf{m}}{dt} = \gamma \mathbf{m} \times \mathcal{B} \equiv -\mathbf{m} \times (\Omega_1 \cos \omega t \mathbf{n}_x + \Omega_1 \sin \omega t \mathbf{n}_y + \Omega_0 \mathbf{n}_z),$$

which is valid in an inertial reference frame, but the modified equation

$$\left. \frac{d\mathbf{m}}{dt} \right|_{\text{rot}} = \frac{d\mathbf{m}}{dt} - \omega \mathbf{n}_z \times \mathbf{m} = -\mathbf{m} \times [\Omega_1 \mathbf{n}_x' + (\Omega_0 - \omega) \mathbf{n}_z] \equiv -\mathbf{m} \times (\Omega_1 \mathbf{n}_x' - \xi \mathbf{n}_z) \equiv -\mathbf{m} \times \mathbf{\Omega},$$

similar to that for a constant magnetic field of the magnitude  $\mathcal{B} = \Omega/\gamma = (\mathcal{B}_0^2 + \mathcal{B}_1^2)^{1/2}$  – see the last figure above. By the way, this fact might be used to calculate the Cartesian components of the vector  $\langle \mathbf{S}' \rangle$  directly from the Bloch equation so modified (just as this was done in the previous problem) and then transfer the results to the lab frame.

**Problem 5.6.\*** Analyze statistics of the spacing  $S \equiv E_+ - E_-$  between energy levels of a two-level system, assuming that all elements  $H_{ij}$  of its Hamiltonian matrix (5.2) are independent random numbers, with equal and constant probability densities within the energy interval of interest. Compare the result



<sup>11</sup> See, e.g., CM Eq. (4.8).

with that for a purely diagonal Hamiltonian matrix, with a similar probability distribution of its random diagonal elements.

*Solution:* According to Eq. (5.6) of the lecture notes,

$$S \equiv E_+ - E_- = 2 \left[ \left( \frac{H_{11} - H_{22}}{2} \right)^2 + H_{12}H_{21} \right]^{1/2}.$$

Since the Hamiltonian has to have real eigenvalues, its matrix has to be Hermitian, i.e. the diagonal elements  $H_{11}$  and  $H_{22}$  have to be real, while the off-diagonal elements  $H_{12}$  and  $H_{21}$  to be complex-conjugate, so we may rewrite the expression for  $S$  as

$$S = 2(X^2 + Y^2)^{1/2},$$

where  $X \equiv (H_{11} - H_{22})/2$  and  $Y \equiv \text{Re}[H_{12}] = \text{Re}[H_{21}]$  are independent random real numbers distributed, each along its axis, with a certain constant probability density  $w_0$ . As a result, the probability for them to be within an elementary interval  $dXdY$  (i.e. an elementary area of the  $[X, Y]$  plane) is

$$dw = w_0^2 dXdY.$$

By introducing, in the standard way, the polar coordinates  $\rho$  and  $\varphi$  on that plane:

$$X \equiv \rho \cos \varphi, \quad Y \equiv \rho \sin \varphi,$$

we get  $dXdY = \rho d\rho d\varphi$  and  $S = 2\rho$ . Hence the probability for the system to be within a small interval  $d\rho$ , regardless of the angle  $\varphi$  (which does not affect  $S$ ) is

$$dW = w_0^2 2\pi\rho d\rho = \frac{\pi}{2} w_0^2 S dS.$$

On the other hand, by the definition of the probability density  $w$  of a 1D variable (in our case,  $S$ ),  $dW$  should be equal to  $w(S)dS$ , so in our case,

$$w(S) = \frac{\pi}{2} w_0^2 S. \quad (*)$$

However, this result may be taken for the genuine probability density of the interlevel spacing only for small  $S$ , because it does not reflect the fact that each two-level system has only one value of  $S$ . (For example, if integrated over  $S$  from 0 to some growing value, Eq. (\*) would eventually give a probability larger than 1.) The standard general way to correct this deficiency is to say that as  $S$  is increased, the probability  $W(S)$  of having the spacing at the interval  $[0, S]$  increases as

$$\frac{dW(S)}{dS} = w(S)[1 - W(S)].$$

Here the additional factor  $[1 - W(S)]$  reflects the fact that only if the spacing is not located on the interval  $[0, S]$ , it may be located at larger values of the spacing. Integrating this simple differential equation with the obvious boundary condition  $W(0) = 0$ , we get

$$W(S) = 1 - \exp \left\{ - \int_0^S w(S') dS' \right\}.$$

Now the genuine probability density of the interlevel spacing may be calculated as

$$\tilde{w}(S) \equiv \frac{dW(S)}{dS} = w(S) \exp \left\{ - \int_0^S w(S') dS' \right\}. \quad (**)$$

As a sanity check, at  $S \rightarrow 0$ , this probability density coincides with the “seed density”  $w(S)$ , but at  $S \rightarrow \infty$ , it drops exponentially, ensuring the automatic convergence of the aggregate probability to have the spacing at one (some) value  $S$ ,

$$W(\infty) = \int_0^{\infty} \tilde{w}(S) dS,$$

to the appropriate (unit) value, for any seed function  $w(S)$ :

$$W(\infty) = \int_0^{\infty} w(S) \exp \left\{ - \int_0^S w(S') dS' \right\} dS = \int_0^{\infty} \exp \left\{ - \int_0^S w(S') dS' \right\} d \left[ \int_0^S w(S') dS' \right] = \int_0^{\infty} \exp \{ - \xi \} d\xi = 1.$$

For our particular case, by plugging Eq. (\*) into the general Eq. (\*\*), we get

$$\tilde{w}(S) = \frac{\pi}{2} w_0^2 S \exp \left\{ - \frac{\pi}{2} w_0^2 \int_0^S S' dS' \right\} = \frac{\pi}{2} w_0^2 S \exp \left\{ - \frac{\pi}{4} w_0^2 S^2 \right\}. \quad (***)$$

This result may be used, in particular, to calculate the average level spacing,<sup>12</sup>

$$\langle S \rangle = \int_0^{\infty} S \tilde{w}(S) dS = \frac{\pi}{2} w_0^2 \int_0^{\infty} S^2 \exp \left\{ - \frac{\pi}{4} w_0^2 S^2 \right\} dS = \frac{4}{\pi^{1/2} w_0} \int_0^{\infty} \xi^2 \exp \{ - \xi^2 \} d\xi = \frac{4}{\pi^{1/2} w_0} \frac{\pi^{1/2}}{4} = \frac{1}{w_0}.$$

The last relation allows one to express the parameter  $w_0$  as  $1/\langle S \rangle$ , and rewrite Eq. (\*\*\*) in its canonical form, as the probability density of the normalized spacing  $s \equiv S/\langle S \rangle$ :<sup>13</sup>

$$\tilde{w}(s) = \frac{dS}{ds} \tilde{w}(S) = \langle S \rangle \tilde{w}(S) = \frac{\pi}{2} s \exp \left\{ - \frac{\pi}{4} s^2 \right\}. \quad (***)$$

This result (called the *Wigner surmise*) shows that the probability of having the two eigenenergies of a random two-level system very close to each other is vanishingly small. This fact, called the *level repulsion*, is perhaps the best-known qualitative result of the field called the *Random Matrix Theory (RMT)*.<sup>14</sup>

To appreciate how nontrivial Eq. (\*\*\*) is, let us compare it with the statistics of spacing between fully independent energy values, which may be described by Eq. (5.2) with  $H_{12} = H_{21} = 0$ , so

$$S = |H_{11} - H_{22}| \equiv 2|X|.$$

<sup>12</sup> Using the well-known Gaussian integral – see, e.g., MA Eq. (6.9c).

<sup>13</sup> The first of these equalities follows from the invariance of the elementary probability  $dW$  with respect to the choice of its argument:  $dW = \tilde{w}(S) dS = \tilde{w}(s) ds$ .

<sup>14</sup> The de-facto bible of the RMT (whose founding father set notably includes E. Wigner and F. Dyson) is the monograph by M. Mehta, *Random Matrices*, Elsevier/Academic Press, 2004. The field was inspired by the experimental observations, in the 1940-50s, of pseudo-random energy spectra of atomic nuclei, but is applicable to many other systems with uncontrollable parameters, for example solid-state “quantum dots” – see, e.g., C. Beenakker, *Rev. Mod. Phys.* **69**, 731 (1997). The general RMT shows that Eq. (\*\*\*) is valid for the so-called *orthogonal ensemble* – just one of three major statistical ensemble types. (The reader interested in this classification and other details of the RMT is referred to the cited sources.)

With the probability density of  $X$  equal to  $w_0 = \text{const}$ , we have  $dW = w(S)dS = 4w_0dX$  (with the additional factor of 2 coming from the contributions from two branches of the function  $S(X)$ , for positive and negative  $X$ ), so the seed density is

$$w(S) = 4w_0 = \text{const}.$$

Plugging this expression into the general Eq. (\*\*), we get a purely exponential distribution:

$$\tilde{w}(S) = 4w_0 \exp\left\{-4w_0 \int_0^S dS'\right\} = 4w_0 \exp\{-4w_0 S\},$$

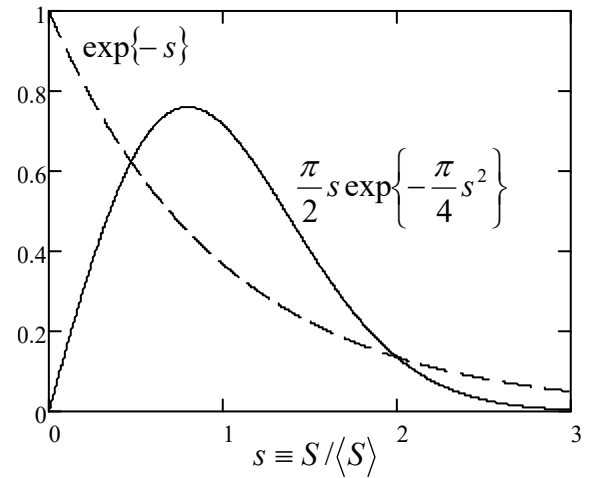
which is usually also recast into that for the normalized spacing  $s$ :

$$\tilde{w}(s) = \exp\{-s\},$$

Where, as above,  $s \equiv S/\langle S \rangle$ , but in this case, with

$$\langle S \rangle = \int_0^\infty S \tilde{w}(S) dS = \frac{1}{4w_0} \int_0^\infty \xi \exp\{-\xi\} d\xi = \frac{1}{4w_0}.$$

This exponential distribution is shown, together with the one given by Eq. (\*\*\*\*), in the figure on the right; please agree that their difference is quite spectacular.



The Wigner surmise may be interpreted as the direct result of the level repulsion at their anticrossing – see, e.g., Fig. 5.1 of the lecture notes.

Let me also note one more interesting aspect of the RMT: its application to the statistics of energy spectra of classically chaotic Hamiltonian systems.<sup>15</sup> Namely, in such systems, the level spacing distribution is closer to the Wigner surmise (\*\*\*\*), while in non-chaotic (“integrable”) systems it is closer to the exponential one. To the best of my knowledge, this *Bohigas-Giannoni-Schmit conjecture* has not received any general proof (yet), but it has been implicitly confirmed by many numerical simulations of particular systems.<sup>16</sup>

**Problem 5.7.** For a periodic motion of a single particle in a confining potential  $U(\mathbf{r})$ , the *virial theorem* of non-relativistic classical mechanics<sup>17</sup> is reduced to the following equality:

$$\bar{T} = \frac{1}{2} \overline{\mathbf{r} \cdot \nabla U},$$

where  $T$  is the particle’s kinetic energy, and the top bar means averaging over the time period of motion. Prove the following quantum-mechanical version of the theorem for an arbitrary stationary state, in the absence of spin effects:

<sup>15</sup> For a brief discussion of the classical deterministic chaos see, e.g., CM Sec. 9.3; for a brief remark on quantum dynamics of classically chaotic systems, see a footnote at the beginning of Sec. 3.5 of the lecture notes.

<sup>16</sup> See, e.g., S. McDonald and A. Kaufmann, *Phys. Rev. Lett.* **42**, 1189 (1979).

<sup>17</sup> See, e.g., CM Problem 1.12.

$$\langle T \rangle = \frac{1}{2} \langle \mathbf{r} \cdot \nabla U \rangle,$$

where the angular brackets denote (as usual in this course) the expectation values of the observables.

*Hint:* Mimicking the proof of the classical virial theorem, consider the time evolution of the following operator:  $\hat{G} \equiv \hat{\mathbf{r}} \cdot \hat{\mathbf{p}}$ .

*Solution:* According to Eq. (4.199), in the Heisenberg picture of quantum dynamics

$$i\hbar \dot{\hat{G}} = [\hat{G}, \hat{H}],$$

where, in the absence of spin effects, the particle's Hamiltonian may be taken in the form (4.237), so

$$\dot{\hat{G}} = \frac{1}{i\hbar} [\hat{G}, \hat{H}] = \frac{1}{i\hbar} \left[ \hat{\mathbf{r}} \cdot \hat{\mathbf{p}}, \frac{\hat{p}^2}{2m} \right] + \frac{1}{i\hbar} [\hat{\mathbf{r}} \cdot \hat{\mathbf{p}}, \hat{U}(\mathbf{r})].$$

Let us use, for each Cartesian coordinate, the commutation relation similar to Eq. (5.27), so that all of them may be summarized as the following vector equality:

$$[\hat{\mathbf{r}}, \hat{p}^2] = 2i\hbar \hat{\mathbf{p}}.$$

If we also use a set of three equations similar to Eqs. (5.33)-(5.34) which give, in the coordinate representation, the following vector relation

$$[\hat{\mathbf{p}}, \hat{U}(\mathbf{r})] = -i\hbar \nabla U, \quad (*)$$

then we get

$$\dot{\hat{G}} = \frac{\hat{p}^2}{m} - \hat{\mathbf{r}} \cdot \nabla U \equiv 2 \left( \hat{T} - \frac{1}{2} \hat{\mathbf{r}} \cdot \nabla U \right).$$

Averaging both sides of this equation over the ensemble of initial quantum states, we get the following relation for the expectation values of the involved variables

$$\langle \dot{\hat{G}} \rangle = 2 \left( \langle T \rangle - \frac{1}{2} \langle \mathbf{r} \cdot \nabla U \rangle \right). \quad (**)$$

Since, by its definition, for any localized motion,  $G$  is a limited variable, the expectation value of its time derivative has to vanish in any stationary state of the system. Hence the right-hand side of Eq. (\*\*) has to equal zero as well, thus proving the quantum virial theorem.

Note that, just as in classical mechanics, the theorem may be generalized as follows,

$$\langle T \rangle = \frac{1}{2} \left\langle \sum_{k=1}^N \hat{\mathbf{r}}_k \cdot \nabla_k U \right\rangle, \quad (***)$$

for a system of  $N$  particles described by the spin-independent Hamiltonian

$$\hat{H} = \sum_{k=1}^N \frac{\hat{p}_k^2}{2m_k} + \hat{U}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2, \dots, \hat{\mathbf{r}}_N).$$

Indeed, the commutators  $[\hat{\mathbf{r}}_k, \hat{p}_{k'}]$  for all particle pairs ( $k \neq k'$ ) vanish because these operators belong to different Hilbert spaces, and Eq. (\*), in the form

$$[\hat{\mathbf{p}}_k, \hat{U}] = -i\hbar \nabla_k U,$$

is valid even if the potential energy depends on the positions of other particles as well, making the proof of Eq. (\*\*\*) similar to that of its single-particle version.

**Problem 5.8.** A non-relativistic 1D particle moves in the spherically symmetric potential  $U(r) = C \ln(r/R)$ . Prove that:

- (i)  $\langle p^2 \rangle$  is the same in each stationary state, and
- (ii) the spacing between the energy levels is independent of the particle's mass.

*Solutions:*

- (i) In this particular case, the virial theorem<sup>18</sup> applied to the  $n^{\text{th}}$  stationary state,

$$\langle T \rangle_n = \frac{1}{2} \langle \mathbf{r} \cdot \nabla U \rangle_n,$$

takes the form

$$\frac{1}{2m} \langle p^2 \rangle_n = \frac{1}{2} \left\langle r \frac{dU}{dr} \right\rangle_n \equiv \frac{1}{2} \langle C \rangle_n \equiv \frac{C}{2}, \quad \text{i.e. } \langle p^2 \rangle_n = Cm, \quad (*)$$

so that  $\langle p^2 \rangle_n$  is fully determined by the constant  $C$  and the particle's mass.

- (ii) Let  $E_n$  be the particle's energy level, and apply to it the Hellmann-Feynman theorem in the form

$$\frac{\partial E_n}{\partial m} = \left\langle \frac{\partial H}{\partial m} \right\rangle_n \equiv \left\langle \frac{\partial}{\partial m} \left[ \frac{p^2}{2m} + U(r) \right] \right\rangle_n = - \left\langle \frac{p^2}{2m^2} \right\rangle_n.$$

Now using Eq. (\*), we get

$$\frac{\partial E_n}{\partial m} = -\frac{C}{2m},$$

so that this derivative does not depend on the stationary state's number  $n$ . Hence for the spacing  $\Delta \equiv E_{n+1} - E_n$  between the energy levels, we may write:

$$\frac{\partial \Delta}{\partial m} = \frac{\partial E_{n+1}}{\partial m} - \frac{\partial E_n}{\partial m} = 0,$$

i.e. it is indeed independent of  $m$ .

Finally, note that this function  $U(r)$  is not as artificial as it may look, despite its divergences at  $r \rightarrow 0$  and  $r \rightarrow \infty$ . For example, it describes the potential energy of a charged particle in the field of a long, thin, straight filament carrying a distributed charge with a constant density<sup>19</sup> – of course, within the limits imposed by a final length and a non-zero thickness of the filament.

**Problem 5.9.** Calculate, in the WKB approximation, the transparency  $\mathcal{T}$  of the following saddle-shaped potential barrier:

<sup>18</sup> See the previous problem.

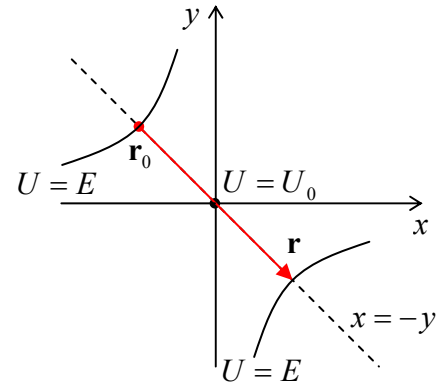
<sup>19</sup> See, e.g., the solutions of EM Problems 1.1 and 1.6.

$$U(x, y) = U_0 \left( 1 + \frac{xy}{a^2} \right),$$

where  $U_0 > 0$  and  $a$  are real constants, for tunneling of a 2D particle with energy  $E < U_0$ .

*Solution:* The equipotential lines of this potential profile, corresponding to  $U(x, y) = E$ , are hyperbolas symmetric with respect to the straight-line diagonals  $y = \pm x$  – see the figure on the right. Hence the quasi-classical instanton trajectory that provides the minimum of the tunneling exponent given by Eq. (5.56) of the lecture notes,

$$I \equiv \int_{\mathbf{r}_0}^{\mathbf{r}} \boldsymbol{\kappa} \cdot d\mathbf{r}, \quad \text{where} \quad \frac{\hbar^2 \boldsymbol{\kappa}^2}{2m} \equiv U(\mathbf{r}) - E,$$



cannot deviate from one of these symmetry axes. If  $U_0 > 0$ , the diagonal connecting classically allowed regions with energies  $E < U(0, 0) = U_0$  is  $y = -x$  – see the red arrow in the figure above. Plugging this relation into the function  $U(x, y)$ , and the resulting function into the above expression for  $\boldsymbol{\kappa}^2$ , we get

$$I = \frac{1}{\hbar} \int_{-l_c}^{+l_c} \left\{ 2m \left[ U_0 \left( 1 - \frac{x^2}{a^2} \right) - E \right] \right\}^{1/2} dl,$$

with  $dl = \sqrt{2}dx$ ,  $l_c = \sqrt{2}x_c$ , where  $\pm x_c$  are the  $x$ -coordinates of the classical turning points  $\mathbf{r}_0$  and  $\mathbf{r}$ , determined by the condition

$$U(x, y)_{y=-x} - E \equiv U_0 \left( 1 - \frac{x_c^2}{a^2} \right) - E = 0.$$

A simple integration yields

$$I = \frac{\pi a}{\hbar} \left( \frac{m}{U_0} \right)^{1/2} (U_0 - E),$$

giving the following WKB transparency (5.58):

$$\mathcal{F} = \exp\{-2I\} = \exp\left\{ -\frac{2\pi a}{\hbar} \left( \frac{m}{U_0} \right)^{1/2} (U_0 - E) \right\}.$$

**Problem 5.10.** In the WKB approximation, calculate the so-called *Gamow factor*<sup>20</sup> for the alpha decay of atomic nuclei, i.e. the exponential factor in the transparency of the potential barrier resulting from the following simple model for the alpha-particle's potential energy as a function of its distance from the nuclear center:

$$U(r) = \begin{cases} U_0 < 0, & \text{for } r < R, \\ \frac{ZZ'e^2}{4\pi\epsilon_0 r}, & \text{for } R < r, \end{cases}$$

<sup>20</sup> Named after G. Gamow, who made this calculation as early as 1928.



where  $Ze = 2e > 0$  is the charge of the particle,  $Z'e > 0$  is that of the nucleus after the decay, and  $R$  is the nucleus' radius.

*Solution:* Evidently, such tunneling is possible only for energies  $E > U(\infty) = 0$ . Due to the spherical symmetry of the potential, the instanton trajectory that minimizes the functional  $I$  given by Eq. (5.56) of the lecture notes, has to be a straight radial line, so

$$I \equiv \int_R^{R'} \kappa(r) dr = \frac{1}{\hbar} \int_R^{R'} \{2m[U(r) - E]\}^{1/2} dr = \frac{1}{\hbar} \int_R^{R'} \left\{ 2m \left[ \frac{ZZ'e^2}{4\pi\epsilon_0 r} - E \right] \right\}^{1/2} dr,$$

where  $R' > R$  is the radius at which the particle of energy  $E$  comes out from under the barrier:

$$U(R') \equiv \frac{ZZ'e^2}{4\pi\epsilon_0 R'} = E.$$

By using this definition to simplify the function under the integral, and then the variable substitution  $r \equiv R' \sin^2 \xi$  (so that  $dr = 2R' \sin \xi \cos \xi d\xi$ ), we get

$$\begin{aligned} I &= \frac{(2mE)^{1/2}}{\hbar} \int_R^{R'} \left( \frac{R'}{r} - 1 \right)^{1/2} dr = \frac{2(2mE)^{1/2} R'}{\hbar} \int_{\sin^{-1}(R/R')}^{\pi/2} \left( \frac{1}{\sin^2 \xi} - 1 \right)^{1/2} \sin \xi \cos \xi d\xi \\ &\equiv \frac{2(2mE)^{1/2} R'}{\hbar} \int_{\sin^{-1}(R/R')}^{\pi/2} \cos^2 \xi d\xi \equiv \frac{2(2mE)^{1/2} R'}{\hbar} \int_{\sin^{-1}(R/R')}^{\pi/2} \frac{1 + \cos 2\xi}{2} d\xi \\ &= \frac{(2mE)^{1/2} R'}{\hbar} \left[ \frac{\pi}{2} - \sin^{-1} \left( \frac{R}{R'} \right)^{1/2} - \left( \frac{R}{R'} \right)^{1/2} \left( 1 - \frac{R}{R'} \right)^{1/2} \right]. \end{aligned}$$

At this point, it is convenient to introduce a natural energy constant,

$$E_0 \equiv \max[U(r)] = U(R) = \frac{ZZ'e^2}{4\pi\epsilon_0 R} \quad \left( \text{so } \frac{R}{R'} = \frac{E}{E_0} \right),$$

to, finally, get

$$\mathcal{F} = e^{-2I} = \exp \left\{ - \frac{2(2mE_0)^{1/2} R}{\hbar} \left[ \frac{\pi}{2} \left( \frac{E_0}{E} \right)^{1/2} - \left( \frac{E_0}{E} \right)^{1/2} \sin^{-1} \left( \frac{E}{E_0} \right)^{1/2} - \left( 1 - \frac{E}{E_0} \right)^{1/2} \right] \right\}.$$

Just for the reader's reference, the typical energies  $E$  of emitted alpha particles are much smaller than  $E_0$ , so the experimental data are reasonably well described by a simpler expression that follows from the last formula after dropping the two last terms in the square brackets:

$$\mathcal{F} \approx \exp \left\{ - \frac{\sqrt{2\pi m}^{1/2} E_0 R}{\hbar E^{1/2}} \right\} \equiv \exp \left\{ - \frac{\sqrt{2\pi m}^{1/2} ZZ'e^2}{\hbar E^{1/2} 4\pi\epsilon_0} \right\} \equiv \exp \left\{ - ZZ' \alpha \left( \frac{2\pi^2 m c^2}{E} \right)^{1/2} \right\},$$

where  $\alpha$  is the fine structure constant. Moreover, the last expression gives reasonable results not only for alpha particles, but for many other nuclear reactions, provided that  $Z$  and  $Z'$  are taken equal to the

numbers of protons in the reacting nuclei, and the particle's mass  $m$  is replaced with the so-called *reduced mass* of the two reacting nuclei.<sup>21</sup>

**Problem 5.11.** Use the WKB approximation to calculate the average time of ionization of a hydrogen atom, initially in its ground state, made metastable by the application of an additional weak, uniform, time-independent electric field  $\mathcal{E}$ . Formulate the conditions of validity of your result.

*Solution:* The net potential energy of the atomic electron's motion is

$$U(\mathbf{r}) = -\frac{q^2}{4\pi\epsilon_0 r} - q\mathcal{E}z,$$

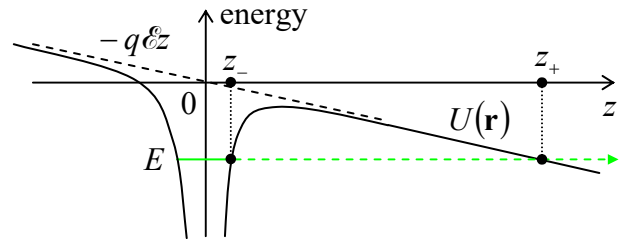
where  $z$  is the electric field's direction. If the field is sufficiently weak,

$$q|\mathcal{E}|r_B \ll E_H, \quad (*)$$

where  $r_B$  is the Bohr radius and  $E_H$  is the Hartree energy (see, respectively, Eqs. (1.10) and (1.13) of the lecture notes), then the field-induced correction to the ground-state energy  $E$  of the electron in the atom is negligible, and we may use for it the unperturbed value (1.12) with  $n = 1$ :

$$E = -\frac{E_H}{2}.$$

The green dashed arrow in the (schematic) figure on the right shows the electron tunneling path leading to the atom's ionization. Due to the axial symmetry of the potential  $U(\mathbf{r})$  and the ground-state wavefunction  $\psi_{100}$ , the instanton trajectory that minimizes the tunnel integral  $I$  (5.56) has to be a straight radial line along the  $z$ -axis (i.e. along the direction shown in the sketch<sup>22</sup>), so



$$I = \int_{z_-}^{z_+} \kappa(z) dz, \quad \text{with} \quad \frac{\hbar^2 \kappa^2(z)}{2m} = U(\mathbf{n}_z z) - E \equiv -\frac{q^2}{4\pi\epsilon_0 z} - q\mathcal{E}z + \frac{E_H}{2}, \quad (**)$$

where  $z_{\pm}$  are the classical turning points that are defined by the condition  $U(\mathbf{n}_z z_{\pm}) = E$  (see the figure above):

$$-\frac{q^2}{4\pi\epsilon_0 z_{\pm}} - q\mathcal{E}z_{\pm} + \frac{E_H}{2} = 0.$$

In the case (\*), there is no need to solve this quadratic equation for  $z_{\pm}$  exactly, because

$$z_- \approx \frac{q^2}{4\pi\epsilon_0} \frac{E_H}{2} \equiv 2r_B, \quad z_+ \approx \frac{E_H}{2} / q\mathcal{E} \gg z_-,$$

<sup>21</sup> See, e.g., CM Sec. 3.4 of the lecture notes, in particular, Eq. (3.35). As will be discussed in Chapter 8 below, this mass renormalization is valid in quantum mechanics as well. For the relatively light alpha particles, this mass renormalization is typically not essential.

<sup>22</sup> Strictly speaking, for the electron's charge  $q = -e < 0$ , all  $z$  in this figure and all the following relations should read  $-z$ , but the final results are still valid, with the replacement  $q \rightarrow +e > 0$ .

and the integral  $I$  may be well approximated by neglecting the Coulomb term in Eq. (\*\*):

$$I \approx \frac{(2m)^{1/2}}{\hbar} \int_0^{z_+} \left( -q\mathcal{E}z + \frac{E_H}{2} \right)^{1/2} dz.$$

This is exactly the same (easy) integral as at the WKB approach to the Fowler-Nordheim tunneling (see Problem 2.12, and also Problem 2.18), with the replacements  $U_0 - E \rightarrow E_H/2$  and  $\mathbf{F} \rightarrow q\mathcal{E}$ , which yields

$$\mathcal{F}_{\text{WKB}} = \exp \left\{ -\frac{4}{3} \frac{(2m)^{1/2}}{\hbar} \frac{(E_H/2)^{3/2}}{q\mathcal{E}} \right\} \equiv \exp \left\{ -\frac{2}{3} \frac{E_H}{q\mathcal{E}r_B} \right\}.$$

Since this expression does not include a possible pre-exponential factor,<sup>23</sup> it does not make much sense to calculate the attempt time  $t_a$  exactly. By taking it at a reasonable value  $\hbar/|E| \equiv 2\hbar/E_H$  and using the general Eq. (2.153), we get the following estimate of the lifetime of the metastable ground state, i.e. of the average ionization time:

$$\tau \equiv \frac{t_a}{\mathcal{F}} \sim \frac{2\hbar}{E_H} \exp \left\{ \frac{2}{3} \frac{E_H}{q\mathcal{E}r_B} \right\}. \quad (***)$$

In the limit (\*), the main (exponential) factor in this result is quantitatively correct and is much larger than 1. This condition is only violated in extremely high electric fields above  $E_H/er_B \sim 10^{12}$  V/m, practically attainable using very intensive laser beams.<sup>24</sup>

**Problem 5.12.** For a 1D harmonic oscillator with mass  $m$  and frequency  $\omega_0$ , calculate:

- (i) all matrix elements  $\langle n | \hat{x}^3 | n' \rangle$ , and
- (ii) the diagonal matrix elements  $\langle n | \hat{x}^4 | n \rangle$ ,

where  $n$  and  $n'$  are arbitrary Fock states.

*Solutions:*

- (i) Breaking  $\hat{x}^3$  into the product of  $\hat{x}$  by  $\hat{x}^2$ , and using the closure relation (4.44), we may write

$$\langle n' | \hat{x}^3 | n \rangle \equiv \langle n | \hat{x} \hat{x}^2 | n' \rangle \equiv \langle n | \hat{x} \hat{I} \hat{x}^2 | n' \rangle = \sum_{n''=0}^{\infty} \langle n' | \hat{x} | n'' \rangle \langle n'' | \hat{x}^2 | n \rangle.$$

Now we may use Eqs. (5.92) and (5.94) of the lecture notes to get

$$\langle n' | \hat{x}^3 | n \rangle = \frac{x_0^3}{\sqrt{8}} \left\{ [n(n-1)(n-2)]^{1/2} \delta_{n',n-3} + 3n^{3/2} \delta_{n',n-1} + 3(n+1)^{3/2} \delta_{n',n+1} + [(n+1)(n+2)(n+3)]^{1/2} \delta_{n',n+3} \right\}.$$

- (ii) Here it is simpler to factor  $\hat{x}^4$  into the product of  $\hat{x}^2$  by  $\hat{x}^2$ , so by using the closure relation again, we get

<sup>23</sup> Calculation of this factor (which in this 3D problem is different from that for the 1D Fowler-Nordheim tunneling discussed in the solution of Problem 2.12) is a good additional exercise for the reader.

<sup>24</sup> This case is used, in particular, for the so-called *High-Harmonic Generation* (HHG) – see, e.g., EM Sec. 10.4 and/or the review paper by M. Lewenstein *et al.*, *Phys. Rev. A* **49**, 2117 (1994).

$$\langle n|\hat{x}^4|n\rangle \equiv \langle n|\hat{x}^2\hat{x}^2|n\rangle \equiv \langle n|\hat{x}^2\hat{I}\hat{x}^2|n\rangle = \sum_{n'=0}^{\infty} \langle n|\hat{x}^2|n'\rangle \langle n'|\hat{x}^2|n\rangle.$$

Now, by using Eq. (5.94) again and keeping only the partial products with equal and opposite differences between the indices  $n$  and  $n'$  (because all other products vanish), we get

$$\langle n|\hat{x}^4|n\rangle = \frac{3}{4}x_0^4(2n^2 + 2n + 1).$$

Note that for  $n = 0$ , this result may be readily calculated in the wave-mechanics approach as well, by using Eq. (2.275) for the ground state wavefunction and the table integral MA Eq. (6.9d):

$$\langle 0|\hat{x}^4|0\rangle = \int \psi_0^* x^4 \psi_0 dx = \frac{1}{\pi^{1/2}x_0} \int_{-\infty}^{+\infty} x^4 \exp\left\{-\frac{x^2}{x_0^2}\right\} dx \equiv \frac{2x_0^4}{\pi^{1/2}} \int_0^{+\infty} \xi^4 \exp\{-\xi^2\} d\xi = \frac{3}{4}x_0^4,$$

but for higher  $n$ , such calculations are harder because of the much more involved form (2.284) of the eigenfunctions  $\psi_n$ .

**Problem 5.13.** Calculate the sum (over all  $n > 0$ ) of the so-called *oscillator strengths*,

$$f_n \equiv \frac{2m}{\hbar^2}(E_n - E_0)|\langle n|\hat{x}|0\rangle|^2,$$

- (i) for a 1D harmonic oscillator, and
- (ii) for a 1D particle confined in an arbitrary stationary potential well.<sup>25</sup>

*Solutions:*

(i) According to Eq. (5.92) of the lecture notes, for a harmonic oscillator, only one of the oscillator strengths is nonvanishing:

$$\langle n|\hat{x}|0\rangle = \left(\frac{\hbar}{2m\omega_0}\right)^{1/2} \delta_{1,n},$$

while  $E_1 - E_0 = \hbar\omega_0$ , so

$$f_n = \frac{2m}{\hbar^2} \hbar\omega_0 \frac{\hbar}{2m\omega_0} \delta_{1,n} \equiv \delta_{1,n},$$

and the sum in question equals 1 indeed.

(ii) According to the Eqs. (4.191) and (4.199) for the Heisenberg picture, the time evolution of a matrix element of an operator  $\hat{A}$  that does not depend on time explicitly, in the basis of stationary states  $n$  of an arbitrary system, is described by the following equation:

$$\begin{aligned} i\hbar\dot{A}_{nn'} &\equiv \langle n|i\hbar\dot{\hat{A}}(t)|n'\rangle = \langle n|[\hat{A}, \hat{H}]|n'\rangle \equiv \langle n|\hat{A}\hat{H}|n'\rangle - \langle n|\hat{H}\hat{A}|n'\rangle \\ &= \langle n|\hat{A}|n'\rangle E_{n'} - E_n \langle n|\hat{A}|n'\rangle \equiv (E_{n'} - E_n)A_{nn'}. \end{aligned}$$

<sup>25</sup> This *Thomas-Reiche-Kuhn sum rule* is important for applications because the coefficients  $f_n$  describe, in particular, the intensity of dipole quantum transitions between the  $n^{\text{th}}$  energy level and the ground state – see, e.g., Sec. 9.2 and also EM Sec. 7.2.

For the matrix element of our current interest,  $x_{n0} \equiv \langle n | \hat{x} | 0 \rangle$ , and its complex conjugate  $x_{0n}$ , this means

$$i\hbar\dot{x}_{n0} = (E_0 - E_n)x_{n0} \equiv -(E_n - E_0)x_{n0}, \quad i\hbar\dot{x}_{0n} = (E_n - E_0)x_{0n}.$$

Now may use these expressions to rewrite the oscillator strengths sum's definition,

$$\sum_{n>0} f_n \equiv \frac{2m}{\hbar^2} \sum_{n>0} (E_n - E_0) |x_{n0}|^2 \equiv \frac{2m}{\hbar^2} \sum_{n>0} (E_n - E_0) x_{0n} x_{n0},$$

in two different forms: either as

$$\sum_{n>0} f_n = \frac{2m}{\hbar^2} \sum_{n>0} (i\hbar\dot{x}_{0n}) x_{n0} = i \frac{2m}{\hbar} \sum_{n>0} \langle 0 | \dot{\hat{x}} | n \rangle \langle n | \hat{x} | 0 \rangle,$$

or as

$$\sum_{n>0} f_n = -\frac{2m}{\hbar^2} \sum_{n>0} x_{0n} (i\hbar\dot{x}_{n0}) = -i \frac{2m}{\hbar} \sum_{n>0} \langle 0 | \hat{x} | n \rangle \langle n | \dot{\hat{x}} | 0 \rangle.$$

Taking the arithmetic average of these two expressions, and using the closure condition (4.44) for the full set of orthonormal stationary states  $n$ , we get

$$\sum_{n>0} f_n = i \frac{m}{\hbar} \langle 0 | (\dot{\hat{x}} - \hat{x}\dot{\hat{x}}) | 0 \rangle. \quad (*)$$

But for a particle with the time-independent Hamiltonian (4.237), we may use Eq. (5.29),

$$\dot{\hat{x}} = \frac{\hat{p}_x}{m},$$

and the Heisenberg's commutation relation (4.238), to transform Eq. (\*) as

$$\sum_{n>0} f_n = \frac{i}{\hbar} \langle 0 | (\hat{p}_x \hat{x} - \hat{x} \hat{p}_x) | 0 \rangle \equiv -\frac{i}{\hbar} \langle 0 | [\hat{x}, \hat{p}_x] | 0 \rangle = \langle 0 | \hat{I} | 0 \rangle = 1,$$

so the Thomas-Reiche-Kuhn sum rule is valid even for 1D systems that are different from the harmonic oscillator.

Note that it is only one of a broad family of very similar *sum rules* – see, e.g., the next problem. Just for the reader's reference, of the rules not used in this course, perhaps the most useful one is

$$\sum_{n'} (E_{n'} - E_n)^2 |\langle n | \hat{x} | n' \rangle|^2 = \frac{\hbar^2}{m^2} \langle n | \hat{p}^2 | n \rangle.$$

Problem 5.14. Prove the so-called *Bethe sum rule*,

$$\sum_{n'} (E_{n'} - E_n) |\langle n | e^{ik\hat{x}} | n' \rangle|^2 = \frac{\hbar^2 k^2}{2m}$$

(where  $k$  is any  $c$ -number constant), valid for a 1D particle moving in an arbitrary time-independent potential  $U(x)$ , and discuss its relation with the Thomas-Reiche-Kuhn sum rule whose derivation was the subject of the previous problem.

*Hint:* Calculate the expectation value, in a stationary state  $n$ , of the double commutator

$$\hat{D} \equiv \left[ \left[ \hat{H}, e^{ik\hat{x}} \right], e^{-ik\hat{x}} \right]$$

in two ways: first, just by spelling out both commutators, and, second, by using the commutation relations between the operators  $\hat{p}_x$  and  $e^{ik\hat{x}}$ , and compare the results.

*Solution:* By spelling out the commutators involved in the definition of  $\hat{D}$ , we get

$$\begin{aligned} \hat{D} &= \left( \hat{H} e^{ik\hat{x}} - e^{ik\hat{x}} \hat{H} \right) e^{-ik\hat{x}} - e^{-ik\hat{x}} \left( \hat{H} e^{ik\hat{x}} - e^{ik\hat{x}} \hat{H} \right) \equiv \left( \hat{H} - e^{ik\hat{x}} \hat{H} e^{-ik\hat{x}} \right) - \left( e^{-ik\hat{x}} \hat{H} e^{ik\hat{x}} - \hat{H} \right) \\ &\equiv 2\hat{H} - \left( e^{ik\hat{x}} \hat{H} e^{-ik\hat{x}} + e^{-ik\hat{x}} \hat{H} e^{ik\hat{x}} \right). \end{aligned}$$

Since the Hamiltonian operator  $\hat{H}$  is Hermitian, the second term inside the last parentheses is just the Hermitian conjugate of the first one, their expectation values are complex conjugates of each other, so

$$D_n \equiv \langle n | \hat{D} | n \rangle = 2E_n - \left( \langle n | e^{ik\hat{x}} \hat{H} e^{-ik\hat{x}} | n \rangle + \text{c.c.} \right).$$

Inserting the identity operator on any side of the Hamiltonian operator, and then using the closure relation (4.44) in the stationary state basis, we may rewrite this relation as

$$\begin{aligned} D_n &= 2E_n - \left( \langle n | e^{ik\hat{x}} \hat{H} e^{-ik\hat{x}} | n \rangle + \text{c.c.} \right) = 2E_n - \sum_{n'} \left( \langle n | e^{ik\hat{x}} \hat{H} | n' \rangle \langle n' | e^{-ik\hat{x}} | n \rangle + \text{c.c.} \right) \\ &= 2E_n - \sum_{n'} E_{n'} \left( \langle n | e^{ik\hat{x}} | n' \rangle \langle n' | e^{-ik\hat{x}} | n \rangle + \text{c.c.} \right) = 2 \left( E_n - \sum_{n'} E_{n'} \left| \langle n | e^{ik\hat{x}} | n' \rangle \right|^2 \right). \end{aligned} \quad (*)$$

Since the eigenenergy  $E_n$  is a  $c$ -number, we may formally represent it as a similar sum:

$$\begin{aligned} E_n &= E_n \langle n | n \rangle = E_n \langle n | e^{ik\hat{x}} e^{-ik\hat{x}} | n \rangle = E_n \langle n | e^{ik\hat{x}} \hat{I} e^{-ik\hat{x}} | n \rangle = \sum_{n'} E_n \langle n | e^{ik\hat{x}} | n' \rangle \langle n' | e^{-ik\hat{x}} | n \rangle \\ &= \sum_{n'} E_n \left| \langle n | e^{ik\hat{x}} | n' \rangle \right|^2, \end{aligned}$$

and then use the last expression to recast Eq. (\*) as

$$D_n = 2 \sum_{n'} (E_n - E_{n'}) \left| \langle n | e^{ik\hat{x}} | n' \rangle \right|^2 \equiv -2 \sum_{n'} (E_{n'} - E_n) \left| \langle n | e^{ik\hat{x}} | n' \rangle \right|^2. \quad (**)$$

On the other hand, the same double commutator  $\hat{D}$  may be calculated by using the explicit form of the particle's Hamiltonian:

$$\hat{H} = \frac{\hat{p}^2}{2m} + U(\hat{x}),$$

where  $\hat{p} \equiv \hat{p}_x$  for brevity. Since the operators  $U(\hat{x})$  and  $e^{\pm ik\hat{x}}$  are all functions of the coordinate operator, and hence commute with each other, the double commutator reduces to

$$\hat{D} = \frac{1}{2m} \left[ \left[ \hat{p}^2, e^{ik\hat{x}} \right], e^{-ik\hat{x}} \right]. \quad (***)$$

By reviewing Eqs. (5.32)-(5.35) of the lecture notes, in which the commutator of the operators  $\hat{p}$  and  $U(\hat{x})$  was calculated, we may see that this calculation is valid for any function  $f(\hat{x})$ :

$$[\hat{p}, f(\hat{x})] = -i\hbar \frac{df(\hat{x})}{d\hat{x}},$$

so for the particular cases  $f(x) = e^{\pm ikx}$ , we get

$$\left[ \hat{p}, e^{\pm ik\hat{x}} \right] = -i\hbar \left( \pm ike^{ik\hat{x}} \right) \equiv \pm \hbar ke^{ik\hat{x}}, \quad \text{i.e. } \hat{p}e^{\pm ik\hat{x}} = e^{\pm ik\hat{x}} \hat{p} \pm \hbar ke^{\pm ik\hat{x}}. \quad (****)$$

Applying the last formula, with the top signs, twice to the inner commutator in Eq. (\*\*\*) , we get

$$\begin{aligned} \left[ \hat{p}^2, e^{ik\hat{x}} \right] &\equiv \hat{p}\hat{p}e^{ik\hat{x}} - e^{ik\hat{x}}\hat{p}\hat{p} = \hat{p} \left( e^{ik\hat{x}}\hat{p} + \hbar ke^{ik\hat{x}} \right) - e^{ik\hat{x}}\hat{p}\hat{p} \equiv \hat{p}e^{ik\hat{x}}\hat{p} + \hbar k\hat{p}e^{ik\hat{x}} - e^{ik\hat{x}}\hat{p}\hat{p} \\ &= \left( e^{ik\hat{x}}\hat{p} + \hbar ke^{ik\hat{x}} \right)\hat{p} + \hbar k\hat{p}e^{ik\hat{x}} - e^{ik\hat{x}}\hat{p}\hat{p} \equiv \hbar k \left( e^{ik\hat{x}}\hat{p} + \hat{p}e^{ik\hat{x}} \right). \end{aligned}$$

With this, Eq. (\*\*\*) becomes

$$\hat{D} = \frac{\hbar k}{2m} \left[ \left( e^{ik\hat{x}}\hat{p} + \hat{p}e^{ik\hat{x}} \right), e^{-ikx} \right] \equiv \frac{\hbar k}{2m} \left( e^{ik\hat{x}}\hat{p}e^{-ik\hat{x}} - e^{-ik\hat{x}}\hat{p}e^{ik\hat{x}} \right).$$

Now applying Eq. (\*\*\*\*) again (with the corresponding signs) to each of these two terms, get finally get

$$\hat{D} = \frac{\hbar k}{2m} \left[ (\hat{p} - \hbar k) - (\hat{p} + \hbar k) \right] \equiv -\frac{\hbar^2 k^2}{m}.$$

So, our operator  $\hat{D}$  is actually just a  $c$ -number, so its expectation value in any state, including any stationary state  $n$ , is the same:

$$D_n \equiv \langle n | \hat{D} | n \rangle = -\frac{\hbar^2 k^2}{m}.$$

Requiring this expression to give the same result as in Eq. (\*\*), we get the Bethe sum rule:

$$\sum_{n'} (E_{n'} - E_n) \left| \langle n | e^{ik\hat{x}} | n' \rangle \right|^2 = \frac{\hbar^2 k^2}{2m}.$$

This relation, which is also valid in higher dimensionalities (with the replacement  $e^{ikx} \rightarrow e^{i\mathbf{k}\cdot\mathbf{r}}$ ), is especially useful for the solid-state theory.<sup>26</sup> As a sanity check, in the limit  $k \rightarrow 0$ , we may expand the exponent inside the matrix element into the Taylor series in  $k$ , and keep only two leading terms:

$$\begin{aligned} \sum_{n'} (E_{n'} - E_n) \left| \langle n | e^{ik\hat{x}} | n' \rangle \right|^2 &\rightarrow \sum_{n'} (E_{n'} - E_n) \left| \langle n | (1 + ik\hat{x}) | n' \rangle \right|^2 = \sum_{n'} (E_{n'} - E_n) \left| \delta_{nn'} + ik \langle n | \hat{x} | n' \rangle \right|^2 \\ &= \sum_{n'} (E_{n'} - E_n) \left( \delta_{nn'}^2 + k^2 \langle n | \hat{x} | n' \rangle^2 \right) = k^2 \sum_{n'} (E_{n'} - E_n) \langle n | \hat{x} | n' \rangle^2, \end{aligned}$$

so the Bethe sum rule is reduced to

$$\sum_{n'} (E_{n'} - E_n) \left| \langle n | \hat{x} | n' \rangle \right|^2 = \frac{\hbar^2}{2m}.$$

<sup>26</sup> See, e.g., Sec. 5.6 in the famous monograph by J. Ziman, *Principles of the Theory of Solids*, 2<sup>nd</sup> ed., Cambridge U. Press, 1979, or any of its later re-printings.

In the particular case  $n = 0$ , and with the replacement  $n' \rightarrow n$ , this result is reduced to the Thomas-Reiche-Kuhn sum rule for the oscillator strength, proved in the previous problem:

$$\sum_n f_n \equiv \sum_n \frac{2m}{\hbar^2} |\langle n | \hat{x} | 0 \rangle|^2 = 1.$$

**Problem 5.15.** Spell out the commutator  $[\hat{a}, \exp\{\lambda \hat{a}^\dagger\}]$ , where  $\hat{a}^\dagger$  and  $\hat{a}$  are the creation-annihilation operators (5.65), and  $\lambda$  is a  $c$ -number.

*Solution:* Let us expand the operator  $\exp\{\lambda \hat{a}^\dagger\}$  into the Taylor series:

$$\exp\{\lambda \hat{a}^\dagger\} = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} (\hat{a}^\dagger)^n \equiv \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} \underbrace{\hat{a}^\dagger \hat{a}^\dagger \dots \hat{a}^\dagger}_{n \text{ times}}.$$

Then we may write

$$\hat{a} \exp\{\lambda \hat{a}^\dagger\} = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} \hat{a} \underbrace{\hat{a}^\dagger \hat{a}^\dagger \dots \hat{a}^\dagger}_{n \text{ times}}, \quad (*)$$

and use the commutation relation (5.71),

$$\hat{a} \hat{a}^\dagger = \hat{a}^\dagger \hat{a} + \hat{I},$$

$n$  times to transform Eq. (\*) as follows:

$$\begin{aligned} \hat{a} \exp\{\lambda \hat{a}^\dagger\} &= \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} (\hat{a} \hat{a}^\dagger)^n \underbrace{\hat{a}^\dagger \dots \hat{a}^\dagger}_{(n-1) \text{ times}} = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} (\hat{a}^\dagger \hat{a} + \hat{I}) \underbrace{\hat{a}^\dagger \dots \hat{a}^\dagger}_{(n-1) \text{ times}} \equiv \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} \left( \hat{a}^\dagger \hat{a} \underbrace{\hat{a}^\dagger \dots \hat{a}^\dagger}_{(n-1) \text{ times}} + \underbrace{\hat{a}^\dagger \dots \hat{a}^\dagger}_{(n-1) \text{ times}} \right) \\ &= \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} \left[ \hat{a}^\dagger (\hat{a} \hat{a}^\dagger) \underbrace{\hat{a}^\dagger \dots \hat{a}^\dagger}_{(n-2) \text{ times}} + \underbrace{\hat{a}^\dagger \dots \hat{a}^\dagger}_{(n-1) \text{ times}} \right] = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} \left[ \hat{a}^\dagger (\hat{a}^\dagger \hat{a} + \hat{I}) \underbrace{\hat{a}^\dagger \dots \hat{a}^\dagger}_{(n-2) \text{ times}} + \underbrace{\hat{a}^\dagger \dots \hat{a}^\dagger}_{(n-1) \text{ times}} \right] \\ &= \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} \left( \underbrace{\hat{a}^\dagger \hat{a}^\dagger}_{2 \text{ times}} \hat{a} \underbrace{\hat{a}^\dagger \dots \hat{a}^\dagger}_{(n-2) \text{ times}} + 2 \underbrace{\hat{a}^\dagger \dots \hat{a}^\dagger}_{(n-1) \text{ times}} \right) = \dots = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} \left( \underbrace{\hat{a}^\dagger \hat{a}^\dagger}_{n \text{ times}} \hat{a} + n \underbrace{\hat{a}^\dagger \dots \hat{a}^\dagger}_{(n-1) \text{ times}} \right) \\ &= \left( \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} \underbrace{\hat{a}^\dagger \hat{a}^\dagger}_{n \text{ times}} \right) \hat{a} + \lambda \sum_{n=1}^{\infty} \frac{\lambda^{n-1}}{(n-1)!} \underbrace{\hat{a}^\dagger \dots \hat{a}^\dagger}_{(n-1) \text{ times}} = \exp\{\lambda \hat{a}^\dagger\} \hat{a} + \lambda \exp\{\lambda \hat{a}^\dagger\}. \end{aligned}$$

From here,

$$[\hat{a}, \exp\{\lambda \hat{a}^\dagger\}] \equiv \hat{a} \exp\{\lambda \hat{a}^\dagger\} - \exp\{\lambda \hat{a}^\dagger\} \hat{a} = \lambda \exp\{\lambda \hat{a}^\dagger\}.$$

**Problem 5.16.** Given Eq. (5.116) of the lecture notes, prove Eq. (5.117) by using the hint given in the accompanying note.

*Solution:* Following the hint, we can write

$$\hat{f}(\lambda) = \hat{f}|_{\lambda=0} + \frac{\lambda}{1!} \frac{\partial \hat{f}}{\partial \lambda} \Big|_{\lambda=0} + \frac{\lambda^2}{2!} \frac{\partial^2 \hat{f}}{\partial \lambda^2} \Big|_{\lambda=0} + \dots \quad (*)$$

Let us calculate the derivatives participating in this expression, for our current case



$$\hat{f}(\lambda) = \exp\{\lambda \hat{A}\} \hat{B} \exp\{-\lambda \hat{A}\}.$$

Since both exponents  $\exp\{\pm \lambda \hat{A}\}$  are defined by their Taylor expansions:

$$\exp\{\pm \lambda \hat{A}\} = \hat{I} \pm \frac{\lambda}{1!} \hat{A} + \frac{\lambda^2}{2!} \hat{A} \hat{A} \pm \frac{\lambda^3}{3!} \hat{A} \hat{A} \hat{A} + \dots,$$

their differentiation over the parameter  $\lambda$  gives

$$\frac{\partial}{\partial \lambda} \exp\{\pm \lambda \hat{A}\} = \pm \hat{A} + \frac{\lambda}{1!} \hat{A} \hat{A} \pm \frac{\lambda^2}{2!} \hat{A} \hat{A} \hat{A} \dots \equiv \pm \hat{A} \left( \hat{I} \pm \frac{\lambda}{1!} \hat{A} + \frac{\lambda^2}{2!} \hat{A} \hat{A} + \dots \right) = \pm \hat{A} \exp\{\pm \lambda \hat{A}\}$$

As a result, the differentiation of the operator  $\hat{f}$  over  $\lambda$  yields

$$\frac{\partial \hat{f}}{\partial \lambda} = \hat{A} \hat{f} - \hat{f} \hat{A} \equiv [\hat{A}, \hat{f}] \quad \frac{\partial^2 \hat{f}}{\partial \lambda^2} \equiv \frac{\partial}{\partial \lambda} \left( \frac{\partial \hat{f}}{\partial \lambda} \right) = \frac{\partial}{\partial \lambda} [\hat{A}, \hat{f}] = [\hat{A}, [\hat{A}, \hat{f}]], \quad \dots,$$

so at  $\lambda = 0$  (when  $\hat{f} = \hat{B}$ ), we may combine this result with Eq. (5.116) to get

$$\left. \frac{\partial \hat{f}}{\partial \lambda} \right|_{\lambda=0} = [\hat{A}, \hat{B}] = \mu \hat{I}, \quad \left. \frac{\partial^2 \hat{f}}{\partial \lambda^2} \right|_{\lambda=0} = [\hat{A}, [\hat{A}, \hat{B}]] = [\hat{A}, \mu \hat{I}] = \hat{0}, \quad \left. \frac{\partial^3 \hat{f}}{\partial \lambda^3} \right|_{\lambda=0} = \hat{0}, \dots$$

Plugging this result into Eq. (\*), we get (for *arbitrary*  $\lambda$ ):

$$\hat{f}(\lambda) = \hat{B} + \frac{\lambda}{1!} \mu \hat{I},$$

for the *particular* case  $\lambda = 1$ , giving Eq. (5.117).

**Problem 5.17.** Use Eqs. (5.116)-(5.117) of the lecture notes to simplify the following operators:

- (i)  $\exp\{+ia\hat{x}\} \hat{p}_x \exp\{-ia\hat{x}\}$ , and
- (ii)  $\exp\{+ia\hat{p}_x\} \hat{x} \exp\{-ia\hat{p}_x\}$ ,

where  $a$  is a  $c$ -number.

*Solutions:*

- (i) Let us apply Eq. (5.117) of the lecture notes,

$$\exp\{+ \hat{A}\} \hat{B} \exp\{- \hat{A}\} = \hat{B} + \mu \hat{I}, \quad (*)$$

where  $\mu$  is the  $c$ -number coefficient in the commutation relation (5.116),

$$[\hat{A}, \hat{B}] = \mu \hat{I}, \quad (**)$$

to the following operators:  $\hat{A} = ia\hat{x}$  and  $\hat{B} = \hat{p}_x$ . Since, according to the Heisenberg uncertainty relation (4.238), for these two operators,

$$[\hat{A}, \hat{B}] \equiv [ia\hat{x}, \hat{p}_x] \equiv ia[\hat{x}, \hat{p}_x] = ia(i\hbar \hat{I}) \equiv -a\hat{I},$$

i.e. Eq. (\*\*) is valid with  $\mu = -a$ , Eq. (\*) yields

$$\exp\{+ia\hat{x}\}\hat{p}_x \exp\{-ia\hat{x}\} = \hat{p}_x - a\hat{I}.$$

(ii) Now applying Eq. (\*) to another pair of operators,  $\hat{A} = ia\hat{p}_x$  and  $\hat{B} = \hat{x}$ :

$$[\hat{A}, \hat{B}] \equiv [ia\hat{p}_x, \hat{x}] \equiv ia[\hat{p}_x, \hat{x}] = ia(-i\hbar\hat{I}) \equiv a\hat{I},$$

so in Eq. (\*\*),  $\mu = +a$ , we get

$$\exp\{+ia\hat{p}_x\}\hat{x} \exp\{-ia\hat{p}_x\} = \hat{x} + a\hat{I}.$$

**Problem 5.18.\*** Derive the commutation relation between the number operator (5.73) and a reasonably defined quantum-mechanical operator describing the harmonic oscillator's phase  $\varphi$ . Write the uncertainty relation for the corresponding observables, and explore its limit at  $N \gg 1$ .

*Solution:* Attempts to introduce the operator  $\hat{\varphi}$  of the phase directly run into the following problem. All operators discussed in Sec. 5.4 of the lecture notes are defined in the Hilbert space of the oscillator's Fock states that are invariant with respect to  $2\pi$ -rotations of the phase plane (see Fig. 5.8); however, the operator  $\hat{\varphi}$  would not have such an invariance. Instead, let us take a clue from the fact that Eq. (5.104) for the classical oscillations may be represented as follows:

$$\alpha(t) = ae^{i\varphi} \exp\{-i\omega_0 t\}, \quad \alpha^*(t) = ae^{-i\varphi} \exp\{+i\omega_0 t\},$$

where  $a$  is the real amplitude of the oscillations and  $\varphi$  is their phase. Comparing these equations with Eqs. (5.141),

$$\hat{a}(t) = a(0)\exp\{-i\omega_0 t\}, \quad \hat{a}^\dagger(t) = \hat{a}^\dagger(0)\exp\{+i\omega_0 t\},$$

we see that according to the correspondence principle, the annihilation and creation operators may be viewed as the quantum-mechanical operators of, respectively,  $ae^{+i\varphi}$  and  $a^*e^{-i\varphi}$ . Next, comparing Eqs. (5.89),

$$\hat{a}|n\rangle = n^{1/2}|n-1\rangle, \quad \hat{a}^\dagger|n\rangle = (n+1)^{1/2}|n+1\rangle, \quad \text{for } n \geq 0, \quad (*)$$

with the combination of Eqs. (5.74) and (5.80),

$$\hat{N}|n\rangle = n|n\rangle,$$

we see that in quantum mechanics, the factors  $(n+1)^{1/2}$  and  $n^{1/2}$  play the role of the (normalized) classical real amplitude  $a \propto E^{1/2} \propto (n+1/2)^{1/2}$  – see Eq. (5.86). Hence, the quantum-mechanical operators that are defined by Eqs. (\*) stripped of these factors:<sup>27</sup>

$$\hat{e}_+|n\rangle = \begin{cases} |n-1\rangle, & \text{for } n > 0, \\ 0|n\rangle, & \text{for } n = 0, \end{cases} \quad \hat{e}_-|n\rangle = |n+1\rangle,$$

<sup>27</sup> The special condition for  $n = 0$  in the first of these definitions is necessary to avoid running into the non-existing state with  $n = -1$ . (As the first of Eqs. (\*) shows, for the corresponding annihilation operator  $\hat{a}$ , this cutoff is automatically provided by the front factor  $n^{1/2}$ .)

are reasonable representations of, respectively,  $e^{+i\varphi}$  and  $e^{-i\varphi}$ .

Let us establish the basic properties of these operators, first of all, by calculating their matrix elements in the Fock state basis:

$$\langle n | \hat{e}_+ | n' \rangle = \begin{cases} \langle n | n' - 1 \rangle = \delta_{n, n' - 1}, & \text{for } n' > 0 \\ 0, & \text{for } n' = 0 \end{cases} \equiv \delta_{n+1, n'}, \quad \langle n | \hat{e}_- | n' \rangle = \langle n | n' + 1 \rangle = \delta_{n, n' + 1}. \quad (**)$$

(Given the implied condition  $n, n' \geq 0$ , the last form of the first formula automatically excludes the special case  $n' = 0$ .) Now we may readily calculate the following matrix elements:

$$\begin{aligned} \langle n | [\hat{N}, \hat{e}_+] | n' \rangle &\equiv \langle n | \hat{N} \hat{e}_+ | n' \rangle - \langle n | \hat{e}_+ \hat{N} | n' \rangle = (n - n') \langle n | \hat{e}_+ | n' \rangle = -\delta_{n+1, n'}, \\ \langle n | [\hat{N}, \hat{e}_-] | n' \rangle &\equiv \langle n | \hat{N} \hat{e}_- | n' \rangle - \langle n | \hat{e}_- \hat{N} | n' \rangle = (n - n') \langle n | \hat{e}_- | n' \rangle = +\delta_{n, n'+1}. \end{aligned}$$

Comparing these results with Eqs. (\*\*), we see that we may write the following operator relations:

$$[\hat{N}, \hat{e}_+] = -\hat{e}_+, \quad [\hat{N}, \hat{e}_-] = \hat{e}_-. \quad (***)$$

We cannot use these commutation relations in Eq. (4.140) directly because since (as Eqs. (\*\*)) show) the operators  $\hat{e}_\pm$  are not Hermitian, they cannot correspond to any real observables. However, let us consider their linear combinations,

$$\hat{c} = \frac{\hat{e}_+ + \hat{e}_-}{2}, \quad \hat{s} = \frac{\hat{e}_+ - \hat{e}_-}{2i},$$

which correspond to the real observables  $\cos\varphi$  and  $\sin\varphi$ , and are Hermitian. Indeed, per Eqs. (\*\*), their only non-zero matrix elements are

$$\langle n-1 | \hat{c} | n \rangle = \langle n | \hat{c} | n-1 \rangle = \frac{1}{2}, \quad \langle n-1 | \hat{s} | n \rangle = \langle n | \hat{s} | n-1 \rangle^* = \frac{1}{2i}, \quad \text{for } n > 0.$$

For these operators, Eqs. (\*\*\*) yield

$$[\hat{N}, \hat{c}] = -i\hat{s}, \quad [\hat{N}, \hat{s}] = i\hat{c},$$

so that Eq. (4.140) gives the following uncertainty relations:

$$\delta N \delta(\cos\varphi) \geq \frac{1}{2} |\langle \sin\varphi \rangle|, \quad \delta N \delta(\sin\varphi) \geq \frac{1}{2} |\langle \cos\varphi \rangle|. \quad (***)$$

In the quasiclassical case  $N \gg 1$ , the uncertainty  $\delta N$  may be much larger than 1, so per Eqs. (\*\*\*), the phase uncertainty  $\delta\varphi$  may be much smaller than 1. In this case, we may use the approximations  $\delta(\cos\varphi) \approx |\sin\varphi| \delta\varphi$  and  $\delta(\sin\varphi) \approx |\cos\varphi| \delta\varphi$ , and both Eqs. (\*\*\*) are reduced to the same inequality:

$$\delta N \delta\varphi \geq \frac{1}{2}.$$

This result is of key importance for the properties of laser radiation (to be discussed in Sec. 9.3 of the lecture notes), which may be interpreted as a coherent set of  $N \gg 1$  photons in the same quantum state – see Sec. 9.3. Moreover, it is also valid for Bose-Einstein condensates of particles with nonzero rest mass, such as Cooper pairs in superconductors – please revisit the last part of Sec. 3.1.

**Problem 5.19.** At  $t = 0$ , a 1D harmonic oscillator was in a state described by the ket-vector

$$|\alpha\rangle = \frac{1}{\sqrt{2}}(|31\rangle + |32\rangle),$$

where  $|n\rangle$  are the ket-vectors of the stationary (Fock) states of the oscillator. Calculate:

- (i) the expectation value of the oscillator's energy, and
- (ii) the time evolution of the expectation values of its coordinate and momentum.

*Solutions:*

(i) In this Hamiltonian system, the energy is conserved, so we may calculate it in the initial moment:

$$\langle E \rangle = \langle \alpha(0) | \hat{H} | \alpha(0) \rangle = \frac{1}{2} (\langle 31 | + \langle 32 |) \hat{H} (|31\rangle + |32\rangle).$$

Using the fact that the Hamiltonian is diagonal in the basis of the Fock states  $n$ , with the diagonal elements equal to  $E_n = \hbar\omega_0(n + 1/2)$ , we get

$$\langle E \rangle = \frac{1}{2} (\langle 31 | \hat{H} | 31 \rangle + \langle 32 | \hat{H} | 32 \rangle) = \frac{\hbar\omega_0}{2} \left[ \left( 31 + \frac{1}{2} \right) + \left( 32 + \frac{1}{2} \right) \right] = 32\hbar\omega_0.$$

(ii) The time evolution of the expectation values of  $x$  and  $p$  may be obtained, for example, from Eqs. (5.36) of the lecture notes, with  $U = m\omega_0^2 x^2/2$ :

$$\langle \dot{x} \rangle = \frac{\langle p \rangle}{m}, \quad \langle \dot{p} \rangle = -m\omega_0^2 \langle x \rangle. \quad (*)$$

These equations (which coincide with the classical equations of motion of the corresponding observables) have the well-known solution<sup>28</sup>

$$\langle x \rangle(t) = \langle x \rangle(0) \cos \omega_0 t + \frac{\langle p \rangle(0)}{m\omega_0} \sin \omega_0 t, \quad \langle p \rangle(t) = \langle p \rangle(0) \cos \omega_0 t - m\omega_0 \langle x \rangle(0) \sin \omega_0 t, \quad (**)$$

so the only thing still to be done is to find the expectation values of these observables at  $t = 0$ . This may be accomplished exactly as has been done above for the energy, but with a little bit more care, because the matrices of the coordinate and momentum operators, in the Fock state basis, are *not* diagonal – see Eqs. (5.92)-(5.93) of the lecture notes:

$$\begin{aligned} \langle x \rangle(0) &= \frac{1}{2} (\langle 31 | + \langle 32 |) \hat{x} (|31\rangle + |32\rangle) = \frac{1}{2} (\langle 31 | \hat{x} | 32 \rangle + \langle 32 | \hat{x} | 31 \rangle) = \frac{1}{2} \frac{x_0}{\sqrt{2}} (\sqrt{32} + \sqrt{32}) = 4x_0, \\ \langle p \rangle(0) &= \frac{1}{2} (\langle 31 | + \langle 32 |) \hat{p} (|31\rangle + |32\rangle) = \frac{1}{2} (\langle 31 | \hat{p} | 32 \rangle + \langle 32 | \hat{p} | 31 \rangle) = \frac{1}{2} \frac{m\omega_0 x_0}{\sqrt{2}} (\sqrt{32} - \sqrt{32}) = 0, \end{aligned}$$

where  $x_0 \equiv (\hbar/m\omega_0)^{1/2}$ . Plugging these expressions into Eq. (\*\*), we get

<sup>28</sup> As a (hopefully, unnecessary) explanation: one can, for example, differentiate one of Eqs. (\*) over time again, and plug the counterpart equation into the result, getting the standard second-order differential equation

$\ddot{\xi} + \omega_0^2 \xi = 0$ , with  $\xi$  being either  $\langle x \rangle$  or  $\langle p \rangle$ . The general solution of this equation is  $\xi(t) = C_c \cos \omega_0 t + C_s \sin \omega_0 t$ . Now calculating the constants  $C_c$  and  $C_s$  from the initial conditions, we arrive at Eqs. (\*\*).

$$\langle x \rangle = 4x_0 \cos \omega_0 t, \quad \langle p \rangle = -4m\omega_0 x_0 \sin \omega_0 t.$$

Note that the exact answer could be different if there was a phase shift between the component Fock states – see, e.g., the solution of Problem 4.17. However, even then, the expectation values of the coordinate and momentum would oscillate harmonically with the oscillator's frequency  $\omega_0$ .

**Problem 5.20.\*** Re-derive the London dispersion force's potential of the interaction of two isotropic 3D harmonic oscillators (already calculated in Problem 3.20), by using the language of mutually-induced polarization.

*Solution:*<sup>29</sup> The solution of Problem 3.20, based on the calculation of the ground-state energy of the system, somewhat obscures the physical nature of the force. A more transparent physical picture of this effect is that the “quantum fluctuations” (whose r.m.s. values are equal to the quantum uncertainties) of the dipole moments  $\mathbf{d}_{1,2}$  of the interacting oscillators cause proportional fluctuating electric fields  $\mathcal{E}_{1,2}(\mathbf{r}) \propto \mathbf{d}_{1,2}$  in their vicinity, including the location of the counterpart oscillator. Each of these fields induces a small additional polarization,  $\tilde{\mathbf{d}}_2 \propto \mathcal{E}_1 \propto \mathbf{d}_1$  and  $\tilde{\mathbf{d}}_1 \propto \mathcal{E}_2 \propto \mathbf{d}_2$ , of the counterpart oscillator, on top of its own spontaneous fluctuations. In contrast to these spontaneous fluctuations  $\mathbf{d}_{1,2}$ , which are statistically independent, the induced parts  $\tilde{\mathbf{d}}_{1,2}$  of the polarization are correlated with their sources:  $\tilde{\mathbf{d}}_2$  with  $\mathbf{d}_1$ , and  $\tilde{\mathbf{d}}_1$  with  $\mathbf{d}_2$ , so their interaction has a nonvanishing average component resulting in a mutual attraction of the oscillators.

Let us make this argumentation quantitative, using the isotropic single-particle model already used for the model solution of Problem 3.20:  $\mathbf{d}_{1,2} = q\mathbf{s}_{1,2}$ , where  $q$  is the electric charge of the effective oscillator's particle and  $\mathbf{s}_{1,2}$  its displacement from the equilibrium position. Since the classical electric field  $\mathcal{E}$  of a dipole is proportional to its moment  $\mathbf{d}$ , the relation between their Heisenberg-picture operators in quantum mechanics is the same, namely<sup>30</sup>

$$\begin{aligned} \hat{\mathcal{E}}_k(\mathbf{r}) &= \frac{1}{4\pi\epsilon_0} \frac{3\mathbf{r}(\mathbf{r} \cdot \hat{\mathbf{d}}_k) - \hat{\mathbf{d}}_k r^2}{r^5} \equiv \frac{1}{4\pi\epsilon_0 r^3} \left( -\hat{d}_{kx} \mathbf{n}_x - \hat{d}_{ky} \mathbf{n}_y + 2\hat{d}_{kz} \mathbf{n}_z \right) \\ &\equiv \frac{q}{4\pi\epsilon_0 r^3} \left( -\hat{x}_k \mathbf{n}_x - \hat{y}_k \mathbf{n}_y + 2\hat{z}_k \mathbf{n}_z \right), \end{aligned} \quad (*)$$

where  $k = 1, 2$  is the dipole number, and  $\{x_k, y_k, z_k\}$  are the Cartesian components of the displacement vector  $\mathbf{s}_k$ , and  $r \gg |\mathbf{s}_k|$  is the distance between the  $k^{\text{th}}$  oscillator and the field observation point. According to Eq. (5.141) of the lecture notes, the coordinate operators change with the oscillator's eigenfrequency, for example

$$\hat{x}_k(t) = \left( \frac{\hbar}{2m\omega_k} \right)^{1/2} \left[ \hat{a}_k(t) + \hat{a}_k^\dagger(t) \right] = \left( \frac{\hbar}{2m\omega_k} \right)^{1/2} \left[ \hat{a}_k(0) \exp\{-i\omega_k t\} + \hat{a}_k^\dagger(0) \exp\{i\omega_k t\} \right]$$

<sup>29</sup> This explanation of the long-range interaction between electroneutral atoms and molecules was suggested by P. Debye in 1921 and quantified by F. London in 1937.

<sup>30</sup> See, e.g., EM Sec. 3.1, in particular Eq. (3.13), which uses a different notation ( $\mathbf{p}$ ) for the electric dipole vector.

$$\equiv \hat{X}_{k\omega} \exp\{-i\omega_k t\} + \hat{X}_{k\omega}^\dagger \exp\{i\omega_k t\} \equiv \hat{X}_{k\omega} \exp\{-i\omega_k t\} + \text{h.c.}, \quad \text{with } \hat{X}_{k\omega} \equiv \left( \frac{\hbar}{2m\omega_k} \right)^{1/2} \hat{a}(0),$$

and similarly for two other Cartesian components,<sup>31</sup> so the electric fields (\*) they induce are similar functions of time.

Let us use these relations for the field at the location of the counterpart dipole, so that  $r$  in Eq. (\*) becomes the distance between the dipoles. Next, since the classical equations of motion of the harmonic oscillator are linear, the Heisenberg equations of motion are also linear, so the complex amplitudes of the induced dipole moment operators may be also calculated using the classical relation<sup>32,33</sup>

$$\tilde{\mathbf{d}}_{k'\omega} \equiv q(\mathbf{n}_x \hat{X}_{k'\omega} + \mathbf{n}_y \hat{Y}_{k'\omega} + \mathbf{n}_z \hat{Z}_{k'\omega}) = \frac{q^2 \hat{\mathcal{E}}_{k\omega}}{m(\omega_{k'}^2 - \omega_k^2)}, \quad (**)$$

where the index  $k'$ , which may be formally defined as  $(3 - k)$ , is used for the notation of the counterpart oscillator. Since these expressions diverge at  $\omega_k \rightarrow \pm\omega_{k'}$ , i.e. at  $\omega_1 \rightarrow \pm\omega_2$ , let us assume for a while that the oscillator eigenfrequencies are not exactly equal.

The energy of interaction of the dipole  $\mathbf{d}_{k'}$  with the external electric field  $\mathcal{E}_k$  is proportional to the scalar product  $\mathbf{d}_{k'} \cdot \mathcal{E}_k$ . In our case, the dipole moment of this oscillator is the sum of two parts: the spontaneous fluctuations  $\mathbf{d}_{k'}$  and the externally induced polarization  $\tilde{\mathbf{d}}_{k'}$ . Only the latter part is correlated with  $\mathcal{E}_k$ , so only it contributes to average interaction energy.<sup>34</sup> Since  $\tilde{\mathbf{d}}_{k'} \propto \mathcal{E}_k$ , the energy needs the factor  $1/2$  before the usual scalar product  $-\tilde{\mathbf{d}}_{k'} \cdot \mathcal{E}_k$ ,<sup>35</sup> so the expectation value of the full time-averaged interaction potential may be calculated as

$$\langle U \rangle = -\frac{1}{2} \overline{\langle \hat{\mathcal{E}}_1 \cdot \tilde{\mathbf{d}}_2 \rangle} - \frac{1}{2} \overline{\langle \hat{\mathcal{E}}_2 \cdot \tilde{\mathbf{d}}_1 \rangle}, \quad (***)$$

where the top bar, as usual, means the time average. Let us spell out, for example, the first average of this sum, using Eq. (\*\*) first and then Eq. (\*) with  $k = 1$  and  $k' = 2$ :

$$\overline{\langle \hat{\mathcal{E}}_1 \cdot \tilde{\mathbf{d}}_2 \rangle} \equiv \overline{\langle \hat{\mathcal{E}}_{1x}(t) \tilde{d}_{2x}(t) + \hat{\mathcal{E}}_{1y}(t) \tilde{d}_{2y}(t) + \hat{\mathcal{E}}_{1z}(t) \tilde{d}_{2z}(t) \rangle} = \frac{q^2}{m(\omega_2^2 - \omega_1^2)} \overline{\langle \hat{\mathcal{E}}_{1x\omega} \hat{\mathcal{E}}_{1x\omega}^\dagger + \hat{\mathcal{E}}_{1y\omega} \hat{\mathcal{E}}_{1y\omega}^\dagger + \hat{\mathcal{E}}_{1z\omega} \hat{\mathcal{E}}_{1z\omega}^\dagger \rangle}$$

<sup>31</sup> Due to the assumed oscillator's isotropy, the frequencies  $\omega_k$  are the same for all 3 coordinates.

<sup>32</sup> If this formula is not immediately evident, see, e.g., CM Sec. 5.1.

<sup>33</sup> This relation between  $d_\omega$  and  $\mathcal{E}_\omega$  defines the complex electric permittivity  $\varepsilon(\omega)$  of the continuous medium of such dipoles, which in turn determines the dispersion of electromagnetic wave propagating in it (see, e.g., EM Sec. 7.2). This fact was apparently the origin of the term *dispersion force*, coined by F. London for the dipole-dipole interaction we are calculating.

<sup>34</sup> Mathematically, the absence of mutual correlation of the main (spontaneous) part  $\mathbf{d}_k$  with  $\mathcal{E}_k \propto \mathbf{d}_k$  at  $\omega_k \neq \omega_{k'}$  is expressed as the difference of their Heisenberg-picture operator frequencies, leading to averaging out of all terms  $\exp\{\pm i(\omega_k \pm \omega_{k'})t\}$  of the  $\mathbf{d}_k \cdot \mathbf{E}_{k'}$  products. The special case  $\omega_k = \omega_{k'}$  (i.e.  $\omega_1 = \omega_2$ ) requires a bit more subtle analysis (based on random phase differences), which leads to the same conclusion.

<sup>35</sup> See, e.g., EM Eq. (3.15b).

$$= \frac{q^2}{m(\omega_2^2 - \omega_1^2)} \left( \frac{q}{4\pi\epsilon_0 r^3} \right)^2 \left\langle \hat{X}_{1\omega} \hat{X}_{1\omega}^\dagger + \hat{Y}_{1\omega} \hat{Y}_{1\omega}^\dagger + 4\hat{Z}_{1\omega} \hat{Z}_{1\omega}^\dagger \right\rangle.$$

Due to the assumed isotropy of the oscillators, all coordinate product averages are equal, so we get

$$\left\langle \hat{\mathcal{E}}_1 \cdot \hat{\mathbf{d}}_2 \right\rangle = \frac{q^2}{m(\omega_2^2 - \omega_1^2)} \left( \frac{q}{4\pi\epsilon_0 r^3} \right)^2 6 \left\langle \hat{X}_{1\omega} \hat{X}_{1\omega}^\dagger \right\rangle \equiv \frac{q^2}{m(\omega_2^2 - \omega_1^2)} \left( \frac{q}{4\pi\epsilon_0 r^3} \right)^2 6 \frac{\hbar}{2m\omega_1} \left\langle \hat{a}(0) \hat{a}^\dagger(0) + \text{h.c.} \right\rangle.$$

The last average may be treated as that of the Schrödinger-picture operators, and according to Eqs. (5.89) of the lecture notes, equals 1 in the ground state of the oscillator, so, finally,

$$\left\langle \hat{\mathcal{E}}_1 \cdot \hat{\mathbf{d}}_2 \right\rangle = \frac{q^2}{m(\omega_2^2 - \omega_1^2)} \left( \frac{q}{4\pi\epsilon_0 r^3} \right)^2 6 \frac{\hbar}{2m\omega_1} \equiv \frac{3q^4 \hbar}{(4\pi\epsilon_0)^2 m^2 r^6} \frac{1}{\omega_1(\omega_2^2 - \omega_1^2)}.$$

The second term in Eq. (\*\*\*) is absolutely similar, with swapped indices 1 and 2, so we finally get<sup>36</sup>

$$\langle U \rangle = -\frac{3q^4 \hbar}{2(4\pi\epsilon_0)^2 m^2 r^6} \left[ \frac{1}{\omega_1(\omega_2^2 - \omega_1^2)} + \frac{1}{\omega_2(\omega_1^2 - \omega_2^2)} \right] \equiv -\frac{3q^4 \hbar}{2(4\pi\epsilon_0)^2 m^2 r^6} \frac{1}{\omega_1 \omega_2 (\omega_1 + \omega_2)}.$$

Now that the terms proportional to  $1/(\omega_1 - \omega_2)$  have cancelled, it is safe to consider the most important case of similar oscillators,  $\omega_1 = \omega_2 \equiv \omega_0$ :

$$U = -\frac{3}{4} \frac{q^4 \hbar}{(4\pi\epsilon_0)^2 m^2 r^6 \omega_0^3} \equiv -\frac{3}{4} \mu^2 \hbar \omega_0, \quad \text{with } \mu \equiv \frac{q^2}{4\pi\epsilon_0 r^3 m \omega_0^2} \ll 1. \quad \text{(***)}$$

This result exactly coincides with the one that was obtained in the model solution of Problem 3.20 by simpler means. However, the current, more lengthy derivation not only gives a clearer physical picture of the London dispersion force but also paves a way toward generalizations of this result to more general models of the interacting atoms/molecules (see Problems 6.19-6.20) and to their interaction at non-zero temperatures (see Problem 7.6).

Finally, let me note that one more popular form of the final result may be obtained by expressing it via the static *atomic polarizability*  $\alpha$ , which may be defined by the relation<sup>37</sup>

$$\hat{\mathbf{d}}_\omega = \alpha \hat{\mathcal{E}}_\omega, \quad \text{at } \omega \rightarrow 0.$$

According to Eq. (\*\*), in our simple oscillator model  $\alpha = q^2/m\omega_0^2$ , so Eq. (\*\*\*) becomes

$$U = -\frac{3}{4} \frac{\alpha^2 \hbar \omega_0}{(4\pi\epsilon_0)^2 r^6}.$$

However, I believe that this form conceals the resonant nature of the London dispersion force, which is so manifest in the above calculation.

<sup>36</sup> To my personal taste, this “miraculous” cancellation of the two divergences, which allows one to pursue the limit  $\omega_1 \rightarrow \omega_2$  without mathematical complications, is one of the most beautiful results of quantum mechanics.

<sup>37</sup> See, e.g., EM Eq. (3.48).

**Problem 5.21.** An external force pulse  $F(t)$ , of a finite time duration  $\mathcal{T}$ , is exerted on a 1D harmonic oscillator, initially in its ground state. Use the Heisenberg-picture equations of motion to calculate:

- (i) the expectation values of the oscillator's coordinate and momentum and their uncertainties, at an arbitrary moment,
- (ii) its total energy after the end of the pulse.

*Solution:* By using the system's Hamiltonian, which is a straightforward generalization of Eq. (5.62) of the lecture notes,

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega_0^2 \hat{x}^2}{2} - F(t)\hat{x},$$

in the Heisenberg equations of motion (4.199), we get

$$i\hbar\dot{\hat{x}} = [\hat{x}, \hat{H}] = \frac{1}{2m}[\hat{x}, \hat{p}^2], \quad i\hbar\dot{\hat{p}} = [\hat{p}, \hat{H}] = \frac{m\omega_0^2}{2}[\hat{p}, \hat{x}^2] - F(t)[\hat{p}, \hat{x}].$$

(Here and below, the index H is just implied.) The right-hand side of the first of these equations, and the first term in the second of them, were already spelled out in Sec. 5.2 of the lecture notes, while the last term in the second equation is just the product of the  $c$ -number function  $F(t)$  by the basic commutator (4.238). As a result, we get the operator equations

$$\dot{\hat{x}} = \frac{\hat{p}}{m}, \quad \dot{\hat{p}} = -m\omega_0^2 \hat{x} + F(t),$$

which have the same form as the classical equations of motion of the corresponding observables.

Due to the linearity of these equations, they are satisfied by the following linear superpositions:

$$\hat{x}(t) = \hat{x}^{(0)}(t) + X(t), \quad \hat{p}(t) = \hat{p}^{(0)}(t) + P(t). \quad (*)$$

Here the upper index (0) marks the solution for  $F(t) = 0$ , which satisfies Eqs. (5.139) and the initial conditions, while  $X$  and  $P$  are the  $c$ -number additions due to the external force  $F(t)$ , which satisfy the similar classical equations of motion:

$$\dot{X} = \frac{P}{m}, \quad \dot{P} = -m\omega_0^2 X + F(t), \quad (**)$$

with zero initial conditions:  $X(0) = P(0) = 0$ , where  $t = 0$  is the moment when the force pulse starts.

(i) For addressing this task, we do not need an explicit solution of Eqs. (\*\*). Indeed, according to the basic Eq. (4.191), the expectation value of any variable is the average of its Heisenberg operator over the quantum ensemble of initial states (not over time!) – in our current case, of the harmonic oscillator's ground state. Per Eqs. (5.92)–(5.93), for the operators  $\hat{x}^{(0)}$  and  $\hat{p}^{(0)}$  (in any picture of quantum dynamics), these averages vanish, so Eqs. (\*) give very simple results:

$$\langle x \rangle(t) = X(t), \quad \langle p \rangle(t) = P(t).$$

Now we may readily calculate the requested variances:

$$\langle \hat{x}(t)^2 \rangle \equiv \langle [\hat{x}(t) - \langle x \rangle]^2 \rangle = \langle [\hat{x}(t) - X(t)]^2 \rangle = \langle (\hat{x}^{(0)})^2 \rangle,$$



$$\langle \hat{p}(t)^2 \rangle \equiv \langle [\hat{p}(t) - \langle p \rangle]^2 \rangle = \langle [\hat{p}(t) - P(t)]^2 \rangle = \langle (\hat{p}^{(0)})^2 \rangle.$$

However, the resulting averages were calculated in Sec. 5.5 for an arbitrary Fock state  $n$  of the oscillator – see Eqs. (5.95) and (5.97). In particular, for the ground state ( $n = 0$ ), those formulas give

$$\langle \hat{x}(t)^2 \rangle = \langle (\hat{x}^{(0)})^2 \rangle = \frac{x_0^2}{2} \equiv \frac{\hbar}{2m\omega_0}, \quad \langle \hat{p}(t)^2 \rangle = \langle (\hat{p}^{(0)})^2 \rangle = (m\omega_0)^2 \frac{x_0^2}{2} \equiv \frac{m\omega_0 \hbar}{2},$$

so the requested uncertainties are not affected by the classical force  $F(t)$ :

$$\delta x \equiv \langle \hat{x}(t)^2 \rangle^{1/2} = \left( \frac{\hbar}{2m\omega_0} \right)^{1/2}, \quad \delta p \equiv \langle \hat{p}(t)^2 \rangle^{1/2} = \left( \frac{m\omega_0 \hbar}{2} \right)^{1/2},$$

and correspond to the smallest product  $\delta x \delta p = \hbar/2$  allowed by Heisenberg's uncertainty relation (1.35).

(ii) Now let us use Eq. (\*) to calculate the Heisenberg “value” of our Hamiltonian at  $t > \mathcal{T}$ , i.e. after the end of the force pulse  $F(t)$ :

$$\begin{aligned} \hat{H}(t) &= \frac{\hat{p}^2(t)}{2m} + \frac{m\omega_0^2 \hat{x}^2(t)}{2} = \left[ \frac{(\hat{p}^{(0)})^2(t)}{2m} + \frac{m\omega_0^2 (\hat{x}^{(0)})^2(t)}{2} \right] + \left[ \frac{P^2(t)}{2m} + \frac{m\omega_0^2 X^2(t)}{2} \right] \\ &+ \frac{1}{m} \hat{p}^{(0)}(t)P(t) + m\omega_0^2 \hat{x}^{(0)}(t)X(t), \quad \text{for } \mathcal{T} \leq t. \end{aligned}$$

After using the results of Task (i), for the expectation value of this Hamiltonian, i.e. the system's energy, we get simply

$$\langle E \rangle \equiv \langle \hat{H} \rangle = \frac{\hbar\omega_0}{2} + E_F,$$

where  $E_F$  is the classical energy acquired by the oscillator by the end of the force's pulse :

$$E_F = \frac{P^2(\mathcal{T})}{2m} + \frac{m\omega_0^2 X^2(\mathcal{T})}{2}.$$

(Obviously, this energy does not change at  $t > \mathcal{T}$  when  $F(t) = 0$ .),

The calculation of  $E_F$  from Eqs. (\*\*) is a task of classical mechanics, but for the reader's benefit, I will still give its solution here.<sup>38</sup> The easiest way to solve this classical system of linear differential equations is to form the complex variable  $A(t) \equiv X(t) + iP(t)/m\omega_0$ ;<sup>39</sup> for it, the system is reduced to just one equation:

$$\dot{A} + i\omega_0 A = i \frac{F(t)}{m\omega_0}.$$

Its solution may be obtained, for example, by the substitution  $A(t) \equiv C(t)\exp\{-i\omega_0 t\}$ .<sup>40</sup> For the new variable  $C(t)$ , the equation is reduced to the form

<sup>38</sup> For a ready solution for  $X(t)$ , see, e.g., CM Eqs. (5.27) and (5.34) with  $\delta = 0$ , so  $\omega_0' = \omega_0$ .

<sup>39</sup> This is of course just a dimensional version of the variable (5.101):  $A(t) \equiv \sqrt{2x_0}\alpha(t)$ . Note that  $A$  differs from the oscillation amplitude  $A$  (participating, e.g., in Eq. (5.104) of the lecture notes), which is just its modulus.

<sup>40</sup> This is just a simple version of the well-known method of variation of constants: with  $C(t) = \text{const}$ , this  $A(t)$  is the solution of the corresponding homogeneous equation.

$$\dot{C} \exp\{-i\omega_0 t\} = \frac{i}{m\omega_0} F(t), \quad \text{i.e. } \dot{C} = \frac{i}{m\omega_0} F(t) \exp\{i\omega_0 t\},$$

which may be readily integrated:

$$C(t) = \frac{i}{m\omega_0} \int_0^t F(t') \exp\{i\omega_0 t'\} dt' + \text{const.}$$

With our initial condition  $Z(0) = 0$  (giving  $C(0) = 0$ ), this relation yields

$$A(t) \equiv C(t) \exp\{-i\omega_0 t\} = \frac{i}{m\omega_0} \int_0^t F(t') \exp\{-i\omega_0(t-t')\} dt', \quad \text{so} \quad (***)$$

$$X(t) \equiv \text{Re}[A(t)] = \frac{1}{m\omega_0} \int_0^t F(t') \sin \omega_0(t-t') dt', \quad P(t) \equiv m\omega_0 \text{Im}[A(t)] = \int_0^t F(t') \cos \omega_0(t-t') dt'.$$

Note that these formulas are valid both during the pulse action (for  $t < \mathcal{T}$ ) and after it (for  $t > \mathcal{T}$ ), but in the latter case, the integrals are only contributed by the interval  $0 < t' < \mathcal{T}$ :

$$A(t) = \frac{i}{m\omega_0} \int_0^{\mathcal{T}} F(t') \exp\{-i\omega_0(t-t')\} dt' \equiv A(\mathcal{T}) \exp\{-i\omega_0(t-\mathcal{T})\}, \quad \text{for } \mathcal{T} < t.$$

Hence, after the end of the pulse, the classical components of the coordinate and momentum perform purely sinusoidal oscillations:

$$X(t) \equiv \text{Re}[A(t)] = X(\mathcal{T}) \cos \omega(t-\mathcal{T}) + \frac{P(\mathcal{T})}{m\omega_0} \sin \omega(t-\mathcal{T}),$$

$$P(t) \equiv m\omega_0 \text{Im}[A(t)] = P(\mathcal{T}) \cos \omega(t-\mathcal{T}) - m\omega_0 X(\mathcal{T}) \sin \omega(t-\mathcal{T}), \quad \text{for } \mathcal{T} < t.$$

Now by using Eqs. (\*\*\*) for  $t = \mathcal{T}$  and the replacement  $t' \rightarrow t$  (just for the notation simplicity), we get the final result:<sup>41</sup>

$$E_F = \frac{P^2(\mathcal{T})}{2m} + \frac{m\omega_0^2 X^2(\mathcal{T})}{2} = \frac{1}{2m} \left\{ \left[ \int_0^{\mathcal{T}} F(t) \cos \omega_0(\mathcal{T}-t) dt \right]^2 + \left[ \int_0^{\mathcal{T}} F(t) \sin \omega_0(\mathcal{T}-t) dt \right]^2 \right\}.$$

To summarize, all results of this solution are in full correspondence with the physical picture of the (Glauber) state of the oscillator, which may be described, at arbitrary  $t$ ,<sup>42</sup> as its ground state with its center being dragged, by the classical force pulse, into a definite point  $\{X(t), P(t)/m\omega_0\}$  on the phase plane – see Fig. 5.8 in the lecture notes.

<sup>41</sup> Alternatively,  $E_F$  may be calculated by integrating over time, from  $t = 0$  to  $t = \mathcal{T}$ , of the instant power  $\mathcal{A}(t) = F(t)V(t) = F(t)P(t)/m$  of the external force, using the last of Eqs. (\*\*\*). (See, e.g., the model solution of CM Problem 5.4.)

<sup>42</sup> The only reason why the problem did not address the oscillator's energy at  $t < \mathcal{T}$  is that whether at  $F \neq 0$ , the last term of the Hamiltonian (which describes the interaction with the force's source) should be included in the calculation, is a matter of convention.

**Problem 5.22.** Use Eqs. (5.144)-(5.145) of the lecture notes to calculate the uncertainties  $\delta x$  and  $\delta p$  for a harmonic oscillator in its squeezed ground state, and in particular, to prove Eqs. (5.143) for the case  $\theta = 0$ .

*Solution:* Let us represent the squeezed annihilation operator (5.144) in the following form, more convenient for calculations:

$$\hat{b} = \mu \hat{a} + \nu \hat{a}^\dagger, \quad \text{where } \mu \equiv \cosh r, \quad \nu \equiv e^{i\theta} \sinh r, \quad (*)$$

where  $r$  and  $\theta$  are the real  $c$ -numbers describing the complex parameter  $\zeta = r e^{i\theta}$  of the operator's eigenstate (5.145). Since the parameter  $\mu$  is real, the Hermitian conjugate of Eq. (\*) is

$$\hat{b}^\dagger = \mu \hat{a}^\dagger + \nu^* \hat{a}. \quad (**)$$

Solving the system of two linear equations (\*) and (\*\*), with the account of the identity  $\mu^2 - \nu \nu^* \equiv \cosh^2 r - \sinh^2 r = 1$ , we get the following reciprocal relations:

$$\hat{a} = \mu \hat{b} - \nu \hat{b}^\dagger, \quad \hat{a}^\dagger = \mu \hat{b}^\dagger - \nu^* \hat{b}.$$

Now, using Eqs. (5.66) of the lecture notes,

$$\hat{x} = \frac{x_0}{\sqrt{2}} (\hat{a} + \hat{a}^\dagger), \quad \hat{p} = \frac{m\omega_0 x_0}{\sqrt{2}i} (\hat{a} - \hat{a}^\dagger),$$

we may express these Hermitian operators via the squeezed creation-annihilation operators:

$$\hat{x} = \frac{x_0}{\sqrt{2}} \left[ (\mu - \nu^*) \hat{b} + (\mu - \nu) \hat{b}^\dagger \right], \quad \hat{p} = \frac{m\omega_0 x_0}{\sqrt{2}i} \left[ (\mu + \nu^*) \hat{b} + (-\mu - \nu) \hat{b}^\dagger \right].$$

Let us use the first of these expressions to calculate the expectation values of the coordinate and its square in some state  $\zeta$ :

$$\begin{aligned} \langle x \rangle &\equiv \langle \zeta | \hat{x} | \zeta \rangle = \frac{x_0}{\sqrt{2}} \left[ (\mu - \nu^*) \langle \zeta | \hat{b} | \zeta \rangle + (\mu - \nu) \langle \zeta | \hat{b}^\dagger | \zeta \rangle \right], \\ \langle x^2 \rangle &= \frac{x_0^2}{2} \left[ (\mu - \nu^*)^2 \langle \zeta | \hat{b}^2 | \zeta \rangle + (\mu - \nu)^2 \langle \zeta | \hat{b}^{\dagger 2} | \zeta \rangle \right. \\ &\quad \left. + (\mu - \nu^*)(\mu - \nu) \left( \langle \zeta | \hat{b} \hat{b}^\dagger | \zeta \rangle + \langle \zeta | \hat{b}^\dagger \hat{b} | \zeta \rangle \right) \right]. \end{aligned} \quad (***)$$

According to Eqs. (5.144)-(5.145) of the lecture notes, for the general squeezed state,

$$\hat{b} | \zeta \rangle = (\alpha \mu + \alpha^* \nu) | \zeta \rangle, \quad \text{so } \langle \zeta | \hat{b}^\dagger = \langle \zeta | (\alpha^* \mu + \alpha \nu^*).$$

However, our task is to discuss only the specific *ground* squeezed state  $\zeta$ , with  $\alpha = 0$ . For this state, the last relations are reduced to

$$\hat{b} | \zeta \rangle = 0, \quad \langle \zeta | \hat{b}^\dagger = 0.$$

With these relations, the first of Eqs. (\*\*\*) immediately gives  $\langle x \rangle = 0$ ,<sup>43</sup> while in the second of these expressions, only one average on the right-hand side survives, giving

$$\langle x^2 \rangle = \frac{x_0^2}{2} (\mu - \nu^*) (\mu - \nu) \langle \zeta | \hat{b} \hat{b}^\dagger | \zeta \rangle.$$

In order to evaluate this expression, let us first use the fact that  $\mu^2 - \nu \nu^* = 1$  to verify that the squeezed creation-annihilation operators satisfy the same commutation relation as the usual creation-annihilation operators – see Eq. (5.68):

$$\left[ \hat{b}, \hat{b}^\dagger \right] = \left[ \left( \mu \hat{a} + \nu \hat{a}^\dagger \right), \left( \mu \hat{a}^\dagger + \nu^* \hat{a} \right) \right] = \mu^2 \left[ \hat{a}, \hat{a}^\dagger \right] + \nu \nu^* \left[ \hat{a}^\dagger, \hat{a} \right] = (\mu^2 - \nu \nu^*) \left[ \hat{a}, \hat{a}^\dagger \right] = \hat{I}.$$

This relation may be rewritten as a convenient operator identity

$$\hat{b} \hat{b}^\dagger = \hat{b}^\dagger \hat{b} + \hat{I}; \quad (****)$$

plugging it into the last expression for  $\langle x^2 \rangle$ , we get

$$\langle x^2 \rangle = \frac{x_0^2}{2} (\mu - \nu^*) (\mu - \nu) \left( \langle \zeta | \hat{b}^\dagger \hat{b} | \zeta \rangle + \langle \zeta | \hat{I} | \zeta \rangle \right) = \frac{x_0^2}{2} (\mu - \nu^*) (\mu - \nu) \langle \zeta | \zeta \rangle.$$

According to its definition (5.142b), the squeezing operator  $\hat{S}_\zeta$  is unitary, and hence the squeezed ground states are normalized to 1:

$$\langle \zeta | \zeta \rangle \equiv \langle 0 | \hat{S}_\zeta^\dagger \hat{S}_\zeta | 0 \rangle = \langle 0 | \hat{I} | 0 \rangle = 1,$$

so, finally,

$$\langle x^2 \rangle = \frac{x_0^2}{2} (\mu - \nu^*) (\mu - \nu),$$

and we may use the general Eqs. (1.33)-(1.34) to calculate

$$\delta x = \left( \langle x^2 \rangle - \langle x \rangle^2 \right)^{1/2} = \frac{x_0}{\sqrt{2}} \left[ (\mu - \nu^*) (\mu - \nu) \right]^{1/2} \equiv \frac{x_0}{\sqrt{2}} \left( \cosh^2 r + \sinh^2 r - 2 \sinh r \cosh r \cos \theta \right)^{1/2}.$$

This general result depends on the phase  $\theta$ , which may be time-dependent (reflecting the rotation of the squeezed state's image on the phase plane, as shown in Fig. 5.8), but for the particular instants when  $\theta$  is equal to 0 (plus any multiple of  $\pi$ ), i.e.  $\cos \theta = 1$ , it takes the minimum value stated in the first of Eqs. (5.143):

$$\delta x = \frac{x_0}{\sqrt{2}} \left( \cosh^2 r + \sinh^2 r - 2 \sinh r \cosh r \right)^{1/2} \equiv \frac{x_0}{\sqrt{2}} (\cosh r - \sinh r) \equiv \frac{x_0}{\sqrt{2}} e^{-r}.$$

The momentum's uncertainty may be calculated absolutely similarly, giving

$$\delta p = \frac{m \omega_0 x_0}{\sqrt{2}} \left( \cosh^2 r + \sinh^2 r + 2 \sinh r \cosh r \cos \theta \right)^{1/2},$$

<sup>43</sup> This result could be readily anticipated from the physical sense of the squeezed ground state – see, e.g., its image in Fig. 5.8 of the lecture notes.

and, in particular, the second of Eqs. (5.143) for the same case when  $\cos\theta = 1$ .

**Problem 5.23.** Calculate the energy of a harmonic oscillator in the squeezed ground state  $\zeta$ .

*Solution:* Let us re-use the expressions

$$\hat{a} = \mu\hat{b} - \nu\hat{b}^\dagger, \quad \hat{a}^\dagger = \mu\hat{b}^\dagger - \nu^*\hat{b},$$

discussed in the solution of the previous problem. Plugging them into Eq. (5.73) of the lecture notes, let us calculate the average  $\langle N \rangle$ , which determines the state's energy  $E \equiv \langle H \rangle = \hbar\omega_0(\langle N \rangle + 1/2)$ , in a squeezed state  $\zeta$ :

$$\begin{aligned} \langle N \rangle &\equiv \langle \hat{N} \rangle_\zeta = \langle \hat{a}^\dagger \hat{a} \rangle_\zeta = \langle \zeta | \hat{a}^\dagger \hat{a} | \zeta \rangle = \langle \zeta | \left( \mu\hat{b}^\dagger - \nu^*\hat{b} \right) \left( \mu\hat{b} - \nu\hat{b}^\dagger \right) | \zeta \rangle \\ &\equiv \mu^2 \langle \zeta | \hat{b}^\dagger \hat{b} | \zeta \rangle + \nu\nu^* \langle \zeta | \hat{b}\hat{b}^\dagger | \zeta \rangle - \mu\nu \langle \zeta | \hat{b}^\dagger \hat{b}^\dagger | \zeta \rangle - \mu\nu^* \langle \zeta | \hat{b}\hat{b} | \zeta \rangle. \end{aligned} \quad (*)$$

Our task is to discuss only the special, ground squeezed state  $\zeta$  with  $\alpha = 0$ . As was discussed in the previous problem's solution, it has the following properties:

$$\hat{b}|\zeta\rangle = 0, \quad \text{and hence } \langle \zeta | \hat{b}^\dagger = 0.$$

Due to these properties, all terms in the last form of Eq. (\*), besides the second one, are equal to zero, so

$$\langle N \rangle = \nu\nu^* \langle \zeta | \hat{b}\hat{b}^\dagger | \zeta \rangle.$$

Applying to this expression the relations derived in the solution of the previous problem,

$$\hat{b}\hat{b}^\dagger = \hat{b}^\dagger\hat{b} + \hat{I}, \quad \text{and } \langle \zeta | \zeta \rangle = 1;$$

we, finally, get

$$\langle N \rangle = \nu\nu^* \langle \zeta | \hat{b}\hat{b}^\dagger | \zeta \rangle = \nu\nu^* \langle \zeta | \left( \hat{b}^\dagger\hat{b} + \hat{I} \right) | \zeta \rangle = \nu\nu^* \langle \zeta | \zeta \rangle = \nu\nu^* \equiv \sinh^2 r,$$

so

$$E = \hbar\omega_0 \left( \sinh^2 r + \frac{1}{2} \right).$$

Note that this result is independent of the parameter  $\theta$ . Actually, this fact could be predicted from the physical sense of that parameter as the angle that only determines the squeezing direction – see Fig. 5.8 of the lecture notes. Also note that at  $r \rightarrow 0$  (no squeezing),  $E \rightarrow \hbar\omega_0/2$ , which is the correct energy of the Fock/Glauber ground state. However, at  $r \gg 1$ ,  $E$  is much larger than  $\hbar\omega_0/2$ , so the adjective “ground” in the name of this squeezed state should not be taken too literally – it is just the lowest-energy state of all squeezed states with the same  $r$ . The same is true for the term *squeezed vacuum* which is frequently used for a set of field oscillators (see Sec. 9.1) in their ground squeezed states  $\zeta$ ; actually, such a “vacuum” may have a lot of energy in it!

**Problem 5.24.\*** Prove that the squeezed ground state described by Eqs. (5.142) and (5.144)-(5.145) of the lecture notes may be sustained by a sinusoidal modulation of a harmonic oscillator's

parameter, and calculate the squeezing factor  $r$  as a function of the parameter modulation depth, assuming that the depth is small and the oscillator's damping is negligible.

*Solution:* The analysis of a dissipation-free classical harmonic oscillator of frequency  $\omega_0$ , with one of its parameters weakly modulated with frequency  $2\omega \approx 2\omega_0$ , gives<sup>44</sup> the following equation of motion of the complex amplitude  $a$  of the oscillations, defined by the relation  $x(t) = \text{Re}[a(t)\exp\{-i\omega t\}]$ :

$$\dot{a} = i\xi a - ima^* , \quad (*)$$

where  $\xi \equiv \omega - \omega_0$  is the detuning, and  $m$  is proportional to the parameter modulation depth. (Eq. (\*) is strictly valid only if  $m$  and  $|\xi|$  are much smaller than  $\omega$ .) A straightforward analysis of this linear differential equation shows that the parametric excitation, i.e. an exponential growth of  $|a(t)|$ , takes place if  $m$  exceeds the critical value

$$m_c = |\xi| ;$$

because of this, let us focus on the case  $m < m_c$ .

Due to the similarity of linear equations of motion of observables in classical mechanics and the corresponding Heisenberg operators in quantum mechanics (see Sec. 5.2 of the lecture notes), we may mimic Eq. (\*) as the so-called RWA equation of the parametric oscillator:

$$\dot{\hat{a}} = i\xi\hat{a} - im\hat{a}^\dagger , \quad \text{and hence } \dot{\hat{a}}^\dagger = -i\xi\hat{a}^\dagger + im\hat{a} .$$

Note that these  $\hat{a}^\dagger$  and  $\hat{a}$  are not exactly the creation-annihilation operators defined by Eqs. (5.65) of the lecture notes in two aspects: first, they are not necessarily properly normalized (which does not matter for this linear system), and second, they include additional factors  $\exp\{\mp i\omega t\}$ ; however, the latter difference also does not affect the forthcoming calculation.

Now, transferring to the mixed operator  $\hat{b}$  defined by Eq. (5.144) of the lecture notes and its Hermitian conjugate, in the form used in the solutions of the two previous problems,

$$\hat{b} = \mu\hat{a} + \nu\hat{a}^\dagger , \quad \hat{b}^\dagger = \mu\hat{a}^\dagger + \nu^*\hat{a} , \quad \text{where } \mu \equiv \cosh r , \quad \nu \equiv e^{i\theta} \sinh r , \quad (**)$$

we get the following equation of motion of the operator  $\hat{b}$ :

$$\dot{\hat{b}} = i \left[ \xi(\mu^2 + \nu\nu^*) + m\mu(\nu + \nu^*) \right] \hat{b} - i \left[ m(\mu^2 + \nu^2) + 2\xi\mu\nu \right] \hat{b}^\dagger , \quad (***)$$

and its Hermitian conjugate for the operator  $\hat{b}^\dagger$ . As this formula shows, this system may indeed sustain a time-independent<sup>45</sup> squeezed state, provided that the second square bracket vanishes. Upon the substitution of the above definitions of the parameters  $\mu$  and  $\nu$ , we see that this condition:

$$m \left( \cosh^2 r + \sinh^2 r e^{2i\theta} \right) + 2\xi \sinh r \cosh r e^{i\theta} = 0 ,$$

is equivalent to two requirements:  $e^{2i\theta} = 1$ , i.e.  $e^{i\theta} = \pm 1$ ,<sup>46</sup> and

<sup>44</sup> See, e.g., CM Eq. (5.78) with  $m \equiv \mu\omega/4$  and  $\delta = 0$ .

<sup>45</sup> Again, besides its rotation, on the phase plane, with a constant frequency close to  $\omega$  and  $\omega_0$  – see Fig. 5.8.

$$\tanh 2r = \frac{m}{|\xi|}.$$

The last result shows that in the absence of the parameter modulation ( $m = 0$ ),  $r$  vanishes, so according to Eq. (\*\*), the operators  $\hat{a}$  and  $\hat{b}$  (and hence their eigenstates) coincide, and the ground squeezed state is just the usual ground state – as it should. On the other hand, as  $m$  approaches its critical value  $m_c = |\xi|$ , the squeezing factor  $r$  tends to infinity, i.e. the squeezing becomes infinitely strong. According to the solution of the previous problem, this also means that in this limit, the energy of the ground squeezed state tends to infinity.

**Problem 5.25.** Use Eqs. (5.148) of the lecture notes to prove that at negligible spin effects, the operators  $\hat{L}_j$  and  $\hat{L}^2$  commute with the Hamiltonian of a particle placed in any central potential field.

*Solution:* The Hamiltonian in question may be represented as

$$\hat{H} = \frac{\hat{p}^2}{2m} + U(\hat{\mathbf{r}}) \equiv \frac{\hat{p}^2}{2m} + f(\hat{r}^2), \quad \text{where } \hat{r}^2 = \sum_{j=1}^3 \hat{r}_j^2, \text{ and } \hat{p}^2 = \sum_{j=1}^3 \hat{p}_j^2. \quad (*)$$

Let us first calculate the commutators of  $\hat{L}_j$  with  $\hat{r}_j^2$  and  $\hat{p}_j^2$ , for arbitrary  $j$  and  $j'$ . For the first of them, we may use Eq. (5.148) of the lecture notes, rewritten as

$$\hat{L}_j \hat{r}_{j'} = \hat{r}_{j'} \hat{L}_j + i\hbar \sum_{j''=1}^3 \hat{r}_{j''} \varepsilon_{jjj''}.$$

Using this relation twice, we get

$$\begin{aligned} [\hat{L}_j, \hat{r}_j^2] &\equiv \hat{L}_j \hat{r}_j^2 - \hat{r}_j^2 \hat{L}_j \equiv (\hat{L}_j \hat{r}_j) \hat{r}_j - \hat{r}_j \hat{r}_j \hat{L}_j = \left( \hat{r}_j \hat{L}_j + i\hbar \sum_{j''=1}^3 \hat{r}_{j''} \varepsilon_{jjj''} \right) \hat{r}_j - \hat{r}_j \hat{r}_j \hat{L}_j \\ &\equiv \hat{r}_j (\hat{L}_j \hat{r}_j) - \hat{r}_j \hat{r}_j \hat{L}_j + i\hbar \sum_{j''=1}^3 \hat{r}_{j''} \hat{r}_j \varepsilon_{jjj''} \\ &= \hat{r}_j \left( \hat{r}_j \hat{L}_j + i\hbar \sum_{j''=1}^3 \hat{r}_{j''} \varepsilon_{jjj''} \right) - \hat{r}_j \hat{r}_j \hat{L}_j + i\hbar \sum_{j''=1}^3 \hat{r}_{j''} \hat{r}_j \varepsilon_{jjj''} \equiv 2i\hbar \sum_{j''=1}^3 \hat{r}_{j''} \hat{r}_j \varepsilon_{jjj''}. \end{aligned} \quad (**)$$

Now we may use this result to calculate

$$[\hat{L}_j, \hat{r}^2] \equiv \left[ \hat{L}_j, \sum_{j'=1}^3 \hat{r}_j^2 \right] = \sum_{j'=1}^3 [\hat{L}_j, \hat{r}_j^2] = 2i\hbar \sum_{j', j''=1}^3 \hat{r}_{j''} \hat{r}_j \varepsilon_{jjj''}.$$

According to the definition of the Levi-Civita symbol, three terms of the last sum, with  $j' = j''$ , equal zero, while the other six terms form three pairs of terms that differ only by the replacements  $j' \leftrightarrow j''$ , and thus are equal and opposite. As a result,

$$[\hat{L}_j, \hat{r}^2] = 0, \quad \text{so } [\hat{L}_j, f(\hat{r}^2)] = 0.$$

<sup>46</sup> In the duality of the solution for the angle  $\theta$ :  $\theta_1 = 0$  and  $\theta_2 = \pi$  (plus any multiples of  $2\pi$ ), we may readily recognize two possible (and equivalent) phases of the degenerate parametric excitation – see, e.g., CM Sec. 5.5.

Since all three operators  $\hat{L}_j$  commute with the function  $f(\hat{r}^2)$ , so do operators  $\hat{L}_j^2$ , and hence the operator  $\hat{L}^2$  that is defined as their sum – see Eq. (5.150).

Next, due to the full similarity of the first and the second of Eqs. (5.149),

$$[\hat{L}_j, \hat{r}_{j'}] = i\hbar \sum_{j''=1}^3 \hat{r}_{j''} \epsilon_{jjj''}, \quad [\hat{L}_j, \hat{p}_{j'}] = i\hbar \sum_{j''=1}^3 \hat{p}_{j''} \epsilon_{jjj''},$$

we may immediately reuse Eq. (\*\*), just replacing  $r_{j'}$  with  $p_{j'}$ :

$$[\hat{L}_j, \hat{p}_{j'}^2] = 2i\hbar \sum_{j''=1}^3 \hat{p}_{j''} \hat{p}_{j'} \epsilon_{jjj''},$$

so the summation over all  $j'$  yields a similar result:

$$[\hat{L}_j, \hat{p}^2] = \sum_{j'=1}^3 [\hat{L}_j, \hat{p}_{j'}^2] = 2i\hbar \sum_{j', j''=1}^3 \hat{p}_{j''} \hat{p}_{j'} \epsilon_{jjj''} = 0.$$

Again, since all three operators  $\hat{L}_j$  commute with  $\hat{p}^2$ , so do operators  $\hat{L}_j^2$ , and hence the operator  $\hat{L}^2$ .

Combining these results with Eq. (\*), we, finally, get

$$[\hat{L}_j, \hat{H}] = \frac{1}{2m} [\hat{L}_j, \hat{p}^2] + [\hat{L}_j, f(\hat{r}^2)] = 0, \quad [\hat{L}^2, \hat{H}] = \frac{1}{2m} [\hat{L}^2, \hat{p}^2] + [\hat{L}^2, f(\hat{r}^2)] = 0.$$

According to Eq. (4.199) of the lecture notes, these equalities guarantee that the Heisenberg-picture operators of  $L_j$  and  $L^2$  do not change in time during the particle's motion in the central field; this quantum-mechanical fact corresponds to the classical-mechanical fact of conservation of these observables in such a field.

**Problem 5.26.** Use Eqs. (5.149)-(5.150) and (5.153) of the lecture notes to prove Eqs. (5.155).

*Solution:* Let us spell out the following operator product:

$$\hat{L}_+ \hat{L}_- \equiv (\hat{L}_x + i\hat{L}_y)(\hat{L}_x - i\hat{L}_y) = \hat{L}_x^2 + \hat{L}_y^2 - i(\hat{L}_x \hat{L}_y - \hat{L}_y \hat{L}_x) \equiv \hat{L}_x^2 + \hat{L}_y^2 - i[\hat{L}_x, \hat{L}_y].$$

But according to the last of Eqs. (5.149) of the lecture notes, the last commutator equals  $i\hbar \hat{L}_z$ , so we get the following equality:

$$\hat{L}_+ \hat{L}_- = \hat{L}_x^2 + \hat{L}_y^2 + \hbar \hat{L}_z. \quad (*)$$

Now, from the definition of the operator  $\hat{L}^2$  given by Eq. (5.150), we may write

$$\hat{L}_x^2 + \hat{L}_y^2 = \hat{L}^2 - \hat{L}_z^2.$$

Plugging the last relation into Eq. (\*), we get the first of Eqs. (5.155). The second of these relations (which was already used in Sec. 5.6 of the lecture notes) may be proved by the absolutely similar transformation of the reversed product,  $\hat{L}_- \hat{L}_+$ .



Problem 5.27. Derive Eq. (5.164) of the lecture notes by using any of the prior formulas.

*Solution:* According to Eqs. (5.159) of the lecture notes and their discussion, the action of the ladder operators upon the common eigenkets  $|l, m\rangle$  of operators  $\hat{L}^2$  and  $\hat{L}_z$  may be described as

$$\hat{L}_\pm |l, m\rangle = L_\pm^{(m)} |l, m \pm 1\rangle, \quad (*)$$

where, at that stage of reasoning,  $L_\pm^{(m)}$  were *some*  $c$ -number coefficients.<sup>47</sup> Let us calculate them, assuming that these eigenstates are normalized:  $\langle l, m | l, m \rangle = 1$ . For that, first of all, let us notice that we are speaking essentially about finding just one rather than two coefficient sets. Indeed, we may use the general rule bra-ket rule (4.25) to write

$$\langle l, m | (\hat{L}_+^\dagger) |l, m+1\rangle = \langle l, m+1 | \hat{L}_+ |l, m\rangle^*.$$

Since, by their definition (5.153), the ladder operators are the Hermitian conjugates of each other, this equality takes the following form:

$$\langle l, m | \hat{L}_- |l, m+1\rangle = \langle l, m+1 | \hat{L}_+ |l, m\rangle^*.$$

By using Eq. (\*) and the state normalization condition, the last equality yields

$$L_-^{(m+1)} = (L_+^{(m)})^*, \quad (**)$$

so the problem is indeed reduced to finding just one of these two coefficient sets – say,  $L_+^{(m)}$ .

This may be done, for example, by using the second of Eqs. (5.155) (whose proof was the subject of the previous problem) for writing a relation similar to the initial form of Eq. (5.163), but for an eigenstate with an arbitrary  $m$ :

$$\hat{L}^2 |l, m\rangle = \hbar \hat{L}_z |l, m\rangle + \hat{L}_z^2 |l, m\rangle + \hat{L}_- \hat{L}_+ |l, m\rangle.$$

Now using the eigenvalues calculated in Sec. 5.6 to evaluate the first three terms, and the definition (\*) of the coefficients  $L_\pm^{(m)}$  in the last term, we get

$$\hbar^2 l(l+1) |l, m\rangle = \hbar^2 m |l, m\rangle + \hbar^2 m^2 |l, m\rangle + \hat{L}_- L_+^{(m)} |l, m+1\rangle = [\hbar^2 m(m+1) + L_-^{(m+1)} L_+^{(m)}] |l, m\rangle.$$

For all existing eigenstates (with  $|m| \leq l$ ), this equality may be true only if the  $c$ -number factors in its first and last forms are equal. Together with Eq. (\*\*), this gives us the final answer:

$$|L_+^{(m)}| = |L_-^{(m+1)}| = \hbar [l(l+1) - m(m+1)]^{1/2}.$$

The other two frequently used forms of the same result are

$$|L_\pm^{(m)}| = \hbar [l(l+1) - m(m \pm 1)]^{1/2} \equiv \hbar [(l \pm m + 1)(l \mp m)]^{1/2};$$

<sup>47</sup> Note that per Eq. (\*), the coefficients  $L_\pm^{(m)}$  are the *only* nonvanishing elements of the ladder operator matrices in the basis of the  $|l, m\rangle$  states with a fixed orbital quantum number  $l$ :

$$(L_\pm)_{m, m'} \equiv \langle l, m | \hat{L}_\pm |l, m'\rangle = L_\pm^{(m)} \delta_{m' \pm 1, m}.$$

the first of these forms, together with Eq. (\*), gives Eq. (5.164) of the lecture notes, which is valid to an arbitrary phase multiplier.

As a sanity check,  $L_+^{(m)}$  turns into zero at  $m = +l$  (thus making the next state  $|l, l + 1\rangle$  properly impossible), while  $L_-^{(m)}$  does the same at  $m = -l$ , thus terminating the state ladder on both sides – see Fig. 5.11.

**Problem 5.28.** Derive the expression  $\langle L^2 \rangle = \hbar^2 l(l + 1)$  from basic statistics, by assuming that all  $(2l + 1)$  values  $L_z = \hbar m$  of a system with a fixed integer number  $l$  have equal probability, and that the system is isotropic. Explain why this statistical picture cannot be used for proof of Eq. (5.163).

*Solution:* In this statistical model, the probability of each value of  $m$  of the set (5.162),

$$-l \leq m \leq l,$$

and hence of having  $L_z = \hbar m$ , is  $W_m = 1/(2l + 1)$ , so according to the general Eq. (1.37), the average value of  $L_z^2$  is

$$\langle L_z^2 \rangle = \sum_{m=-l}^{+l} W_m L_z^2 = \sum_{m=-l}^{+l} W_m (\hbar m)^2 \equiv \frac{\hbar^2}{2l + 1} \sum_{m=-l}^{+l} m^2.$$

The last sum equals  $l(l + 1)(2l + 1)/3$ ,<sup>48</sup> so

$$\langle L_z^2 \rangle = \frac{\hbar^2 l(l + 1)}{3}.$$

If the system we are considering is isotropic, this formula should be also valid for the averages  $\langle L_x^2 \rangle$  and  $\langle L_y^2 \rangle$ , and we get

$$\langle L^2 \rangle \equiv \langle L_x^2 + L_y^2 + L_z^2 \rangle = 3\langle L_z^2 \rangle = \hbar^2 l(l + 1),$$

i.e. exactly the value given by Eq. (5.163).

As it follows from the discussion of Eq. (5.163) in the lecture notes, this naïve statistical picture catches a glimpse of the angular momentum's uncertainty responsible for the difference between the quantum-mechanical factor  $l(l + 1)$  and the classically expected value  $(m_{\max})^2 = l^2$ . However, the importance of its result should not be exaggerated. Indeed, the actual quantum-mechanical average (i.e. the expectation value) of  $L^2$  equals  $\hbar^2 l(l + 1)$  for *any* distribution of a system with fixed  $l$  between its possible states of  $L_z = \hbar m$ , in particular in the case when the system has a definite value of  $m$ , i.e. is described by just a single  $|l, m\rangle$  ket.

**Problem 5.29.** In the basis of the common eigenstates of the operators  $\hat{L}_z$  and  $\hat{L}^2$ , described by kets  $|l, m\rangle$ :

(i) calculate the matrix elements  $\langle l, m_1 | \hat{L}_x | l, m_2 \rangle$  and  $\langle l, m_1 | \hat{L}_x^2 | l, m_2 \rangle$ ,

(ii) spell out your results for the diagonal matrix elements (with  $m_1 = m_2$ ) and their y-axis counterparts, and

<sup>48</sup> See, e.g., MA Eq. (2.6a).

(iii) calculate the diagonal matrix elements  $\langle l, m | \hat{L}_x \hat{L}_y | l, m \rangle$  and  $\langle l, m | \hat{L}_y \hat{L}_x | l, m \rangle$ .

*Solutions:*

(i) The definition (5.153) of the ladder operators yields the reciprocal relations

$$\hat{L}_x = \frac{\hat{L}_+ + \hat{L}_-}{2}, \quad \hat{L}_y = \frac{\hat{L}_+ - \hat{L}_-}{2i}, \quad (*)$$

so by using Eq. (5.164) of the lecture notes (whose proof was the subject of the previous problem), we may calculate the matrix elements of the operator  $\hat{L}_x$  in two equivalent forms:

$$\begin{aligned} \langle l, m_1 | \hat{L}_x | l, m_2 \rangle &= \frac{1}{2} \langle l, m_1 | \hat{L}_+ | l, m_2 \rangle + \frac{1}{2} \langle l, m_1 | \hat{L}_- | l, m_2 \rangle \\ &= \frac{\hbar}{2} \left\{ [(l + m_2 + 1)(l - m_2)]^{1/2} \delta_{m_2, m_1 - 1} + [(l - m_2 + 1)(l + m_2)]^{1/2} \delta_{m_2, m_1 + 1} \right\} \\ &\equiv \frac{\hbar}{2} \left\{ [(l + m_1)(l - m_1 + 1)]^{1/2} \delta_{m_1, m_2 + 1} + [(l - m_1)(l + m_1 + 1)]^{1/2} \delta_{m_1, m_2 - 1} \right\}. \quad (**)$$

For the calculation of the matrix elements of  $\hat{L}_x^2$ , it is instrumental to represent this operator as the product  $\hat{L}_x \hat{L}_x$ , and then act by the first of them (a Hermitian operator!) upon the bra-vector, and with the second one, upon the ket-vector, using Eq. (\*\*) twice – each time in a more convenient form:

$$\begin{aligned} \langle l, m_1 | \hat{L}_x^2 | l, m_2 \rangle &\equiv \langle l, m_1 | \hat{L}_x \hat{L}_x | l, m_2 \rangle \\ &= \frac{\hbar}{2} \langle l, m_1 - 1 | \left\{ [(l + m_1)(l - m_1 + 1)]^{1/2} + \langle l, m_1 + 1 | [(l - m_1)(l + m_1 + 1)]^{1/2} \right\} \\ &\quad \times \frac{\hbar}{2} \left\{ [(l + m_2 + 1)(l - m_2)]^{1/2} | l, m_2 + 1 \rangle + [(l - m_2 + 1)(l + m_2)]^{1/2} | l, m_2 - 1 \rangle \right\} \\ &= \frac{\hbar^2}{4} \times \left\{ \begin{aligned} & \left\{ [(l + m_1)(l - m_1 + 1)(l - m_2 + 1)(l + m_2)]^{1/2} \right. \\ & \left. + [(l - m_1)(l + m_1 + 1)(l + m_2 + 1)(l - m_2)]^{1/2} \right\} \delta_{m_1, m_2} \\ & + [(l + m_1)(l - m_1 + 1)(l + m_2 + 1)(l - m_2)]^{1/2} \delta_{m_1 - 1, m_2 + 1} \\ & + [(l - m_1)(l + m_1 + 1)(l - m_2 + 1)(l + m_2)]^{1/2} \delta_{m_1 + 1, m_2 - 1} \end{aligned} \right\}. \end{aligned}$$

These expressions show that operator  $\hat{L}_x^2$  “connects” only the states whose magnetic quantum numbers either do not differ at all or differ by  $\pm 2$ , in a clear analogy with the operator  $\hat{x}^2$  in a harmonic oscillator – see Eq. (5.94).

(ii) For the diagonal matrix elements (with  $m_1 = m_2 \equiv m$ ), these general formulas yield:

$$\begin{aligned} \langle l, m | \hat{L}_x | l, m \rangle &= 0, \\ \langle l, m | \hat{L}_x^2 | l, m \rangle &= \frac{\hbar^2}{4} [(l + m)(l - m + 1) + (l - m)(l + m + 1)] \equiv \frac{\hbar^2}{2} [l(l + 1) - m^2]. \end{aligned}$$

Carrying out absolutely similar calculations for the operator  $\hat{L}_y$  and its square, we get similar results:

$$\begin{aligned}\langle l, m_1 | \hat{L}_y | l, m_2 \rangle &= \frac{1}{2i} \langle l, m_1 | \hat{L}_+ | l, m_2 \rangle - \frac{1}{2i} \langle l, m_1 | \hat{L}_- | l, m_2 \rangle \\ &= \frac{\hbar}{2i} \left\{ [(l + m_2 + 1)(l - m_2)]^{1/2} \delta_{m_2, m_1 - 1} - [(l - m_2 + 1)(l + m_2)]^{1/2} \delta_{m_2, m_1 + 1} \right\} \quad (***) \\ &\equiv \frac{\hbar}{2i} \left\{ [(l + m_1)(l - m_1 + 1)]^{1/2} \delta_{m_1, m_2 + 1} - [(l - m_1)(l + m_1 + 1)]^{1/2} \delta_{m_1, m_2 - 1} \right\}, \\ \langle l, m | \hat{L}_y | l, m \rangle &= 0, \quad \langle l, m | \hat{L}_y^2 | l, m \rangle = \frac{\hbar^2}{2} [l(l+1) - m^2].\end{aligned}$$

(iii) By using Eqs. (\*\*) and (\*\*\*) in the same way as for the calculation of the matrix elements of  $\hat{L}_x^2$  and  $\hat{L}_y^2$ , for the mixed products of the component operators, we get

$$\langle l, m | \hat{L}_x \hat{L}_y | l, m \rangle = \frac{i}{2} \hbar^2 m, \quad \langle l, m | \hat{L}_y \hat{L}_x | l, m \rangle = -\frac{i}{2} \hbar^2 m. \quad (****)$$

As a sanity check, let us verify this result by using Eq. (5.158) to calculate the diagonal matrix elements of the commutator given by the last of Eqs. (5.149):

$$\langle l, m | [\hat{L}_x, \hat{L}_y] | l, m \rangle = i\hbar \langle l, m | \hat{L}_z | l, m \rangle = i\hbar \langle l, m | \hbar m | l, m \rangle = i\hbar^2 m.$$

This is exactly the result following from the subtraction of two Eqs. (\*\*\*\*) from each other.

**Problem 5.30.** For the state described by the common eigenket  $|l, m\rangle$  of the operators  $\hat{L}_z$  and  $\hat{L}^2$  in a reference frame  $\{x, y, z\}$ , calculate the expectation values  $\langle L_{z'} \rangle$  and  $\langle L_{z'}^2 \rangle$  in the reference frame whose  $z'$ -axis forms angle  $\theta$  with the  $z$ -axis.

*Solutions:* Basic trigonometry tells us that if a  $c$ -number geometric vector  $\mathbf{L}$  has Cartesian components  $L_x, L_y, L_z$  in a certain reference frame  $\{x, y, z\}$ , its projection to the  $z'$ -axis equals<sup>49</sup>

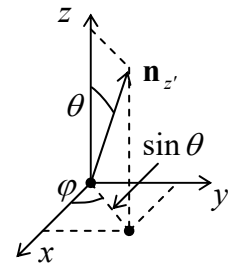
$$L_{z'} = L_x \sin \theta \cos \varphi + L_y \sin \theta \sin \varphi + L_z \cos \theta,$$

where the angles  $\theta$  and  $\varphi$  are defined as at the usual introduction of the spherical coordinates – see the figure on the right. As was discussed in Sec. 1.2 of the lecture notes, all quantum-mechanical vector operators, by definition, follow the same geometric relations as the  $c$ -number geometric vectors, so we may write

$$\hat{L}_{z'} = \hat{L}_x \sin \theta \cos \varphi + \hat{L}_y \sin \theta \sin \varphi + \hat{L}_z \cos \theta. \quad (*)$$

To find  $\langle L_{z'} \rangle$ , it is sufficient to calculate the expectation value of the right-hand side of Eq. (\*):

$$\langle L_{z'} \rangle \equiv \langle l, m | \hat{L}_{z'} | l, m \rangle = \langle l, m | \hat{L}_x | l, m \rangle \sin \theta \cos \varphi + \langle l, m | \hat{L}_y | l, m \rangle \sin \theta \sin \varphi + \langle l, m | \hat{L}_z | l, m \rangle \cos \theta,$$



<sup>49</sup> This formula may be readily derived by representing  $L_{z'}$  as the scalar product  $\mathbf{L} \cdot \mathbf{n}_{z'}$ , with  $\mathbf{L} = \mathbf{n}_x L_x + \mathbf{n}_y L_y + \mathbf{n}_z L_z$  and  $\mathbf{n}_{z'} = \mathbf{n}_x \sin \theta \cos \varphi + \mathbf{n}_y \sin \theta \sin \varphi + \mathbf{n}_z \cos \theta$ . (The last relation follows either from MA Eq. (10.7) with  $\mathbf{r} \rightarrow \mathbf{n}_{z'}$ , i.e. with  $r = 1$ , or just directly from the figure, taking into account that the length of the unit vector  $\mathbf{n}'$  equals 1.)

and take into account that according to the solution of the previous problem, the first two matrix elements on the right-hand side of this expression equal zero, while per Eq. (5.158) of the lecture notes, the last of them is equal to  $\hbar m$ . Hence,

$$\langle L_{z'} \rangle = \hbar m \cos \theta.$$

Now using Eq. (\*) again, we may write (being careful not to swap non-commuting operators):

$$\begin{aligned} \hat{L}_{z'}^2 &\equiv \hat{L}_{z'} \hat{L}_{z'} = \left( \hat{L}_x \sin \theta \cos \varphi + \hat{L}_y \sin \theta \sin \varphi + \hat{L}_z \cos \theta \right) \left( \hat{L}_x \sin \theta \cos \varphi + \hat{L}_y \sin \theta \sin \varphi + \hat{L}_z \cos \theta \right) \\ &= \hat{L}_x^2 \sin^2 \theta \cos^2 \varphi + \hat{L}_y^2 \sin^2 \theta \sin^2 \varphi + \hat{L}_z^2 \cos^2 \theta + \left( \hat{L}_x \hat{L}_y + \hat{L}_y \hat{L}_x \right) \sin^2 \theta \sin \varphi \cos \varphi + \\ &\quad + \left( \hat{L}_x \hat{L}_z + \hat{L}_z \hat{L}_x \right) \sin \theta \cos \theta \cos \varphi + \left( \hat{L}_y \hat{L}_z + \hat{L}_z \hat{L}_y \right) \sin \theta \cos \theta \sin \varphi. \end{aligned}$$

The expectation values of the first two operators participating in the last expression were calculated in the previous problem:

$$\langle L_x^2 \rangle = \langle L_y^2 \rangle = \frac{\hbar^2}{2} [l(l+1) - m^2],$$

while that of the  $\hat{L}_z^2 \equiv \hat{L}_z \hat{L}_z$  may be readily calculated using the fact that, according to Eq. (5.158) of the lecture notes,  $|l, m\rangle$  is an eigenket of the operator  $\hat{L}_z$ , with the eigenvalue  $\hbar m$ :

$$\langle L_z^2 \rangle \equiv \langle l, m | \hat{L}_z \hat{L}_z | l, m \rangle = \langle l, m | \hat{L}_z \hbar m | l, m \rangle = \hbar m \langle l, m | \hat{L}_z | l, m \rangle = \hbar^2 m^2.$$

The expectation values of all other operator combinations vanish, as it follows from the other results of the previous problem and (in the last two cases) from the same Eq. (5.158):

$$\begin{aligned} \langle L_x L_y + L_y L_x \rangle &\equiv \langle l, m | \hat{L}_x \hat{L}_y | l, m \rangle + \langle l, m | \hat{L}_y \hat{L}_x | l, m \rangle = \frac{i}{2} \hbar^2 m - \frac{i}{2} \hbar^2 m = 0, \\ \langle L_x L_z + L_z L_x \rangle &\equiv \langle l, m | \hat{L}_x \hat{L}_z | l, m \rangle + \langle l, m | \hat{L}_z \hat{L}_x | l, m \rangle = \hbar m \langle l, m | \hat{L}_x | l, m \rangle + \langle l, m | \hat{L}_x | l, m \rangle = 0, \\ \langle L_y L_z + L_z L_y \rangle &\equiv \langle l, m | \hat{L}_y \hat{L}_z | l, m \rangle + \langle l, m | \hat{L}_z \hat{L}_y | l, m \rangle = \hbar m \langle l, m | \hat{L}_y | l, m \rangle + \hbar m \langle l, m | \hat{L}_y | l, m \rangle = 0, \end{aligned}$$

so finally we get

$$\begin{aligned} \langle L_{z'}^2 \rangle &= \frac{\hbar^2}{2} [l(l+1) - m^2] \sin^2 \theta \cos^2 \varphi + \frac{\hbar^2}{2} [l(l+1) - m^2] \sin^2 \theta \sin^2 \varphi + \hbar^2 m^2 \cos^2 \theta \\ &\equiv \hbar^2 \left[ \frac{l(l+1) - m^2}{2} \sin^2 \theta + m^2 \cos^2 \theta \right]. \end{aligned}$$

Note that the angle  $\varphi$  shown in the figure above, i.e. the direction of the axes  $x$  and  $y$  of the initial reference frame, as well as the direction of the axes  $x'$  and  $y'$  of the “primed” reference frame (at fixed axes  $z$  and  $z'$ ) do not affect the result. In hindsight, this looks very natural and means that the above solution might be simplified by taking, for example,  $\varphi = 0$  from the very beginning.

**Problem 5.31.** Write down the matrices of the following angular momentum operators:  $\hat{L}_x$ ,  $\hat{L}_y$ ,  $\hat{L}_z$ , and  $\hat{L}_\pm$ , in the  $z$ -basis of the  $\{l, m\}$  states with  $l = 1$ .

*Solution:* Since, according to Eqs. (5.153), (5.158), and (5.164) of the lecture notes, the action of all these operators on the ket- (or bra-) vectors of the  $\{l, m\}$  states does not change the orbital quantum number  $l$ , their matrices consist of the elements with the same value of  $l$  (in our particular case,  $l = 1$ ):

$$A_{mm'} = \langle l = 1, m | \hat{A} | l = 1, m' \rangle.$$

Since for  $l = 1$ , there are 3 possible values of the quantum number  $m$  (+1, 0, and -1), so these are  $3 \times 3$  matrices. Of them, the matrix of the operator  $\hat{L}_z$  is the simplest one, because according to Eq. (5.158) of the lecture notes, it has only diagonal elements equal to  $\hbar m$ , so by numbering the states in the order accepted above, we may write

$$L_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

Next, according to Eq. (5.164),

$$(L_\pm)_{mm'} = L_\pm^{(m')} \delta_{m' \pm 1, m}, \quad \text{with } |L_\pm^{(m)}| = \hbar [l(l+1) - m(m \pm 1)]^{1/2},$$

so in our case  $l = 1$ , the only two nonvanishing matrix elements of each operator have the following magnitudes:

$$\begin{aligned} |(L_+)_{1,0}| &= \hbar [1 \cdot 2 - 0 \cdot 1]^{1/2} = \sqrt{2}\hbar, & |(L_+)_{0,-1}| &= \hbar [1 \cdot 2 - (-1) \cdot 0]^{1/2} = \sqrt{2}\hbar, \\ |(L_-)_{0,1}| &= \hbar [1 \cdot 2 - 1 \cdot 0]^{1/2} = \sqrt{2}\hbar, & |(L_-)_{-1,0}| &= \hbar [1 \cdot 2 - 0 \cdot (-1)]^{1/2} = \sqrt{2}\hbar. \end{aligned} \quad (*)$$

Note that the elements may be multiplied by phase factors  $\exp\{i\varphi\}$ , but their phases  $\varphi$  need to be related to keep the operators of observable momentum components,

$$\hat{L}_x = \frac{\hat{L}_+ + \hat{L}_-}{2} \quad \text{and} \quad \hat{L}_y = \frac{\hat{L}_+ - \hat{L}_-}{2i}, \quad (**)$$

Hermitian, i.e. to have Eqs. (4.65) of the lecture notes satisfied for their matrix elements. An elementary calculation using Eqs. (\*\*) shows that this requires

$$(L_+)_{m'm} = (L_-)_{mm'}^*, \quad \text{i.e. } (L_+)_{1,0} = (L_-)_{0,1}^* \quad \text{and} \quad (L_+)_{0,-1} = (L_-)_{-1,0}^*.$$

This requirement is satisfied, for example, for the simplest choice  $\varphi = 0$ . In this case, we may represent our result as

$$L_+ = \sqrt{2}\hbar \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \quad L_- = \sqrt{2}\hbar \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

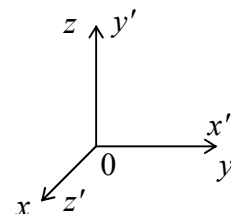
Finally, using Eqs. (\*\*) (which have to be obeyed by each of the matrix elements as well), we get

$$L_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad L_y = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}.$$

**Problem 5.32.** Calculate the angular factor of the orbital wavefunction of a particle with a definite value of  $L^2$ , equal to  $6\hbar^2$ , and the largest possible definite value of  $L_x$ . What is this value?

*Solution:* Let us introduce a new set of Cartesian coordinates  $\{x', y', z'\}$ , with the same origin as the initial one  $\{x, y, z\}$ , but rotated relative to it as the figure on the right shows:

$$x' \equiv y, \quad y' \equiv z, \quad z' \equiv x, \quad \text{so } r' = r. \quad (*)$$



In this reference frame, the state we are looking for has the same fixed value of  $L^2$ , and the largest definite value of  $L_{z'}$ . According to Eqs. (5.158) and (5.163) of the lecture notes, such state is described by the ket  $|l', m'\rangle$  with  $m' = l' = 2$ , and corresponds to  $L_{z'} = m'\hbar = 2\hbar$  and  $L^2 = \hbar^2 l'(l' + 1) = 6\hbar^2$ . But according to the last of Eqs. (3.176), the angular wavefunction corresponding to such a state is

$$\psi = \left( \frac{15}{32\pi} \right)^{1/2} \sin^2 \theta' e^{2i\varphi'},$$

where the primed angles are related to the primed Cartesian coordinates (\*) in the usual way:

$$\sin \theta' \cos \varphi' = \frac{x'}{r'}, \quad \sin \theta' \sin \varphi' = \frac{y'}{r'}, \quad \cos \theta' = \frac{z'}{r'}. \quad (**)$$

To use these relations, let us express  $\psi$  in terms of trigonometric functions of the single angle  $\varphi'$ :

$$\begin{aligned} \psi &\equiv \left( \frac{15}{32\pi} \right)^{1/2} \sin^2 \theta' (\cos 2\varphi' + i \sin 2\varphi') \equiv \left( \frac{15}{32\pi} \right)^{1/2} \sin^2 \theta' (\cos^2 \varphi' - \sin^2 \varphi' + 2i \sin \varphi' \cos \varphi') \\ &\equiv \left( \frac{15}{32\pi} \right)^{1/2} (\sin^2 \theta' \cos^2 \varphi' - \sin^2 \theta' \sin^2 \varphi' + 2i \sin^2 \theta' \sin \varphi' \cos \varphi'). \end{aligned}$$

Now plugging Eqs. (\*\*) into this result, then using Eq. (\*) to replace the coordinates back to the initial Cartesian ones, and, finally, to the initial (in our notation, non-primed) spherical angles, we get

$$\begin{aligned} \psi &= \left( \frac{15}{32\pi} \right)^{1/2} \frac{1}{r'^2} (x'^2 - y'^2 + 2ix'y') \equiv \left( \frac{15}{32\pi} \right)^{1/2} \frac{1}{r^2} (y^2 - z^2 + 2iyz) \\ &\equiv \left( \frac{15}{32\pi} \right)^{1/2} (\sin^2 \theta \sin^2 \varphi - \cos^2 \theta + 2i \sin \theta \sin \varphi \cos \theta). \end{aligned}$$

Naturally, this coordinate replacement does not change the value  $L_x = L_{z'} = 2\hbar$ .

**Problem 5.33.** For the state with the wavefunction  $\psi = Cxye^{-\lambda r}$ , with a real positive  $\lambda$ , calculate:

- (i) the expectation values of the observables  $L_x, L_y, L_z$ , and  $L^2$ , and
- (ii) the normalization constant  $C$ .

*Solutions:*

(i) Rewriting the given wavefunction in the spherical coordinates:

$$\psi = Cr^2 e^{-\lambda r} \sin^2 \theta \sin \varphi \cos \varphi = Cr^2 e^{-\lambda r} \sin^2 \theta \frac{\sin 2\varphi}{2} = Cr^2 e^{-\lambda r} \sin^2 \theta \frac{e^{2i\varphi} - e^{-2i\varphi}}{4i},$$

and comparing the result with the top and bottom lines of Eq. (3.176), we see that

$$\psi = \mathcal{R}(r) \times \frac{1}{\sqrt{2}} [Y_2^2(\theta, \varphi) - Y_2^{-2}(\theta, \varphi)], \quad (*)$$

where

$$\mathcal{R}(r) \equiv -2i \left( \frac{\pi}{15} \right)^{1/2} Cr^2 e^{-\lambda r}. \quad (**)$$

As Eq. (\*) shows, the state is a linear superposition, with equal and opposite weights (and hence equal probabilities  $W_+ = W_- = 1/2$ ), of two angularly-orthogonal states: one with  $l = 2$  and  $m = 2$ , and another one with  $l = 2$  and  $m = -2$ . Hence, according to Eq. (5.158), the expectation value of  $L_z$  is

$$\langle L_z \rangle = \hbar(+2)W_+ + \hbar(-2)W_- = 0,$$

while according to Eq. (5.163), that of  $L^2$  is

$$\langle L^2 \rangle = \hbar^2 2(2+1)W_+ + \hbar^2 2(2+1)W_- = 6\hbar^2.$$

Finally, by using Eq. (5.164) of the lecture notes, it is straightforward to check that in the linear superposition (\*), the expectation values of  $L_{\pm}$ , and hence of both  $L_x = (L_+ - L_-)/2$  and  $L_y = (L_x - L_y)/2i$ , are equal to zero.

(ii) Since all spherical harmonics are already normalized (see Eq. (3.173) of the lecture notes), so is the whole angular factor of the wavefunction (\*), and it is sufficient to require the normalization of its radial part – cf. Eq. (3.194):

$$\int_0^{\infty} \mathcal{R}^*(r) \mathcal{R}(r) r^2 dr = 1.$$

Per Eq. (\*\*), this equality gives the following condition for the constant  $C$ :

$$|C|^{-2} = \frac{4\pi}{15} \int_0^{\infty} r^6 e^{-2\lambda r} dr \equiv \frac{4\pi}{15} \left( \frac{1}{2\lambda} \right)^7 \int_0^{\infty} \xi^6 e^{-\xi} d\xi.$$

This dimensionless integral<sup>50</sup> equals  $6! \equiv 720$ , so we finally get

$$|C| = \left[ \frac{4\pi}{15} \left( \frac{1}{2\lambda} \right)^7 720 \right]^{-1/2} \equiv \left( \frac{2}{3\pi} \right)^{1/2} \lambda^{7/2}.$$

(Just as a reminder, any normalization constant is defined up to a phase multiplier  $e^{i\varphi}$  with any real  $\varphi$ .)

**Problem 5.34.** An angular state of a spinless particle is described by the following ket-vector:

<sup>50</sup> See, e.g., MA Eq. (6.7d) with  $n = 6$ .



$$|\alpha\rangle = \frac{1}{\sqrt{2}}(|l=3, m=0\rangle + |l=3, m=1\rangle).$$

Calculate the expectation values of the  $x$ - and  $y$ -components of its angular momentum. Is the result sensitive to a possible phase shift between the component eigenkets?

*Solution:* Let us start with calculating the expectation values of the ladder operators:

$$\langle L_{\pm} \rangle = \langle \alpha | \hat{L}_{\pm} | \alpha \rangle = \frac{1}{2} (\langle 3,0 | \hat{L}_{\pm} | 3,0 \rangle + \langle 3,0 | \hat{L}_{\pm} | 3,1 \rangle + \langle 3,1 | \hat{L}_{\pm} | 3,0 \rangle + \langle 3,1 | \hat{L}_{\pm} | 3,1 \rangle).$$

Per Eq. (5.164) of the lecture notes, the diagonal matrix elements vanish, while each of the off-diagonal terms contributes to only one expectation value:

$$\begin{aligned} \langle L_+ \rangle &= \frac{1}{2} \langle 3,1 | \hat{L}_+ | 3,0 \rangle = \frac{\hbar}{2} [l(l+1) - m(m+1)]_{l=3, m=0}^{1/2} = \sqrt{3}\hbar, \\ \langle L_- \rangle &= \frac{1}{2} \langle 3,0 | \hat{L}_- | 3,1 \rangle = \frac{\hbar}{2} [l(l+1) - m(m-1)]_{l=3, m=1}^{1/2} = \sqrt{3}\hbar, \end{aligned}$$

so

$$\langle L_x \rangle = \frac{1}{2} (\langle L_+ \rangle + \langle L_- \rangle) = \sqrt{3}\hbar, \quad \langle L_y \rangle = \frac{1}{2i} (\langle L_+ \rangle - \langle L_- \rangle) = 0.$$

However, this result is valid only if the phase shift between the two components of the linear superposition is exactly zero. For an arbitrary phase shift, for example

$$|\alpha\rangle = \frac{1}{\sqrt{2}}(|3,0\rangle + e^{i\varphi}|3,1\rangle), \quad \text{so } \langle \alpha | = \frac{1}{\sqrt{2}}(\langle 3,0 | + e^{-i\varphi} \langle 3,1 |),$$

the result becomes:

$$\langle L_+ \rangle = \sqrt{3}\hbar e^{-i\varphi}, \quad \langle L_- \rangle = \sqrt{3}\hbar e^{i\varphi},$$

so

$$\langle L_x \rangle = \sqrt{3}\hbar \cos \varphi, \quad \langle L_y \rangle = -\sqrt{3}\hbar \sin \varphi$$

– the formulas to be compared with the solutions of Problems 19 and 4.17.

**Problem 5.35.** A particle is in a quantum state  $\alpha$  with the orbital wavefunction proportional to the spherical harmonic  $Y_1^1(\theta, \varphi)$ . Find the angular dependence of the wavefunctions corresponding to the following ket-vectors:

$$(i) \hat{L}_x |\alpha\rangle, \quad (ii) \hat{L}_y |\alpha\rangle, \quad (iii) \hat{L}_z |\alpha\rangle, \quad (iv) \hat{L}_+ \hat{L}_- |\alpha\rangle, \quad \text{and } (v) \hat{L}^2 |\alpha\rangle.$$

*Solution:* According to the discussion of Sec. 5.6, the given ket  $|\alpha\rangle$  is the shared eigenket  $|l, m\rangle$  of the operators  $\hat{L}^2$  and  $\hat{L}_z$ , with  $l = 1$  and  $m = +1$ , i.e.  $|\alpha\rangle \propto |l=1, m=1\rangle \equiv |1, 1\rangle$ . Hence the operators  $\hat{L}^2$  and  $\hat{L}_z$ , acting upon the ket-vector of the state, do not change the angular dependence of its wavefunction, which is proportional to  $\sin\theta \exp\{i\varphi\}$  – see, e.g., the last line of Eq. (3.175) of the lecture notes. The same is true for the ladder operator product  $\hat{L}_+ \hat{L}_-$  because, per Eq. (5.164), its right operand

changes the initial state to  $|1, 0\rangle$  (multiplied by a  $c$ -number coefficient), but the left operand, acting next, returns the ket to its initial form  $|1, 1\rangle$ .

The results of the action of the two remaining operators,  $\hat{L}_x$  and  $\hat{L}_y$ , may be most simply obtained by expressing them via the ladder operators  $\hat{L}_\pm$ . From Eq. (5.153) we readily get

$$\hat{L}_x = \frac{1}{2}(\hat{L}_+ + \hat{L}_-), \quad \hat{L}_y = \frac{1}{2i}(\hat{L}_+ - \hat{L}_-).$$

According to the same Eq. (5.164) (see also Fig. 5.11),

$$\hat{L}_+|1, 1\rangle = 0, \quad \hat{L}_-|1, 1\rangle = \text{const} \times |1, 0\rangle,$$

so the wavefunctions corresponding to  $\hat{L}_x|\alpha\rangle$  and  $\hat{L}_y|\alpha\rangle$  are both proportional to the spherical harmonic with  $l = 1$  and  $m = 0$ , i.e. to  $Y_1^0(\theta, \varphi) \propto \cos\theta$ , albeit with different coefficients.

**Problem 5.36.** A charged spinless 2D particle of mass  $m$  is trapped in the potential well  $U(x, y) = m\omega_0^2(x^2 + y^2)/2$ . Calculate its energy spectrum in the presence of a uniform magnetic field  $\mathcal{B}$  normal to the  $[x, y]$ -plane of the particle's motion

*Solution:* Due to the evident axial symmetry of the problem, it may be most simply solved by the selection of the vector-potential not in the Landau form (3.44), but in the axially symmetric form

$$\mathbf{A} = \frac{1}{2}\mathcal{B} \times \mathbf{p} \equiv \mathbf{n}_\varphi \frac{\mathcal{B}\rho}{2},$$

where  $\mathbf{p} \equiv \{x, y\}$  is the 2D radius vector. (Indeed, using the expression for the curl of a vector in the cylindrical coordinates,<sup>51</sup> it is easy to check that this expression does satisfy the vector-potential's definition,  $\nabla \times \mathbf{A} = \mathcal{B}$ , with  $\mathcal{B} = \mathbf{n}_z \mathcal{B} = \text{const.}$ ) The Cartesian components of this vector are

$$A_x = -\frac{\mathcal{B}}{2}y, \quad A_y = \frac{\mathcal{B}}{2}x,$$

so the 2D form of the Hamiltonian (3.26), with the due replacement  $q\phi \rightarrow U(x, y)$ , is

$$\hat{H} = -\frac{\hbar^2}{2m} \left[ \mathbf{n}_x \left( \frac{\partial}{\partial x} + i \frac{q\mathcal{B}}{2\hbar} y \right) + \mathbf{n}_y \left( \frac{\partial}{\partial y} - i \frac{q\mathcal{B}}{2\hbar} x \right) \right]^2 + \frac{m\omega_0^2}{2}(x^2 + y^2).$$

Squaring the brackets and using the cyclotron frequency definition (3.48) but with a definite sign:  $\omega_c \equiv -q\mathcal{B}/m$  (in order for the vector  $\boldsymbol{\omega}_c = \mathbf{n}_z \omega_c$  to have the correct direction corresponding to that of classical Lorentz force  $\mathbf{F}_L = q\mathbf{v} \times \mathcal{B}$ ), we get

$$\hat{H} = -\frac{\hbar^2}{2m} \left[ \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{m\omega_c}{2\hbar^2} \times i\hbar \left( y \frac{\partial}{\partial x} - x \frac{\partial}{\partial y} \right) \right] + \frac{m\omega^2}{2}(x^2 + y^2),$$

where  $\omega$  is defined as follows:

<sup>51</sup> See, e.g., MA Eq. (10.5).

$$\omega^2 \equiv \omega_0^2 + \frac{1}{4}\omega_c^2. \quad (*)$$

But according to Eq. (5.152) of the lecture notes, the factor following the  $\times$  sign inside the square brackets is just the coordinate representation of the operator  $\hat{L}_z$ , so we may write

$$\hat{H} = \hat{H}_{\text{osc}} + \frac{\omega_c}{2}\hat{L}_z.$$

The first component of this Hamiltonian,

$$\hat{H}_{\text{osc}} \equiv -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + \frac{m\omega^2}{2}(x^2 + y^2) \equiv \frac{1}{2m}(\hat{p}_x^2 + \hat{p}_y^2) + \frac{m\omega^2}{2}(\hat{x}^2 + \hat{y}^2).$$

is just that of an effective 2D (planar) harmonic oscillator, with the frequency re-normalized by the field – see Eq. (\*). Its energy spectrum is given by Eq. (3.124) with  $d = 2$ :

$$E_{\text{osc}} = \hbar\omega(n+1), \quad \text{with } n \equiv n_x + n_y = 0, 1, 2, \dots \quad (**)$$

The second component of the Hamiltonian also has a simple physical sense: in the classical limit, this is just the energy

$$E_{\text{mag}} = \frac{\omega_c}{2}L_z \equiv -\frac{q\mathcal{B}}{2m}L_z = -\mathbf{m} \cdot \mathcal{B}$$

of the classical orbital magnetic moment  $\mathbf{m} = q\mathbf{L}/2m$  in the external field  $\mathcal{B}$ .<sup>52</sup> Using the commutation relations (5.149), it is straightforward to verify that the operator  $\hat{L}_z$  commutes with the operators  $(\hat{p}_x^2 + \hat{p}_y^2)$  and  $(\hat{x}^2 + \hat{y}^2)$ , and hence with the operator  $\hat{H}_{\text{osc}}$ , so these two operators share common eigenfunctions. As we may conclude from Sec. 2.9 (see, e.g., Fig. 2.35), the change of  $n$  is associated with a substantial change of the radial structure of these eigenfunctions. On the other hand, as Eq. (5.152) shows, in this axially-symmetric system, the angular momentum operator cannot change the radial structure, affecting only the angular phase shift of the wavefunctions, and has the eigenvalues  $\hbar m$ , with an integer magnetic quantum number  $m$  – see, e.g., Eqs. (3.129) or (5.158).<sup>53</sup> As a result, the total energy of the system may take the following values:

$$E_{n,m} = \hbar\omega(n+1) + \frac{\hbar\omega_c}{2}m \equiv \hbar\left(\omega_0^2 + \frac{\omega_c^2}{4}\right)^{1/2} (n+1) + \frac{\hbar\omega_c}{2}m. \quad (***)$$

The solid lines in the figure below show the few lowest of these energy levels as functions of the ratio  $\omega_c/2\omega_0$ , i.e. of the normalized magnetic field, with their colors coding the quantum numbers  $n$ : black for  $n = 0$ , red for  $n = 1$ , and blue for  $n = 2$ , while the dashed lines show their high-field trends. The reader should agree that the spectrum evolution is very spectacular, with some energy levels first going down and then up as the field is increased, and levels re-grouping in that process. The spectrum of possible magnetic quantum numbers  $m$  is also nontrivial, with the step between the adjacent values equal to 2 rather than 1.

<sup>52</sup> See, e.g., EM Eq. (5.95).

<sup>53</sup> Note that anticipating the appearance of this magnetic quantum number with its traditional notation  $m$ , I again (just as in the last sections of Chapter 3) used a fancy font to denote the particle's mass  $m$ .

Let us start the interpretation of these results from the field-free limit when the energy spectrum is reduced to the  $n$ -sequence (\*\*). The ground energy level, with  $n = 0$ , corresponds to the only possible combination of the partial quantum numbers,  $n_x = n_y = 0$ , and hence is degenerate. Its eigenfunction is the product of two 1D wavefunctions of the type (2.275):

$$\begin{aligned}\psi_g &= \psi_0(x)\psi_0(y) = \frac{1}{\pi^{1/2}x_0} \exp\left\{-\frac{x^2 + y^2}{2x_0^2}\right\} \\ &\equiv \frac{1}{\pi^{1/2}x_0} \exp\left\{-\frac{\rho^2}{2x_0^2}\right\}.\end{aligned}$$

As the last form of Eq. (5.152) clearly shows, the operator  $\hat{L}_z$  gives zero when acting on such an axially symmetric wavefunction, i.e. it is an eigenfunction of this operator with  $m = 0$ . Hence the action of the magnetic field on the ground state is reduced to the effective frequency re-normalization (\*), gradually increasing its eigenenergy.

The next (first excited) energy level, with  $n = 1$ , corresponds to two different eigenstates, with  $\{n_x = 1, n_y = 0\}$  and  $\{n_x = 0, n_y = 1\}$ , whose eigenfunctions may be represented as the products  $\psi_1(x)\psi_0(y)$  and  $\psi_0(x)\psi_1(y)$ , respectively, where the component wavefunctions are described by Eq. (2.284). As that formula, together with the second of Eqs. (2.282) show, they are proportional to

$$x \exp\left\{-\frac{x^2 + y^2}{2x_0^2}\right\} \equiv \rho \cos \varphi \exp\left\{-\frac{\rho^2}{2x_0^2}\right\} \quad \text{and} \quad y \exp\left\{-\frac{x^2 + y^2}{2x_0^2}\right\} \equiv \rho \sin \varphi \exp\left\{-\frac{\rho^2}{2x_0^2}\right\}.$$

Of these two wavefunctions, we may readily form two linear combinations

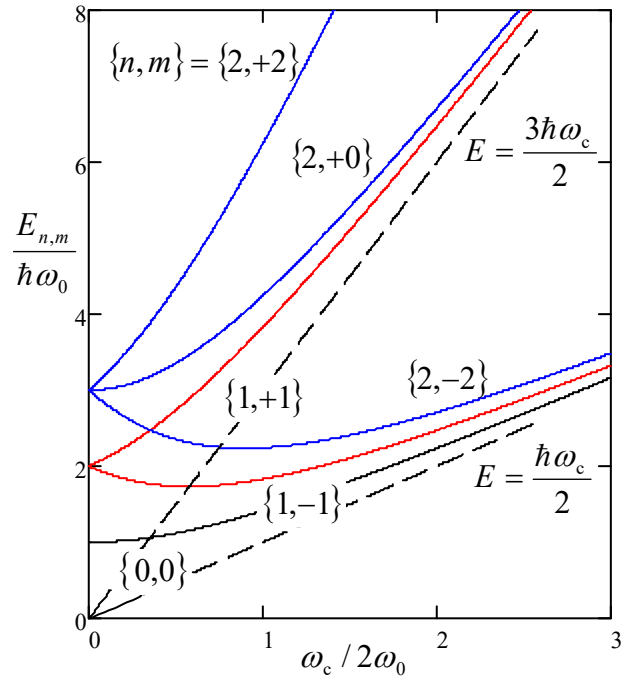
$$\psi_{\pm 1} \propto \rho \exp\left\{-\frac{\rho^2}{2x_0^2}\right\} e^{\pm i\varphi},$$

which are eigenfunctions of  $\hat{L}_z$  with the eigenvalues  $\pm\hbar$  corresponding to  $m = \pm 1$ . As Eq. (\*\*\*) shows, even a low magnetic field lifts this degeneracy, inducing equal and opposite shifts linear in  $\omega_c$ :<sup>54</sup>

$$E_{\text{mag}} = \pm \frac{\hbar\omega_c}{2},$$

so the difference between the adjacent values of  $m$  is indeed 2 rather than 1.

This result ( $\Delta m = 2$ ) persists for higher values of  $n$  as well. For example, in the opposite high-field limit, when  $\omega \rightarrow \omega_c/2$ , Eq. (\*\*\*) tends to Landau's result (3.50):<sup>55</sup>



<sup>54</sup> The linear *decrease* of the eigenenergy  $E_{1,-1}$  with the growing field, described by this formula with the minus sign, competes with its quadratic *increase* due to the frequency renormalization (\*), resulting in the non-monotonic function shown in the figure above.

<sup>55</sup> This result is shown with the dashed straight lines in the figure above.

$$E_N \rightarrow \hbar \omega_c \left| N + \frac{1}{2} \right|, \quad \text{with } N = 0, 1, \dots,$$

with the integer  $N$  equal to  $(n \pm m)/2$ , where the sign before  $m$  is determined by that of the product  $q\mathcal{B}$ . This correspondence means, in particular, that for a fixed  $n$ , the smallest step of the magnetic quantum number  $m$  is 2, in order to keep  $N$  integer.

As a sanity check, in the absence of the magnetic field, the  $n^{\text{th}}$  energy level of the 2D oscillator is  $(n + 1)$ -degenerate, with any of the component quantum numbers  $n_x$  and  $n_y$  taking values  $0, 1, \dots, n$ . The applied magnetic field lifts this degeneracy, so there should be  $g = n + 1$  possible different values of  $m$ . The  $n + 1$  steps, of the size  $\Delta m = 2$  each, make the magnetic quantum number cover the range from  $-n$  to  $+n$  without making  $N$  negative. This zero-centered spectrum of  $m$ , which might be expected for this axially symmetric system, remains the same as in *spherically* symmetric systems – see Eq. (3.162).

**Problem 5.37.** Solve the previous problem for a spinless 3D particle placed (in addition to a uniform magnetic field  $\mathcal{B}$ ) into a spherically-symmetric potential well  $U(\mathbf{r}) = m\omega_0^2 r^2/2$ .

*Solution:* Directing the axis  $z$  along the applied magnetic field, let us select its vector potential just as was done in the (very similar) previous problem,

$$\mathbf{A} = \frac{1}{2} \mathcal{B} \times \boldsymbol{\rho},$$

where  $\boldsymbol{\rho} \equiv \{x, y\}$  is the 2D radius vector. The Cartesian components of this vector are

$$A_x = -\frac{\mathcal{B}}{2} y, \quad A_y = \frac{\mathcal{B}}{2} x,$$

so Eq. (3.27), with the due replacement  $q\phi \rightarrow U(\mathbf{r})$ , takes the form

$$\hat{H} = -\frac{\hbar^2}{2m} \left[ \mathbf{n}_x \left( \frac{\partial}{\partial x} + i \frac{q\mathcal{B}}{\hbar} y \right) + \mathbf{n}_y \left( \frac{\partial}{\partial y} - i \frac{q\mathcal{B}}{\hbar} x \right) + \mathbf{n}_z \frac{\partial}{\partial z} \right]^2 + \frac{m\omega_0^2}{2} (x^2 + y^2 + z^2).$$

Let us represent this Hamiltonian as a sum:

$$\hat{H} = \hat{H}_{x,y} + \hat{H}_z,$$

where  $\hat{H}_{x,y}$  is the Hamiltonian discussed in the solution of the previous problem,

$$\hat{H}_{x,y} = -\frac{\hbar^2}{2m} \left[ \mathbf{n}_x \left( \frac{\partial}{\partial x} + i \frac{q\mathcal{B}}{\hbar} y \right) + \mathbf{n}_y \left( \frac{\partial}{\partial y} - i \frac{q\mathcal{B}}{\hbar} x \right) \right]^2 + \frac{m\omega_0^2}{2} (x^2 + y^2),$$

with the energy spectrum given by Eq. (\*\*\*) of that solution:

$$E_{n,m} = \hbar \left( \omega_0^2 + \frac{\omega_c^2}{4} \right)^{1/2} (n+1) + \frac{\hbar\omega_c}{2} m, \quad \text{where } n = 0, 1, 2, \dots, \text{ and } m = -n, -n+2, \dots, +n,$$

while  $\hat{H}_z$  is the Hamiltonian of a 1D harmonic oscillator:

$$\hat{H}_z = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + \frac{m\omega_0^2}{2} z^2,$$

with eigenenergies  $E_z = \hbar\omega_0(n_z + 1/2)$ , where  $n_z = 0, 1, 2, \dots$ . These two Hamiltonians describe two independent systems defined in different Hilbert spaces, so their eigenvalues (i.e. the system's energy components) just add up. As a result, the full energy spectrum of the system is

$$E = E_{n,m} + E_z = \hbar \left( \omega_0^2 + \frac{\omega_c^2}{4} \right)^{1/2} (n+1) + \frac{\hbar\omega_c}{2} m + \hbar\omega_0 \left( n_z + \frac{1}{2} \right). \quad (*)$$

In the limit of vanishing magnetic field ( $\omega_c \rightarrow 0$ ), this result tends to Eq. (3.124) of the lecture notes, with  $d = 3$ , for an isotropic 3D oscillator

$$E \rightarrow \hbar\omega_0(n+1) + \hbar\omega_0 \left( n_z + \frac{1}{2} \right) \equiv \hbar\omega_0 \left( n' + \frac{3}{2} \right), \quad \text{with } n' \equiv n + n_z = 0, 1, 2, \dots$$

In the opposite limit  $\omega_0 \ll \omega_c$ , the relative smallness of the coefficient  $\hbar\omega_0$  in the last term of Eq. (\*) may be compensated by (possibly, very large) values of the quantum number  $n_z$ , so for energies of the order of  $\hbar\omega_c$ , the result may be approximately represented as the sum,

$$E = \hbar|\omega_c| \left( N + \frac{1}{2} \right) + E_z,$$

of the discrete Landau levels (3.50), with  $N \equiv (n \pm m)/2 \geq 0$ , and a quasi-continuous energy  $E_z$  of the essentially classical harmonic oscillations along the  $z$ -axis.<sup>56</sup>

**Problem 5.38.** Calculate the spectrum of rotational energies of an axially symmetric rigid macroscopic body.

*Solution:* According to classical mechanics,<sup>57</sup> the rotational energy of an axially symmetric rigid body, frequently called the *symmetric top*,<sup>58</sup> is related to the principal-axis components of its angular momentum as

$$E = \frac{L_x^2 + L_y^2}{2I_1} + \frac{L_z^2}{2I_3},$$

where  $I_3$  is the principal moment of inertia for rotation about the axis of symmetry (taken here for the  $z$ -axis), and  $I_1 \equiv I_x = I_y$  is that for rotation about any axis normal to  $z$ . According to the correspondence principle, in quantum mechanics, the rotation may be described by the similar Hamiltonian:

$$\hat{H} = \frac{\hat{L}_x^2 + \hat{L}_y^2}{2I_1} + \frac{\hat{L}_z^2}{2I_3}.$$

According to Eq. (5.150) of the lecture notes, this Hamiltonian may be rewritten as

<sup>56</sup> Note that the last displayed formula also describes the spectrum of a 3D particle moving in a 2D quadratic potential  $U(x, y) = m\omega_0^2(x^2 + y^2)/2$ ; in this case,  $E_z$  is a fully continuous energy  $\hbar^2 k_z^2/2m$  of the free motion in the  $z$ -direction.

<sup>57</sup> See, e.g., CM Sec. 4.2, in particular, Eqs. (4.25)-(4.26).

<sup>58</sup> Note that the set of symmetric tops, with two equal principal moments of inertia, is not limited to the axially-symmetric bodies; for example, any uniform cylinder with an equilateral-triangle base (see, e.g., CM Fig. 4.3) also belongs to this class. As a result, the energy spectrum calculated in this solution is even more general than the problem's assignment specifies.

$$\hat{H} = \frac{\hat{L}^2 - \hat{L}_z^2}{2I_1} + \frac{\hat{L}_z^2}{2I_3} \equiv \frac{\hat{L}^2}{2I_1} + \frac{1}{2} \left( \frac{1}{I_3} - \frac{1}{I_1} \right) \hat{L}_z^2.$$

Since, according to Eq. (5.151), the operator  $\hat{L}^2$  commutes with the operator  $\hat{L}_z$ , and hence with its square, they share the eigenstates described by the ket-vectors  $|l, m\rangle$  that were discussed in Sec. 5.6 of the lecture notes. As a result, we may use the corresponding eigenvalues given by Eqs. (5.158) and (5.163) to immediately write the corresponding eigenvalues of our Hamiltonian, i.e. the energy spectrum of the system:

$$E_{l,m} = \frac{\hbar^2 l(l+1)}{2I_1} + \frac{1}{2} \left( \frac{1}{I_3} - \frac{1}{I_1} \right) \hbar^2 m^2, \quad \text{with } l = 0, 1, 2, \dots; \quad -l \leq m \leq +l.$$

Note that the second term of this expression may be either positive (for bodies stretched along the symmetry axis  $z$ , and hence having with  $I_1 > I_3$  – see CM Eq. (4.24) of the lecture notes), or equal zero (for a particular case of a *spherical top*, with all principal moment of inertia equal), or even negative (at  $I_1 < I_3$ ). However, due to the condition  $-l \leq m \leq +l$ , even in the latter case, all energies  $E_{l,m}$  are still non-negative.

Note also that this calculation implies that the body is “macroscopic” in the sense that its rotation about the  $z$ -axis by any angle different from a  $2\pi$ -multiple leads to a physically distinguishable position. As a result, the above result may be only partially valid for such microscopic objects as axially symmetric (e.g., diatomic) molecules; for their discussion, see Chapter 8.

**Problem 5.39.** Simplify the double commutator  $[\hat{r}_j, [\hat{L}^2, \hat{r}_j]]$ .

*Solution:* Using Eq. (5.150) of the lecture notes, we may write

$$\hat{A}_{jj'} \equiv [\hat{r}_j, [\hat{L}^2, \hat{r}_{j'}]] \equiv \left[ \hat{r}_j, \left[ \sum_{j''=1}^3 \hat{L}_{j''}^2, \hat{r}_{j'} \right] \right] \equiv \sum_{j''=1}^3 [\hat{r}_j, [\hat{L}_{j''}, \hat{L}_{j''}, \hat{r}_{j'}]]. \quad (*)$$

Let us start with spelling out the internal commutator in this expression. The calculations may be shortened a bit using the easily provable operator identity

$$[\hat{B}\hat{C}, \hat{D}] = \hat{B}[\hat{C}, \hat{D}] + [\hat{B}, \hat{D}]\hat{C}. \quad (**)$$

Indeed, taking  $\hat{B} = \hat{C} = \hat{L}_{j''}$  and  $\hat{D} = \hat{r}_{j'}$ , we get

$$[\hat{L}_{j''}, \hat{L}_{j''}, \hat{r}_{j'}] = \hat{L}_{j''}[\hat{L}_{j''}, \hat{r}_{j'}] + [\hat{L}_{j''}, \hat{r}_{j'}]\hat{L}_{j''}.$$

Now by applying Eq. (5.148), in the form

$$[\hat{L}_{j''}, \hat{r}_{j'}] = i\hbar \sum_{j'''=1}^3 \hat{r}_{j'''} \varepsilon_{j''j'''j'''} , \quad (***)$$

to both commutators on the right-hand side, we get

$$[\hat{L}_{j''}, \hat{L}_{j''}, \hat{r}_{j'}] = \hat{L}_{j''} i\hbar \sum_{j'''=1}^3 \hat{r}_{j'''} \varepsilon_{j''j'''j'''} + i\hbar \sum_{j'''=1}^3 \hat{r}_{j'''} \varepsilon_{j''j'''j'''} \hat{L}_{j''} \equiv i\hbar \sum_{j'''=1}^3 \varepsilon_{j''j'''j'''} (\hat{L}_{j''} \hat{r}_{j'''} + \hat{r}_{j'''} \hat{L}_{j''}).$$

With this, the external commutator in Eq. (\*) becomes

$$[\hat{r}_j, [\hat{L}_{j''} \hat{L}_{j'''}, \hat{r}_j]] = i\hbar \sum_{j''=1}^3 \varepsilon_{j''j'''} \left( [\hat{r}_j, \hat{L}_{j''} \hat{r}_{j''}] + [\hat{r}_j, \hat{r}_{j''} \hat{L}_{j''}] \right) \equiv i\hbar \sum_{j''=1}^3 \varepsilon_{j''j'''} \left( [\hat{L}_{j''} \hat{r}_{j''}, \hat{r}_j] + [\hat{r}_{j''} \hat{L}_{j''}, \hat{r}_j] \right).$$

(Note the swap of the indices  $j'$  and  $j'''$  in the Levi-Civita symbol in the last expression, which compensates for the sign reversal due to the swap of operands in both commutators.) Now we may apply the identity (\*\*) again to both commutators on the right-hand side: in the first case, with  $\hat{B} = \hat{L}_{j''}$ ,  $\hat{C} = \hat{r}_{j''}$ , and  $\hat{D} = \hat{r}_j$ , and in the second case, with  $\hat{B} = \hat{r}_{j''}$ ,  $\hat{C} = \hat{L}_{j''}$ , and  $\hat{D} = \hat{r}_j$ . This gives

$$\begin{aligned} [\hat{r}_j, [\hat{L}_{j''} \hat{L}_{j'''}, \hat{r}_j]] &= i\hbar \sum_{j''=1}^3 \varepsilon_{j''j'''} \left( \hat{L}_{j''} [\hat{r}_{j''}, \hat{r}_j] + [\hat{L}_{j''}, \hat{r}_j] \hat{r}_{j''} + \hat{r}_{j''} [\hat{L}_{j''}, \hat{r}_j] + [\hat{r}_{j''}, \hat{r}_j] \hat{L}_{j''} \right) \\ &= i\hbar \sum_{j''=1}^3 \varepsilon_{j''j'''} \left( [\hat{L}_{j''}, \hat{r}_j] \hat{r}_{j''} + \hat{r}_{j''} [\hat{L}_{j''}, \hat{r}_j] \right), \end{aligned}$$

because the Cartesian coordinate operators commute regardless of their indices.

Let us apply to the commutator on the right-hand side of the last expression the basic Eq. (\*\*\*) again, now in the form

$$[\hat{L}_{j''}, \hat{r}_j] = i\hbar \sum_{j'''=1}^3 \hat{r}_{j'''} \varepsilon_{j''j'''}.$$

The result is

$$[\hat{r}_j, [\hat{L}_{j''} \hat{L}_{j'''}, \hat{r}_j]] = i\hbar \sum_{j''=1}^3 \varepsilon_{j''j'''} \left( i\hbar \hat{r}_{j'''} \varepsilon_{j''j'''} \hat{r}_{j''} + \hat{r}_{j''} i\hbar \hat{r}_{j'''} \varepsilon_{j''j'''} \right) \equiv -2\hbar^2 \sum_{j''=1}^3 \varepsilon_{j''j'''} \varepsilon_{j''j'''} \hat{r}_{j''} \hat{r}_{j'''},$$

so the double commutator in question is reduced to

$$\hat{A}_{jj'} = -2\hbar^2 \sum_{j''=1}^3 \varepsilon_{j''j'''} \varepsilon_{j''j'''} \hat{r}_{j''} \hat{r}_{j'''} \quad (****)$$

Generally, the Levi-Civita product sums over a similar index (in our case,  $j''$ ) may be calculated using the so-called “contracted epsilon identity”,<sup>59</sup> but in our simple case, it is easier to use a more pedestrian way.

(i) If  $j' = j$ , then the “productive” values of the indices  $j''$  and  $j'''$  (meaning those giving nonvanishing contributions to the sum) are equal to each other for any  $j''$ , so the Levi-Civita index product in the sum (\*\*\*\*) equals  $(-1)$  in both terms with  $j'' \neq j$ . In the remaining two terms, with  $j'' = j$ , the “productive” common indices can take both values not equal to  $j$  (and hence to  $j'$ ), and the terms cancel. The total result may be conveniently represented as

$$\hat{A}_{jj} = 2\hbar^2 (\hat{r}^2 - \hat{r}_j^2).$$

(ii) If  $j = j' \pm 1$ ,<sup>60</sup> the sum in Eq. (\*\*\*\*) has not two but just one nonvanishing term because the Levi-Civita symbols kill the terms with both  $j'' = j'$  and  $j'' = j = j' \pm 1$ . In the only remaining term of the

<sup>59</sup> See, e.g., MA Eq. (13.3b).



sum,  $j'' = j' \mp 1$ , and hence, by its definition as the complementary one to  $j'$  and  $j''$ , the “productive” value of  $j'''$  is equal to  $j' \pm 1 = j$ , while such value of  $j''''$ , by its definition as the complementary one to  $j$  and  $j''$ , equals  $j'$ . As a result, Eq. (\*\*\*) is reduced to

$$\hat{A}_{jj'} = -2\hbar^2 \varepsilon_{(j\mp 1)(j\pm 1)j'} \varepsilon_{(j\mp 1)(j\pm 1)j'} \hat{r}_j \hat{r}_{j'} = -2\hbar^2 \hat{r}_j \hat{r}_{j'}, \quad \text{for } j \neq j'.$$

These results may be summarized as

$$\hat{A}_{jj'} = 2\hbar^2 (\hat{r}^2 \delta_{jj'} - \hat{r}_j \hat{r}_{j'}).$$

By the way, the reader may have noticed an interesting analogy between this result and the well-known classical expression for the contribution of an elementary mass  $dm$  of a rigid body to its inertia tensor:<sup>61</sup>

$$dI_{jj'} = dm (r^2 \delta_{jj'} - r_j r_{j'}).$$

**Problem 5.40.** Prove the following commutation relation:

$$[\hat{L}^2, [\hat{L}^2, \hat{r}_j]] = 2\hbar^2 (\hat{r}_j \hat{L}^2 + \hat{L}^2 \hat{r}_j).$$

*Solution:* We may start from the following by-product of the model solution of the previous problem (with the number of primes in each  $j$ -index reduced by one, for the notation simplicity):

$$[\hat{L}_{j'}^2, \hat{r}_j] = i\hbar \sum_{j''=1}^3 \varepsilon_{jjj''} (\hat{L}_{j'} \hat{r}_{j''} + \hat{r}_{j''} \hat{L}_{j'}) \equiv -i\hbar \sum_{j''=1}^3 \varepsilon_{jjj''} (\hat{L}_{j'} \hat{r}_{j''} + \hat{r}_{j''} \hat{L}_{j'}).$$

Since the Levi-Civita symbol vanishes if any two of the indices  $j, j'$ , and  $j''$  coincide, we get only two non-zero contributions to the full inner commutator

$$[\hat{L}^2, \hat{r}_j] \equiv \sum_{j'=1}^3 [\hat{L}_{j'}^2, \hat{r}_j] = -i\hbar \sum_{j', j''=1}^3 \varepsilon_{jjj''} (\hat{L}_{j'} \hat{r}_{j''} + \hat{r}_{j''} \hat{L}_{j'}) = -i\hbar \left[ (\hat{L}_{j+1} \hat{r}_{j+2} + \hat{r}_{j+2} \hat{L}_{j+1}) - (\hat{L}_{j+2} \hat{r}_{j+1} + \hat{r}_{j+1} \hat{L}_{j+2}) \right], (*)$$

where the sums  $(j+1)$  and  $(j+2)$  are understood by modulo 3, i.e. the sums  $(3+1)$  and  $(2+2)$  are taken for 1, and  $(3+2)$  for 2. Now using Eq. (5.148) of the lecture notes to write

$$\hat{L}_{j+1} \hat{r}_{j+2} = \hat{r}_{j+2} \hat{L}_{j+1} + i\hbar \hat{r}_j, \quad \text{and} \quad \hat{L}_{j+2} \hat{r}_{j+1} = \hat{r}_{j+1} \hat{L}_{j+2} - i\hbar \hat{r}_j,$$

we may rewrite Eq. (\*) in a shorter form:

$$[\hat{L}^2, \hat{r}_j] = -2i\hbar (\hat{r}_{j+2} \hat{L}_{j+1} - \hat{r}_{j+1} \hat{L}_{j+2} + i\hbar \hat{r}_j). \quad (**)$$

Plugging this expression for the internal commutator into the left-hand side of the identity to be proved, and taking into account that per Eq. (5.151), the operator of  $L^2$  commutes with the operators of all Cartesian components  $L_j$ , we get

<sup>60</sup> If  $j' + 1 = 4$ , such a sum means 1, and if  $j' - 1 = 0$ , the difference means 3. (In math speak, we define the combinations  $j' \pm 1$  “modulo 3”.)

<sup>61</sup> See, e.g., CM Eq. (4.16).

$$[\hat{L}^2, [\hat{L}^2, \hat{r}_j]] = -2i\hbar [\hat{L}^2, (\hat{r}_{j+2}\hat{L}_{j+1} - \hat{r}_{j+1}\hat{L}_{j+2} + i\hbar\hat{r}_j)] = -2i\hbar \{ [\hat{L}^2, \hat{r}_{j+2}] \hat{L}_{j+1} - [\hat{L}^2, \hat{r}_{j+1}] \hat{L}_{j+2} + i\hbar [\hat{L}^2, \hat{r}_j] \}.$$

Now using Eq. (\*\*) again for the first two commutators (with the corresponding replacements of the index  $j$ ), we get

$$\begin{aligned} [\hat{L}^2, [\hat{L}^2, \hat{r}_j]] &= -2i\hbar \{ [-2i\hbar(\hat{r}_{j+1}\hat{L}_j - \hat{r}_j\hat{L}_{j+1} + i\hbar\hat{r}_{j+2})] \hat{L}_{j+1} - [-2i\hbar(\hat{r}_j\hat{L}_{j+2} - \hat{r}_{j+2}\hat{L}_j + i\hbar\hat{r}_{j+1})] \hat{L}_{j+2} + i\hbar [\hat{L}^2, \hat{r}_j] \} \\ &\equiv 4\hbar^2 (-\hat{r}_{j+1}\hat{L}_j\hat{L}_{j+1} + \hat{r}_j\hat{L}_{j+1}\hat{L}_{j+1} - i\hbar\hat{r}_{j+2}\hat{L}_{j+1} + \hat{r}_j\hat{L}_{j+2}\hat{L}_{j+2} - \hat{r}_{j+2}\hat{L}_j\hat{L}_{j+2} + i\hbar\hat{r}_{j+1}\hat{L}_{j+2}) + 2\hbar^2 (\hat{L}^2\hat{r}_j - \hat{r}_j\hat{L}^2). \end{aligned}$$

Adding to and subtracting from the right-hand side of this relation the following expression:

$$4\hbar^2 \hat{r}_j \hat{L}^2 \equiv 4\hbar^2 \hat{r}_j (\hat{L}_j \hat{L}_j + \hat{L}_{j+1} \hat{L}_{j+1} + \hat{L}_{j+2} \hat{L}_{j+2}),$$

we get

$$[\hat{L}^2, [\hat{L}^2, \hat{r}_j]] = 4\hbar^2 [ -(\hat{r}_{j+1}\hat{L}_j + i\hbar\hat{r}_{j+2})\hat{L}_{j+1} - (\hat{r}_{j+2}\hat{L}_j - i\hbar\hat{r}_{j+1})\hat{L}_{j+2} - \hat{r}_j\hat{L}_j\hat{L}_j ] + 2\hbar^2 (\hat{L}^2\hat{r}_j + \hat{r}_j\hat{L}^2).$$

With the commutation relation (5.148) applied to each term in the square brackets,

$$\hat{r}_{j+1}\hat{L}_j + i\hbar\hat{r}_{j+2} = \hat{L}_j\hat{r}_{j+1}, \quad \hat{r}_{j+2}\hat{L}_j - i\hbar\hat{r}_{j+1} = \hat{L}_j\hat{r}_{j+2}, \quad \hat{r}_j\hat{L}_j = \hat{L}_j\hat{r}_j,$$

this expression is reduced to

$$\begin{aligned} [\hat{L}^2, [\hat{L}^2, \hat{r}_j]] &= 4\hbar^2 (-\hat{L}_j\hat{r}_{j+1}\hat{L}_{j+1} - \hat{L}_j\hat{r}_{j+2}\hat{L}_{j+2} - \hat{L}_j\hat{r}_j\hat{L}_j) + 2\hbar^2 (\hat{L}^2\hat{r}_j + \hat{r}_j\hat{L}^2) \\ &\equiv -4\hbar^2 \hat{L}_j (\hat{r}_j\hat{L}_j + \hat{r}_{j+1}\hat{L}_{j+1} + \hat{L}_j\hat{r}_{j+2}\hat{L}_{j+2}) + 2\hbar^2 (\hat{L}^2\hat{r}_j + \hat{r}_j\hat{L}^2). \end{aligned}$$

But according to Eq. (5.147), the sum in the first parentheses equals zero:

$$\hat{r}_j\hat{L}_j + \hat{r}_{j+1}\hat{L}_{j+1} + \hat{r}_{j+2}\hat{L}_{j+2} \equiv \hat{\mathbf{r}} \cdot \hat{\mathbf{L}} \equiv \hat{\mathbf{r}} \cdot (\hat{\mathbf{r}} \times \hat{\mathbf{p}}) = 0,$$

so we indeed get

$$[\hat{L}^2, [\hat{L}^2, \hat{r}_j]] \equiv 2\hbar^2 (\hat{L}^2\hat{r}_j + \hat{r}_j\hat{L}^2).$$

**Problem 5.41.** Use the commutation relation proved in the previous problem and Eq. (5.148) of the lecture notes to prove the orbital electric-dipole transition selection rules mentioned in Sec. 5.6.

*Solution:* First, let us calculate the matrix elements of both sides of the identity proved in the previous problem,

$$[\hat{L}^2, [\hat{L}^2, \hat{r}_j]] = 2\hbar^2 (\hat{r}_j\hat{L}^2 + \hat{L}^2\hat{r}_j), \quad (*)$$

in the basis of the  $\{l, m\}$  states discussed in Sec. 5.6 of the lecture notes, i.e. the common eigenstates of the operators  $\hat{L}^2$  and  $\hat{L}_z$ . For the left-hand side, we get

$$\langle l, m | [\hat{L}^2, [\hat{L}^2, \hat{r}_j]] | l', m' \rangle \equiv \langle l, m | \hat{L}^2 [\hat{L}^2, \hat{r}_j] | l', m' \rangle - \langle l, m | [\hat{L}^2, \hat{r}_j] \hat{L}^2 | l', m' \rangle.$$

According to Eq. (5.163) of the lecture notes, the action of the rightmost operator  $\hat{L}^2$  on the rightmost ket-vector gives the same ket but multiplied by  $\hbar^2 l'(l' + 1)$ , while the action of the similar (Hermitian!) operator in the leftmost position on the leftmost bra-vector gives the same vector but multiplied by  $\hbar^2 l(l + 1)$ . As a result, we may continue as follows:

$$\begin{aligned}\langle l, m | [\hat{L}^2, [\hat{L}^2, \hat{r}_j]] | l', m' \rangle &= \hbar^2 [l(l+1) - l'(l'+1)] \langle l, m | [\hat{L}^2, \hat{r}_j] | l', m' \rangle \\ &\equiv \hbar^2 [l(l+1) - l'(l'+1)] \langle l, m | (\hat{L}^2 \hat{r}_j - \hat{r}_j \hat{L}^2) | l', m' \rangle.\end{aligned}$$

Now a similar simplification of the last bracket gives

$$\langle l, m | [\hat{L}^2, [\hat{L}^2, \hat{r}_j]] | l', m' \rangle = \hbar^4 [l(l+1) - l'(l'+1)]^2 \langle l, m | \hat{r}_j | l', m' \rangle.$$

The matrix elements of the right-hand side of Eq. (\*) may be calculated in a similar way:

$$\begin{aligned}\langle l, m | 2\hbar^2 (\hat{r}_j \hat{L}^2 + \hat{L}^2 \hat{r}_j) | l', m' \rangle &\equiv 2\hbar^2 [\langle l, m | \hat{r}_j \hat{L}^2 | l', m' \rangle + \langle l, m | \hat{L}^2 \hat{r}_j | l', m' \rangle] \\ &= 2\hbar^4 \langle l, m | \hat{r}_j | l', m' \rangle [l'(l'+1) + l(l+1)].\end{aligned}$$

Due to the identity (\*), these matrix elements have to be equal, giving the result

$$\langle l, m | \hat{r}_j | l', m' \rangle f(l, l') = 0, \quad \text{where } f(l, l') \equiv [l(l+1) - l'(l'+1)]^2 - 2[l'(l'+1) + l(l+1)].$$

This means that the matrix element of the  $j^{\text{th}}$  Cartesian coordinate has to vanish unless the function  $f(l, l')$  equals zero. Rewriting this function as

$$f(l, l') \equiv [(l+l'+1)(l-l')]^2 - [(l+l'+1)^2 + (l'-l)^2 - 1] \equiv [(l+l'+1)^2 - 1][(l-l')^2 - 1],$$

and taking into account that  $l$  and  $l'$  cannot be negative, we see that  $f(l, l')$  equals zero only if either  $l = l' = 0$  (when the first square bracket of the last expression vanishes), or if  $(l-l')^2 = 1$ , i.e. if

$$l' = l \pm 1.$$

Since, according to Eq. (3.174), the angular wavefunction of the state with  $l = 0$  (and hence  $m = 0$ ) is a constant, the matrix elements

$$\langle l = 0, m = 0 | \hat{r}_j | l = 0, m = 0 \rangle \propto \oint \hat{r}_j d\Omega,$$

corresponding to the first case ( $l = l' = 0$ ), vanish due to symmetry, the above equality  $l' = l \pm 1$  gives the necessary condition to have at least some matrix element(s)  $\langle l, m | \hat{r}_j | l', m' \rangle$  different from zero.

In order to get the second necessary condition, let us calculate the similar matrix elements of both parts of Eq. (5.148), written for the operator of  $L_3 \equiv L_z$ ,

$$[\hat{L}_3, \hat{r}_j] = i\hbar \sum_{j'=1}^3 \hat{r}_{j'} \varepsilon_{3jj'}. \quad (**)$$

For the left-hand side, we may write

$$\langle l, m | [\hat{L}_3, \hat{r}_j] | l', m' \rangle \equiv \langle l, m | \hat{L}_3 \hat{r}_j | l', m' \rangle - \langle l, m | \hat{r}_j \hat{L}_3 | l', m' \rangle.$$

Per Eq. (5.158), the action of the rightmost operator  $\hat{L}_3 \equiv \hat{L}_z$  on the right ket-vector gives the same vector but multiplied by  $\hbar m'$ , while the action of the similar (Hermitian!) operator in the leftmost position on the ket-vector gives the same vector but multiplied by  $\hbar m$ , so

$$\langle l, m | [\hat{L}_3, \hat{r}_j] | l', m' \rangle \equiv \hbar(m - m') \langle l, m | \hat{r}_j | l', m' \rangle. \quad (***)$$

The similar matrix element of the right-hand side of Eq. (\*\*) is just

$$\langle l, m | i\hbar \sum_{j'=1}^3 \hat{r}_{j'} \varepsilon_{3jj'} | l', m' \rangle \equiv i\hbar \sum_{j'=1}^3 \varepsilon_{3jj'} \langle l, m | \hat{r}_{j'} | l', m' \rangle,$$

so according to Eq. (\*\*),

$$(m - m') \langle l, m | \hat{r}_j | l', m' \rangle = i \sum_{j'=1}^3 \varepsilon_{3jj'} \langle l, m | \hat{r}_{j'} | l', m' \rangle. \quad (****)$$

First, let us consider the case when the index  $j$  is not equal to 3. In this case, the sum on the right-hand side has only one nonzero term:

$$(m - m') \langle l, m | \hat{r}_j | l', m' \rangle = i \varepsilon_{3jj'} \langle l, m | \hat{r}_{j'} | l', m' \rangle, \quad \text{for } j' \neq j, 3.$$

Multiplying this equation by a similar one but written for the complementary index:

$$(m - m') \langle l, m | \hat{r}_{j'} | l', m' \rangle = i \varepsilon_{3jj'} \langle l, m | \hat{r}_j | l', m' \rangle, \quad \text{for } j \neq j', 3,$$

and taking into account that by the Levi-Civita symbol's definition,  $\varepsilon_{3jj'} \varepsilon_{3j'j} = -1$ , we get

$$\left[ (m - m')^2 - 1 \right] \langle l, m | \hat{r}_j | l', m' \rangle \langle l, m | \hat{r}_{j'} | l', m' \rangle = 0.$$

From here, the second necessary condition to have at least some matrix element(s)  $\langle l, m | \hat{r}_j | l', m' \rangle$  with  $j \neq 3$ , different from zero is  $(m - m')^2 = 1$ , i.e.

$$m' = m \pm 1.$$

Finally, let us consider the case  $j = 3$ . In this case, the commutator (\*\*) equals zero, so Eq. (\*\*\*) yields

$$(m - m') \langle l, m | \hat{r}_3 | l', m' \rangle = 0.$$

From here, we may conclude that this particular matrix element may be different from zero only if

$$m = m',$$

thus completing the proof of the selection rules formulated in Sec. 5.6.

As will be discussed in Sec. 9.3, these rules, applied to the emission/absorption of electric-dipole radiation coupled to the orbital motion of a quantum system, express the conservation of the total angular momentum of the system, including that of the emitted/absorbed photon.

Note that these selection rules may be also obtained in a purely wave-mechanical way by using the following recurrence relations for the spherical harmonics (which are given here just for the reader's reference):

$$\begin{aligned}\cos\theta Y_l^m(\theta, \varphi) &= \left[ \frac{(l+1+m)(l+1-m)}{(2l+1)(2l+3)} \right]^{1/2} Y_{l+1}^m(\theta, \varphi) + \left[ \frac{(l+m)(l-m)}{(2l+1)(2l-1)} \right]^{1/2} Y_{l-1}^m(\theta, \varphi), \\ \sin\theta Y_l^m(\theta, \varphi) &= \left\{ - \left[ \frac{(l+1-m)(l+2-m)}{(2l+1)(2l+3)} \right]^{1/2} Y_{l+1}^{m-1}(\theta, \varphi) + \left[ \frac{(l+m)(l-1+m)}{(2l+1)(2l-1)} \right]^{1/2} Y_{l-1}^{m+1}(\theta, \varphi) \right\} e^{i\varphi}.\end{aligned}$$

**Problem 5.42.** Express the commutators listed in Eq. (5.179) of the lecture notes,  $[\hat{J}^2, \hat{L}_z]$  and  $[\hat{J}^2, \hat{S}_z]$ , via  $\hat{L}_j$  and  $\hat{S}_j$ .

*Solution:* By using Eq. (5.181) and then the second of Eqs. (5.176), we may transform the first commutator as

$$[\hat{J}^2, \hat{L}_z] = [\hat{L}^2 + \hat{S}^2 + 2\hat{\mathbf{L}} \cdot \hat{\mathbf{S}}, \hat{L}_z] = 2[\hat{\mathbf{L}} \cdot \hat{\mathbf{S}}, \hat{L}_z] \equiv 2[\hat{L}_x \hat{S}_x + \hat{L}_y \hat{S}_y + \hat{L}_z \hat{S}_z, \hat{L}_z] = 2\hat{S}_x [\hat{L}_x, \hat{L}_z] + 2\hat{S}_y [\hat{L}_y, \hat{L}_z].$$

Now using the first of Eqs. (5.176), we get

$$[\hat{J}^2, \hat{L}_z] = 2i\hbar(-\hat{S}_x \hat{L}_y + \hat{S}_y \hat{L}_x).$$

Acting absolutely similarly, we can obtain

$$[\hat{J}^2, \hat{S}_z] = 2i\hbar(\hat{S}_x \hat{L}_y - \hat{S}_y \hat{L}_x).$$

We see that indeed, neither of these commutators vanishes – though their sum, equal to  $[\hat{J}^2, \hat{J}_z]$ , does.

**Problem 5.43.** Find the operator  $\hat{\mathcal{T}}_\phi$  describing a quantum state's rotation by angle  $\phi$  about a certain axis, by using the similarity of this operation with the shift of a Cartesian coordinate, discussed in Sec. 5.5 of the lecture notes. Then use this operator to calculate the probabilities of measurements of spin- $1/2$  components of particles with  $z$ -polarized spin, by a Stern-Gerlach instrument turned by angle  $\theta$  within the  $[z, x]$  plane, where  $y$  is the axis of particle propagation – see Fig. 4.1.<sup>62</sup>

*Solution:* In the course of our discussion of the Glauber states in Sec. 5.5, we proved that the operator defined by Eq. (5.111),

$$\hat{\mathcal{T}}_x = \exp\left\{-i \frac{\hat{p}_x}{\hbar} X\right\},$$

provides the wavefunction's translation by the distance  $X$  along the  $x$ -axis. From Sec. 5.6, we know that at a planar rotation about the  $z$ -axis, the product  $L_z \varphi$  plays the same role as the product  $p_x x$  at the linear motion along axis  $x$ . Hence, the operator

<sup>62</sup> Note that the last task is just a particular case of Problem 4.18 (see also Problem 1).

$$\hat{\tau}_\varphi = \exp\left\{-i\frac{\hat{L}_z}{\hbar}\varphi\right\}$$

rotates any orbital wavefunction by the angle  $\varphi$  about the  $z$ -axis. It is straightforward to generalize this relation to the rotation by angle  $\phi$  about an arbitrary axis with the unit vector  $\mathbf{n}$ :

$$\hat{\tau}_\phi = \exp\left\{-i\frac{\hat{\mathbf{L}} \cdot \mathbf{n}}{\hbar}\phi\right\}.$$

Since all the commutation properties of the spin operator  $\hat{\mathbf{S}}$  are identical to those of  $\hat{\mathbf{L}}$  (see Sec. 5.7), the spin rotation should be described by a similar operator:

$$\hat{\tau}_\phi = \exp\left\{-i\frac{\hat{\mathbf{S}} \cdot \mathbf{n}}{\hbar}\phi\right\}$$

so for spin- $1/2$  particles, with  $\hat{\mathbf{S}} = (\hbar/2)\hat{\boldsymbol{\sigma}}$ ,

$$\hat{\tau}_\phi = \exp\left\{-i\hat{\boldsymbol{\sigma}} \cdot \mathbf{n} \frac{\phi}{2}\right\}.$$

The last relation may be recast into a simpler form by the expansion of the exponent into the Taylor series, separating the odd- and even-numbered terms:

$$\hat{\tau}_\phi = \exp\left\{-i\hat{\boldsymbol{\sigma}} \cdot \mathbf{n} \frac{\phi}{2}\right\} = \sum_{k=2m} \frac{1}{k!} \left(-i\hat{\boldsymbol{\sigma}} \cdot \mathbf{n} \frac{\phi}{2}\right)^{2m} - i\hat{\boldsymbol{\sigma}} \cdot \mathbf{n} \frac{\phi}{2} \sum_{k=2m+1} \frac{1}{k!} \left(-i\hat{\boldsymbol{\sigma}} \cdot \mathbf{n} \frac{\phi}{2}\right)^{2m}.$$

Since, as we know from Chapter 4,

$$(\hat{\boldsymbol{\sigma}} \cdot \mathbf{n})^2 = (\hat{\sigma}_x n_x)^2 + (\hat{\sigma}_x n_y)^2 + (\hat{\sigma}_x n_z)^2 = (n_x^2 + n_y^2 + n_z^2)\hat{I} = \hat{I},$$

we may write

$$(\hat{\boldsymbol{\sigma}} \cdot \mathbf{n})^{2m} = \hat{I}, \quad \text{so} \quad \hat{\tau}_\phi = \hat{I} \sum_{k=2m} \frac{1}{k!} (-1)^m \left(\frac{\phi}{2}\right)^k - i\hat{\boldsymbol{\sigma}} \cdot \mathbf{n} \sum_{k=2m+1} \frac{1}{k!} (-1)^m \left(\frac{\phi}{2}\right)^k.$$

But these sums are just the Taylor expansions of the functions  $\cos(\phi/2)$  and  $\sin(\phi/2)$ , respectively, so

$$\hat{\tau}_\phi = \hat{I} \cos \frac{\phi}{2} - i\hat{\boldsymbol{\sigma}} \cdot \mathbf{n} \sin \frac{\phi}{2}.$$

If the unit vector  $\mathbf{n}$  of rotation is directed along the particle's propagation axis (in our particular case, the  $y$ -axis), then  $\hat{\boldsymbol{\sigma}} \cdot \mathbf{n} = \hat{\sigma}_y$ , and the operator's matrix in the  $z$ -basis becomes very simple:

$$T_\phi = \begin{pmatrix} \cos(\phi/2) & -\sin(\phi/2) \\ \sin(\phi/2) & \cos(\phi/2) \end{pmatrix},$$

where  $\phi$  is now the angle between the final direction of the state's rotation and its initial direction. If the latter direction is the  $z$ -axis, then  $\phi$  is just the polar angle  $\theta$  of the final direction. The rotation of a Stern-Gerlach instrument from the  $z$ -direction by an angle  $\theta$  is evidently equivalent to the spin's rotation by an equal but opposite angle. Hence the probabilities of the two outcomes of the SG measurements of the  $z$ -polarized spin beam are

$$W(\theta_{\uparrow}) = |(T_{-\theta})_{11}|^2 = \cos^2 \frac{\theta}{2}, \quad W(\theta_{\downarrow}) = |(T_{-\theta})_{21}|^2 = \sin^2 \frac{\theta}{2},$$

– the same result as was obtained earlier in the solutions of Problems 1 and 4.18.

**Problem 5.44.** The rotation operator  $\hat{\tau}_{\phi}$  analyzed in the previous problem and the linear translation operator  $\hat{\tau}_X$  discussed in Sec. 5.5 of the lecture notes have a similar structure:

$$\hat{\tau}_{\lambda} = \exp \left\{ -i \frac{\hat{C}\lambda}{\hbar} \right\},$$

where  $\lambda$  is a real  $c$ -number scaling the translation and  $\hat{C}$  is a Hermitian operator that does not explicitly depend on time.

(i) Prove that such operators are unitary.

(ii) Prove that if the shift by  $\lambda$ , induced by the operator  $\hat{\tau}_{\lambda}$ , leaves the Hamiltonian of some system unchanged for any  $\lambda$ , then  $\langle C \rangle$  is a constant of motion for any initial state of the system.

(iii) Discuss what the last conclusion means for the particular operators  $\hat{\tau}_X$  and  $\hat{\tau}_{\phi}$ .

*Solutions:*

(i) As was repeatedly discussed in the lecture notes, the exponent of an operator is defined by its Taylor expansion. In our current case, such expansion is

$$\hat{\tau}_{\lambda} \equiv \exp \left\{ -i \frac{\hat{C}\lambda}{\hbar} \right\} = \sum_{k=0}^{\infty} \frac{1}{k!} \left( -i \frac{\hat{C}\lambda}{\hbar} \right)^k \equiv \sum_{k=0}^{\infty} \frac{1}{k!} (-i)^k \left( \frac{\lambda}{\hbar} \right)^k \hat{C}^k.$$

The Hermitian conjugate of this expression is

$$\hat{\tau}_{\lambda}^{\dagger} \equiv \sum_{k=0}^{\infty} \frac{1}{k!} [(-i)^k]^* \left[ \left( \frac{\lambda}{\hbar} \right)^k \right]^* (\hat{C}^k)^{\dagger} = \sum_{k=0}^{\infty} \frac{1}{k!} i^k \left( \frac{\lambda}{\hbar} \right)^k \hat{C}^k, \quad (*)$$

because the Hermitian conjugation of a  $c$ -number is reduced to its complex conjugation, the ratio  $\lambda/\hbar$  is real, and since the operator  $\hat{C}$  is Hermitian, i.e.  $\hat{C}^{\dagger} = \hat{C}$ , so are all operators  $\hat{C}^k$ , with  $k = 0, 1, 2, \dots$  (Indeed, by applying the relation

$$(\hat{A}\hat{B})^{\dagger} = \hat{B}^{\dagger}\hat{A}^{\dagger},$$

whose proof was the subject of Problem 4.1(iii), to the operators  $\hat{A} \equiv \hat{C}^{k-1}$  and  $\hat{B} \equiv \hat{C}$ , we get

$$(\hat{C}^k)^{\dagger} \equiv (\hat{C}^{k-1}\hat{C})^{\dagger} = \hat{C}^{\dagger}(\hat{C}^{k-1})^{\dagger} = \hat{C}(\hat{C}^{k-1})^{\dagger}.$$

Repeating this operation  $(k-1)$  more times, we get  $(\hat{C}^k)^{\dagger} = \hat{C}^k$ .

Now returning to Eq. (\*), we may see that its last form is just the Taylor expansion of the following operator:

$$\exp\left\{+i\frac{\hat{C}\lambda}{\hbar}\right\} = \sum_{k=1}^{\infty} \frac{1}{k!} \left(i\frac{\hat{C}\lambda}{\hbar}\right)^k \equiv \sum_{k=1}^{\infty} \frac{1}{k!} i^k \left(\frac{\lambda}{\hbar}\right)^k \hat{C}^k.$$

Thus we have proved that

$$\hat{\tau}^\dagger = \exp\left\{+i\frac{\hat{C}\lambda}{\hbar}\right\}, \quad \text{i.e. that } \exp\left\{+i\frac{\hat{C}\lambda}{\hbar}\right\} = \left(\exp\left\{-i\frac{\hat{C}\lambda}{\hbar}\right\}\right)^\dagger.$$

Let us apply to these two operators the general Eq. (5.117) of the lecture notes, with  $\hat{A} \equiv i\hat{C}\lambda/\hbar$  and  $\hat{B} \equiv \hat{I}$ . Since the identity operator commutes with any other operator, Eq. (5.116) is valid with  $\mu = 0$ , so Eq. (5.117) becomes

$$\exp\left\{+i\frac{\hat{C}\lambda}{\hbar}\right\} \exp\left\{-i\frac{\hat{C}\lambda}{\hbar}\right\} = \hat{I}, \quad \text{i.e. } \hat{\tau}_\lambda^\dagger \hat{\tau}_\lambda = \hat{I},$$

i.e. the translation operator  $\hat{\tau}_\lambda$  is indeed unitary.

(ii) Let us spell out the commutator  $[\hat{H}, \hat{\tau}_\lambda]$ , using the Taylor expansion of the latter operator:

$$[\hat{H}, \hat{\tau}_\lambda] = \left[\hat{H}, \exp\left\{-i\frac{\hat{C}\lambda}{\hbar}\right\}\right] = \left[\hat{H}, \sum_{k=1}^{\infty} \frac{1}{k!} \left(-i\frac{\hat{C}\lambda}{\hbar}\right)^k\right] \equiv \sum_{k=1}^{\infty} \alpha_k \lambda^k, \quad (**)$$

where

$$\alpha_k \equiv \frac{1}{k!} \left(-i\frac{1}{\hbar}\right)^k [\hat{H}, \hat{C}^k].$$

According to Eq. (4.93) of the lecture notes, a Hamiltonian's invariance under a unitary transform may be expressed as

$$\hat{U}^\dagger \hat{H} \hat{U} = \hat{H}.$$

Acting by the operator  $\hat{U}$  on both sides of this relation, and taking into account that  $\hat{U}\hat{U}^\dagger \hat{H} \equiv \hat{H} \hat{U} \equiv \hat{H}$ , we see that this relation is equivalent to

$$\hat{H}\hat{U} = \hat{U}\hat{H}, \quad \text{i.e. } [\hat{H}, \hat{U}] = 0.$$

Since we have proved that the operator  $\hat{\tau}_\lambda$  is unitary, the commutator  $[\hat{H}, \hat{\tau}_\lambda]$  equals zero (i.e. is a null operator) for any value of the parameter  $\lambda$ . But according to Eq. (\*\*), this is only possible when each coefficient  $\alpha_k$  in the Taylor expansion of this expression equals zero, including  $\alpha_1$ . This requirement gives

$$[\hat{H}, \hat{C}] = 0. \quad (***)$$

Since, by the problem's conditions, the operator  $\hat{C}$  does not depend on time explicitly,  $\partial\hat{C}/\partial t = 0$ , we may use the key Eq. (4.199) of the lecture notes, together with Eq. (\*\*\*), to calculate its full time derivative in the Heisenberg picture of quantum dynamics:

$$i\hbar \frac{d\hat{C}}{dt} = [\hat{C}, \hat{H}] = 0.$$



According to the basic relation of the Heisenberg picture, Eq. (4.191), this means that  $\langle C \rangle$  does not depend on time, for any initial state of the system.

(iii) For the linear translation operator  $\hat{\tau}_x$  defined by Eq. (5.111),

$$\hat{\tau}_x \equiv \exp\left\{-i\frac{\hat{p}X}{\hbar}\right\},$$

the observable  $C$  is the linear momentum  $p$  (or rather its Cartesian component in the shift's direction  $x$ ). Hence, the invariance of the Hamiltonian of a system with respect to such a shift means the conservation of  $\langle p \rangle$  during an arbitrary motion of the system – the result well-known in classical mechanics (where we speak about the invariance of the Hamiltonian function rather than the operator). Similarly, if the rotations of a system about some axis  $\mathbf{n}$ , by an arbitrary angle  $\phi$ , described by the operators

$$\hat{\tau}_\phi \equiv \exp\left\{-i\frac{\hat{\mathbf{L}} \cdot \mathbf{n}}{\hbar}\phi\right\} \quad \text{and/or} \quad \hat{\tau}_\phi \equiv \exp\left\{-i\frac{\hat{\mathbf{S}} \cdot \mathbf{n}}{\hbar}\phi\right\}$$

do not alter the Hamiltonian of a system (in particular, this is valid for any system symmetric with respect to rotation about the axis  $\mathbf{n}$ ), then the expectation values of the components of the orbital/spin angular momenta along axis  $\mathbf{n}$  are conserved. For the orbital momentum vector  $\mathbf{L}$ , this conclusion is also well known in classical mechanics (see, e.g., CM Sec. 1.4), and it is only natural that the same fact holds for the spin vector  $\mathbf{S}$ , because its operator is defined by similar commutation relations – cf. Eqs. (5.168) and (5.176).

**Problem 5.45.** A particle with spin  $s$  is in a state with definite quantum numbers  $l$  and  $j$ . Prove that the observable  $\mathbf{L} \cdot \mathbf{S}$  also has a definite value and calculate it.

*Solution:* According to Eq. (5.177) of the lecture notes, in any state with a definite value of  $l$ , the variable  $L^2$  has a definite value equal to

$$L^2 = \hbar^2 l(l+1).$$

(This is true even if the state does not have a definite value of  $m_l$ ,<sup>63</sup> because such a state may be always represented as a linear superposition of states with different  $m_l$  but the same  $l$ .)

Similarly (and because the spin  $s$  of a particle is always fixed), Eqs. (5.169) and (5.175) show that for the specified state, the observables  $J^2$  and  $S^2$  also have definite values, respectively:

$$J^2 = \hbar^2 j(j+1), \quad \text{and} \quad S^2 = \hbar^2 s(s+1).$$

Hence, according to Eq. (5.181) of the lecture notes,

$$2\hat{\mathbf{L}} \cdot \hat{\mathbf{S}} = (\hat{J}^2 - \hat{L}^2 - \hat{S}^2),$$

in our state, the scalar product  $\mathbf{L} \cdot \mathbf{S}$  also has a definite value:

<sup>63</sup> As it is the case, for example, for the base states  $\{j, m_j\}$  of the coupled representation – see, e.g., Fig. 5.12 and Eq. (5.183).

$$\mathbf{L} \cdot \mathbf{S} = \frac{\hbar^2}{2} [j(j+1) - l(l+1) - s(s+1)].$$

**Problem 5.46.** For a spin- $\frac{1}{2}$  particle in a state with definite quantum numbers  $l$ ,  $m_l$ , and  $m_s$ , calculate the expectation value of the observable  $J^2$  and the probabilities of all its possible values. Interpret your results in terms of the Clebsch-Gordan coefficients (5.190).

*Solution:* Averaging the first form of Eq. (5.181) of the lecture notes, we may write

$$\langle J^2 \rangle = \langle L^2 \rangle + \langle S^2 \rangle + 2\langle \mathbf{L} \cdot \mathbf{S} \rangle \equiv \langle L^2 \rangle + \langle S^2 \rangle + 2\langle L_x S_x \rangle + 2\langle L_y S_y \rangle + 2\langle L_z S_z \rangle.$$

According to the second of Eqs. (5.177), a state with a definite quantum number  $l$  is an eigenstate of the operator  $\hat{L}^2$ , so the first term on the right-hand side of the last expression is equal to the corresponding eigenvalue,  $\hbar^2 l(l+1)$ . Since the spin quantum number  $s$  of a particle is always definite (fixed), Eq. (5.169) allows us to make a similar conclusion about the second term:  $\langle S^2 \rangle = \hbar^2 s(s+1) = \hbar^2 \cdot \frac{1}{2} \cdot (\frac{1}{2} + 1) = (3/4) \hbar^2$ .

Next, the fact that not only the squares of the vectors  $\mathbf{L}$  and  $\mathbf{S}$  but also their  $z$ -components,  $L_z = \hbar m_l$  and  $S_z = \hbar m_s$ , have definite values in the given quantum state means that these vectors are uncoupled,<sup>64</sup> so we may write  $\langle L_x S_x \rangle = \langle L_x \rangle \langle S_x \rangle$ , etc., where the first averaging is over the Hilbert space of the orbital states, while the second one is over that of the spin states. But as we know from Sec. 4.5 of the lecture notes (see, e.g., Eq. (4.134), which is valid, in the nomenclature of Sec. 4.7, for  $m_s = +\frac{1}{2}$ ), in a state with a definite  $m_s$ , the averages  $\langle S_x \rangle$  and  $\langle S_y \rangle$  equal zero, so the only nonvanishing product of the component averages is  $\langle L_z \rangle \langle S_z \rangle = (\hbar m_l)(\hbar m_s)$ . Thus, we get

$$\langle J^2 \rangle = \hbar^2 \left[ l(l+1) + \frac{3}{4} + 2m_l m_s \right]. \quad (*)$$

Now, according to Eq. (5.189) of the lecture notes, in the quantum-statistical ensemble with a definite  $l$  (and  $s = \frac{1}{2}$ ), the quantum number  $j$ , and hence the variable  $J^2 = \hbar^2 j(j+1)$ , may take only two values each:

$$j_{\pm} = l \pm \frac{1}{2}, \quad J_{\pm}^2 = \hbar^2 j_{\pm}(j_{\pm} + 1) = \hbar^2 \left( l \pm \frac{1}{2} \right) \left( l + 1 \pm \frac{1}{2} \right) \equiv \hbar^2 \left[ l(l+1) + \frac{1}{4} \pm \frac{2l+1}{2} \right]. \quad (**)$$

Hence there are only two nonvanishing probabilities,  $W_+$  and  $W_- = 1 - W_+$ , to calculate, and the general Eq. (1.37) takes the form

$$\langle J^2 \rangle = W_+ J_+^2 + W_- J_-^2 = W_+ J_+^2 + (1 - W_+) J_-^2 \equiv J_-^2 + W_+ (J_+^2 - J_-^2),$$

so

$$W_+ = \frac{\langle J^2 \rangle - J_-^2}{J_+^2 - J_-^2}, \quad \text{and} \quad W_- = 1 - W_+ = \frac{\langle J^2 \rangle - J_+^2}{J_-^2 - J_+^2}.$$

Plugging into these expressions the relations (\*) and (\*\*), we get

<sup>64</sup> More strictly, in the terms of Sec. 5.7 of the lecture notes, such a state is a member of the uncoupled-representation basis – see, e.g., Fig. 5.12 and the first line of Eq. (5.182).

$$W_+ = \frac{l+1+2m_l m_s}{2l+1}, \quad W_- = \frac{l-2m_l m_s}{2l+1}, \quad \text{i.e. } W_{\pm} = \frac{l+\frac{1}{2} \pm \frac{1}{2} \pm 2m_l m_s}{2l+1}.$$

Finally, note that using the relation proved in Sec. 5.7,  $m_l = m_j - m_s$ , and the fact that for spin- $\frac{1}{2}$  particles,  $(m_s)^2 = (\pm\frac{1}{2})^2 = \frac{1}{4}$ , we may recast the last formula in the form

$$W_{\pm} = \frac{l \pm 2m_j m_s + \frac{1}{2}}{2l+1} \equiv \frac{1}{2l+1} \times \begin{cases} l \pm m_j + \frac{1}{2}, & \text{for } m_s = +\frac{1}{2}, \\ l \mp m_j + \frac{1}{2}, & \text{for } m_s = -\frac{1}{2}. \end{cases}$$

Comparing this formula with Eqs. (5.190), we see that  $W_{\pm}$  are just the squared moduli of the Clebsch-Gordan coefficients – as they should be. So, if we need only the moduli of these coefficients (as we do for most applications), this solution presents a simple alternative way to calculate them.

**Problem 5.47.** Derive general recurrence relations for the Clebsch-Gordan coefficients for a particle with spin  $s$ .

*Hint:* By using the similarity of the commutation relations discussed in Sec. 5.7, write the relations similar to Eqs. (5.164) of the lecture notes, for other components of the angular momentum, and then apply them to Eq. (5.170).

*Solution:* The definition (5.170) of the total momentum means that the ladder operators of its components, defined similarly to Eq. (5.153), are related simply as

$$\hat{J}_{\pm} = \hat{L}_{\pm} + \hat{S}_{\pm}.$$

Let us act by these operators on the corresponding sides of Eq. (5.183), keeping in mind that the brackets  $\langle m_l, m_s | j, m_j \rangle$  in that relation are just the  $c$ -numbers (the Clebsch-Gordan coefficients) and hence are not affected by the operator action:

$$\hat{J}_{\pm} | j, m_j \rangle = \sum_{m_l, m_s} \langle m_l, m_s | j, m_j \rangle (\hat{L}_{\pm} + \hat{S}_{\pm}) | m_l, m_s \rangle, \quad (*)$$

where in both representations, the common quantum numbers  $l$  and  $s$  are just implied.

In order to spell out the left-hand and right-hand sides of this equality, let us recall that Eq. (5.164) of the lecture notes could be derived directly from the commutation relations (5.176), without any appeal to the wave-mechanics form of the orbital angular momentum operator. (See the solution of Problem 27.) Since, according to Eqs. (5.168) and (5.174), the commutation relations for the operators  $\hat{S}$  and  $\hat{J}$  are similar to those of  $\hat{L}$ , we may repeat all the arguments to get similar formulas for the similarly defined ladder operators. In the notation of Sec. 5.6, Eq. (5.164) takes the form

$$\hat{L}_{\pm} | m_l, m_s \rangle = \hbar [(l \pm m_l + 1)(l \mp m_l)]^{1/2} | m_l \pm 1, m_s \rangle,$$

so in the same uncoupled-representation basis, we get<sup>65</sup>

<sup>65</sup> For the most important case of spin- $\frac{1}{2}$  ( $s = \frac{1}{2}$ , and  $m_s = \pm\frac{1}{2}$ ), Eq. (\*\*) is much simplified:

$$\hat{S}_+ | m_l, m_s = +\frac{1}{2} \rangle = \hat{S}_- | m_l, m_s = -\frac{1}{2} \rangle = 0, \quad \hat{S}_{\pm} | m_l, m_s = \mp\frac{1}{2} \rangle = \hbar | m_l, m_s = \pm\frac{1}{2} \rangle.$$

$$\hat{S}_{\pm} |m_l, m_s\rangle = \hbar [(s \pm m_s + 1)(s \mp m_s)]^{1/2} |m_l, m_s \pm 1\rangle, \tag{**}$$

while for the coupled-representation eigenstates,

$$\hat{J}_{\pm} |j, m_j\rangle = \hbar [(j \pm m_j + 1)(j \mp m_j)]^{1/2} |j, m_j \pm 1\rangle.$$

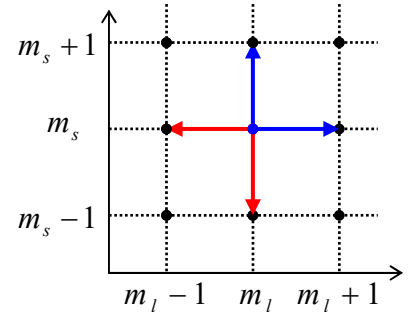
Plugging these expressions into Eq. (\*), with the temporary notation replacements  $m_l \rightarrow \mu_l$  and  $m_s \rightarrow \mu_s$  (the reason for it will be clear in just a moment), we get:

$$[(j \pm m_j + 1)(j \mp m_j)]^{1/2} |j, m_j \pm 1\rangle = \sum_{\mu_l, \mu_s} \langle \mu_l, \mu_s | j, m_j \rangle \times \left\{ \begin{aligned} & [(l \pm \mu_l + 1)(l \mp \mu_l)]^{1/2} |\mu_l \pm 1, \mu_s\rangle \\ & + [(s \pm \mu_s + 1)(s \mp \mu_s)]^{1/2} |\mu_l, \mu_s \pm 1\rangle \end{aligned} \right\}.$$

Now let us inner-multiply both sides of this relation by the bra-vector  $\langle m_l, m_s |$ . Since the vectors of any basis (including that of the uncoupled representation) are assumed to be orthonormal, the first term in the figure brackets gives a nonzero result only for  $\mu_l = m_l \mp 1$  and  $\mu_s = m_s$ , while the second term, for  $\mu_l = m_l$  and  $\mu_s = m_s \mp 1$ . As a result, the summation on that side is reduced to just two terms, and we get

$$[(j \pm m_j + 1)(j \mp m_j)]^{1/2} \langle m_l, m_s | j, m_j \pm 1\rangle = \left\{ \begin{aligned} & [(l \pm m_l)(l \mp m_l + 1)]^{1/2} \langle m_l \mp 1, m_s | j, m_j \rangle \\ & + [(s \pm m_s)(s \mp m_s + 1)]^{1/2} \langle m_l, m_s \mp 1 | j, m_j \rangle \end{aligned} \right\}. \tag{***}$$

The red and blue arrows in the figure on the right show the sets of the uncoupled-representation states related by Eqs. (\*\*\*) with, respectively, the upper and lower signs, on the rectangular lattice similar to the one that was shown in Fig. 5.14 of the lecture notes – in that case, for  $s = 1/2$ . These relations enable one to derive explicit formulas for the Clebsch-Gordan coefficients, similar to Eqs. (5.190), for an arbitrary spin  $s$ , starting from one of the two particular “corner” states with  $m_l = \pm l$  and  $m_s = \pm s$ , which may be represented by single ket-vectors in both the uncoupled and coupled representations.

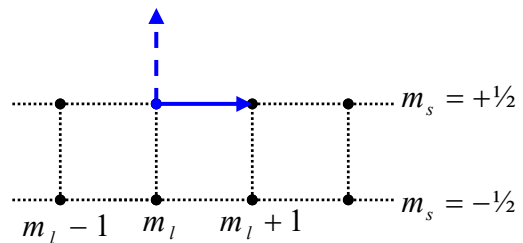


**Problem 5.48.** Use the recurrence relations derived in the previous problem to prove Eqs. (5.190) of the lecture notes for the spin- $1/2$  Clebsch-Gordan coefficients.

**Solution:** Eqs. (5.190) is the set of four expressions corresponding to two independent signs in the relations  $m_s = \pm 1/2$  and  $j - l = \pm 1/2$ ; as an example, let us consider the case

$$m_s = +1/2, \quad j = l + 1/2. \tag{*}$$

For our case  $s = 1/2$ , the rectangular diagram on the  $[m_l, m_s]$  plane has the form shown in Fig. 5.14 of the lecture notes – see its simplified version in the figure on the right. If we apply the recurrence relations derived in the solution of the previous problem, with the lower signs, to an arbitrary point  $\{m_l, +1/2\}$  of the upper row, we may expect one of the  $c$ -number



This means that the ladder operators of the proper sign just flip the spin orientation. The orbital quantum number  $m_l$  aside, this is exactly the result we could get for the ladder operators  $\hat{S}_{\pm} \equiv \hat{S}_x \pm i\hat{S}_y$  directly from Eqs. (4.128).

coefficients on the right-hand side of these relations (corresponding to the dashed arrow on the diagram) to vanish, giving a direct recurrence relation between two adjacent Clebsch-Gordan coefficients of the upper row – in the figure above, corresponding to the points connected by the solid arrow.

Indeed, let us use Eq. (\*\*\*) of the solution with the proper (lower) sign in each term. For the selected values (\*) of  $m_s$  and  $j$ , making the replacement  $m_j \rightarrow m_l + \frac{1}{2} + 1$ ,<sup>66</sup> it yields

$$\begin{aligned} & [(l - m_l)(l + m_l + 2)]^{1/2} \langle m_l, +\frac{1}{2} | l + \frac{1}{2}, m_l + \frac{1}{2} \rangle \\ &= [(l - m_l)(l + m_l + 1)]^{1/2} \langle m_l + 1, +\frac{1}{2} | l + \frac{1}{2}, m_l + \frac{1}{2} + 1 \rangle + [(0) \cdot (2)]^{1/2} \langle m_l, +\frac{1}{2} + 1 | l + \frac{1}{2}, m_l + \frac{1}{2} \rangle, \end{aligned} \quad (**)$$

so the coefficient before the last bracket (whose ket-vector would describe an impossible state with  $m_s = \frac{1}{2} + 1 > s$ ) vanishes as it has to, and we get a direct, simple recurrence relation

$$\langle m_l, +\frac{1}{2} | l + \frac{1}{2}, m_l + \frac{1}{2} \rangle = \left( \frac{l + m_l + 1}{l + m_l + 2} \right)^{1/2} \langle m_l + 1, +\frac{1}{2} | l + \frac{1}{2}, m_l + \frac{1}{2} + 1 \rangle, \quad (***)$$

which is valid for all  $m_l$  that give positive factors  $(l - m_l)$ ,  $(l + m_l + 1)$ , and  $(l + m_l + 2)$ , i.e. for any point of the rectangular diagram, besides its rightmost points. As was discussed in the lecture notes, in the rightmost upper point, the only Clebsch-Gordan coefficient should equal 1:

$$\langle l, +\frac{1}{2} | l + \frac{1}{2}, l + \frac{1}{2} \rangle = 1,$$

so applying Eq. (\*\*\*) sequentially to the points further and further left in that upper row, we get:

$$\text{for } m_l = l - 1: \langle l - 1, +\frac{1}{2} | l + \frac{1}{2}, l - \frac{1}{2} \rangle = \left( \frac{2l}{2l + 1} \right)^{1/2} \langle l, +\frac{1}{2} | l + \frac{1}{2}, l + \frac{1}{2} \rangle = \left( \frac{2l}{2l + 1} \right)^{1/2},$$

$$\text{for } m_l = l - 2: \langle l - 2, +\frac{1}{2} | l + \frac{1}{2}, l - \frac{1}{2} - 1 \rangle = \left( \frac{2l - 1}{2l} \right)^{1/2} \langle l - 1, +\frac{1}{2} | l + \frac{1}{2}, l - \frac{1}{2} \rangle = \left( \frac{2l}{2l + 1} \cdot \frac{2l - 1}{2l} \right)^{1/2},$$

etc., with both the numerator and denominator decreasing by 1 in each next fraction. Continuing this sequence to an arbitrary  $m_l$ , we finally get

$$\langle m_l, +\frac{1}{2} | l + \frac{1}{2}, m_l + \frac{1}{2} \rangle = \left( \frac{2l}{2l + 1} \cdot \frac{2l - 1}{2l} \cdot \frac{2l - 2}{2l - 1} \cdots \frac{l + m_l + 2}{l + m_l + 3} \cdot \frac{l + m_l + 1}{l + m_l + 2} \right)^{1/2} \equiv \left( \frac{l + m_l + 1}{2l + 1} \right)^{1/2},$$

because all intermediate factors in the numerator and denominator cancel. Now rewriting this result in terms of  $m_j = m_l + \frac{1}{2}$ , we obtain

$$\langle m_j - \frac{1}{2}, +\frac{1}{2} | l + \frac{1}{2}, m_j \rangle = \left( \frac{l + m_j + \frac{1}{2}}{2l + 1} \right)^{1/2},$$

i.e. the shorthand of the first line of Eqs. (5.190), for the proper (upper) sign of the difference  $(j - l)$ .

The proofs of the relations for other signs of  $m_s$  and  $(j - l)$  are completely similar.

<sup>66</sup> The last replacement presented a difficulty for some of my students, because it apparently contradicts the general equality (5.187):  $m_j = m_l + m_s$  in our case,  $m_j = m_l + \frac{1}{2}$ . However, it is necessary exactly to have that general equality satisfied for each state in the initial recurrent relations (with the proper lower signs), and hence in our result.

**Problem 5.49.** A spin- $\frac{1}{2}$  particle is in a state with definite values of  $L^2$ ,  $J^2$ , and  $J_z$ . Find all possible values of the observables  $S^2$ ,  $S_z$ , and  $L_z$ , the probability of each listed value, and the expectation value for each of these observables.

*Solution:* Evidently, such a state is a common eigenstate of the operators  $\hat{L}^2$ ,  $\hat{J}^2$ , and  $\hat{J}_z$ , with definite values of the corresponding quantum numbers  $l$ ,  $j$ , and  $m_j$ , such that

$$L^2 = \hbar^2 l(l+1), \quad J^2 = \hbar^2 j(j+1), \quad \text{and} \quad J_z = \hbar m_j.$$

According to Eqs. (5.175), (5.177), and (5.189) of the lecture notes, these numbers should satisfy the following conditions:

$$l \geq 0, \quad j = l \pm \frac{1}{2}, \quad -j \leq m_j \leq +j.$$

As was discussed in Sec. 5.7 of the lecture notes (see, e.g., Fig. 5.12), this state is one of the basis states of the *coupled* representation, which may be represented by the ket-vector  $|j, m_j\rangle$ , where the definite quantum numbers  $l$  and  $s$  are implied. Using Eqs. (5.190) of the lecture notes, any such ket may be expressed via the kets  $|m_l, m_s\rangle$  of the *uncoupled* representation:

$$\begin{aligned} |j = l \pm \frac{1}{2}, m_j\rangle = & \pm \left( \frac{l \pm m_j + \frac{1}{2}}{2l+1} \right)^{1/2} |m_l = m_j - \frac{1}{2}, m_s = +\frac{1}{2}\rangle \\ & + \left( \frac{l \mp m_j + \frac{1}{2}}{2l+1} \right)^{1/2} |m_l = m_j + \frac{1}{2}, m_s = -\frac{1}{2}\rangle. \end{aligned} \quad (*)$$

Now we are ready to start answering the posed questions. First of all, according to the second of Eqs. (5.169), for the fixed  $s = \frac{1}{2}$ , the observable  $S^2$  may have only one value,  $S^2 = \hbar^2 s(s + \frac{1}{2}) = (3/4)\hbar^2$ , so its probability is 100%, and

$$\langle S^2 \rangle = \frac{3}{4} \hbar^2,$$

regardless of the quantum state of the particle.

Next, due to the first of Eqs. (5.169), the possible values of  $S_z$  are  $\hbar m_s = \pm \hbar/2$ , and for the state (\*), their probabilities are given by the squares of the corresponding Clebsch-Gordan coefficients:

$$W_{\uparrow} = \frac{l \pm m_j + \frac{1}{2}}{2l+1}, \quad W_{\downarrow} = \frac{l \mp m_j + \frac{1}{2}}{2l+1}, \quad (**)$$

giving the expectation value

$$\langle S_z \rangle = \frac{\hbar}{2} \times \frac{l \pm m_j + \frac{1}{2}}{2l+1} - \frac{\hbar}{2} \times \frac{l \mp m_j + \frac{1}{2}}{2l+1} \equiv \pm \frac{\hbar m_j}{2l+1}, \quad (***)$$

where the sign, as in Eq. (\*), is determined by that in the relation  $j = l \pm \frac{1}{2}$ . In any orbital  $s$ -state ( $l = 0$ ), this result is reduced to the obvious formula  $\langle S_z \rangle = \pm \hbar m_j = \pm \hbar/2$  because in this case, the total orbital moment  $J$  is due to the particle's spin  $S$  alone.

Finally, the observable  $L_z$  may take values  $\hbar m_l$ . According to Eq. (\*), for fixed  $j$  and  $m_j$ , the sign in the relation  $m_l = m_j \mp \frac{1}{2}$  is always opposite to that in relation  $m_s = \pm \frac{1}{2}$ . This means that the probabilities (\*\*\*) also describe those of these two possible values  $m_l$ :

$$W_{m_l=m_j-1/2} = \frac{l \pm m_j + 1/2}{2l+1}, \quad W_{m_l=m_j+1/2} = \frac{l \mp m_j + 1/2}{2l+1},$$

and the expectation value of the observable  $L_z$  is

$$\langle L_z \rangle = \hbar \left( m_j - \frac{1}{2} \right) \frac{l \pm m_j + 1/2}{2l+1} + \hbar \left( m_j + \frac{1}{2} \right) \frac{l \mp m_j + 1/2}{2l+1} \equiv \hbar m_j \left( 1 \mp \frac{1}{2l+1} \right).$$

Alternatively, the last formula may be obtained by averaging the operator equality (5.171):

$$\langle L_z \rangle = \langle J_z \rangle - \langle S_z \rangle = \hbar m_j - \langle S_z \rangle,$$

and plugging Eq. (\*\*\*) for  $\langle S_z \rangle$  into it.

**Problem 5.50.** Re-solve the Landau-level problem discussed in Sec. 3.2 of the lecture notes, now for a spin- $1/2$  particle. Discuss the result for the particular case of an electron.

*Solution:* The problem may be described by the Hamiltonian which is the sum of that of the orbital 2D motion (see Eq. (3.26) of the lecture notes, with  $\phi = 0$  and  $\partial/\partial z = 0$ ) and the Pauli Hamiltonian (4.163), describing the interaction between its spin and the field:

$$\hat{H} = -\frac{\hbar^2}{2m} \left( \mathbf{n}_x \frac{\partial}{\partial x} + \mathbf{n}_y \frac{\partial}{\partial y} - i \frac{q}{\hbar} \mathbf{A} \right)^2 - \gamma \hat{\mathbf{S}} \cdot \mathcal{B},$$

Since the orbital and spin states are defined in different Hilbert spaces and, in this case, do not interact, the total eigenenergy of the system is just a sum of the independent contributions from these two parts of the Hamiltonian – the first one given by Eq. (3.50), and another one, by Eq. (4.167):

$$E = \hbar \omega_c \left( n + \frac{1}{2} \right) \pm \frac{\hbar \Omega}{2}, \quad \text{with } n = 0, 1, 2, \dots$$

This expression shows that the spin-field interaction splits each Landau level into two sub-levels with different spin orientations. However, as was discussed in Sec. 4.6, for an electron, the frequencies  $\omega_c \equiv e\mathcal{B}/m_e$  and  $|\Omega| \equiv |\gamma\mathcal{B}| = |g_e e\mathcal{B}/2m_e|$  are very close because its  $g$ -factor  $g_e$  is very close to 2, so that the above result may be very closely approximated as

$$E = \hbar \omega_c \left( n + \frac{1}{2} \pm \frac{1}{2} \right),$$

i.e. the energy values are integer multiples of  $\hbar\omega_c$ . In this picture, besides the ground-state energy  $E_g = 0$ , each other energy level is doubly degenerate, with its two states having not only different spin directions but also adjacent values of the orbital quantum number  $n$ .

**Problem 5.51.** In the Heisenberg picture of quantum dynamics, find an explicit relation between the operators of velocity  $\hat{\mathbf{v}} \equiv d\hat{\mathbf{r}}/dt$  and acceleration  $\hat{\mathbf{a}} \equiv d\hat{\mathbf{v}}/dt$  of a non-relativistic particle with an electric charge  $q$ , moving in an arbitrary external electromagnetic field. Compare the result with the corresponding classical expression.

*Hint:* For the orbital motion's description, you may use Eq. (3.26) of the lecture notes.

*Solution:* The Hamiltonian of the particle in the field may be composed as the sum of the orbital Hamiltonian (3.26) and the Pauli Hamiltonian (4.163) corresponding to the magnetic field  $\mathcal{B} = \nabla \times \mathbf{A}$ :

$$\hat{H} = \frac{1}{2m} (\hat{\mathbf{P}} - q\hat{\mathbf{A}})^2 + q\hat{\phi} - \gamma\hat{\mathbf{S}} \cdot (\nabla \times \hat{\mathbf{A}}).$$

Here the operator signs over the scalar and vector potentials are spelled out as reminders that the potentials are generally functions of not only time but also of the particle's position, which, in this calculation, should be treated as an operator. Hence the potentials should be also treated as linear operators (commuting with  $\hat{\mathbf{r}}$ ), even if the quantum properties of the electromagnetic field itself are negligible – as they are considered to be in this course before Chapter 9.

The orbital operators  $\hat{\mathbf{r}}$  and  $\hat{\mathbf{P}}$  are defined in a Hilbert space different from that of the spin operator  $\hat{\mathbf{S}}$ , and hence commute with it. On the other hand, similar Cartesian components of the orbital operators do not commute. However, the commutation relation (4.238), valid for an arbitrary  $j^{\text{th}}$  component,

$$[\hat{r}_j, \hat{p}_j] = i\hbar, \quad (*)$$

is not affected by the addition, to the kinetic momentum operator  $\hat{\mathbf{p}}$ , of the field part  $q\hat{\mathbf{A}}(\hat{\mathbf{r}})$  because the latter commutes with the coordinate operator  $\hat{\mathbf{r}}$ , so

$$[\hat{r}_j, \hat{P}_j] = i\hbar. \quad (**)$$

As a result, the equation of motion of the coordinate operator components is given by Eq. (5.29) of the lecture notes even in the field. In the vector form,

$$\hat{\mathbf{v}} \equiv \frac{d\hat{\mathbf{r}}}{dt} = \frac{\hat{\mathbf{p}}}{m} = \frac{\hat{\mathbf{P}} - q\hat{\mathbf{A}}}{m}, \quad (***)$$

so our Hamiltonian may be rewritten in the form<sup>67</sup>

$$\hat{H} = \frac{m\hat{\mathbf{v}}^2}{2} + q\hat{\phi} - \gamma\hat{\mathbf{S}} \cdot (\nabla \times \hat{\mathbf{A}}).$$

Plugging these two expressions into the general Eq. (4.199), we may calculate the acceleration operator:

$$\hat{\mathbf{a}} \equiv \frac{d\hat{\mathbf{v}}}{dt} = \frac{1}{i\hbar} [\hat{\mathbf{v}}, \hat{H}] = \frac{1}{i\hbar} \frac{1}{m} [\hat{\mathbf{p}}, q\hat{\phi}] + \frac{1}{i\hbar} \frac{m}{2} [\hat{\mathbf{v}}, \hat{\mathbf{v}}^2].$$

Due to the similarity of Eqs. (\*) and (\*\*), the Cartesian components of the first term may be calculated exactly as it was done in Sec. 5.2 of the lecture notes, giving the vector version of Eq. (5.35) with the replacement

$$-\frac{\partial}{\partial \hat{r}_j} U(\hat{\mathbf{r}}) \rightarrow -q \frac{\partial}{\partial \hat{r}_j} \hat{\phi}(\hat{\mathbf{r}}) = q\hat{\mathcal{E}}_j(\hat{\mathbf{r}}),$$

where  $\hat{\mathcal{E}} = -\nabla\hat{\phi}$  is the vector operator of the electric field. Calculating the  $j^{\text{th}}$  Cartesian component of the second commutator,

<sup>67</sup> Note also that Eq. (\*\*\*) allows us to rewrite Eq. (3.28) in a very simple and natural form:  $\mathbf{j} = \psi^* \hat{\mathbf{v}} \psi$ .



$$[\hat{\mathbf{v}}, \hat{\mathbf{v}}^2]_j \equiv \left[ \hat{\mathbf{v}}, \sum_{j'=1}^3 \hat{\mathbf{v}}_{j'}^2 \right]_j \equiv \sum_{j'=1}^3 \mathbf{n}_j [\hat{\mathbf{v}}_j, \hat{\mathbf{v}}_{j'}^2],$$

we should remember that the  $j^{\text{th}}$  component of the vector potential  $\mathbf{A}$  may be (and most typically is) a function of *all* Cartesian coordinates  $r_j$ , and as a result, the Cartesian components of the velocity operator (\*\*\*) do not commute:

$$\begin{aligned} [\hat{\mathbf{v}}_j, \hat{\mathbf{v}}_{j'}] &= \frac{1}{m^2} \left[ (\hat{P} - q\hat{A})_j, (\hat{P} - q\hat{A})_{j'} \right] = \frac{1}{m^2} \left[ \left( -i\hbar \frac{\partial}{\partial r_j} - q\hat{A}_j \right), \left( -i\hbar \frac{\partial}{\partial r_{j'}} - q\hat{A}_{j'} \right) \right] \\ &= \frac{i\hbar q}{m^2} \left( \left[ \frac{\partial}{\partial r_j}, \hat{A}_{j'} \right] + \left[ \hat{A}_j, \frac{\partial}{\partial r_{j'}} \right] \right) = \frac{i\hbar q}{m^2} \left( \frac{\partial \hat{A}_{j'}}{\partial r_j} - \frac{\partial \hat{A}_j}{\partial r_{j'}} \right), \end{aligned}$$

where, in the last expression, the derivatives act only upon the components of the vector potential  $\mathbf{A}$ , but not upon the wavefunction these operators act upon. But the last combination of two derivatives is just the  $j^{\text{th}}$  component of the magnetic field  $\mathcal{B} = \nabla \times \mathbf{A}$ , multiplied by the proper Levi-Civita symbol,<sup>68</sup> so

$$[\hat{\mathbf{v}}_j, \hat{\mathbf{v}}_{j'}] = \frac{i\hbar q}{m^2} \sum_{j''=1}^3 \hat{\mathcal{B}}_{j''} \varepsilon_{jjj''}, \quad \text{i.e. } \hat{\mathbf{v}}_j \hat{\mathbf{v}}_{j'} = \hat{\mathbf{v}}_{j'} \hat{\mathbf{v}}_j + \frac{i\hbar q}{m^2} \sum_{j''=1}^3 \hat{\mathcal{B}}_{j''} \varepsilon_{jjj''},$$

Applying the last relation twice, we get

$$\begin{aligned} [\hat{\mathbf{v}}, \hat{\mathbf{v}}^2]_j &\equiv \sum_{j'=1}^3 [\hat{\mathbf{v}}_j, \hat{\mathbf{v}}_{j'}^2] \equiv \sum_{j'=1}^3 (\hat{\mathbf{v}}_j \hat{\mathbf{v}}_{j'} \hat{\mathbf{v}}_{j'} - \hat{\mathbf{v}}_{j'} \hat{\mathbf{v}}_{j'} \hat{\mathbf{v}}_j) = \sum_{j'=1}^3 \left( \hat{\mathbf{v}}_{j'} \hat{\mathbf{v}}_j \hat{\mathbf{v}}_{j'} + \frac{i\hbar q}{m^2} \sum_{j''=1}^3 \hat{\mathcal{B}}_{j''} \varepsilon_{jjj''} \hat{\mathbf{v}}_{j'} - \hat{\mathbf{v}}_{j'} \hat{\mathbf{v}}_{j'} \hat{\mathbf{v}}_j \right) \\ &= \sum_{j'=1}^3 \left( \hat{\mathbf{v}}_{j'} \hat{\mathbf{v}}_j \hat{\mathbf{v}}_{j'} + \hat{\mathbf{v}}_{j'} \frac{i\hbar q}{m^2} \sum_{j''=1}^3 \hat{\mathcal{B}}_{j''} \varepsilon_{jjj''} + \frac{i\hbar q}{m^2} \sum_{j''=1}^3 \hat{\mathcal{B}}_{j''} \varepsilon_{jjj''} \hat{\mathbf{v}}_{j'} - \hat{\mathbf{v}}_{j'} \hat{\mathbf{v}}_{j'} \hat{\mathbf{v}}_j \right) \equiv \frac{i\hbar q}{m^2} \sum_{j', j''=1}^3 (\hat{\mathbf{v}}_{j'} \hat{\mathcal{B}}_{j''} + \hat{\mathcal{B}}_{j''} \hat{\mathbf{v}}_{j'}) \varepsilon_{jjj''}. \end{aligned}$$

But per the same Eq. (5.18), the last double sum is just the  $j^{\text{th}}$  Cartesian component of the vector operator  $(\hat{\mathbf{v}} \times \hat{\mathcal{B}} - \hat{\mathcal{B}} \times \hat{\mathbf{v}})$ . As a result, merging three such scalar expressions into the vector form, we finally get

$$\hat{\mathbf{a}} = \frac{q}{m} \left( \hat{\mathcal{E}} + \frac{\hat{\mathbf{v}} \times \hat{\mathcal{B}} - \hat{\mathcal{B}} \times \hat{\mathbf{v}}}{2} \right). \quad \text{****}$$

Perhaps the most important feature of this result is that the operators of the particle's velocity and acceleration (and hence its orbital motion) are not affected by the particle's spin. (This conclusion is valid only if the relativistic effect of the spin-orbit interaction<sup>69</sup> is ignored – as they are in the Pauli Hamiltonian). Also, note that Eq. (\*\*\*\*) formally coincides with the well-known formula for the Lorentz-force-induced acceleration in classical electromagnetism, rewritten in the form

$$\mathbf{a} = \frac{\mathbf{F}_L}{m}, \quad \mathbf{F}_L = q(\mathcal{E} + \mathbf{v} \times \mathcal{B}) \equiv q \left( \mathcal{E} + \frac{\mathbf{v} \times \mathcal{B} - \mathcal{B} \times \mathbf{v}}{2} \right).$$

<sup>68</sup> See, e.g., Eq. (5.18) of the lecture notes.

<sup>69</sup> See, e.g., Secs. 6.3 and 9.7.

However, making the transition to quantum mechanics from the first form of this classical formula for  $\mathbf{F}_L$  would give a wrong result because, as we have just seen, the operators  $\hat{\mathbf{v}}$  and  $\hat{\mathcal{B}}$  do not commute.

**Problem 5.52.** One byproduct of the solution of Problem 47 was the following relation for the spin operators (valid for any spin  $s$ ):

$$\langle m_s \pm 1 | \hat{S}_{\pm} | m_s \rangle = \hbar [(s \pm m_s + 1)(s \mp m_s)]^{1/2}.$$

Use this result to spell out the matrices  $S_x$ ,  $S_y$ ,  $S_z$ , and  $S^2$  of a particle with  $s = 1$ , in the  $z$ -basis – defined as the basis in which the matrix  $S_z$  is diagonal.

*Solution:* According to Eqs. (5.169) of the lecture notes, the matrices  $S_z$  and  $S^2$  are diagonal in the basis of the states with definite quantum numbers  $m_s$ . For  $s = 1$ , this is a three-function basis with  $m_s = +1, 0$ , and  $-1$ . In this basis, these relations (with  $s = 1$  and hence  $s(s + 1) = 2$ ) give

$$S_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad S^2 = 2\hbar^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

while the formula given in the assignment yields

$$S_+ = \sqrt{2}\hbar \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \quad S_- = \sqrt{2}\hbar \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

Since the operators  $\hat{S}_{\pm}$  are defined via the Cartesian component operators as  $\hat{S}_{\pm} \equiv \hat{S}_x \pm i\hat{S}_y$ , for the component matrices we get

$$S_x \equiv \frac{S_+ + S_-}{2} = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S_y \equiv \frac{S_+ - S_-}{2i} = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}.$$

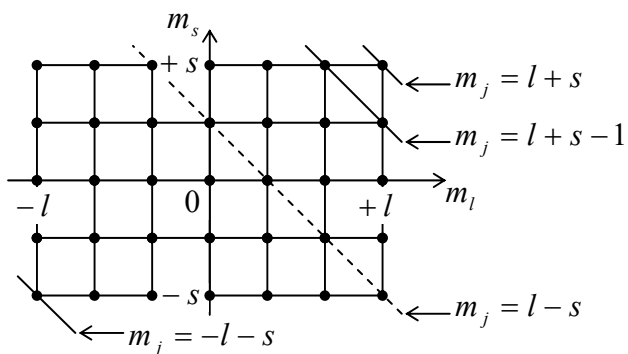
Note that the calculated matrices are fully similar to those calculated in the solution of Problem 31 for the orbital momentum with the definite quantum number  $l = 1$ . (This similarity is natural due to that of the commutation relations valid for these operators.) Note also that finding the eigenvalues of a matrix similar to  $S_x$  (without the front factor) was one of the tasks of Problem 4.23.

**Problem 5.53.\*** For a particle with an arbitrary spin  $s$ , find the quantum numbers  $m_j$  and  $j$  that are necessary to describe, in the coupled-representation basis:

- (i) all states with a definite quantum number  $l$ , and
- (ii) a state with definite values of not only  $l$  but also  $m_l$  and  $m_s$ .

Give an interpretation of your results in terms of a classical vector diagram – see, e.g., Fig. 5.13 of the lecture notes.

*Solutions:* For arbitrary  $l$  and  $s$ , the “rectangular diagram” of the basis states (see Fig. 5.14 of the lecture notes), looks as shown in the figure on the right.<sup>70</sup> Here each point corresponds to one of  $N_m = (2l+1) \times (2s+1)$  basis states of the uncoupled representation, each with definite quantum numbers  $m_l$  and  $m_s$ , while each tilted straight line connects the states contributing to the basis states of the coupled representation, with definite quantum numbers  $j$  and  $m_j = m_l + m_s$ .



(i) The diagram immediately shows that for the set of quantum numbers  $m_s$  and  $m_l$ , following from Eqs. (5.169) and (5.177), namely  $-s \leq m_s \leq +s$  and  $-l \leq m_l \leq +l$ , the range of possible numbers  $m_j$  is

$$-l - s \leq m_j \leq l + s,$$

but the range of possible numbers  $j$  is a bit less evident. To calculate it, we may use the fact that in order to have a unique set of linearly independent relations (5.183),

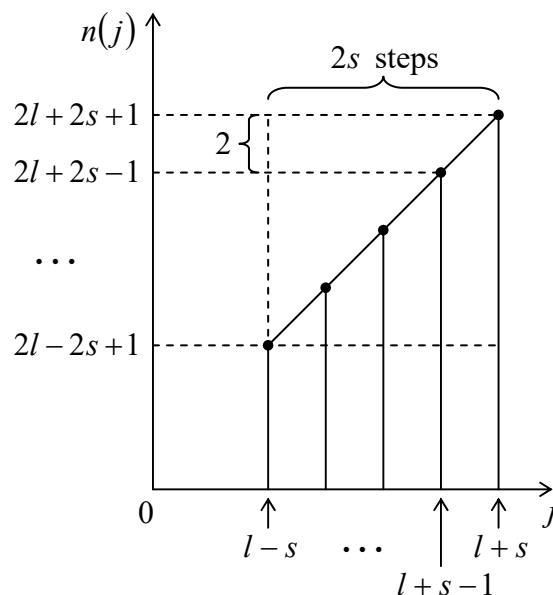
$$|j, m_j\rangle = \sum_{m_l, m_s} |m_l, m_s\rangle \langle m_l, m_s | j, m_j\rangle,$$

the number of the basis ket vectors (and hence the basis states) in both representations should be equal. Let us count the number of states of the coupled representation, starting from the top right corner of the above diagram. Evidently, there is only one such state corresponding to the single uncoupled-representation state with quantum numbers  $m_l = +l$  and  $m_s = +s$ , i.e. that with  $m_j = (m_j)_{\max} \equiv (m_l + m_s)_{\max} = l + s$ . Per the last of Eqs. (5.175) of the lecture notes,  $-j \leq m_j \leq j$ , the quantum number  $j$  has to be exactly equal to this maximum value of  $m_j$ , so

$$j_{\max} = l + s. \quad (*)$$

According to the same relation  $-j \leq m_j \leq j$ , the full set of the basis states of the coupled representation should include  $n(j_{\max}) = 2(m_j)_{\max} + 1 = 2l + 2s + 1$  states corresponding to  $j = j_{\max}$  – see the rightmost vertical line in the figure on the right, in which we will gradually plot the number of the coupled-representation basis states as a function of  $j$ .

Moving down to the next value,  $m_j = l + s - 1$ , the rectangular diagram above shows two  $\{m_l, m_s\}$  states, both with  $m_j \equiv m_l + m_s = (m_j)_{\max} - 1 \equiv l + s - 1$ , which need, for their linear representation, two different  $\{j, m_j\}$  states. Since both these states have the same  $m_j$ , they cannot be described by the same  $j = j_{\max}$ . Hence we need one more



<sup>70</sup> For clarity, I had to draw the diagram for certain values of  $l$  and  $s$ , but none of the expressions below uses these particular values, besides the assumed restriction  $s \leq l$ ; the opposite case will be discussed below. Also, note that all the formulas below are valid whether  $s$  is an integer or a half-integer – e.g., as in Fig. 5.14 of the lecture notes.

value of  $j$ ; repeating the discussion above, we see that this value has to be equal to the current value of  $m_j$ , i.e. to  $l + s - 1$ , i.e. is less than  $j_{\max} = l + s$  by 1. The overall number of  $m_j$ -states, corresponding to this new value  $j = j_{\max} - 1$  is  $n(j_{\max} - 1) = 2(l + s - 1) + 1 \equiv 2l + 2s - 1$ , i.e. by 2 less than  $n(j_{\max})$  – see the second vertical line from the right in the state counting diagram above.

Repeating this process again and again, we may move to the left on both diagrams by unit steps, each time reducing  $m_j$  by one and getting one more new value of  $j$ , which is also less than the smallest previous value by one, and has the number of  $m_j$ -states lower by 2 – see the figure above. This process breaks only after  $2s$  steps, when on the rectangular diagram, the tilted line of equal  $m_j$  hits the lower right corner – with  $m_l = l$ ,  $m_s = -s$ , i.e. with  $m_j \equiv m_l + m_s = l - s$ , and the value of  $j$  equal to

$$j_{\min} = j_{\max} - 2s \equiv l - s \geq 0, \quad (**)$$

responsible for  $n(j_{\min}) = 2l - 2s - 1$  states with different values of  $m_j$ . (See the dashed line in the first figure above.)

Let us count the total number  $N_j$  of the basis states of the coupled representation, which correspond to the already covered values of  $j$ , within the interval  $j_{\min} \leq j \leq j_{\max}$ . From the number-of-state diagram above, we get

$$N_j \equiv \sum_{j=j_{\min}}^{j_{\max}} n(j) = \sum_{j=j_{\min}}^{j_{\max}} [n(j_{\min}) + 2(j - j_{\min})] = \sum_{j=l-s}^{l+s} [(2l - 2s + 1) + 2(j - l + s)] \equiv \sum_{j=l-s}^{l+s} (1 + 2j).$$

This is just the sum of  $(2s + 1)$  terms equal to 1, plus a difference between two standard arithmetic progressions, so using the well-known formula for the progression,<sup>71</sup> we get

$$N_j = (2s + 1) + 2 \sum_{j=1}^{l+s} j - 2 \sum_{j=1}^{l-s-1} j = (2s + 1) + 2 \frac{(l+s)(l+s+1)}{2} - 2 \frac{(l-s-1)(l-s)}{2} \equiv (2s + 1)(2l + 1).$$

But this number is exactly equal to  $N_m$ ; hence we have reached the state number equality in both representations without involving lower values of  $j$ . (The states on the left of the dashed tilted line on the rectangular diagram are covered by the already counted values of  $j$ ; for example, the left bottom corner state with  $m_j = -s - l \equiv -j_{\max}$  is obviously described by  $j = j_{\max}$ .)

Hence Eqs. (\*) and (\*\*) indeed give the boundaries of the range of  $j$  for all  $N \equiv N_m = N_j$  states of the system in the case  $s \leq l$ ; in the opposite case  $l \leq s$ , it is sufficient to repeat all the above arguments after transposing the rectangular diagram, getting the same result besides the reversal  $s \leftrightarrow l$ , so  $j_{\min} = s - l$  is again non-negative. Both cases may be summarized as follows:

$$|l - s| \leq j \leq l + s. \quad (***)$$

(ii) If the quantum numbers  $m_l$  and  $m_s$  are fixed, and hence the sum  $m_j \equiv m_l + m_s$  is fixed as well, we may repeat all the process of motion from the top right corner of the rectangular diagram, which was discussed above. However, if  $m_j$  is positive and larger than  $|l - s|$ , i.e. the point  $\{m_l, m_s\}$  is located to the right of the dashed tilted line on the diagram, we may stop the process as soon as we have reached this point, because the state in question has been, by construction, covered by the already accounted values of  $j$ . Similarly, if  $m_j$  is negative, and its magnitude is larger than  $|l - s|$ , we may repeat the process by

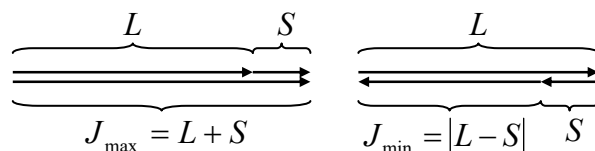
<sup>71</sup> See, e.g., MA Eq. (2.5).

starting from the lower left corner, and again stop it when the tilted line of fixed  $m_j$  has reached the given point  $\{m_l, m_s\}$ . Summarizing these cases, we get the following range of  $j$ :

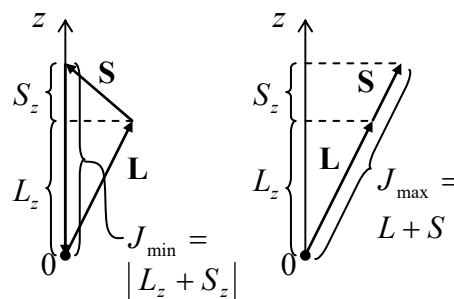
$$\max[|l-s|, |m_l + m_s|] \leq j \leq l + s. \quad (****)$$

The above results of Tasks (i) and (ii) may be readily interpreted using the classical vector diagrams, such as those shown in Fig. 5.13 of the lecture notes. As a reminder, on such diagrams, the products  $\hbar m_l$ ,  $\hbar m_s$ , and  $\hbar m_j$  are associated with the  $z$ -components,  $L_z$ ,  $S_z$ , and  $J_z$ , of the angular momentum vectors  $\mathbf{L}$ ,  $\mathbf{S}$ , and  $\mathbf{J}$ , respectively, while  $\hbar l$ ,  $\hbar s$ , and  $\hbar j$ , with the lengths  $L$ ,  $S$ , and  $J$  of these vectors, i.e. the differences between  $l$  and  $[l(l+1)]^{1/2}$ , etc. (which are of a purely quantum origin) are ignored.

In case (i), when the  $z$ -components of the angular momentum vectors are not fixed, the largest length of the vector  $\mathbf{J} \equiv \mathbf{L} + \mathbf{S}$  corresponds to the parallel alignment of the vectors  $\mathbf{L}$  and  $\mathbf{S}$ :  $J_{\max} = L + S$ , while its smallest value, to their antiparallel alignment:  $J_{\min} = |L - S|$  (see the figure on the right), in full agreement with the quantum Eq. (\*\*\*)



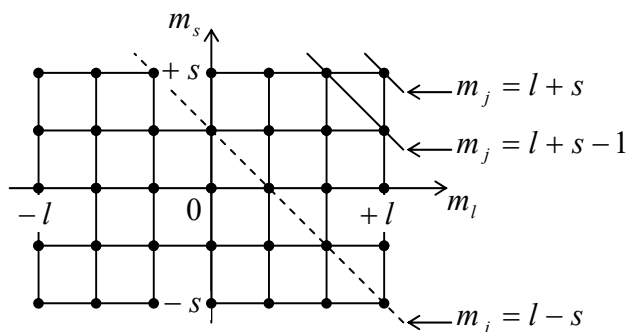
In case (ii), when  $L_z$  and  $S_z$  are fixed (in addition to definite  $L$  and  $S$ ), the classical picture (see the figure on the right) shows an additional limitation imposed at  $J$  from below:  $J_{\min} = |L_z + S_z|$ , provided that  $|L_z + S_z| > |L - S|$ , in agreement with the left inequality in Eq. (\*\*\*) . Note, however, that in the classical picture, the exact parallel alignment of the vectors  $\mathbf{L}$  and  $\mathbf{S}$  necessary to reach the maximum value  $J_{\max} = L + S$ , implied by the right part of Eq. (\*\*\*) , is possible only at a certain exact proportion between their  $z$ -components and lengths:  $S_z/L_z = S/L$ . In quantum mechanics, there is no such exact restriction – the fact that again emphasizes the limitations of the classical vector model. Only in the limit  $l, s \rightarrow \infty$ , the asymptotic correspondence to classical mechanics is achieved, by the Clebsch-Gordan coefficients  $\langle m_l, m_s | j, m_j \rangle$  tending to zero everywhere at the rectangular diagram besides very close to its diagonal, i.e. at  $m_s/m_l \approx s/l$ , approaching the classical restriction.



**Problem 5.54.** For a particle with spin  $s$ , find the range of the quantum numbers  $j$  necessary to describe, in the coupled-representation basis, all states with definite quantum numbers  $l$  and  $m_l$ .

*Solution:* Two similar tasks, but either without the fixation of  $m_l$  or with the simultaneous fixation of both  $m_l$  and  $m_s$ , were analyzed in the solution of the previous problem, by using the rectangular state diagram – see the figure on the right, again for the case  $s < l$ .

For the first of those tasks, a simple procedure of simultaneously listing the values of  $j$ , and counting the coupled-representation basis states, by moving the tilted line of fixed  $m_j \equiv m_l + m_s$  sequentially, in unit



steps, from the top right corner of the diagram (where  $m_j = l + s$ ) toward the dashed line passing through the lower right corner (where  $m_j = l - s$ ), showed that by the time the dashed line has been reached, the state number has already reached that,  $N_m = (2l + 1)(2s + 1)$ , of the uncoupled representation basis. This means that the range of the values of  $j$ , accumulated by that point, namely

$$|l - s| \leq j \leq l + s, \quad (*)$$

would not be further expanded, and the counting may be stopped.

In the second of those tasks, the process could be stopped even earlier, and hence the range of  $j$  is reduced in comparison with Eq. (\*), if the fixed point  $\{m_l, m_s\}$  is on the right of the dashed line in the figure above, i.e. if  $m_l + m_s > l - s$ . The generalization of this argumentation to all possible signs of the combinations  $(l - s)$  and  $(m_l + m_s)$  gave the following condition of the reduction:

$$|m_l + m_s| > |l - s|. \quad (**)$$

Now proceeding to our current task, we see that the set of the uncoupled-representation states with fixed  $m_l$ , located on one vertical line of the rectangular diagram, contains all the numbers  $m_s$  within the range  $[-s, +s]$ , so the set always has at least one state that does *not* satisfy Eq. (\*\*). (For example, if  $(l - s) > 0$ , we may use the rectangular diagram drawn above to see that each vertical line has at least one point that is *not* on the right side of the dashed line.) As a result, the state counting process cannot be stopped before the dashed line has been reached, and the range of necessary quantum numbers  $j$  is given by Eq. (\*).

Note that the same conclusion is valid if  $m_s$ , rather than  $m_l$ , is fixed.

**Problem 5.55.** A particle of mass  $m$ , with electric charge  $q$  and spin  $s$ , free to move along a planar circle of radius  $R$ , is placed into a constant uniform magnetic field  $\mathcal{B}$  directed normally to the circle's plane. Calculate the energy spectrum of the system. Explore and interpret the particular form the result takes when the particle is an electron with the  $g$ -factor  $g_e \approx 2$ .

*Solution:* Directing the  $z$ -axis parallel to the field, i.e. normally to the circle's plane, we may describe the problem by a Hamiltonian which is the sum of the rotor's kinetic energy in the presence of the magnetic field (see Eq. (3.131) of the lecture notes, with the convenient, axially symmetric choice (3.132) of the vector potential), and the Pauli Hamiltonian (4.163) of the interaction between the particle's spin and the field:

$$\hat{H} = -\frac{1}{2m} \left( -i \frac{\hbar}{R} \frac{\partial}{\partial \varphi} - qA_\varphi \right)^2 - \gamma \mathcal{B} \hat{S}_z \equiv \frac{1}{2m} \left( \frac{\hat{L}_z}{R} - q \frac{\mathcal{B}R}{2} \right)^2 - \gamma \mathcal{B} \hat{S}_z,$$

where  $\gamma$  is the gyromagnetic ratio of the particle.

As the Hamiltonian shows, in this system, the orbital and spin degrees of freedom both interact with the external magnetic field, but not with each other. Moreover, each of the involved operators  $\hat{L}_z$  and  $\hat{S}_z$  commutes with this Hamiltonian, and hence their eigenstates (in the corresponding Hilbert spaces) are eigenstates of the total Hamiltonian as well. As a result, the total energy of the system is just the sum of the independent contributions from these two parts of the Hamiltonian, with the observables  $S_z$  and  $L_z$  quantized independently in accordance with Eqs. (5.169) and (5.177):

$$E = \frac{1}{2m} \left( \frac{\hbar m_l}{R} - q \frac{\mathcal{B}R}{2} \right)^2 - \gamma \mathcal{B} \hbar m_s, \quad \text{with } m_l = 0, \pm 1, \pm 2, \dots, \text{ and } -s \leq m_s \leq +s. \quad (*)$$

This expression shows that each orbital level (with a particular magnetic quantum number  $m_l$ ) is split into  $(2s + 1)$  equidistant spin sub-levels numbered by the spin magnetic number  $m_s$ .

For an electron,  $q = -e$ ,  $\gamma = \gamma_e \equiv qg_e/2m_e \approx -e/m_e$ ,  $m_s = \pm 1/2$ , so Eq. (\*) may be well approximated as

$$E \approx \frac{1}{2m_e} \left( \frac{\hbar m_l}{R} + \frac{e\mathcal{B}R}{2} \right)^2 \pm \frac{e\mathcal{B}\hbar}{2m_e} \equiv \frac{\hbar^2 m_l^2}{2m_e R^2} + \frac{e\hbar}{2m_e} (m_l \pm 1) \mathcal{B} + \frac{e^2 \mathcal{B}^2 R^2}{8m_e}.$$

The first term of the last expression is the electron's quantized kinetic energy in the absence of a magnetic field, while the next two terms describe the field's effects. The second term, linear in  $\mathcal{B}$  and hence dominating in weak fields (with the magnetic flux  $\Phi \equiv \pi R^2 |\mathcal{B}|$  through the circle's area much smaller than the "normal" field quantum  $\Phi_0' \equiv 2\pi\hbar/e$ ), may be interpreted as a result of the field's interaction with the pre-existing magnetic moment of the system, with the normal ( $z$ -) component

$$m_z = -\frac{e\hbar}{2m_e} (m_l \pm 1) \equiv -\frac{e}{2m_e} (L_z + 2S_z).$$

This double contribution of the electron's spin to the magnetic moment, and hence to its interaction with the external magnetic field, is responsible for all the intricacies of the Zeeman effect – see Sec. 6.4 of the lecture notes.

Finally, the last term of Eq. (\*), quadratic in  $\mathcal{B}$  and hence dominating at  $\Phi \gg \Phi_0'$ , describes the essentially classical (and hence independent of both quantum numbers) effect of the orbital diamagnetism of the system, i.e. the energy of the field's interaction with the magnetic moment it has induced.<sup>72</sup>

Note also a close similarity between this problem and Problem 50.

<sup>72</sup> See, e.g., EM Sec. 5.5 – in particular the model solution of EM Problem 5.18(i), with the appropriate replacement  $\langle x^2 \rangle + \langle y^2 \rangle \rightarrow R^2$ .

## Chapter 6. Perturbative Approaches

**Problem 6.1.** Use Eq. (6.14) of the lecture notes to prove the following general form of the Hellmann-Feynman theorem:<sup>73</sup>

$$\frac{\partial E_n}{\partial \lambda} = \langle n | \frac{\partial \hat{H}}{\partial \lambda} | n \rangle,$$

where  $\lambda$  is an arbitrary  $c$ -number parameter.

*Solution:* In the basic Eq. (6.1), let us take

$$\hat{H}^{(0)} = \hat{H} \Big|_{\lambda=\lambda_0}, \quad \hat{H}^{(1)} = \frac{\partial \hat{H}}{\partial \lambda} \Big|_{\lambda=\lambda_0} (\lambda - \lambda_0),$$

where  $\lambda_0$  is arbitrary but the difference  $(\lambda - \lambda_0)$  is small. In the first approximation in this difference, the eigenenergy perturbation may be also expressed by the linear term of the Taylor series:

$$E_n(\lambda) - E_n(\lambda_0) = E^{(1)} = \frac{\partial E_n}{\partial \lambda} \Big|_{\lambda=\lambda_0} (\lambda - \lambda_0).$$

Plugging these relations into Eq. (6.14), with  $n^{(0)}$  being the eigenstate  $n$  at  $\lambda = \lambda_0$ , we get the Hellmann-Feynman theorem at this particular value of  $\lambda$  (which, again, is arbitrary).

As was discussed in the solution of Problem 3.43, this theorem may be used, for example, for the proof of the first of Eqs. (3.211).

**Problem 6.2.** Establish a relation between Eq. (6.16) of the lecture notes and the result of the classical theory of weakly anharmonic (“nonlinear”) oscillations at negligible damping.

*Hint:* You may like to use N. Bohr’s reasoning that was discussed in Problem 1.1.

*Solution:* Following N. Bohr’s arguments, let us use Eqs. (2.262) and (6.16) to calculate the frequency of quantum transitions between the adjacent high energy levels of the anharmonic oscillator ( $n \gg 1$ ):

$$\omega \equiv \frac{1}{\hbar} (E_{n+1} - E_n) \approx \frac{1}{\hbar} \frac{dE_n}{dn} \approx \frac{1}{\hbar} \frac{d(E_n^{(0)} + E_n^{(1)})}{dn} = \omega_0 + \frac{3}{2} \frac{\beta x_0^4}{\hbar} (2n + 1).$$

Since the correction to the frequency  $\omega_0$  is already proportional to the small parameter  $\beta$ , we may combine this result with the expression for the effective real amplitude  $A$  of the coordinate’s sinusoidal oscillations, defined as

$$\frac{A^2}{2} \equiv \langle x^2 \rangle,$$

by using the unperturbed expression (5.95). This gives  $A^2 = x_0^2(2n + 1)$ , so we may write

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<sup>73</sup> As a reminder, proof of its wave-mechanics form was the task of Problem 1.7.



$$\omega \approx \omega_0 + \frac{3}{2} \frac{\beta x_0^2}{\hbar} A^2 \equiv \omega_0 + \frac{3}{2} \frac{\beta}{m\omega_0} A^2. \quad (*)$$

On the other hand, the classical theory of weakly nonlinear oscillations at negligible damping, described by the differential equation<sup>74</sup>

$$\ddot{x} + \omega_0^2 x = \alpha_{\text{cl}} x^3, \quad (**)$$

gives the following approximate (but at  $\alpha_{\text{cl}} \rightarrow 0$ , asymptotically correct) expression for the oscillation frequency as a function of the amplitude  $A$  of nearly-sinusoidal oscillations  $x(t)$ :<sup>75</sup>

$$\omega \approx \omega_0 - \frac{3}{8} \frac{\alpha_{\text{cl}}}{\omega_0} A^2. \quad (***)$$

In order to reveal the relation between the coefficients  $\alpha_{\text{cl}}$  and  $\beta$ , let us write the classical Lagrangian function corresponding to the Hamiltonian (6.2) with  $\alpha = 0$ :

$$L \equiv T - U = \frac{m\dot{x}^2}{2} - \left( \frac{m\omega_0^2}{2} x^2 + \beta x^4 \right).$$

The corresponding Lagrange equation of motion is

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = 0, \quad \text{giving } m\ddot{x} + m\omega_0^2 x + 4\beta x^3 = 0.$$

The comparison of this equation and Eq. (\*\*) shows that they coincide if  $\alpha_{\text{cl}} = -4\beta/m$ . But with this substitution, Eq. (\*\*\*) exactly coincides with Eq. (\*).

So, in the limit  $n \rightarrow \infty$ , the quantum and classical theories yield the same result – as they should by the correspondence principle.

**Problem 6.3.** An additional weak time-independent force  $F$  is exerted on a 1D particle that had been placed into a hard-wall potential well

$$U(x) = \begin{cases} 0, & \text{for } 0 < x < a, \\ +\infty, & \text{otherwise.} \end{cases}$$

Calculate, sketch, and discuss the 1<sup>st</sup>-order perturbation of its ground-state wavefunction.

*Solution:* The unperturbed wavefunctions and energy levels of the problem have been calculated in Sec. 1.7 of the lecture notes – see Eqs. (1.84)-(1.85); in the notation of Sec. 6.1:

$$\psi_n^{(0)} = \left( \frac{2}{a} \right)^{1/2} \sin \frac{\pi n x}{a}, \quad E_n^{(0)} = \frac{\pi^2 \hbar^2}{2m} n^2 \equiv E_1^{(0)} n^2, \quad \text{with } n = 1, 2, \dots$$

<sup>74</sup> See, e.g., CM Eq. (5.43) with  $\delta = 0$ ,  $f_0 = 0$ , and  $\omega \approx \omega_0$ , so  $\xi \equiv \omega - \omega_0 \approx (\omega - \omega_0)^2 / 2\omega_0$ . (The index “cl” is attached to the constant  $\alpha$  just to avoid any chance of confusion with that participating in Eq. (6.2) of the lecture notes of this, QM course.)

<sup>75</sup> See, e.g., CM Eq. (5.49).

The 1<sup>st</sup>-order perturbation of the ground-state wavefunction may be calculated using the coordinate representation of Eq. (6.18) with  $n = 1$  and the notation change  $n' \rightarrow n$ :

$$\psi_g^{(1)} \equiv \psi_g^{(1)} = \sum_{n=2}^{\infty} \frac{H_{1,n}^{(1)}}{E_1^{(0)} - E_n^{(0)}} \psi_n^{(0)}, \quad (*)$$

where  $H_{1,n}^{(1)}$  are the matrix elements (6.8) of the perturbation Hamiltonian  $\hat{H}^{(1)} = -Fx$ :

$$H_{1,n}^{(1)} \equiv \int \psi_1^{(0)*}(x) \hat{H}^{(1)} \psi_n^{(0)}(x) dx = -\frac{2F}{a} \int_0^a \sin \frac{\pi x}{a} x \sin \frac{\pi n x}{a} dx = -\frac{2F}{a} \left( \frac{a}{\pi} \right)^2 I,$$

where

$$I \equiv \int_0^{\pi} \xi \sin \xi \sin n \xi d\xi, \quad \text{and } \xi \equiv \frac{\pi x}{a}.$$

The last integral may be re-written using MA Eq. (3.3c):

$$I \equiv \int_0^{\pi} \xi \sin \xi \sin n \xi d\xi = \frac{I_- - I_+}{2}, \quad \text{where } I_{\pm} \equiv \int_0^{\pi} \xi \cos(n \pm 1) \xi d\xi.$$

Now the integrals  $I_{\pm}$  may be worked out by parts,

$$I_{\pm} = \int_{\xi=0}^{\xi=\pi} \xi \frac{d[\sin(n \pm 1)\xi]}{(n \pm 1)} = \left[ \xi \frac{\sin(n \pm 1)\xi}{(n \pm 1)} \right]_{\xi=0}^{\xi=\pi} - \frac{1}{(n \pm 1)} \int_0^{\pi} \sin(n \pm 1)\xi d\xi = \frac{1}{(n \pm 1)^2} [\cos(n \pm 1)\pi - 1],$$

so

$$I = \frac{1}{2} \left\{ \frac{1}{(n-1)^2} [\cos(n-1)\pi - 1] - \frac{1}{(n+1)^2} [\cos(n+1)\pi - 1] \right\} = -\frac{4n}{(n^2-1)^2} \times \begin{cases} 1, & \text{for } n \text{ even,} \\ 0, & \text{for } n \text{ odd.} \end{cases}$$

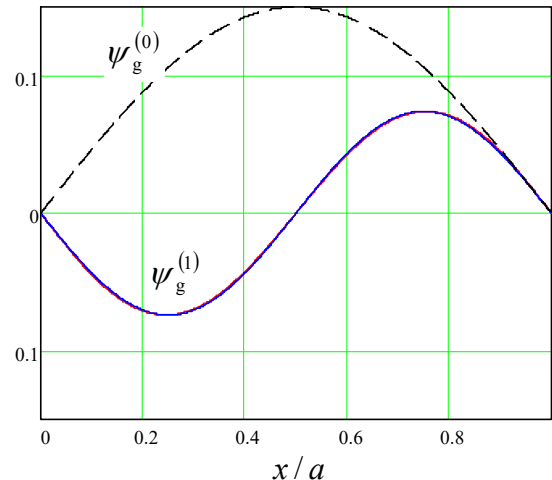
As a result, Eq. (\*) yields

$$\psi_g^{(1)} = -\frac{8}{\pi^2} \frac{Fa}{E_1^{(0)}} \sum_{n=2,4,\dots}^{\infty} \frac{n}{(n^2-1)^3} \psi_n^{(0)}. \quad (**)$$

The numerical fraction under the sum is a rapidly decreasing function of  $n$ : its first value, for  $n = 2$ , is  $2/27 \approx 0.0741$ , while the next nonvanishing value, for  $n = 4$ , is already  $4/512 \approx 0.0012$ . So, a very good approximation of the result is given by the first term alone:

$$\begin{aligned} \psi_g^{(1)} &\approx -\frac{8}{\pi^2} \frac{Fa}{E_1^{(0)}} \frac{2}{(2^2-1)^3} \psi_2^{(0)} \\ &= -\frac{32}{27\pi^4} \frac{Fa}{\hbar^2/m} \left( \frac{2}{a} \right)^{1/2} \sin \frac{2\pi x}{a}. \end{aligned} \quad (***)$$

The red line in the figure on the right shows this function, while the exact result (\*\*) is shown with the blue line. These lines virtually overlap, showing how good the approximation (\*\*\*) is. The dashed line in the same figure



shows (not to scale!) the unperturbed ground-state wavefunction  $\psi_g^{(0)} \equiv \psi_1^{(0)}$ . Sketching its sum with the small perturbation, we may see that the external force  $F$  shifts the total wavefunction in its direction (if  $F > 0$ , then to the right) – as it should. (A good additional exercise for the reader: use the above results to calculate the resulting shift of the expectation value  $\langle x \rangle$  from its unperturbed value  $a/2$ .)

One more additional exercise: calculate the corresponding shift of the ground state energy, in the first nonvanishing approximation.

**Problem 6.4.** A time-independent force  $\mathbf{F} = \mu(\mathbf{n}_x y + \mathbf{n}_y x)$ , where  $\mu$  is a small constant, is applied to a 3D isotropic harmonic oscillator of mass  $m$  and frequency  $\omega_0$ , located at the origin. Calculate, in the first order of the perturbation theory, the effect of the force upon the ground-state energy of the oscillator and its lowest excited energy level. How small should the constant  $\mu$  be for your results to be quantitatively correct?

*Solution:* Any potential force  $\mathbf{F} = \mathbf{F}(\mathbf{r})$  may be described by an additional potential energy  $U(\mathbf{r})$ , such that  $\mathbf{F} = -\nabla U$ . In our particular case, independent integrations of the force  $\mathbf{F}$  along each of the three coordinates yield the results

$$U = -\int F_x dx + f_1(y, z) = -\int \mu y dx + f_1(y, z) = -\mu xy + f_1(y, z),$$

$$U = -\int F_y dy + f_2(x, z) = -\int \mu x dy + f_2(x, z) = -\mu xy + f_2(x, z),$$

$$U = -\int F_z dz + f_3(x, y) = -\int 0 dz + f_3(x, y) = f_3(x, y),$$

which are compatible only if  $f_3(x, y) = -\mu xy + \text{const}$ , and  $f_1(y, z) = f_2(x, z) = \text{const}$ . Dropping this inconsequential constant, we may use the resulting  $U$  as the perturbation Hamiltonian:

$$\hat{H}^{(1)} = -\mu xy. \quad (*)$$

As was discussed at the beginning of Sec. 3.5 of the lecture notes, unperturbed eigenstates of the 3D isotropic harmonic oscillator may be described by the products of the eigenfunctions of 1D similar harmonic oscillators:

$$\psi_{klm}^{(0)}(\mathbf{r}) = \psi_k(x)\psi_l(y)\psi_m(z),$$

with each of the indices  $\{k, l, m\}$  taking independent integer values 0, 1, 2, .... The corresponding unperturbed energies are

$$E_{klm}^{(0)} = \hbar\omega_0 \left( k + l + m + \frac{3}{2} \right),$$

so there is only one ground state with the wavefunction  $\psi_{000}$  and energy  $E_0 = (3/2)\hbar\omega_0$ , and three lowest excited states with the wavefunctions  $\psi_{100}$ ,  $\psi_{010}$ , and  $\psi_{001}$ , all three with the same energy  $E_1 = (5/2)\hbar\omega_0$ .

According to Eq. (2.275), the (non-degenerate) ground state of the oscillator is described by an even function of all its arguments:

$$\psi_{000}^{(0)}(\mathbf{r}) = \psi_0(x)\psi_0(y)\psi_0(z) \propto \exp\left\{-\frac{x^2 + y^2 + z^2}{2x_0^2}\right\}, \quad \text{with } x_0 \equiv \left(\frac{\hbar}{m\omega_0}\right)^{1/2},$$

so the first-order shift (6.14) of its energy,

$$E_{000}^{(1)} = \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \int_{-\infty}^{+\infty} dz \psi_{000}^{(0)*}(\mathbf{r}) \hat{H}^{(1)} \psi_{000}^{(0)}(\mathbf{r}),$$

vanishes for the perturbation (\*), which is an odd function of  $x$  and  $y$ . Similarly, all *diagonal* matrix elements (6.8) for the lowest excited states also vanish because each of  $\psi_{100}$ ,  $\psi_{010}$ , and  $\psi_{001}$  is an odd function of one coordinate, but an even function of the other two coordinates. For example, according to Eqs. (2.282) and (2.284),

$$\psi_{100}(\mathbf{r}) = \psi_1(x)\psi_0(y)\psi_0(z) = \frac{1}{\sqrt{2}} \frac{2x}{\pi^{3/4} x_0^{3/2}} \exp\left\{-\frac{x^2 + y^2 + z^2}{2x_0^2}\right\},$$

so

$$E_{100}^{(1)} = \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \int_{-\infty}^{+\infty} dz \psi_{100}^{(0)*}(\mathbf{r}) \hat{H}^{(1)} \psi_{100}^{(0)}(\mathbf{r}) \propto \int_{-\infty}^{+\infty} y \exp\left\{-\frac{y^2}{x_0^2}\right\} dy = 0,$$

and similarly for two other eigenstates. However, since the excited eigenstates are degenerate, the *off-diagonal* matrix elements are also important, and one pair of these elements (not involving the eigenfunction  $\psi_{001}$ ) is different from zero. For example,

$$\begin{aligned} H_{100,010}^{(1)} &\equiv \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \int_{-\infty}^{+\infty} dz \psi_{100}^{(0)*}(\mathbf{r}) \hat{H}^{(1)} \psi_{010}^{(0)}(\mathbf{r}) \\ &= -\mu \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \int_{-\infty}^{+\infty} dz \psi_1^*(x) \psi_0^*(y) \psi_1^*(z) xy \psi_0(x) \psi_1(y) \psi_0(z) \\ &= -\mu \frac{1}{2\pi^{3/2} x_0^3} \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \int_{-\infty}^{+\infty} dz xy \frac{2x}{x_0} \frac{2y}{x_0} \exp\left\{-\frac{x^2 + y^2 + z^2}{x_0^2}\right\} \\ &= -\mu \frac{2x_0^2}{\pi^{3/2}} \left( \int_{-\infty}^{+\infty} \xi^2 \exp\{-\xi^2\} d\xi \right)^2 \left( \int_{-\infty}^{+\infty} \exp\{-\xi^2\} d\xi \right). \end{aligned}$$

These are two standard Gaussian integrals<sup>76</sup> equal, respectively, to  $\pi^{1/2}/2$  and  $\pi^{1/2}$ , so

$$H_{100,010}^{(1)} = -\frac{\mu x_0^2}{2} \equiv -\frac{\mu \hbar}{2m\omega_0},$$

and absolutely similarly for  $H_{010,100}^{(1)}$ .

Hence the characteristic equation (6.26) for the states  $\{100\}$  and  $\{010\}$  has the form

$$\begin{vmatrix} H_{100,100}^{(1)} - E^{(1)} & H_{010,100}^{(1)} \\ H_{100,010}^{(1)} & H_{010,010}^{(1)} - E^{(1)} \end{vmatrix} \equiv \begin{vmatrix} -E^{(1)} & -\mu \hbar / 2m\omega_0 \\ -\mu \hbar / 2m\omega_0 & -E^{(1)} \end{vmatrix} = 0,$$

and has two roots

$$E_{\pm}^{(1)} = \pm \frac{\mu \hbar}{2m\omega_0}. \quad (**)$$

<sup>76</sup> See, e.g., MA Eq. (6.9).

Their difference describes lifting the degeneracy of these two states, while the state  $\{001\}$  is not involved in the interaction, and its energy is not changed.

The above calculation is asymptotically exact if the energy correction (\*\*\*) is much smaller than the basic level spacing  $\hbar\omega_0$ :

$$\left| \frac{\mu\hbar}{2m\omega_0} \right| \ll \hbar\omega_0, \quad \text{i.e. if } |\mu| \ll 2m\omega_0^2.$$

Note the Planck constant has dropped from this condition, so it has a classical character. This happens because the perturbation (\*) is a quadratic form of the coordinates, just as the unperturbed potential energy of the oscillator,

$$U^{(0)} = \frac{m\omega_0^2}{2}(x^2 + y^2 + z^2),$$

so the relation of their magnitudes does not depend on the oscillator's quantum length scale  $x_0$ . This fact also enables an easy exact solution of this problem, similar to that of Problem 3.20. The reader is recommended to carry out this solution and compare its result with Eq. (\*\*).

**Problem 6.5.** A 1D particle of mass  $m$  is localized in a very short potential well that may be approximated with a delta function:

$$U(x) = -w\delta(x), \quad \text{with } w > 0.$$

Calculate the change of its ground state energy by an additional weak time-independent force  $F$ , in the first nonvanishing approximation of the perturbation theory. Discuss the limits of validity of this result, taking into account that at  $F \neq 0$ , the localized state of the particle is metastable.

*Solution:* As was discussed at the beginning of Sec. 2.6 of the lecture notes (see also Sec. 6.6), the unperturbed Hamiltonian of this system has just one localized state – with a negative energy

$$E_g^{(0)} = -\frac{\hbar^2 \kappa^2}{2m} = -\frac{m w^2}{2\hbar^2},$$

and an exponentially decaying wavefunction

$$\psi_g^{(0)} = \kappa^{1/2} e^{-\kappa|x|}, \quad \text{where } \kappa = \frac{m w}{\hbar^2}.$$

Treating the force  $F$  as a perturbation, with

$$\hat{H}^{(1)} = -Fx, \quad (*)$$

we immediately see from Eq. (6.14) that the first-order correction to the ground state energy vanishes, because the function under the corresponding integral is odd:

$$E_g^{(1)} = \langle \mathbf{g}^{(0)} | \hat{H}^{(1)} | \mathbf{g}^{(0)} \rangle = \int_{-\infty}^{+\infty} \psi_g^{(0)*} \hat{H}^{(1)} \psi_g^{(0)} dx = -F\kappa \int_{-\infty}^{+\infty} x e^{-\kappa|x|} dx = 0.$$

Hence, we need to proceed to the 2<sup>nd</sup> order perturbation (6.20), which includes all unperturbed states:

$$E_g^{(2)} \equiv E_0^{(2)} = \sum_{n \neq 0} \frac{|H_{n0}^{(1)}|^2}{E_0^{(0)} - E_n^{(0)}}. \quad (**)$$

At this point, we need to notice that the unperturbed system has a continuum of positive-energy eigenstates, with energies

$$E_n^{(0)} = \frac{\hbar^2 k_n^2}{2m}.$$

As was discussed in Sec. 6.6 of the lecture notes, the only consequential states of this set, with eigenfunctions

$$\psi_n^{(0)} = \left(\frac{2}{l}\right)^{1/2} \sin k_n x,$$

where  $l \gg 1/\kappa$ ,  $1/k_n$  is the length of the artificial normalization segment, are not affected by the delta-functional potential of the well. The matrix elements we need,

$$H_{n0}^{(1)} \equiv \langle n^{(0)} | \hat{H}^{(1)} | g^{(0)} \rangle = \int_{-\infty}^{+\infty} \psi_n^{(0)*} \hat{H}^{(1)} \psi_g^{(0)} dx = -2F \left(\frac{2\kappa}{l}\right)^{1/2} \frac{2\kappa k_n}{(\kappa^2 + k_n^2)^2},$$

were also calculated in Sec. 6.6. (The factor-of-two difference between the above expression and Eq. (6.130) is due to the similar difference between the operator  $\hat{H}^{(1)}$  given by Eq. (\*), and the operator  $\hat{A}$  defined by Eq. (6.123) of the lecture notes.) As a result, Eq. (\*\*) yields

$$E_g^{(2)} = \sum_{n \neq 0} \frac{|H_{n0}^{(1)}|^2}{E_0^{(0)} - E_n^{(0)}} = -\frac{64mF^2\kappa^3}{\hbar^2 l} \sum_{n>0} \frac{k_n^2}{(\kappa^2 + k_n^2)^5}.$$

In the limit  $\kappa l \rightarrow \infty$ , the distance between the adjacent values of  $k_n$  becomes much less than  $\kappa$ , so using the density of the final states (see Eq. (1.93) and also Sec. 6.6):

$$\frac{dn}{dk_n} = \frac{l}{2\pi},$$

the sum over  $n$  may be well approximated by the corresponding integral:<sup>77</sup>

$$E_g^{(2)} = -\frac{64mF^2\kappa^3}{\hbar^2 l} \int_0^\infty \frac{k_n^2}{(\kappa^2 + k_n^2)^5} dn = -\frac{64mF^2\kappa^3}{\hbar^2 l} \int_0^\infty \frac{k_n^2}{(\kappa^2 + k_n^2)^5} \frac{dn}{dk_n} dk_n = -\frac{32mF^2}{\pi \hbar^2 \kappa^4} I, \quad (***)$$

where

$$I \equiv \int_0^\infty \frac{\xi^2 d\xi}{(1 + \xi^2)^5}, \quad \text{with } \xi \equiv \frac{k_n}{\kappa}.$$

The dimensionless integral  $I$  may be worked out, for example, by reducing it to a table one by *integration over a parameter* – the trick so simple and so frequently used that, as an exception, I will

<sup>77</sup> This cancellation of the artificial length  $l$  is a necessary condition of the correctness of such a normalization procedure.

demonstrate it here – despite all my focus on physics rather than math. Let us define the following function:

$$J(\lambda) \equiv \int_0^{\infty} \frac{d\zeta}{(1 + \lambda\zeta^2)^4}.$$

Then, on one hand, we may write

$$\frac{dJ}{d\lambda} = \int_0^{\infty} \frac{\partial}{\partial \lambda} \left[ \frac{1}{(1 + \lambda\zeta^2)^4} \right] d\zeta = -4 \int_0^{\infty} \frac{\zeta^2 d\zeta}{(1 + \lambda\zeta^2)^5}, \quad \text{so our } I = -\frac{1}{4} \frac{dJ}{d\lambda} \Big|_{\lambda=1}.$$

On the other hand, introducing a new integration variable  $\xi \equiv \lambda^{1/2} \zeta$ , so  $d\zeta = \lambda^{-1/2} d\xi$  and  $\lambda\zeta^2 = \xi^2$ ,  $J(\lambda)$  may be readily reduced to a well-known table integral<sup>78</sup>:

$$J(\lambda) \equiv \int_0^{\infty} \frac{d\zeta}{(1 + \lambda\zeta^2)^4} = \lambda^{-1/2} \int_0^{\infty} \frac{d\xi}{(1 + \xi^2)^4} = \lambda^{-1/2} \frac{\pi}{2} \cdot \frac{1 \cdot 3 \cdot 5}{2 \cdot 4 \cdot 6} \equiv \frac{5\pi}{32} \lambda^{-1/2},$$

so

$$\frac{dJ}{d\lambda} = -\frac{5\pi}{64} \lambda^{-3/2},$$

and, finally, the integral we need is

$$I = -\frac{1}{4} \frac{dJ}{d\lambda} \Big|_{\lambda=1} = -\frac{1}{4} \cdot \left( -\frac{5\pi}{64} \right) \equiv \frac{5\pi}{256}.$$

With this, Eq. (\*\*\*) yields the following final result for the ground-state energy's shift:

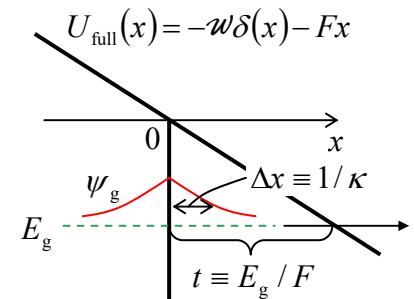
$$E_g^{(2)} = -\frac{32mF^2}{\pi\hbar^2\kappa^4} \cdot \frac{5\pi}{256} \equiv -\frac{5mF^2}{8\hbar^2\kappa^4}.$$

As was discussed in Sec. 6.1 of the lecture notes, the necessary condition of the perturbation theory's validity is that this shift is much smaller than the unperturbed energy. In our case, this condition, apart from numerical factors of the order of 1, reads

$$\frac{mF^2}{\hbar^2\kappa^4} \ll \frac{\hbar^2\kappa^2}{m}, \quad \text{giving } \frac{|F|}{\kappa} \ll \frac{\hbar^2\kappa^2}{m}, \quad \text{i.e. } |F|\Delta x \ll |E_g|, \quad \text{where } \Delta x \equiv \frac{1}{\kappa}. \quad \text{(***)}$$

The physics of the last condition is very clear: the potential work of the force  $F$  moving the particle within the localization region, of the effective width  $\Delta x = 1/\kappa$ , has to be much smaller than the unperturbed energy of the localized state.

Now let us discuss whether this condition is affected by one more feature of this system: as the figure on the right shows, for any  $F \neq 0$ , the localized state is separated from the continuum of states with  $E > U_{\text{full}}(x)$  by a triangular potential barrier of the height  $|E_g|$  and the width  $t = |E_g/F|$ , so the state is metastable, with a finite lifetime  $\tau$ . The calculation of this lifetime, within the modified WKB approximation, was the subject of Problem 2.18, and the result was



<sup>78</sup> See, e.g., MA Eq. (6.5b) with  $n = 4$ .

$$\tau = \frac{\hbar^3}{m\omega^2} \exp\left\{\frac{2m^2\omega^3}{3\hbar^4|F|}\right\}.$$

As was discussed in Sec. 2.5 of the lecture notes, the very notion of the energy of such a metastable state lifetime is well defined only if its lifetime is much longer than the attempt time's scale  $t_a \sim \hbar/|E_g| = 2\hbar^3/m\omega^2$ . This condition is satisfied if the above exponent is much larger than 1, i.e. if

$$|F| \ll \frac{m^2\omega^3}{\hbar^4}.$$

But given the above relation between  $\omega$  and  $\kappa$ , this is the same condition as given by Eq. (\*\*\*)<sup>79</sup>. Hence, the ground state's metastability does not affect the above result for its energy – within the range (\*\*\*) of validity of the perturbative approach to the problem.

Note also the ground-state energy shift calculated above is quadratic rather than exponential in  $F$ , and hence (in our small-force approximation) is much larger than the energy's uncertainty  $\hbar/\tau$ .

**Problem 6.6.** Use Eq. (6.16) of the lecture notes to calculate the eigenvalues of the operator  $\hat{L}^2$ , in the limit  $|m| \approx l \gg 1$ , by purely wave-mechanical means.

*Hint:* You may like to use the following substitution:  $\Theta(\theta) = f(\theta)/\sin^{1/2}\theta$ .

*Solution:* According to Eqs. (5.146) and (5.166) of the lecture notes, in the coordinate representation, the eigenproblem for the operator  $\hat{L}^2$  may be reduced to solving the following equation,

$$\hbar^2 \left[ -\frac{1}{\sin\theta} \frac{d}{d\theta} \left( \sin\theta \frac{d\Theta}{d\theta} \right) + \frac{m^2}{\sin^2\theta} \Theta \right] = L^2 \Theta,$$

for the polar-angle factor  $\Theta(\theta)$  of the eigenfunction. Here  $L^2$  is the (at this stage, unknown) eigenvalue of the operator, and  $m$  is the “magnetic” quantum number.

Plugging in the substitution suggested in the *Hint*, and multiplying all terms by  $(\sin^{1/2}\theta)/\hbar^2$ , we get the following differential equation for the new function  $f(\theta)$ :

$$-\frac{d^2 f}{d\theta^2} + u(\theta)f = \varepsilon f, \quad \text{where } u(\theta) \equiv \left( \frac{m^2 - 1/4}{\sin^2\theta} - \frac{1}{4} \right) \text{ and } \varepsilon \equiv \frac{L^2}{\hbar^2}. \quad (*)$$

The structure of this equation is the same as of the Schrödinger equation for a 1D particle, with the function  $u(\theta)$  playing the role of the effective potential energy. At  $m^2 \gg 1$ , this function has a deep minimum at  $\theta \approx \pi/2$ , so the lowest-energy wavefunctions of the system are localized near this minimum. To calculate these eigenfunctions (and corresponding eigenvalues  $\varepsilon$ ), we may approximate the effective potential energy by Taylor-expanding the function  $u(\theta)$  with respect to the small deviation

$$\tilde{\theta} \equiv \theta - \frac{\pi}{2}, \quad \text{so } \sin^2\theta = \cos^2\tilde{\theta},$$

and keeping only the leading terms of this expansion:

<sup>79</sup> Note that this condition may be also written in another, very intuitive form:  $t \gg \Delta x$  – see the figure above.



$$u(\theta) \equiv -\frac{1}{4} + \left(m^2 - \frac{1}{4}\right) \frac{1}{\cos^2 \tilde{\theta}} \approx -\frac{1}{4} + \left(m^2 - \frac{1}{4}\right) \left(1 + \tilde{\theta}^2 + \frac{2}{3} \tilde{\theta}^4\right), \quad \text{for } |\tilde{\theta}| \ll 1.$$

In this approximation, Eq. (\*) takes the form

$$-\frac{d^2 f}{d\theta^2} + \left[ \left(m^2 - \frac{1}{4}\right) \tilde{\theta}^2 + \frac{2}{3} \left(m^2 - \frac{1}{4}\right) \tilde{\theta}^4 \right] f = \left(\varepsilon - m^2 + \frac{1}{2}\right) f,$$

so it is similar to the Schrödinger equation,<sup>80</sup>

$$-\frac{\hbar^2}{2m_{\text{ef}}} \frac{d^2 \psi}{dx^2} + \left( \frac{m_{\text{ef}} \omega_{\text{ef}}^2}{2} x^2 + \alpha_{\text{ef}} x^3 + \beta_{\text{ef}} x^4 \right) \psi = E_{\text{ef}} \psi,$$

of the anharmonic oscillator described by the Hamiltonian (6.2), and fully coincides with it if we take

$$\begin{aligned} m_{\text{ef}} &= \frac{\hbar^2}{2}, & \frac{m_{\text{ef}} \omega_{\text{ef}}^2}{2} &= m^2 - \frac{1}{4} \approx m^2, & \text{so } \hbar \omega_{\text{ef}} &\approx 2|m|, \\ \alpha_{\text{ef}} &= 0, & \beta_{\text{ef}} &= \frac{2}{3} \left(m^2 - \frac{1}{4}\right) \approx \frac{2}{3} m^2, & \text{and } E_{\text{ef}} &= \varepsilon - m^2 + \frac{1}{2}, \end{aligned} \quad (**)$$

where the approximations are justified by our initial assumption  $m^2 \gg 1$ . According to Eq. (6.16) of the lecture notes, with  $x_0 \equiv (\hbar/m_{\text{ef}}\omega_{\text{ef}})^{1/2}$ , in the 1<sup>st</sup>-order of the perturbation theory, the energy spectrum of such an oscillator is

$$E_{\text{ef}} = E_n^{(0)} + E_n^{(1)} = \hbar \omega_{\text{ef}} \left(n + \frac{1}{2}\right) + \frac{3}{4} \beta_{\text{ef}} \frac{\hbar^2}{m_{\text{ef}}^2 \omega_{\text{ef}}^2} (2n^2 + 2n + 1),$$

with  $n$  taking values 0, 1, 2, ... Plugging into this expression the effective oscillator's parameters (\*\*), we get a surprisingly simple result:

$$\varepsilon \equiv E_{\text{ef}} + m^2 - \frac{1}{2} = m^2 + 2|m|n + |m| + n^2 + n \equiv (|m| + n)(|m| + n + 1),$$

Now taking the sum  $|m| + n$ , which can take integer values  $|m|$ ,  $|m| + 1$ ,  $|m| + 2$ , ..., for a new quantum number  $l$ , we get the result,

$$L^2 \equiv \hbar^2 \varepsilon = \hbar^2 l(l+1), \quad (***)$$

which coincides with Eq. (5.163).

The above derivation of this formula is valid only if the height,  $\hbar \omega_{\text{ef}}(n + \frac{1}{2}) = |m|(2n + 1)$ , of the  $n^{\text{th}}$  energy level of the effective oscillator, over the bottom of the potential well  $u(\theta)$ , is much smaller than its depth  $\sim m^2$ , i.e. only if

$$1, n \ll |m|,$$

so  $l \equiv |m| + n$  is relatively close to  $|m|$ :  $l - |m| \ll |m|$ . As was shown in Sec. 5.6 of the lecture notes, operator methods allow a derivation of Eq. (\*\*\*) more easily, and for arbitrary  $m$  and  $l$ . However, the above calculation has its value, at least because it illuminates, from one more standpoint, the notorious difference between the square of the largest eigenvalue of the observable  $L_z$ , equal to  $\hbar^2(m^2)_{\text{max}} = \hbar^2 l^2$ ,

<sup>80</sup> Let me hope that the subscript “ef” excludes any possibility of confusion between the effective mass and the magnetic quantum number.

and that of  $L^2$ , equal to  $\hbar^2 l(l+1) \geq \hbar^2 l^2$ , which was repeatedly discussed in the lecture notes. Indeed, in the picture developed above, this difference is due to the nonvanishing spread, even at  $n=0$  (i.e. at  $|m|=l \equiv m_{\max}$ ), of the function  $f(\theta)$ , and hence of the probability to find the system near the point  $\theta = \pi/2$ .<sup>81</sup> As a result of this spread, the angular momentum vector  $\mathbf{L}$  is never definitely directed along the  $z$ -axis, so the expectation values of  $L_x^2$  and  $L_y^2$  do not vanish even at  $m = \pm l$ , making  $L^2 = L_x^2 + L_y^2 + L_z^2$  larger than  $L_z^2$ .

**Problem 6.7.** In the lowest nonvanishing order of the perturbation theory, calculate the shift of the ground-state energy of an electrically charged spherical rotor (i.e. a particle of mass  $m$ , free to move over a spherical surface of radius  $R$ ) due to a weak uniform time-independent electric field  $\mathcal{E}$ .

*Solution:* As was discussed in Sec. 6.2 of the lecture notes, in the coordinate representation with the  $z$ -axis directed along the applied field, the field-induced perturbation Hamiltonian is proportional to the cosine of the polar angle  $\theta$ , and is independent of the azimuthal angle  $\varphi$ :

$$\hat{H}^{(1)} = -q\mathcal{E}z = -q\mathcal{E}R \cos \theta, \quad (*)$$

where  $q$  is the rotor's electric charge. On the other hand, as was discussed in Sec. 3.6 of the lecture notes, the unperturbed ground-state wavefunction of the rotor is independent of both angles:

$$\psi_g^{(0)}(\theta, \varphi) = Y_0^0(\theta, \varphi) = \frac{1}{(4\pi)^{1/2}} = \text{const.}$$

As a result, the 1<sup>st</sup>-order correction (6.14) to the ground-state energy vanishes:

$$E_g^{(1)} = H_{gg}^{(1)} \equiv \langle g^{(0)} | \hat{H}^{(1)} | g^{(0)} \rangle \equiv \int_0^{2\pi} d\varphi \int_0^\pi \sin \theta d\theta \psi_g^{(0)*} \hat{H}^{(1)} \psi_g^{(0)} = -\frac{q\mathcal{E}R}{2} \int_0^\pi \cos \theta \sin \theta d\theta = 0.$$

In the expression for the 2<sup>nd</sup>-order correction, which follows from Eq. (6.20),

$$E_g^{(2)} = \sum_{n \neq g} \frac{|H_{gn}^{(1)}|^2}{E_g^{(0)} - E_n^{(0)}} = \sum_{n \neq g} \frac{1}{E_g^{(0)} - E_n^{(0)}} \left| \int_0^{2\pi} d\varphi \int_0^\pi \sin \theta d\theta \psi_n^{(0)*} (-q\mathcal{E}R \cos \theta) Y_0^0(\theta) \right|^2, \quad (**)$$

where, per Eq. (3.163) with  $l=0$ ,  $E_g^{(0)} = 0$ . Since, according to Eq. (3.175),  $Y_0^0(\theta, \varphi) = \text{const}$ ,  $\cos \theta$  is proportional to another spherical harmonic:

$$Y_1^0(\theta, \varphi) = \left( \frac{3}{4\pi} \right)^{1/2} \cos \theta,$$

and the spherical harmonics are orthogonal in the sense of Eq. (3.173), the only nonvanishing contribution to the sum in Eq. (\*\*) comes from the wavefunction  $\psi_n^{(0)}$  that is equal to the same  $Y_1^0(\theta, \varphi)$ , corresponding to the eigenenergy (3.163) with  $l=1$ :

$$E_1^{(0)} = \frac{\hbar^2}{mR^2}.$$

<sup>81</sup> Besides analytical results, this spread is clearly visible on the rightmost and leftmost plots in Fig. 3.20 of the lecture notes.

With these substitutions, Eq. (\*\*) yields

$$\begin{aligned} E_g^{(2)} &= \frac{1}{0 - \hbar^2 / mR^2} \left| \frac{q\mathcal{E}R}{(4\pi)^{1/2}} \int_0^{2\pi} d\varphi \int_0^\pi \sin\theta d\theta \left[ \left( \frac{3}{4\pi} \right)^{1/2} \cos\theta \right] \cos\theta \right|^2 = -\frac{3mR^2 (q\mathcal{E}R)^2}{4\hbar^2} \left| \int_0^\pi \cos^2\theta \sin\theta d\theta \right|^2 \\ &= -\frac{3mR^2 (q\mathcal{E}R)^2}{4\hbar^2} \left| \int_{-1}^1 \cos^2\theta d(\cos\theta) \right|^2 = -\frac{3mR^2 (q\mathcal{E}R)^2}{4\hbar^2} \left( \frac{2}{3} \right)^2 \equiv -\frac{(q\mathcal{E}R)^2}{3(\hbar^2/mR^2)} \equiv -\frac{(q\mathcal{E}R)^2}{3E_1^{(0)}}. \end{aligned}$$

Note that this energy shift is negative, as it should be for the 2<sup>nd</sup>-order correction to the ground state energy of any system – see the discussion in Sec. 6.1 of the lecture notes.

**Problem 6.8.** Use the perturbation theory to evaluate the effect of a time-independent uniform electric field  $\mathcal{E}$  on the ground-state energy  $E_g$  of a hydrogen atom. In particular:

- (i) calculate the 2<sup>nd</sup>-order shift of  $E_g$ , neglecting the extended unperturbed states with  $E > 0$ , and bring the result to the simplest analytical form you can,
- (ii) find the lower and the upper bounds on the shift, and
- (iii) discuss the simplest experimental manifestation of this *quadratic Stark effect*.

*Solutions:*

- (i) The perturbation Hamiltonian is the same as in the previous problem:

$$\hat{H}^{(1)} = -q\mathcal{E}r \cos\theta \equiv e\mathcal{E}r \cos\theta.$$

As was shown in Sec. 6.2 of the lecture notes, in this case, the diagonal element of the perturbation matrix (6.8), corresponding to the ground state of the atom (with the quantum numbers  $n = 1$ ,  $l = 0$ , and  $m = 0$ ), equals zero – see Eq. (6.34). Hence, according to Eq. (6.14), the 1<sup>st</sup>-order correction to the ground-state energy vanishes. To calculate its shift  $\Delta E_g$  in the 2<sup>nd</sup> order, we may use Eq. (6.20) of the lecture notes. For the hydrogen atom, neglecting the extended unperturbed states with  $E > 0$ , the summation index  $n'$  on the right-hand side of that relation should be understood as a shorthand for the set of quantum numbers  $n$ ,  $l$ , and  $m$  (with  $0 \leq l \leq n-1$ , and  $-l \leq m \leq +l$ ), so we may write

$$\Delta E_g = \sum_{n=2}^{\infty} \frac{1}{E_1^{(0)} - E_n^{(0)}} \sum_{l=0}^{n-1} \sum_{m=-l}^{+l} \left| \langle 1, 0, 0 | e\mathcal{E}r \cos\theta | n, l, m \rangle \right|^2, \quad (*)$$

where the unperturbed state vectors are denoted with the sets of their quantum numbers. Neglecting the small fine-structure effects discussed in Sec. 6.3, for the unperturbed eigenenergies, we may use Eq. (3.201) with  $E_0 = E_H$ , where  $E_H$  is the Hartree energy (1.13),

$$E_n^{(0)} = -\frac{E_H}{2n^2},$$

so the first fraction in Eq. (\*) is

$$\frac{1}{E_1^{(0)} - E_n^{(0)}} = -\frac{1}{E_H} \left( -\frac{1}{2} + \frac{1}{2n^2} \right)^{-1} \equiv -\frac{2}{E_H} \frac{n^2}{n^2 - 1}.$$

Plugging this expression, using Eqs. (3.171), (3.200) for the unperturbed wavefunctions of the atom, and taking into account that for  $n = 1$  and  $l = m = 0$ ,  $P_l^m(\cos\theta) = 1$  and  $e^{im\varphi} = 1$ , we may write

$$\Delta E_g = -\frac{2e^2\mathcal{E}^2}{E_H} \sum_{n=2}^{\infty} \frac{n^2}{n^2-1} \sum_{l=0}^{n-1} \left( \int_0^{\infty} \mathcal{R}_{n,l}(r) \mathcal{R}_{1,0}(r) r^3 dr \right)^2 \times \frac{(2l+1)}{4\pi} \sum_{m=-l}^{+l} \frac{(l-m)!}{(l+m)!} \left| \int_0^{\pi} P_l^m(\cos\theta) \cos\theta \sin\theta d\theta \int_0^{2\pi} e^{-im\varphi} d\varphi \right|^2.$$

This expression may be simplified because the integral over  $\varphi$  equals  $2\pi$  for  $m=0$  and vanishes for all other  $m$ , so the sum over  $m$  gives just one term:

$$\begin{aligned} \Delta E_g &= -\frac{2e^2\mathcal{E}^2}{E_H} \sum_{n=2}^{\infty} \frac{n^2}{n^2-1} \sum_{l=0}^{n-1} \left( \int_0^{\infty} \mathcal{R}_{n,l}(r) \mathcal{R}_{1,0}(r) r^3 dr \right)^2 \frac{(2l+1)}{2} \left| \int_0^{\pi} P_l^0(\cos\theta) \cos\theta \sin\theta d\theta \right|^2 \\ &\equiv -\frac{2e^2\mathcal{E}^2}{E_H} \sum_{n=2}^{\infty} \frac{n^2}{n^2-1} \sum_{l=0}^{n-1} \left( \int_0^{\infty} \mathcal{R}_{n,l}(r) \mathcal{R}_{1,0}(r) r^3 dr \right)^2 \frac{(2l+1)}{2} \left| \int_{-1}^{+1} P_l(\xi) \xi d\xi \right|^2, \end{aligned}$$

where  $P_l(\xi) = P_l^0(\xi)$  are the Legendre polynomials (3.165). Since per Eq. (3.167), the polynomials are orthonormal, and according to the second of Eqs. (3.166),  $\xi$  in the last integral may be considered  $P_1(\xi)$ , the sum over  $l$  also reduces to just one term, with  $l=1$ ,<sup>82</sup> giving

$$\begin{aligned} \Delta E_g &= -\frac{2e^2\mathcal{E}^2}{E_H} \sum_{n=2}^{\infty} \frac{n^2}{n^2-1} \left( \int_0^{\infty} \mathcal{R}_{n,1}(r) \mathcal{R}_{1,0}(r) r^3 dr \right)^2 \frac{(2 \cdot 1 + 1)}{2} \left| \int_{-1}^{+1} \xi^2 d\xi \right|^2 \\ &\equiv -\frac{4e^2\mathcal{E}^2}{3E_H} \sum_{n=2}^{\infty} \frac{n^2}{n^2-1} \left( \int_0^{\infty} \mathcal{R}_{n,1}(r) \mathcal{R}_{1,0}(r) r^3 dr \right)^2. \end{aligned}$$

(In accordance with a general remark made in Sec. 6.1 of the lecture notes, the 2<sup>nd</sup>-order correction to the ground state energy is negative.)

(ii) For finding the lower and upper bounds of the shift, we may notice that since the fraction under the sum changes only within a narrow interval,

$$1 < \frac{n^2}{n^2-1} \Big|_{n \geq 2} \leq \frac{4}{3}, \quad \text{i.e.} \quad \frac{2}{E_H} < \left| \frac{1}{E_1^{(0)} - E_n^{(0)}} \right|_{n \geq 2} \leq \frac{4}{3} \frac{2}{E_H},$$

Eq. (\*) may be used to get the following bounds for the energy shift magnitude:

$$\frac{2e^2\mathcal{E}^2}{E_H} \Sigma < |\Delta E_g| \leq \frac{4}{3} \frac{2e^2\mathcal{E}^2}{E_H} \Sigma,$$

where

$$\Sigma \equiv \sum_{\substack{n>1 \\ l=1, m=0}} \left| \langle 1,0,0 | r \cos\theta | n,l,m \rangle \right|^2 \equiv \sum_{\substack{n>1 \\ l=1, m=0}} \langle 1,0,0 | r \cos\theta | n,l,m \rangle \langle n,l,m | r \cos\theta | 1,0,0 \rangle.$$

<sup>82</sup> Such disappearance of all terms with  $m \neq 0$  and  $l \neq 1$  is one of the manifestations of the general quantum-transition selection rules, which were repeatedly discussed in this course – see, e.g., Problem 5.35.

This sum would not change if we add to it similar terms with  $n = 1$  (and hence with  $l = m = 0$ ) and with  $l \neq 1$  (and any  $n$  and  $m$ ), because, as was discussed above, these matrix elements equal zero. Hence we may write

$$\Sigma = \sum_{\substack{\text{all possible} \\ n,l,m}} \langle 1,0,0 | r \cos \theta | n,l,m \rangle \langle n,l,m | r \cos \theta | 1,0,0 \rangle.$$

But due to the completeness of the unperturbed state set, we may apply to this sum the closure condition (4.44), getting the following simple expression:

$$\Sigma = \langle 1,0,0 | (r \cos \theta)^2 | 1,0,0 \rangle \equiv \frac{1}{4\pi} \int_0^\infty \mathcal{R}_{1,0}^2(r) r^4 dr \int_0^\pi \cos^2 \theta \sin \theta d\theta \int_0^{2\pi} d\varphi,$$

Now using Eq. (3.208), variable replacements  $\zeta \equiv 2r/r_B$ ,  $\xi \equiv \cos \theta$ , and a table integral over  $\zeta$ ,<sup>83</sup> we get

$$\Sigma = \frac{1}{2} \frac{4}{r_B^3} \int_0^\infty e^{-2r/r_B} r^4 dr \int_{-1}^{+1} \cos^2 \theta d(\cos \theta) = \frac{1}{2} \frac{4}{r_B^3} \left( \frac{r_B}{2} \right)^5 \int_0^\infty e^{-\zeta} \zeta^4 d\zeta \int_{-1}^{+1} \xi^2 d\xi = \frac{1}{2} 4 \frac{1}{2^5} 4! \frac{2}{3} r_B^2 \equiv r_B^2,$$

so, finally, the 2<sup>nd</sup>-order correction is confined to a relatively narrow interval

$$2 \frac{e^2 \mathcal{E}^2 r_B^2}{E_H} < |\Delta E_g| \leq \frac{8}{3} \frac{e^2 \mathcal{E}^2 r_B^2}{E_H}. \quad (**)$$

Just for the reader's reference, the exact theory<sup>84</sup> gives a value,

$$\Delta E_g = -\frac{9}{4} \frac{e^2 \mathcal{E}^2 r_B^2}{E_H}, \quad (***)$$

indeed within the interval (\*\*).

(iii) The above result means that if the temperature is not extremely high, so an atom is reliably in its ground state, the change of its energy in the electric field is negative and proportional to  $\mathcal{E}^2$ . This fact may be expressed in the following traditional form:

$$\Delta E = -\alpha \frac{\mathcal{E}^2}{2}.$$

The most significant manifestation of this effect is that, according to the theory of electric polarization,<sup>85</sup> the coefficient  $\alpha$  in the last formula is just the *atomic* (or “molecular”) *polarizability*, which relates the induced dipole moment  $\mathbf{d}$  of an atom/molecule to the applied field,<sup>86</sup>

$$\mathbf{d} = \alpha \mathcal{E} \quad \text{so} \quad \Delta E = -\frac{\mathbf{d} \cdot \mathcal{E}}{2} = -\alpha \frac{\mathcal{E}^2}{2},$$

<sup>83</sup> See, e.g., MA Eq. (6.7d) with  $n = 4$ .

<sup>84</sup> See, e.g., A. Dalgarno and J. Lewis, *Proc. Roy. Soc.* **A233**, 70 (1956). This result may be also obtained using the 2<sup>nd</sup>-order perturbation theory but with the account of contributions from all extended states with  $E > 0$  – which turn out to be relatively small.

<sup>85</sup> See, e.g., EM Sec. 3.1, in particular, Eqs. (3.15b) and (3.48). (In that part of my series, following tradition, the electric dipole moment is denoted as  $\mathbf{p}$ , rather than  $\mathbf{d}$  as in this part.)

<sup>86</sup> Alternatively,  $\mathbf{d}$  may be calculated as the expectation value of  $q\mathbf{r} = -e\mathbf{r}$ , using the 1<sup>st</sup>-order approximation (6.18) for the state perturbations – giving the same result.

and hence determines the electric susceptibility  $\chi_e$  (and the dielectric constant  $\kappa \equiv 1 + \chi_e$ ) of a medium (e.g., of a gas) with a relatively low volumic density  $n$  of such atoms/molecules, making their interaction negligible:<sup>87</sup>

$$\chi_e = \frac{\alpha n}{\epsilon_0}, \quad \kappa = 1 + \frac{\alpha n}{\epsilon_0}.$$

According to Eq. (1.13), the Hartree energy may be represented as  $E_H = e^2/4\pi\epsilon_0 r_B$ , so  $e^2 r_B^2/E_H = 4\pi\epsilon_0 r_B^3$ , and Eq. (\*\*\*) may be rewritten as

$$\Delta E_g = -4\pi\epsilon_0 \left( \frac{9}{2} r_B^3 \right) \frac{\mathcal{E}^2}{2}.$$

This means that the atomic polarizability of the hydrogen atom, in its ground state, is

$$\alpha = 4\pi\epsilon_0 \frac{9}{2} r_B^3 \approx 4\pi\epsilon_0 (1.651 r_B)^3$$

– the result to be compared with  $\alpha = 4\pi\epsilon_0 R^3$  for a sphere of a hypothetical material that perfectly screens out the external electric field.<sup>88</sup> (Good metals do that, but only if  $R$  is much larger than  $r_B$  – see, e.g., EM Sec. 2.1.)

**Problem 6.9.** A particle of mass  $m$ , with electric charge  $q$ , is in its ground  $s$ -state with a given energy  $E_g < 0$ , being localized by a very-short-range, spherically symmetric potential well. Calculate its static electric polarizability.

*Solution:* As was discussed in the solution of the previous problem, the electric polarizability  $\alpha$  is directly related to the quadratic shift of the ground-state energy of the system, caused by a weak external electric field  $\mathcal{E}$ :

$$\Delta E_g = -\alpha \frac{\mathcal{E}^2}{2}.$$

(The linear shift, given by Eq. (6.14) of the lecture notes,

$$E_g^{(1)} = \int \psi_g^*(\mathbf{r}) \hat{H}^{(1)} \psi_g(\mathbf{r}) d^3r \propto \mathcal{E},$$

evidently vanishes for our perturbation Hamiltonian (6.29),

$$\hat{H}^{(1)} = -q\mathcal{E}z = -q\mathcal{E}r \cos\theta,$$

due to the spherical symmetry of the ground-state wavefunction  $\psi_g(\mathbf{r}) = \psi_g(r)$ .)

As Eq. (6.20) shows, to calculate  $\Delta E_g = E_g^{(2)}$ , we need to evaluate all matrix elements

$$H_{gn}^{(1)} = \int \psi_g^*(\mathbf{r}) \hat{H}^{(1)} \psi_n(\mathbf{r}) d^3r = -q\mathcal{E} \int \psi_g^*(r) r \cos\theta \psi_n(\mathbf{r}) d^3r = -q\mathcal{E} \oint d\Omega \int_0^\infty r^2 dr \psi_g^*(r) r \cos\theta \psi_n(\mathbf{r}).$$

<sup>87</sup> See, e.g., EM Eqs. (3.44) and (3.50).

<sup>88</sup> See, e.g., EM Eq. (3.11).

Since, according to Eqs. (3.166) and (3.171),  $\cos\theta$  may be represented as  $P_1^0(\cos\theta) \propto Y_1^0(\theta, \varphi)$ , and all spherical harmonics are orthogonal in the sense of Eq. (3.173), in our case only the wavefunctions with  $l = 1$  and  $m = 0$ ,

$$\psi_n(r) = \mathcal{R}_{1,k}(r) Y_1^0(\theta, \varphi) \equiv \mathcal{R}_{1,k}(r) \left( \frac{3}{4\pi} \right)^{1/2} \cos\theta, \quad (*)$$

give nonvanishing matrix elements of the perturbation Hamiltonian:

$$\begin{aligned} H_{gn}^{(1)} &= -q\mathcal{E} \left( \frac{3}{4\pi} \right)^{1/2} \oint \cos^2\theta d\Omega \int_0^\infty r^2 dr \psi_g^*(r) r \mathcal{R}_{1,k}(r) d^3r \\ &= -q\mathcal{E} \left( \frac{4\pi}{3} \right)^{1/2} \int_0^\infty r^2 dr \psi_g^*(r) r \mathcal{R}_{1,k}(r). \end{aligned} \quad (**)$$

The radial eigenfunctions of the states with  $l = 1$  and  $m = 0$  in a spherically symmetric region with  $U(r) = 0$  have been already discussed in Sec. 3.6 (where they have been valid for  $r < R$ ) – see Eq. (3.186)

$$\mathcal{R}_{1,k}(r) = C_k j_1(kr) \equiv C_k \left( \frac{\sin kr}{k^2 r^2} - \frac{\cos kr}{kr} \right).$$

For the normalization of these functions, let us introduce (just as it was done in the course repeatedly, starting from Sec. 1.7) an auxiliary, sufficiently large volume, to which these wavefunctions would be confined. It is convenient, in our current case, to take it in the form of a sphere of a radius  $R \gg 1/k_0$ , where  $k_0$  is the characteristic scale of the wave numbers  $k$  – still to be determined. Then the normalization (3.194) of wavefunctions with  $k \sim k_0$ , i.e.  $kR \gg 1$ , requires

$$|C_k|^{-2} = \int_0^R \left( \frac{\sin kr}{k^2 r^2} - \frac{\cos kr}{kr} \right)^2 r^2 dr \approx \frac{1}{k^2} \int_0^R \cos^2 kr dr \approx \frac{R}{2k^2}, \quad \text{for } kR \gg 1,$$

so we may take<sup>89</sup>

$$\mathcal{R}_{1,k}(r) = \left( \frac{2}{R} \right)^{1/2} \left( \frac{\sin kr}{kr^2} - \frac{\cos kr}{r} \right).$$

Note that the confinement makes the spectrum of the wave vectors  $k$  discrete; at  $kR \gg 1$ , the distance between the eigenvalues is constant:

$$kR = \frac{\pi}{2} + n\pi, \quad \text{i.e. } k = \frac{\pi}{2R} + n \frac{\pi}{R}, \quad \text{for } n \gg 1. \quad (***)$$

Now proceeding to the ground-state wavefunction  $\psi_g$ : as was discussed in the model solution of Problem 3.28, it has the form

$$\psi_g = C_g \frac{\exp\{-\kappa r\}}{r}, \quad \text{with } \frac{\hbar^2 \kappa^2}{2m} = -E_g > 0, \quad \text{for } r \geq R';$$

<sup>89</sup> Just as a reminder, we may multiply the wavefunction by  $\exp\{i\varphi\}$ , where  $\varphi$  is any real constant, but since Eq. (6.20) includes only the matrix element moduli, the phase factor is inconsequential, and the choice  $\varphi = 0$  is the most convenient one.

in our current limit of a very small well ( $R' \rightarrow 0$ ), this form may be used for any  $r \neq 0$ , so the normalization condition,

$$\int \psi_g^*(\mathbf{r})\psi_g(\mathbf{r})d^3r \equiv 4\pi \int_0^\infty r^2 dr |\psi_g|^2 \equiv 4\pi |C_g|^2 \int_0^\infty e^{-2\kappa r} dr = 1,$$

after an elementary integration, yields  $|C_g|^2 = \kappa/2\pi$ , and (again ignoring the phase factor) we may take

$$\psi_g = \left(\frac{\kappa}{2\pi}\right)^{1/2} \frac{\exp\{-\kappa r\}}{r}.$$

Now we can, finally, calculate the nonvanishing matrix elements (\*\*):

$$\begin{aligned} H_{gn}^{(1)} &= -q\mathcal{E} \left(\frac{4\pi}{3}\right)^{1/2} \int_0^\infty r^2 dr \left(\frac{\kappa}{2\pi}\right)^{1/2} \frac{\exp\{-\kappa r\}}{r} \left(\frac{2}{R}\right)^{1/2} \left(\frac{\sin kr}{kr^2} - \frac{\cos kr}{r}\right) \\ &\equiv -q\mathcal{E} \left(\frac{4\kappa}{3R}\right)^{1/2} \left[ \frac{1}{k} \text{Im} \int_0^\infty e^{(ik-\kappa)r} dr - \text{Re} \int_0^\infty r e^{(ik-\kappa)r} dr \right] \\ &= -q\mathcal{E} \left(\frac{4\kappa}{3R}\right)^{1/2} \left[ \frac{1}{k} \text{Im} \frac{\exp\{(ik-\kappa)r\}}{(ik-\kappa)} + \text{Re} \frac{\exp\{(ik-\kappa)r\}}{(ik-\kappa)^2} \right]_0^\infty \equiv -q\mathcal{E} \left(\frac{4\kappa}{3R}\right)^{1/2} \frac{2k^2}{(k^2 + \kappa^2)^2}. \end{aligned}$$

Next, note that according to the solution of Problem 3.28, the unperturbed eigenenergy of the state (\*) is just  $\hbar^2 k^2/2m$ . With this, and the above expressions for  $E_g$  and  $H_{gn}^{(1)}$ , Eq. (6.20) of the lecture notes for the ground state energy takes the following form:

$$\Delta E_g = E_g^{(2)} = \sum_{n>0} \frac{|H_{gn}^{(1)}|^2}{E_n^{(0)} - E_g^{(0)}} = -\frac{32q^2 \mathcal{E}^2 \kappa m}{3R\hbar^2} \sum_{n>0} \frac{k^4}{(k^2 + \kappa^2)^5},$$

where  $k$  and  $n$  are related by Eq. (\*\*\*). Since our result for  $E_g^{(2)}$  is only valid for  $kR \gg 1$ , i.e.  $n \gg 1$ , we may transfer from the summation to integration over  $n$  and then to that over  $k$ , with  $dk = (\pi/R)dn$ , i.e.  $dn = (R/\pi)dk$ :

$$\Delta E_g = -\frac{32q^2 \mathcal{E}^2 \kappa m}{3R\hbar^2} \int_0^\infty \frac{k^4 dn}{(k^2 + \kappa^2)^5} = -\frac{32q^2 \mathcal{E}^2 \kappa m}{3\pi\hbar^2} \int_0^\infty \frac{k^4 dk}{(k^2 + \kappa^2)^5} \equiv -\frac{32q^2 \mathcal{E}^2 m}{3\pi\kappa^4 \hbar^2} \int_0^\infty \frac{\xi^4 d\xi}{(1 + \xi^2)^5},$$

with  $\xi \equiv k/\kappa$ .<sup>90</sup> The last integral may be readily worked out by recasting its numerator as a sum of three terms proportional to different powers of the sum  $(1 + \xi^2)$ :

$$\xi^4 \equiv [(1 + \xi^2) - 1]^2 = (1 + \xi^2)^2 - 2(1 + \xi^2) + 1,$$

and hence representing the integral as a sum of three terms, all proportional to integrals of the same type MA Eq. (6.5b), but with different  $n$  (equal to 3, 4, and 5, respectively):

<sup>90</sup> Note that the auxiliary bounding radius  $R \gg 1/k_0 \sim 1/\kappa$  has dropped out of the result, thus satisfying a necessary condition of the self-consistency of this state-counting procedure.



$$\int_0^{\infty} \frac{\xi^4 d\xi}{(1+\xi^2)^5} = \int_0^{\infty} \frac{d\xi}{(1+\xi^2)^3} - 2 \int_0^{\infty} \frac{d\xi}{(1+\xi^2)^4} + \int_0^{\infty} \frac{d\xi}{(1+\xi^2)^5} = \frac{\pi}{2} \frac{1 \cdot 3}{2 \cdot 4} \left[ 1 - 2 \frac{5}{6} + \frac{5 \cdot 7}{6 \cdot 8} \right] \equiv \frac{3\pi}{256}.$$

As a result, for the energy shift by the electric field, we get<sup>91</sup>

$$\Delta E_g = -\frac{q^2 \mathcal{E}^2 m}{8\kappa^4 \hbar^2} \equiv -\frac{q^2 \hbar^2}{16mE_g^2} \frac{\mathcal{E}^2}{2},$$

so the electric polarizability of the system is

$$\alpha = \frac{q^2 \hbar^2}{16mE_g^2} \equiv \frac{q^2 m}{4\kappa^4 \hbar^2}.$$

The first of the expressions for  $\alpha$  shows that the larger the unperturbed  $|E_g|$ , the smaller the electric field effect. This is natural because the stronger the particle's confinement (the larger  $|E_g|$ ), the smaller the effective radius  $r_{\text{ef}} \equiv 1/\kappa \propto |E_g|^{-1/2}$  of the ground-state wavefunction  $\psi_g$ , and hence the smaller the effective potential energy difference  $\delta E \sim q\mathcal{E}r_{\text{ef}}$  created by the external field for the localized particle.

**Problem 6.10.** In some atoms, the effect of nuclear charge screening by electrons on the motion of each of them may be reasonably well approximated by the replacement of the Coulomb potential (3.190),  $U = -C/r$ , with the so-called *Hulthén potential*

$$U = -\frac{C/a}{\exp\{r/a\}-1} \rightarrow -C \times \begin{cases} 1/r, & \text{for } r \ll a, \\ \exp\{-r/a\}/a, & \text{for } a \ll r. \end{cases}$$

Assuming that the effective screening radius  $a$  is much larger than  $r_0 \equiv \hbar^2/mC$ , use the perturbation theory to calculate the energy spectrum of a single particle of mass  $m$ , moving in this potential, in the lowest order needed to lift the  $l$ -degeneracy of the energy levels.

*Solution:* As was discussed in Sec. 3.7 of the lecture notes, the radial extension of the eigenfunctions of an electron in a hydrogen-like atom/ion scales as  $n^2 r_0$ , where  $n$  is the principal quantum number. Hence, if  $n$  is not too high ( $n^2 \ll a/r_0$ ), we may treat the difference between the Hulthén and Coulomb potentials as a small perturbation:

$$\hat{H}^{(1)} \equiv -\frac{C/a}{\exp\{r/a\}-1} - \left(-\frac{C}{r}\right) \equiv \frac{C}{r} \left[ 1 - \frac{r/a}{\exp\{r/a\}-1} \right] \ll \frac{C}{r}, \quad \text{for } r \ll a,$$

and limit the Taylor expansion of the function in the square brackets, in the small parameter  $\xi \equiv r/a$ :

$$1 - \frac{\xi}{e^\xi - 1} = \frac{\xi}{2} - \frac{\xi^2}{12} + \frac{\xi^4}{720} - \dots$$

to its two leading terms,<sup>92</sup> so

<sup>91</sup> Note that this expression may be represented in a form similar to Eq. (\*\*\*) of the model solution of the previous problem:  $\Delta E_g = -(q\mathcal{E}r_{\text{ef}})^2/8E_g$ , where  $r_{\text{ef}} \equiv 1/\kappa$  is the particle localization radius.

$$\hat{H}^{(1)} \approx C \left( \frac{1}{2a} - \frac{r}{12a^2} \right), \quad \text{for } r \ll a.$$

With this perturbation, Eq. (6.14) of the lecture notes takes the form

$$E_{n,l,m}^{(1)} = \langle n, l, m | \hat{H}^{(1)} | n, l, m \rangle = C \left( \frac{1}{2a} - \frac{\langle n, l, m | \hat{r} | n, l, m \rangle}{12a^2} \right) \equiv \frac{C}{2a} - \frac{C \langle r \rangle_{n,l,m}}{12a^2},$$

where  $\{n, l, m\}$  are the unperturbed states of the Bohr atom. Now using Eq. (3.210) of the lecture notes, we immediately get

$$E_{n,l,m}^{(1)} = \frac{C}{2a} + \frac{Cr_0}{24a^2} [-3n^2 + l(l+1)].$$

This expression describes the sought-after effect of lifting the energy level degeneracy, with higher values of the orbital quantum number  $l$  giving higher energy – the effect already mentioned in Sec. 3.7 and pertinent to virtually any realistic perturbation of the Coulomb potential – see, for example, Sec. 6.3, in particular, Eqs. (6.51) and (6.60), and Fig. 6.4.

**Problem 6.11.** In the lowest nonvanishing order of the perturbation theory, calculate the correction to energies of the ground state and all lowest excited states of a hydrogen-like atom/ion, due to the electron's penetration into the nucleus, by modeling the latter as a spinless, uniformly charged sphere of radius  $R \ll r_B/Z$ .

*Solution:* The electrostatic potential  $\phi$  inside a uniformly charged sphere of radius  $R$ , with the total charge  $Q = Ze$ , may be readily calculated either using the Gauss law or solving the corresponding Poisson equation. The result is<sup>93</sup>

$$\phi(r) = \frac{Ze}{4\pi\epsilon_0 R} \left( \frac{3}{2} - \frac{r^2}{2R^2} \right), \quad \text{for } r \leq R.$$

The constant in this expression is selected so that at  $r = R$ , the potential coincides with the usual form of the Coulomb potential outside the sphere (which is the same as that of the point charge  $Ze$ ):

$$\phi_0(r) = \frac{Ze}{4\pi\epsilon_0 r}, \quad \text{for } R \leq r, \quad (*)$$

tending to zero at  $r \rightarrow \infty$ . Since the potential (\*) has already been taken into account in the solution of the basic Bohr atom problem (see, e.g., Sec. 3.6 of the lecture notes), the perturbation Hamiltonian of our current problem is due to their difference:

$$\hat{H}^{(1)} = U^{(1)}(\mathbf{r}) = -e[\phi(r) - \phi_0(r)] = -\frac{Ze^2}{4\pi\epsilon_0 R} \times \begin{cases} \left( \frac{3}{2} - \frac{r^2}{2R^2} - \frac{R}{r} \right), & \text{for } r \leq R, \\ 0, & \text{for } R \leq r. \end{cases}$$

<sup>92</sup> If we kept just the first term, the resulting (constant) shift  $C/2a$  of the energy levels would not lift the  $l$ -degeneracy.

<sup>93</sup> See, e.g., EM Eq. (1.51).

Since the spatial extension scale of the unperturbed wavefunctions  $\psi^{(0)}(\mathbf{r})$  of the atom/ion is given by the radius  $r_0 = r_B/Z \ll R$ , in the first order in the parameter  $R/r_0 \ll 1$  (in actual atoms, as small as  $\sim 10^{-5}$ ) we may approximate this potential with a 3D delta function:

$$U^{(1)}(\mathbf{r}) \approx w\delta(\mathbf{r}),$$

with the weight

$$\begin{aligned} w &= \int U^{(1)}(\mathbf{r})d^3r = -\frac{Ze^2}{4\pi\epsilon_0 R} \int_{r \leq R} \left( \frac{3}{2} - \frac{r^2}{2R^2} - \frac{R}{r} \right) d^3r = -\frac{Ze^2}{4\pi\epsilon_0 R} 4\pi \int_0^R \left( \frac{3}{2} - \frac{r^2}{2R^2} - \frac{R}{r} \right) r^2 dr \\ &\equiv -\frac{Ze^2}{4\pi\epsilon_0 R} 4\pi R^3 \int_0^1 \left( \frac{3}{2} - \frac{\xi^2}{2} - \frac{1}{\xi} \right) \xi^2 d\xi = -\frac{Ze^2 R^2}{4\pi\epsilon_0} 4\pi \left( \frac{3}{2} \cdot \frac{1}{3} - \frac{1}{2} \cdot \frac{1}{5} - \frac{1}{2} \right) \equiv \frac{Ze^2 R^2}{4\pi\epsilon_0} 4\pi \frac{1}{10}. \end{aligned}$$

As a result, the matrix elements (6.8) of the perturbation may be calculated as

$$\hat{H}_{n'n''}^{(1)} \equiv \int \psi_{n'}^{(0)*}(\mathbf{r}) \hat{H}^{(1)} \psi_{n''}^{(0)}(\mathbf{r}) d^3r \approx w \psi_{n'}^{(0)*}(0) \psi_{n''}^{(0)}(0), \quad (**)$$

where each of the indices  $n'$  and  $n''$  encodes the whole appropriate set of quantum numbers – in the case of the hydrogen-like atom,  $n$ ,  $l$ , and  $m$  – see Sec. 3.7 of the lecture notes.

For the ground state ( $n = 1$ ,  $l = m = 0$ ), Eqs. (3.174), (3.200), and (3.208) yield

$$\psi_g^{(0)}(0) = \frac{1}{(4\pi)^{1/2}} \frac{2}{r_0^{3/2}}.$$

Since this state is non-degenerate, the 1<sup>st</sup>-order correction to its energy may be calculated using the simple Eq. (6.14):

$$E_g^{(1)} = H_{gg}^{(1)} = w \psi_g^{(0)*}(0) \psi_g^{(0)}(0) = \frac{Ze^2 R^2}{4\pi\epsilon_0} 4\pi \frac{1}{10} \frac{1}{4\pi} \frac{4}{r_0^3} \equiv 0.4 \frac{Ze^2}{4\pi\epsilon_0 r_0} \left( \frac{R}{r_0} \right)^2 \equiv 0.4 E_0 \left( \frac{R}{r_0} \right)^2,$$

where the energy scale  $E_0$  and the spatial scale  $r_0$  are defined by Eqs. (3.192) with  $C = Ze^2/4\pi\epsilon_0$ . For the generic hydrogen atom, with  $Z = 1$ ,  $E_0$  is just the Hartree energy  $E_H \approx 27.2$  eV, while  $r_0$  is the Bohr radius  $r_B$  – see Eqs. (1.13).

Generally, for the four lowest excited states (all with  $n = 2$ , but with either  $l = m = 0$  or  $l = 1$  and  $m = 0, \pm 1$ ) we should be more accurate because in the absence of perturbation, they are degenerate, so the perturbation that may lift their degeneracy should be treated using the approach discussed in the last part of Sec. 6.1 of the lecture notes. However, according to the second of Eqs. (3.209), all  $2p$ -states with  $l = 1$  have  $\psi^{(0)}(0) = 0$ , so within the approximation (\*\*), all the matrix elements involving these states vanish. According to the first of Eqs. (3.209), this is not true for the  $2s$ -state (with  $n = 2$  and  $l = 0$ ):

$$\psi_s^{(0)}(0) = \frac{1}{(4\pi)^{1/2}} \frac{2}{(2r_0)^{3/2}},$$

so this perturbation causes the shift of the  $2s$ -state's energy by

$$E_s^{(1)} = H_{ss}^{(1)} = w \psi_s^{(0)*}(0) \psi_s^{(0)}(0) = \frac{Ze^2 R^2}{4\pi\epsilon_0} 4\pi \frac{1}{10} \frac{4}{4\pi (2r_0)^3} = 0.05 \frac{Ze^2}{4\pi\epsilon_0 r_0} \left( \frac{R}{r_0} \right)^2 \equiv 0.05 E_0 \left( \frac{R}{r_0} \right)^2,$$

i.e. by the magnitude, 8 times lower than the ground state's shift. For actual atoms, with their small  $R$ , both shifts are very small, of the order of  $10^{-10}E_H \sim 10^{-9}$  eV.<sup>94</sup>

**Problem 6.12.** A particle of mass  $m$  is placed inside a hard-wall ellipsoid whose surface is described by the equation

$$\frac{x^2 + y^2}{a^2} + \frac{z^2}{b^2} = 1, \quad \text{with } b = (1 + \varepsilon)a, \quad |\varepsilon| \ll 1.$$

Calculate its ground-state energy in the 1<sup>st</sup> order in the small parameter  $\varepsilon$ , and interpret the result.

*Solution:* The system may be described by the following potential:

$$U(r) = \begin{cases} 0, & \text{for } \frac{x^2 + y^2}{a^2} + \frac{z^2}{b^2} \leq 1, \\ +\infty, & \text{otherwise.} \end{cases}$$

Let us introduce new coordinates

$$x' \equiv x, \quad y' \equiv y, \quad z' \equiv \frac{a}{b}z \equiv \frac{1}{1 + \varepsilon}z, \quad \text{so } z = (1 + \varepsilon)z'.$$

In them, the particle's motion region is just a sphere of radius  $a$ :

$$U(r) = \begin{cases} 0, & \text{for } x'^2 + y'^2 + z'^2 \equiv r'^2 \leq a^2, \\ +\infty, & \text{otherwise,} \end{cases}$$

and the stationary Schrödinger equation inside this volume is

$$-\frac{\hbar^2}{2m} \left[ \frac{\partial^2}{\partial x'^2} + \frac{\partial^2}{\partial y'^2} + \frac{\partial^2}{\partial z'^2} \right] \psi = E \psi.$$

In the first order in the small parameter,  $1/(1 + \varepsilon)^2 \approx 1 - 2\varepsilon$ , so we may rewrite this equation as

$$-\frac{\hbar^2}{2m} \nabla'^2 \psi + \hat{H}^{(1)} \psi = E \psi, \quad \text{with } \hat{H}^{(1)} = 2\varepsilon \frac{\hbar^2}{2m} \frac{\partial^2}{\partial z'^2}, \quad (*)$$

where the prime sign is now dropped for the notation brevity.

This is just the standard Schrödinger equation for a particle that moves freely inside a sphere of radius  $a$ , besides the perturbation described by the Hamiltonian  $\hat{H}^{(1)}$ . Its solution, in the 0<sup>th</sup> approximation (i.e. for  $\varepsilon = 0$ ), was discussed at the end of Sec. 3.6 of the lecture notes. In particular, the ground-state's wavefunction  $\psi_g^{(0)}$  is spherically symmetric, and the corresponding energy is

$$E_g^{(0)} = E_{0,1} = \frac{\pi^2 \hbar^2}{2ma^2}. \quad (**)$$

Plugging the perturbation  $\hat{H}^{(1)}$  into the coordinate representation of Eq. (6.14),

<sup>94</sup> A calculation in the next approximation in  $R/r_0 \ll 1$  (highly recommended to the reader as an additional exercise) shows that the  $2p$ -states' energy shift is even smaller by an additional factor of  $\sim 10^{-3}(R/r_0)^2 \sim 10^{-10}$ .

$$E_n^{(1)} = \int (\psi_n^{(0)})^* \hat{H}^{(1)} \psi_n^{(0)} d^3r,$$

and assuming that the wavefunction is normalized,

$$\int (\psi_g^{(0)})^* \psi_g^{(0)} d^3r = 1, \quad (***)$$

we get

$$E_g^{(1)} = \int_{r \leq a} (\psi_g^{(0)})^* \hat{H}^{(1)} \psi_g^{(0)} d^3r = -2\varepsilon \int_{r \leq a} (\psi_g^{(0)})^* \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} \psi_g^{(0)} \right] d^3r.$$

The simplest way to calculate this integral is to notice that due to the spherical symmetry of the wavefunction  $\psi_g(0)$ , the integral would not change if we replaced  $z$  with either  $x$  or  $y$ , so

$$E_g^{(1)} = -\frac{2\varepsilon}{3} \int_{r \leq a} (\psi_g^{(0)})^* \left[ -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi_g^{(0)} \right] d^3r = -\frac{2\varepsilon}{3} \int_{r \leq a} (\psi_g^{(0)})^* \left[ -\frac{\hbar^2}{2m} \nabla^2 \psi_g^{(0)} \right] d^3r.$$

But according to Eq. (\*) with  $\varepsilon = 0$ , the expression in the square brackets is just  $E_g^{(0)} \psi_g^{(0)}$ , so

$$E_g^{(1)} = -\frac{2\varepsilon}{3} E_g^{(0)} \int_{r \leq a} (\psi_g^{(0)})^* \psi_g^{(0)} d^3r.$$

Now using Eqs. (\*\*) and (\*\*\*), we finally get

$$E_g^{(1)} = -\frac{2\varepsilon}{3} E_g^{(0)} = -\frac{2\varepsilon}{3} \frac{\pi^2 \hbar^2}{2ma^2}, \quad \text{i.e. } E_g = E_g^{(0)} + E_g^{(1)} = \left( 1 - \frac{2\varepsilon}{3} \right) \frac{\pi^2 \hbar^2}{2ma^2}.$$

The simplicity of this relation between  $E_g^{(1)}$  and  $E_g^{(0)}$ , and its independence of the exact form of the wavefunction  $\psi_g^{(0)}$ , suggest that there is some deep reason behind it. To reveal it, let us note that according to basic geometry, the volume of our axially symmetric ellipsoid is

$$V = \frac{4\pi}{3} a^2 b = \frac{4\pi}{3} a^3 (1 + \varepsilon).$$

Let us calculate the radius  $R$  of an exact sphere with the same volume:

$$\frac{4\pi}{3} R^3 = V = \frac{4\pi}{3} a^3 (1 + \varepsilon), \quad \text{i.e. } R = a(1 + \varepsilon)^{1/3} \approx a \left( 1 + \frac{\varepsilon}{3} \right).$$

Per Eq. (\*\*), the ground-state energy of the particle inside a spherical surface with this radius would be

$$E'_g = \frac{\pi^2 \hbar^2}{2mR^2} = \frac{\pi^2 \hbar^2}{2ma^2 (1 + \varepsilon/3)^2} \approx \frac{\pi^2 \hbar^2}{2ma^2} \left( 1 - \frac{2\varepsilon}{3} \right),$$

i.e., to the first order in the small parameter  $\varepsilon$ , the same energy as we have calculated.

This coincidence implies that  $E_g$  may depend only on the volume inside the deformed spherical surface rather than on the type of its deformation, provided that this deformation is relatively small. Indeed, a quantum particle placed inside a closed surface exerts certain forces on it even in the ground

state.<sup>95</sup> For a spherical surface, these forces have to be isotropic and hence may be described by the scalar pressure

$$\mathcal{P} = -\frac{\partial E}{\partial V}.$$

Rewriting this expression as

$$dE = -\mathcal{P}dV,$$

we see that it gives  $dE = 0$  for any small deformation that keeps the volume constant.

**Problem 6.13.** Prove that the relativistic correction operator (6.48) indeed has only diagonal matrix elements in the basis of unperturbed Bohr atom states (3.200).

*Solution:* In an expression similar to Eq. (6.49) of the lecture notes, but with two arbitrary stationary states  $\{n, l, m\}$  and  $\{n', l', m'\}$ , let us act by the first of the two similar (Hermitian) operators  $\hat{H}^{(0)} - \hat{U}(r)$  upon the bra-vector, and by the second one, on the ket-vector. Since these vectors describe the eigenstates of  $\hat{H}^{(0)}$ , and the corresponding eigenvalues depend only on the principal quantum number  $n$ , we get

$$\begin{aligned} \langle nlm | \hat{H}^{(1)} | n'l'm' \rangle &= -\frac{1}{4mc^2} \langle nlm | (E_n - \hat{U}(r))(E_{n'} - \hat{U}(r)) | n'l'm' \rangle \\ &\equiv -\frac{1}{4mc^2} \left[ E_n^2 \delta_{nlm, n'l'm'} - (E_n + E_{n'}) \langle nlm | \hat{U}(r) | n'l'm' \rangle + \langle nlm | \hat{U}^2(r) | n'l'm' \rangle \right]. \end{aligned}$$

The operators of the spherically-symmetric functions  $U(r)$  and  $U^2(r)$  can act only on the radial factors  $\mathcal{R}_{n,l}(r)$  of the wavefunctions  $\psi_{n,l,m}$ . As a result, due to the orthogonality of all angular factors, both long brackets with either  $m \neq m'$  or  $l \neq l'$  (or both) vanish, and so does the first term.

**Problem 6.14.** Calculate the lowest-order relativistic correction to the ground-state energy of a 1D harmonic oscillator.

*Solution:* The perturbation Hamiltonian for this problem is the same as in Eq. (6.47) of the lecture notes:

$$\hat{H}^{(1)} = -\frac{1}{8m^3 c^2} \hat{p}^4,$$

besides that in our current case,  $\hat{p}$  should be understood as a 1D operator, so it may be expressed via the creation–annihilation operators – see Eq. (5.66):

$$\hat{p} = \frac{(\hbar m \omega_0)^{1/2}}{\sqrt{2}i} (\hat{a} - \hat{a}^\dagger).$$

Since the energy levels of the unperturbed oscillator are non-degenerate, the first-order correction to the ground state energy may be calculated using Eq. (6.14) of the lecture notes:

<sup>95</sup> See, e.g., the model solution of Problem 1.11.

$$E_g^{(1)} = \langle 0 | \hat{H}^{(1)} | 0 \rangle = -\frac{1}{8m^3c^2} \langle 0 | \hat{p}^4 | 0 \rangle \equiv -\frac{(\hbar\omega_0)^2}{32mc^2} I, \quad \text{with } I \equiv \langle 0 | (\hat{a} - \hat{a}^\dagger)^4 | 0 \rangle. \quad (*)$$

The long bracket  $I$  may be calculated either as  $\langle n | x^4 | n \rangle$  was calculated in the model solution of Problem 5.12(ii) (i.e. using Eq. (5.93) of the lecture notes) or even simpler – using the fact that according to Eqs. (5.89),

$$\hat{a}|0\rangle = 0, \quad \text{so } \langle 0|\hat{a}^\dagger = 0.$$

As a result, if, in the last form of the expression

$$I = \langle 0 | \left( \hat{a} - \hat{a}^\dagger \right)^2 \left( \hat{a} - \hat{a}^\dagger \right)^2 | 0 \rangle \equiv \langle 0 | \left( \hat{a}^2 - \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} + \hat{a}^{\dagger 2} \right) \left( \hat{a}^2 - \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} + \hat{a}^{\dagger 2} \right) | 0 \rangle,$$

we act by the operators in the first parentheses upon the bra-vector, and by those in the second parentheses, upon the ket-vector, two of each four terms vanish, giving

$$I = \langle 0 | \left( \hat{a}^2 - \hat{a}\hat{a}^\dagger \right) \left( -\hat{a}\hat{a}^\dagger + \hat{a}^{\dagger 2} \right) | 0 \rangle \equiv \langle 0 | \left( -\hat{a}^3\hat{a}^\dagger + \hat{a}^2\hat{a}^{\dagger 2} + \hat{a}\hat{a}^\dagger\hat{a}\hat{a}^\dagger - \hat{a}\hat{a}^{\dagger 3} \right) | 0 \rangle.$$

According to Eqs. (5.89), the first and the last terms in the parentheses of the last expression yield zero contributions to the expectation value because they have different powers of the creation and annihilation operators, so their sequential action on, say, the ket-vector gives a non-ground ket-vector, orthogonal to the ground-state bra-vector. The remaining two terms may be calculated directly, by using the same Eqs. (5.89):

$$\begin{aligned} I &= \langle 0 | \left( \hat{a}^2\hat{a}^{\dagger 2} + \hat{a}\hat{a}^\dagger\hat{a}\hat{a}^\dagger \right) | 0 \rangle \equiv \langle 0 | \hat{a} \left( \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} \right) \hat{a}^\dagger | 0 \rangle = \langle 1 | \left( \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} \right) | 1 \rangle = \\ &\equiv \langle 1 | \hat{a}\hat{a}^\dagger | 1 \rangle + \langle 1 | \hat{a}^\dagger\hat{a} | 1 \rangle = \langle 2 | \sqrt{2} \cdot \sqrt{2} | 2 \rangle + \langle 0 | \sqrt{1} \cdot \sqrt{1} | 0 \rangle = 3, \end{aligned}$$

so, finally, Eq. (\*) yields

$$E_g^{(1)} = -\frac{3}{32} \frac{(\hbar\omega_0)^2}{mc^2}.$$

As usual in the stationary perturbation theory, this expression is quantitatively valid only if this correction is much smaller than the unperturbed ground-state energy  $E_g^{(0)} = \hbar\omega_0/2$ , i.e. if  $\hbar\omega_0 \ll mc^2$ . Since, according to Eq. (5.97),  $\hbar\omega_0$  also gives the scale of the kinetic energy  $T$  of the particle in this state, this requirement is essentially the same as was discussed in Sec. 6.3 of the lecture notes:  $T \ll mc^2$ .

**Problem 6.15.** Use the perturbation theory to calculate the contribution to the magnetic susceptibility  $\chi_m$  of a dilute gas, that is due to the orbital motion of a single electron inside each gas particle. Spell out your result for a spherically symmetric ground state of the electron, and give an estimate of the magnitude of this *orbital susceptibility*.

*Solution:* According to basic electrodynamics,<sup>96</sup> the magnetic energy  $u$  per unit volume of a linear, isotropic medium may be expressed as

<sup>96</sup> See, e.g., EM Sec. 5.5, in particular, Eqs. (5.112) and (5.140).

$$u = \frac{\mathcal{B}^2}{2\mu},$$

where  $\mathcal{B}$  is the applied magnetic field, while  $\mu$  is the magnetic permeability, which is related to the magnetic susceptibility as  $\mu = \mu_0(1 + \chi_m)$ . For a dilute gas, the susceptibility is small in comparison with 1; in this case, we may separate the energy density  $u$  into a sum of the energy  $\mathcal{B}^2/2\mu_0$  of the magnetic field in free space and a small correction  $u_m$  proportional to  $\chi_m$ :

$$u_m \equiv \frac{\mathcal{B}^2}{2\mu} - \frac{\mathcal{B}^2}{2\mu_0} = \frac{\mathcal{B}^2}{2\mu_0} \left( \frac{1}{1 + \chi_m} - 1 \right) \approx -\chi_m \frac{\mathcal{B}^2}{2\mu_0},$$

On the other hand, for a medium of non-interacting particles with a spatial density  $n$ ,  $u_m$  should be equal to  $n\langle E_m \rangle$ , where  $E_m$  is the change of the energy of one particle due to its magnetization. Comparing these two formulas, we see that in this case the susceptibility may be calculated as<sup>97</sup>

$$\chi_m = -\frac{2\mu_0 \langle E_m \rangle}{\mathcal{B}^2} n. \quad (*)$$

In order to calculate the single electron energy contribution from its orbital motion in a spherically symmetric confining potential, we may use the Hamiltonian (6.63), neglecting the term linear in the field,<sup>98</sup> but keeping the term quadratic in the vector-potential  $\mathbf{A}$ . By using Eq. (6.64), we may represent this term in the convenient form

$$\hat{H}_m = \frac{e^2}{2m_e} \hat{\mathbf{A}}^2 = \frac{e^2}{8m_e} |\mathcal{B} \times \hat{\mathbf{r}}|^2 = \frac{e^2 \mathcal{B}^2}{8m_e} (\hat{x}^2 + \hat{y}^2),$$

where  $x$  and  $y$  are the Cartesian coordinates perpendicular to the field's direction (taken for the  $z$ -axis). If the field is not too high, this Hamiltonian may be used as  $\hat{H}^{(1)}$  in the formulas of the perturbation theory. For the electron in its ground state 0 (which is always non-degenerate), we may immediately use Eq. (6.14) to get

$$\langle E_m \rangle = \frac{e^2 \mathcal{B}^2}{8m_e} \langle 0 | \hat{x}^2 + \hat{y}^2 | 0 \rangle,$$

so Eq. (\*) yields

$$\chi_m = -\frac{\mu_0 n e^2}{4m_e} \langle 0 | \hat{x}^2 + \hat{y}^2 | 0 \rangle.$$

We see that such  $\chi_m$  is always negative – the effect that is called the *orbital* (or “Larmor”) *diamagnetism*. For the motion in a central field, in which the ground state's wavefunction is spherically

<sup>97</sup> An alternative way to get the same Eq. (\*) is to combine the expression  $E_m = -\mathbf{m} \cdot \mathcal{B}/2$  for the energy of interaction between the magnetic field  $\mathcal{B}$  and the magnetic dipole  $\mathbf{m}$  it has induced, the definition of  $\chi_m$  as  $\mathcal{M}/\mathcal{H}$ , where the magnetization  $\mathcal{M}$  of a dilute medium may be calculated as  $\mathcal{M} = n\mathbf{m}$ , and the fact that if  $|\chi_m| \ll 1$ , then  $\mathcal{H} \approx \mu_0 \mathcal{B}$  – see, e.g., EM Sec. 5.5. (In quantum mechanics,  $\mathbf{m}$ ,  $\mathcal{M}$ , and  $E_m$  in these relations have to be understood either as the operators of these observables or as their expectation values, i.e. their averages over the ensemble of the corresponding quantum states.)

<sup>98</sup> That term, while contributing to the energy level splitting by the field, i.e. the Zeeman effect (see Sec. 6.4), gives zero contribution to the energy of  $s$ -states with no spontaneous angular momentum, in particular, of the spherically symmetric ground state.



symmetric (see Sec. 3.6), this expression may be further simplified by noting that the averages of all Cartesian components squared have to be equal, so

$$\langle 0 | \hat{x}^2 | 0 \rangle = \langle 0 | \hat{y}^2 | 0 \rangle = \frac{1}{3} \langle 0 | \hat{r}^2 | 0 \rangle \equiv \frac{1}{3} \langle r^2 \rangle, \quad \text{so } \chi_m = -\frac{\mu_0 n e^2}{6 m_e} \langle r^2 \rangle. \quad (**)$$

Remarkably, this formula coincides with the one calculated using a reasonable classical model – see, e.g., EM Problem 5.18(i). It gives a good semi-quantitative description of experimental data for gases, and even for liquids and solids of some multi-electron atoms (especially those with filled electron shells, whose net spontaneous orbital and spin momenta vanish), by assuming that the contributions of all atom's electrons add up independently.

In order to estimate the magnitude of the effect described by Eq. (\*\*), note that according to the definition of the electromagnetic constants  $\epsilon_0$  and  $\mu_0$ , the latter of them equals  $1/\epsilon_0 c^2$ , where  $c$  is the speed of light in free space, so our result for the susceptibility (which is dimensionless by its definition) may be rewritten as

$$\chi_m = -\frac{4\pi}{6} \frac{e^2}{4\pi\epsilon_0} \frac{1}{m_e c^2} n \langle r^2 \rangle \equiv -\frac{2\pi}{3} \alpha^2 n r_B \langle r^2 \rangle,$$

where  $\alpha \equiv e^2/4\pi\epsilon_0\hbar c \approx 1/137 \ll 1$  is the fine structure constant (6.62), and  $r_B$  is the Bohr radius (1.10). Since  $r_B^2$  gives a fair scale of  $\langle r^2 \rangle$  in atoms and (not very large) molecules, we may write the following crude estimate:

$$|\chi_m| \sim \alpha^2 n r_B^3 \ll n r_B^3. \quad (***)$$

This estimate shows that the orbital diamagnetism is so weak that it corresponds to pushing out of the atom only a tiny part of the order of  $\alpha^2 \sim 10^{-4}$  of the magnetic field lines – while a perfect diamagnetic (for example, a bulk superconductor) would push out all of them. Note that an uncompensated net spin of atoms/molecules may give them, due to the spin's polarization by the field, a different, *paramagnetic* contribution to the magnetic susceptibility – see, e.g., EM Sec. 5.5 and Problem 5.18(ii). At sufficiently low temperatures, this *spin paramagnetism* may be much higher than the orbital diamagnetism (\*\*) – see, e.g., SM Problems 2.4 and 3.10.

**Problem 6.16.** A certain energy level degeneracy is not lifted in the 1<sup>st</sup> order of the stationary perturbation theory. Calculate its lifting in the 2<sup>nd</sup> order of the theory. Apply the result to a planar rotor of mass  $m$  and radius  $R$ , with electric charge  $q$ , placed into a weak, uniform, time-independent electric field  $\mathcal{E}$ .

*Solution:* If all first-order matrix elements  $H_{n'n''}$  connecting the states that correspond to some degenerate energy level, i.e. participating in Eqs. (6.24)-(6.26) of the lecture notes, vanish in the first order of the perturbation theory, we need to calculate them in the second order. For that, it is sufficient to repeat the calculation that was used to derive Eq. (6.19) starting from the exact system of equations (6.7) and the expansions (6.9)-(6.10). If all  $H_{n'n''}^{(1)} = 0$ , then according to Eq. (6.14),  $E_n^{(1)} = 0$  as well, and the balance of the terms  $O(\mu^2)$  in Eq. (6.7) gives us a system of equations similar to Eq. (6.24), but with the very natural replacement

$$H_{n'n''}^{(1)} \rightarrow H_{n'n''}^{(2)} \equiv \langle n^{(0)} | \hat{H}^{(1)} | n''^{(1)} \rangle,$$

where  $n^{(1)}$  is the state  $n''$  calculated in the first order. It is described by Eq. (6.18), so renaming the quantum numbers in that formula ( $n \rightarrow n''$ ,  $n' \rightarrow n$ ), we get

$$H_{n'n''}^{(2)} \equiv \sum_{n \neq n''} \frac{H_{m''}^{(1)}}{E_{n''}^{(0)} - E_n^{(0)}} \langle n^{(0)} | \hat{H}^{(1)} | n^{(0)} \rangle \equiv \sum_{n \neq n''} \frac{H_{n'n}^{(1)} H_{m''}^{(1)}}{E_{n''}^{(0)} - E_n^{(0)}}. \quad (*)$$

(In the particular case  $n' = n''$ , this expression is reduced to Eq. (6.20) of the lecture notes.)

The basic properties of the unperturbed ( $\mathcal{E} = 0$ ) planar rotor were discussed in Sec. 3.5 of the lecture notes. In the coordinate representation, the rotor's Hamiltonian (3.126) is

$$\hat{H}^{(0)} = -\frac{1}{2mR^2} \frac{\partial^2}{\partial \varphi^2},$$

its eigenfunctions (3.129) are<sup>99</sup>

$$\psi_m^{(0)} = \frac{1}{(2\pi)^{1/2}} e^{im\varphi},$$

and the energy spectrum (3.130) is

$$E_m^{(0)} = m^2 E_1, \quad \text{where } E_1 \equiv \frac{\hbar^2}{2mR^2}.$$

All these energy values, besides the ground state ( $m = 0$ ), are doubly degenerate:

$$E_{-m}^{(0)} = E_m^{(0)}.$$

This degeneracy is lifted by the perturbation created by the applied electric field,

$$\hat{H}^{(1)} = -q\mathcal{E}x \equiv -q\mathcal{E}R \cos \varphi, \quad (**)$$

where  $\mathcal{E}$  is the electric field's component within the rotor's plane, and the  $x$ -axis is directed along that component. However, calculating the first-order matrix elements (6.8) of the perturbation (with the natural notation replacement  $n \rightarrow m$ ):

$$\begin{aligned} H_{m'm''}^{(1)} &= \int_0^{2\pi} \psi_{m'}^{(0)*} \hat{H}^{(1)} \psi_{m''}^{(0)} d\varphi \equiv \frac{1}{2\pi} \int_0^{2\pi} e^{-im'\varphi} (-q\mathcal{E}R \cos \varphi) e^{im''\varphi} d\varphi = -\frac{q\mathcal{E}R}{2\pi} \int_0^{2\pi} e^{-im'\varphi} \frac{e^{i\varphi} + e^{-i\varphi}}{2} e^{im''\varphi} d\varphi \\ &= -\frac{q\mathcal{E}R}{2} (\delta_{m',m''-1} + \delta_{m',m''+1}), \end{aligned}$$

we see that they connect only the states with the quantum numbers  $m$  different by  $\pm 1$ , while the difference between these numbers for each degenerate state couple is  $2|m| > 1$ . Hence, the level degeneracy is not lifted in the first order of the theory.<sup>100</sup>

<sup>99</sup> See also Eq. (5.146). The  $m^{\text{th}}$  unperturbed eigenfunction corresponds to the eigenvalue  $(L_z)_m = m\hbar$  – see Eq. (5.158).

<sup>100</sup> Note that this fact is not generally true for the rotor in a substantial additional *magnetic* field. Indeed, as Eq. (3.134) and Fig. 3.18 of the lecture notes show, if the magnetic flux  $\Phi$  piercing rotor's area is exactly a half-multiple of the flux quantum  $\Phi_0 \equiv 2\pi\hbar/q$ , the lowest unperturbed energy levels  $E_m = E_1(m - 1/2)^2 = E_1/4$  are equal for the states with  $\Delta m = 1$ , for example,  $m = 1$  and  $m = 0$ . This degeneracy is lifted by the electric field already in the first order of the perturbation theory. Note also the analogy between this problem and the 1D band theory (see Sec. 2.7 of the lecture notes), where the role of the magnetic field is played by the quasimomentum  $\hbar q$ , and each

Proceeding to its second order, let us spell out Eq. (\*) for the two states of each degenerate pair, i.e. for  $n' = m'$  and  $n'' = \pm m'$ :

$$H_{m',\pm m'}^{(2)} = \sum_{m \neq m'} \frac{H_{m'm}^{(1)} H_{m,\pm m'}^{(1)}}{E_m^{(0)} - E_{m'}^{(0)}} = \frac{1}{E_1} \left( \frac{q\mathcal{E}R}{2} \right)^2 \sum_{m \neq m'} \frac{(\delta_{m',m+1} + \delta_{m',m-1})(\delta_{m,\pm m'+1} + \delta_{m,\pm m'-1})}{m'^2 - m^2}.$$

This expression yields nonvanishing *diagonal* matrix elements for any  $m'$  (with the sum contributed by two terms, with  $m = m' \pm 1$ ):

$$H_{m'm'}^{(2)} = \frac{1}{E_1} \left( \frac{q\mathcal{E}R}{2} \right)^2 \left[ \frac{1}{m'^2 - (m'+1)^2} + \frac{1}{m'^2 - (m'-1)^2} \right] \equiv \frac{1}{E_1} \left( \frac{q\mathcal{E}R}{2} \right)^2 \frac{2}{4m'^2 - 1}, \quad (***)$$

but *off-diagonal* matrix elements only for  $m' = \pm 1$  (with the sum limited to only one term, with  $m = 0$ ):

$$H_{1,-1}^{(2)} = H_{-1,1}^{(2)} = \frac{1}{E_1} \left( \frac{q\mathcal{E}R}{2} \right)^2. \quad (***)$$

Hence all the energy levels  $E_{m'}$  with  $m' \neq \pm 1$  are just shifted by the amount given by Eq. (\*\*\*), but for the states with  $m' = \pm 1$ , we get a system of two linear equations whose matrix consists of two equal off-diagonal elements (\*\*\*) and two equal diagonal elements (\*\*\*):

$$H_{1,1}^{(2)} = H_{-1,-1}^{(2)} = \frac{2}{3E_1} \left( \frac{q\mathcal{E}R}{2} \right)^2.$$

Solving the corresponding characteristic equation that replaces the similar Eq. (6.26):

$$\begin{vmatrix} H_{1,1}^{(2)} - E_1^{(2)} & H_{1,-1}^{(2)} \\ H_{-1,1}^{(2)} & H_{-1,-1}^{(2)} - E_1^{(2)} \end{vmatrix} = 0, \quad \text{which gives} \quad \begin{vmatrix} \frac{2}{3} - \lambda & 1 \\ 1 & \frac{2}{3} - \lambda \end{vmatrix} = 0, \quad \text{for } \lambda \equiv E_1^{(2)} / \frac{1}{E_1} \left( \frac{q\mathcal{E}R}{2} \right)^2,$$

we get two roots,  $\lambda_{\pm} = 2/3 \pm 1$ , showing that in the second order of the perturbation theory, the double degeneracy of this level is indeed lifted:

$$(E_1)_{\pm} = E_1^{(0)} + E_1^{(2)} = E_1 + \frac{1}{E_1} \left( \frac{q\mathcal{E}R}{2} \right)^2 \left( \frac{2}{3} \pm 1 \right) \equiv E_1 \left[ 1 + \left( \frac{q\mathcal{E}R}{2E_1} \right)^2 \times \begin{Bmatrix} 5/3 \\ -1/3 \end{Bmatrix} \right].$$

This expression is quantitatively valid only at  $q\mathcal{E}R/2 \ll E_1 \equiv \hbar^2/2mR^2$ , i.e. in sufficiently low applied electric fields.

**Problem 6.17.\*** The Hamiltonian of a quantum system is slowly changed over time.

(i) Develop a theory of quantum transitions in the system, and spell out its result in the 1<sup>st</sup> approximation in the speed of the change.

(ii) Use this approximation to calculate the probability that a finite-time pulse of a slowly changing force  $F(t)$  drives a 1D harmonic oscillator, initially in its ground state, into an excited state.

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Fourier harmonic of the periodic potential  $U(x)$ , with amplitude  $U_l$ , acts similarly to the sinusoidal perturbation (\*\*). Indeed, the weak-potential limit explored in Sec. 2.7(ii) of the lecture notes is just a particular case of the 1<sup>st</sup>-order perturbation theory in small  $U_l$ .

(iii) Compare the last result with the exact one.

*Solutions:*

(i) Let us solve the Schrödinger equation (4.158),

$$i\hbar \frac{\partial}{\partial t} |\alpha\rangle = \hat{H} |\alpha\rangle,$$

for a system described by a Hamiltonian  $\hat{H}$ , which is slowly changed in time. In the 0<sup>th</sup> approximation in the speed of the change, when the evolution is fully adiabatic, its general solution may be represented as the sum

$$|\alpha\rangle = \sum_n a_n e^{i\varphi_n(t)} |n\rangle,$$

where

$$\varphi_n(t) \equiv -\frac{1}{\hbar} \int_0^t E_n(t') dt', \quad \text{i.e. } \dot{\varphi}_n \equiv -E_n / \hbar,$$

the energies  $E_n(t)$  are defined, at each moment  $t$ , by the pseudo-stationary Schrödinger equation

$$\hat{H} |n\rangle = E_n |n\rangle, \quad (*)$$

and while  $a_n$  are constant  $c$ -numbers. (The physical sense of each  $a_n$  is the probability amplitude of our system being, at time  $t$ , in the instant state  $|n\rangle$  defined by that equation for the same  $t$ .) If the Hamiltonian changes in time, so are  $E_n$  and  $|n\rangle$ , and the 0<sup>th</sup> approximation is not the *exact* solution of the genuine Schrödinger equation, but we may look for such a solution in the same form, with  $E_n$ ,  $|n\rangle$ , and  $\varphi_n$  still defined by the above expressions at each particular instant, but with the probability amplitudes  $a_n$  also being some slow functions of time.

Plugging this form into the time-dependent Schrödinger equation, we get

$$i\hbar \sum_n (\dot{a}_n |n\rangle - i a_n \dot{\varphi}_n |n\rangle + a_n |\dot{n}\rangle) e^{i\varphi_n(t)} = \sum_n \hat{H} a_n |n\rangle e^{i\varphi_n(t)}.$$

According to the above definitions of  $E_n$ ,  $|n\rangle$ , and  $\varphi_n$ , the right-hand side of this relation cancels with the second term on its left-hand side, and the equation, rewritten for the index  $n'$ , reduces to

$$i\hbar \sum_{n'} (\dot{a}_{n'} |n'\rangle + a_{n'} |\dot{n}'\rangle) e^{i\varphi_{n'}(t)} = 0.$$

Now inner-multiplying the left-hand side by  $\langle n | \exp\{-i\varphi_n\}$  with an arbitrary  $n$ , and using the orthonormality of the kets  $n$  at any instant  $t$ , we get the following equation for the time evolution of the coefficients  $a_n$ :

$$\dot{a}_n = -\sum_{n'} a_{n'} \langle n | \dot{n}' \rangle e^{i(\varphi_{n'} - \varphi_n)}.$$

In order to spell out the inner product on the right-hand side of this expression, let us take the partial time derivative of Eq. (\*), also rewritten for the same index  $n'$ :

$$\dot{\hat{H}} |n'\rangle + \hat{H} |\dot{n}'\rangle = \dot{E}_{n'} |n'\rangle + E_{n'} |\dot{n}'\rangle,$$

where the dot over the Hamiltonian operator means its differentiation over its explicit time dependence. Inner-multiplying both parts of this equation by  $\langle n|$ , we get

$$\dot{\hat{H}}_{nn'} + \langle n|\dot{\hat{H}}|\dot{n}'\rangle = \langle n|\dot{E}_{n'}|n'\rangle + \langle n|E_{n'}|\dot{n}'\rangle, \quad \text{where } \dot{\hat{H}}_{nn'} \equiv \langle n|\dot{\hat{H}}_{nn'}|n'\rangle.$$

Both  $E_{n'}$  and its time derivative are just (time-dependent)  $c$ -numbers and may be taken out of the corresponding long brackets, so acting by the Hamiltonian (a Hermitian operator!) in the second term upon the bra-vector on its left, we may reduce this relation to

$$\dot{\hat{H}}_{nn'} + E_n \langle n|\dot{n}'\rangle = \dot{E}_n \langle n|n'\rangle + E_{n'} \langle n|\dot{n}'\rangle.$$

For any  $n' \neq n$ , the first term on the right-hand side vanishes due to the same orthonormality of the set  $n$ , and we get

$$\langle n|\dot{n}'\rangle = -\frac{\dot{\hat{H}}_{nn'}}{E_n - E_{n'}}, \quad \text{for } n' \neq n.$$

On the other hand, for  $n' = n$ , we may differentiate over time the normalization condition  $\langle n|n\rangle = 1$ , getting

$$\langle n|\dot{n}\rangle + \langle \dot{n}|n\rangle \equiv \langle n|\dot{n}\rangle + \langle n|\dot{n}\rangle^* \equiv 2 \operatorname{Re} \langle n|\dot{n}\rangle = 0. \quad (**)$$

This equality means that  $\langle n|\dot{n}\rangle$  is always purely imaginary, i.e. equal to  $i\phi(t)$ , with some real  $\phi(t)$ . But we may always select the phase of the ket  $|n\rangle$ , defined by Eq. (\*), arbitrarily for any time instant. In other words, we may make the replacement  $|n\rangle \rightarrow |n\rangle \exp\{i\Phi(t)\}$  with arbitrary real  $\Phi(t)$ . At such a replacement, the inner product we are discussing changes as

$$\langle n|\dot{n}\rangle \rightarrow (\langle n|\exp\{-i\Phi\}) \frac{\partial}{\partial t} (|n\rangle \exp\{i\Phi\}) \equiv (\langle n|\exp\{-i\Phi\}) (|\dot{n}\rangle + |n\rangle i\dot{\Phi}) \exp\{i\Phi\} \equiv \langle n|\dot{n}\rangle + i\dot{\Phi} \equiv i(\phi + \dot{\Phi}).$$

Hence, with the proper choice of the function  $\Phi(t)$ , we may always make the product  $\langle n|\dot{n}\rangle$  real,<sup>101</sup> so Eq. (\*\*) yields

$$\langle n|\dot{n}\rangle = 0.$$

As a result, we get

$$\dot{a}_n = \sum_{n' \neq n} a_{n'} \frac{\dot{\hat{H}}_{nn'}}{E_n - E_{n'}} e^{i(\varphi_{n'} - \varphi_n)}. \quad (***)$$

So far, this is an exact result, equivalent to the initial Schrödinger equation. (In this aspect, Eq. (\*\*\*) is similar to Eqs. (6.84) of the “usual” perturbation theory, though these two relations are based on different approaches, each of them being more convenient in its own domain of applications.) Now let us reduce Eq. (\*\*\*) to an approximate form for the case when at  $t < 0$  the system was definitely in its ground state ( $n' = 0$ ). Then, in the 1<sup>st</sup> approximation in the Hamiltonian’s change speed, on the right-hand side of Eqs. (\*\*\*), we may take  $a_0 = 1$ , and all other  $a_{n'} = 0$ , so

<sup>101</sup> It would be, however, an error to say that  $|n\rangle$  itself may be made real in any representation. For example, in the coordinate representation, the corresponding wavefunction  $\psi_n \equiv \langle \mathbf{r}|n\rangle$  cannot be made real in many cases – see, for example, the wavefunctions (3.129) with  $m \neq 0$ , or more generally any eigenstate with a nonvanishing density  $\mathbf{j}$  of probability current – see Eq. (1.49).

$$\dot{a}_n(t) = \frac{\dot{H}_{n0}}{E_n - E_0} \exp\{i[\varphi_0(t) - \varphi_n(t)]\} \equiv \frac{\dot{H}_{n0}}{E_n - E_0} \exp\left\{\frac{i}{\hbar} \int_0^t [E_n(t') - E_0(t')] dt'\right\}.$$

(ii) For a 1D harmonic oscillator under the effect of an additional force  $F(t)$ ,

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega_0^2 \hat{x}^2}{2} - F(t)\hat{x}, \quad \text{so that } \dot{\hat{H}} \equiv \frac{\partial}{\partial t} \hat{H} = -\dot{F}(t)\hat{x}, \quad \text{i.e. } \dot{H}_{n0} = -\dot{F}(t)x_{n0}.$$

As Eq. (5.92) of the lecture notes shows, in the harmonic oscillator, only one of these matrix elements, namely  $x_{10} = x_0/\sqrt{2}$ , is different from zero, so in the 1<sup>st</sup> approximation in speed, only the first excited state ( $n = 1$ ) has a non-zero probability amplitude  $a_n = a_1$ . Taking into account also that for the harmonic oscillator, even biased by an additional force,  $E_1 - E_0 = \hbar\omega_0 = \text{const}$ , we get

$$\dot{a}_1 = -\frac{\dot{F}(t)}{E_1 - E_0} \frac{x_0}{\sqrt{2}} \exp\left\{\frac{i}{\hbar} \int_0^t [E_1(t') - E_0(t')] dt'\right\} \equiv -\frac{x_0}{\sqrt{2}\hbar\omega_0} \dot{F}(t) e^{i\omega_0 t},$$

so, taking into account that  $x_0 \equiv (\hbar/m\omega_0)^{1/2} = \text{const}$ , the probability of finding the oscillator in the first excited state at time  $t$  is

$$W_1(t) \equiv |a_1(t)|^2 = \frac{x_0^2}{2\hbar^2\omega_0^2} \left| \int_0^t \dot{F}(t') e^{i\omega_0 t'} dt' \right|^2 \equiv \frac{1}{2\hbar m\omega_0^3} \left| \int_0^t \dot{F}(t') e^{i\omega_0 t'} dt' \right|^2.$$

For a finite-time pulse of force, we may always select a time interval  $[0, t]$  so broad that  $F(t) = 0$  outside it, and it makes sense to work out the involved integral by parts:

$$\int_{-\infty}^{+\infty} \dot{F}(t) e^{i\omega_0 t} dt = \int_{t=-\infty}^{t=+\infty} e^{i\omega_0 t} d[F(t)] = \left[ F(t) e^{i\omega_0 t} \right]_{t=-\infty}^{t=+\infty} - \int_{t=-\infty}^{t=+\infty} F(t) d(e^{i\omega_0 t}) \equiv 0 - i\omega_0 \int_{t=-\infty}^{t=+\infty} F(t) e^{i\omega_0 t} dt,$$

so we may rewrite the expression for the final value of  $W_1$  in a more convenient form:

$$W_1 = \frac{|I|^2}{2\hbar m\omega_0}, \quad \text{with } I \equiv \int_{-\infty}^{+\infty} F(t) e^{i\omega_0 t} dt. \quad \text{(***)}$$

By construction of the 1<sup>st</sup> approximation, this result is only valid if  $W_1 \ll 1$ .

(iii) For this particular system (the harmonic oscillator, initially in its ground state), the exact solution, valid for *any*  $W_1$ , is also possible. Indeed, as was discussed in the model solution of Problem 5.21, if the oscillator was in the ground state (which is one of the Glauber states) initially, then even at an arbitrary time  $t$ , it remains in the Glauber state (5.107) with the time-dependent central point

$$X(t) = \frac{1}{m\omega_0} \int_0^t F(t') \sin \omega_0(t-t') dt', \quad P(t) = \int_0^t F(t') \cos \omega_0(t-t') dt',$$

i.e. with the dimensionless complex amplitude (defined by Eq. (5.102) of the lecture notes)

$$\alpha(t) \equiv \left( \frac{m\omega_0}{2\hbar} \right)^{1/2} \left[ X(t) + i \frac{P(t)}{m\omega_0} \right] = i \left( \frac{1}{2m\hbar\omega_0} \right)^{1/2} \int_0^t F(t') e^{i\omega_0(t-t')} dt'$$

$$\equiv i \left( \frac{1}{2m\hbar\omega_0} \right)^{1/2} e^{i\omega_0 t} \int_0^t F(t') e^{-i\omega_0 t'} dt'.$$

According to this formula, after the end of the pulse (formally, at  $t = +\infty$ ), the Poisson distribution parameter  $\langle n \rangle$  defined by Eq. (5.137) is

$$\langle n \rangle \equiv |\alpha(+\infty)|^2 = \frac{|I|^2}{2m\hbar\omega_0},$$

where  $I$  is the same integral as in Eq. (\*\*\*\*). Now we may use Eq. (5.135) of the lecture notes to calculate the probability of the oscillator's transfer, by the pulse, into the first excited Fock state:

$$W_1 = \langle n \rangle e^{-\langle n \rangle} \equiv \frac{|I|^2}{2m\hbar\omega_0} \exp \left\{ -\frac{|I|^2}{2m\hbar\omega_0} \right\}.$$

In the limit of small  $I$ , this (exact) result reduces to Eq. (\*\*\*\*), thus confirming its correctness.<sup>102</sup>

**Problem 6.18.\*** Use the single-particle model to calculate the complex electric permittivity  $\varepsilon(\omega)$  of a dilute gas of similar atoms, due to their induced electric polarization by a weak external ac field, for a field frequency  $\omega$  very close to one of the quantum transition frequencies  $\omega_{nn'}$ . Based on the result, calculate and estimate the absorption cross-section of each atom.

*Hint:* In the single-particle model, the atom's properties are determined by  $Z$  similar, non-interacting electrons, each moving in a similar static attracting potential, generally different from the Coulomb one, because it is contributed not only by the nucleus but also by other electrons.

*Solution:* According to the complex electric permittivity's definition,<sup>103</sup> in the approximation of non-interacting atoms, it may be calculated as

$$\varepsilon(\omega) \equiv \frac{\mathcal{D}_\omega}{\mathcal{E}_\omega} = \frac{\varepsilon_0 \mathcal{E}_\omega + n d_\omega}{\mathcal{E}_\omega} \equiv \varepsilon_0 + n \frac{d_\omega}{\mathcal{E}_\omega},$$

where  $n$  is the number of atoms per unit volume,<sup>104</sup> and  $d_\omega$  is the complex amplitude of the time-dependent expectation value of the electric dipole moment of one atom,

$$\langle d \rangle = d_\omega e^{-i\omega t} + d_\omega^* e^{i\omega t},$$

induced by the applied weak classical ac field<sup>105</sup>

<sup>102</sup> According to the same Eq. (5.135), the probability of exciting the  $n^{\text{th}}$  Fock state, in the same limit  $I \rightarrow 0$  (i.e.  $\langle n \rangle \rightarrow 0$ ), scales as  $W_n \propto \langle n \rangle^n \propto |I|^{2n}$ , explaining why all  $W_n$  with  $n > 1$  vanish in the 1<sup>st</sup> approximation in  $|I|^2$ .

<sup>103</sup> See, e.g., EM Secs. 3.3 and 7.2 (where the electric dipole moment is denoted as  $\mathbf{p}$ ). Note that generally,  $\mathcal{E}(t)$  and  $\langle \mathbf{d}(t) \rangle$  are vectors with different directions, not necessarily proportional to each other – see, e.g., EM Secs. 3.1-3.2. Dielectric properties of a medium may be described by a scalar, field-independent function  $\varepsilon(\omega)$  only if these vectors are essentially parallel (which is true for any disordered matter) and proportional to each other (which is always true for sufficiently low fields, in the absence of spontaneous polarization). Since the problem assignment asks for such a scalar function, we may safely assume that these conditions are satisfied.

<sup>104</sup> This fancy font for  $n$  is used here to avoid confusion with the quantum state number  $n$ .

$$\mathcal{E} = \mathcal{E}_\omega e^{-i\omega t} + \mathcal{E}_\omega^* e^{i\omega t}.$$

In the single-particle model,  $d$  may be calculated as  $Zqx$ , where  $q = -e$  is the single electron charge,  $Z$  is the number of electrons per atom, and  $x$  is the electron's coordinate along the applied field's direction, so in the Schrödinger picture, its expectation value in the time-dependent quantum state  $\alpha(t)$  may be calculated as

$$\langle d \rangle = Zq \langle \alpha(t) | \hat{x} | \alpha(t) \rangle. \quad (*)$$

According to the analysis in Sec. 6.5 of the lecture notes, if the field's frequency  $\omega$  is very close to that of a quantum transition between two eigenstates, in the expansion of the bra- and ket-vectors of the state  $\alpha$  into a series over eigenstate vectors, we may keep only the corresponding two terms. At weak applied fields and not extremely high temperatures, the atoms spend most of the time in their ground state (due to unavoidable energy relaxation – see Chapter 7 for its discussion), so one of the involved states, with the probability amplitude very close to 1, has to be the ground state of the system. As a result, by using Eq. (6.82), we may approximate the state vectors as

$$|\alpha(t)\rangle = |0\rangle \exp\left\{-i\frac{E_0 t}{\hbar}\right\} + a(t)|n\rangle \exp\left\{-i\frac{E_n t}{\hbar}\right\}, \quad \langle\alpha(t)| = \langle 0| \exp\left\{i\frac{E_0 t}{\hbar}\right\} + a^*(t)\langle n| \exp\left\{i\frac{E_n t}{\hbar}\right\},$$

where the coefficient  $a(t)$  is proportional to the applied field, and hence small.<sup>106</sup> Plugging this expression into Eq. (\*) and keeping only the terms proportional to  $a$  (and hence to  $\mathcal{E}_\omega$ ), we get

$$\begin{aligned} \langle d \rangle &= Zq \left[ a(t) \exp\left\{i\frac{E_0 - E_n}{\hbar}t\right\} x_{0n} + a^*(t) \exp\left\{i\frac{E_n - E_0}{\hbar}t\right\} x_{n0} \right], \\ &= Zq \left[ a(t) \exp\{-i\omega_{n0}t\} x_{0n} + a^*(t) \exp\{i\omega_{n0}t\} x_{n0} \right] \end{aligned}$$

where  $\omega_{n0} \equiv (E_n - E_0)/\hbar$ , while  $x_{0n}$  and  $x_{n0}$  are time-independent matrix elements of the Hermitian operator of the coordinate:

$$x_{0n} \equiv \langle 0 | \hat{x} | n \rangle = \langle n | \hat{x} | 0 \rangle^* \equiv x_{n0}^*.$$

Generally, the time evolution of the probability amplitude  $a(t)$  of the excited state  $n$  has to be found from the system of equations (6.88), with the Hamiltonian's amplitude

$$\hat{A}_\omega = -q\mathcal{E}_\omega \hat{x},$$

corresponding to the perturbation (6.29), with  $z$  duly replaced with  $x$ . However, in our resonant case when  $\omega \approx \omega_{n0}$ , we may reuse the approximate solution of the system, expressed by the first term of Eq. (6.90), with  $n' = 0$  and  $A_{nn'} = A_{n0} = -q\mathcal{E}_\omega x_{n0}$ . As a result, we get

<sup>105</sup> Note that these relations between  $d(t)$  and  $\mathcal{E}(t)$  and their complex amplitudes differ (by a factor of 2) from the usual relations accepted in this series, e.g.,  $x(t) = \text{Re}[x_\omega \exp\{-i\omega t\}]$ , etc. This notation, accepted here just to better correspond to Eq. (6.86) of the lecture notes, does not change the  $d_\omega/\mathcal{E}_\omega$  ratio of our interest.

<sup>106</sup> Here I assume that  $|a(t)| \ll 1$  – the relation that should be used to derive the qualitative condition of the electric field's smallness necessary for the result's validity.



$$\begin{aligned}\langle d \rangle &= \frac{ZqA_{n,0}}{\hbar(\omega - \omega_{n0})} [\exp\{i(\omega_{n0} - \omega)t\} - 1] \exp\{-i\omega_{n0}t\} x_{0n} + \text{c.c.} \\ &\equiv -\frac{Zq^2 \mathcal{E}_\omega}{\hbar(\omega - \omega_{n0})} x_{n0} x_{0n} [\exp\{-i\omega t\} - \exp\{-i\omega_{n0}t\}] + \text{c.c.}\end{aligned}$$

This means that the complex amplitude of the only frequency component we are interested in (changing in time as  $\exp\{-i\omega t\}$ , i.e. with the same frequency as the field, and hence giving a nonvanishing average contribution to the electric permittivity)<sup>107</sup> is

$$d_\omega = -\frac{Zq^2 |x_{n0}|^2}{\hbar(\omega - \omega_{n0})} \mathcal{E}_\omega \equiv \frac{Zq^2 |x_{n0}|^2}{\hbar(\omega_{n0} - \omega)} \mathcal{E}_\omega.$$

(As a parenthetic remark: note that this result enables the calculation of the average energy of the field-atom interaction:

$$\langle \bar{U} \rangle = -\frac{1}{2} \overline{\langle d \rangle(t) \cdot \mathcal{E}(t)} = -\frac{1}{4} \text{Re}(d_\omega^* \mathcal{E}_\omega) = \frac{Zq^2 |x_{n0}|^2}{4\hbar(\omega - \omega_{n0})} \mathcal{E}_\omega \mathcal{E}_\omega^*.$$

This formula shows that the resulting average force  $\bar{\mathbf{F}} = -\nabla \bar{U}$  exerted on the atom by a standing-wave field pushes it to the field's *maximum* at  $\omega < \omega_{n0}$ , and to its *minimum* in the opposite case.<sup>108</sup>)

Finally, summing the contributions from all excited states  $n$ , we get the following formal result:

$$\varepsilon(\omega) = \varepsilon_0 + nZ \frac{q^2}{\hbar} \sum_{n>0} \frac{|x_{n0}|^2}{\omega_{n0} - \omega}, \quad (**)$$

though it is strictly valid only in a close vicinity of each transition frequency  $\omega_{n0}$  – namely, at  $|\omega - \omega_{n0}| \ll |\omega_{n0}|$ . It describes odd-resonant, diverging responses of the system near each quantum transition frequency  $\omega_{n0}$ .

In the particular case when the atom may be modeled by a 1D harmonic oscillator of an eigenfrequency  $\omega_0$ , we may use Eq. (5.92) to get  $|x_{n0}|^2 = (\hbar/2m\omega_0)\delta_{n0}$ , and hence the function  $\varepsilon(\omega)$ , at positive frequencies, has only one such singularity (*pole*):

$$\varepsilon(\omega) = \varepsilon_0 + nZ \frac{q^2}{2m\omega_0(\omega_0 - \omega)}, \quad \text{at } \omega \approx \omega_0. \quad (***)$$

Remarkably, this result coincides *exactly* with the one of classical theory for a set of  $nZ$  similar harmonic oscillators, with negligible damping, per unit volume,<sup>109</sup> illustrating again that the harmonic oscillator is “the most classical” of all spatially-confined quantum systems, due to the linearity of its

<sup>107</sup> Re-examining the analysis of Sec. 6.5, we may see that the second term in this result, having a different frequency, is the artifact of the zero initial conditions assumed at the sharp turning on of the interaction Hamiltonian – see Eq. (6.86). In real systems with unavoidable nonvanishing (if very small) dissipation, this component decays with time, and the whole atomic response retains only one frequency ( $\omega$ ), representing the quantum version of the classical forced oscillations – see, e.g., CM Sec. 5.1.

<sup>108</sup> A discussion of the physics of this force, for a particular case of a free classical particle, may be found, e.g. in the model solution of EM Problem 7.5.

<sup>109</sup> See, e.g., EM Eq. (7.32) with  $n$  replaced with  $nZ$ ,  $\delta = 0$  and  $\omega \rightarrow \omega_0$ .

Heisenberg equations of motion. (Due to this property, Eq. (\*\*\*) might be obtained much simpler – just using the fact that due to the linearity of Eqs. (5.36) with  $U = m\omega_0^2 x^2/2 - q\mathcal{E}x$ , the expectation value of the coordinate of the oscillator follows the classical equations of motion.)

Now returning to the general quantum-mechanical result (\*\*), valid for an arbitrary confining potential, we may notice that it has a structure similar to Eq. (\*\*\*), and may be rewritten in the form inspired by it:

$$\varepsilon(\omega) = \varepsilon_0 + nZ \frac{q^2}{2m} \sum_{n>0} \frac{f_n}{\omega_{n0}(\omega_{n0} - \omega)}, \quad \text{where } f_n \equiv \frac{2m}{\hbar} \omega_{n0} |x_{n0}|^2 \equiv \frac{2m}{\hbar^2} (E_n - E_0) |x_{n0}|^2.$$

Due to the analogy with Eq. (\*\*\*), the coefficient  $f_n$  is called the *oscillator strength* of the atomic excitation from its ground state to the  $n^{\text{th}}$  energy level. According to Eq. (\*\*\*), for a harmonic oscillator only one such of these coefficients,  $f_1 = 1$ , is different from zero. For an arbitrary confining potential, this is not true, but the sum of all  $f_n$  still equals 1 – see the solution of Problem 5.13.

The above results may leave the impression that the complex electric permittivity is a purely real function of frequency. However, the *Kramers-Kronig dispersion relations*, based on very general causality arguments, and hence valid for the results of the quantum-mechanical analysis as well, show that the real and imaginary parts of the function  $\varepsilon(\omega) = \varepsilon'(\omega) + i\varepsilon''(\omega)$  are always related.<sup>110</sup> In particular, each pole of  $\varepsilon'(\omega)$  at a certain frequency corresponds to a proportional delta function of the imaginary part  $\varepsilon''(\omega)$  of this function, which characterizes energy loss in the medium:<sup>111</sup>

$$\frac{1}{\omega_{n0} - \omega} \text{ in } \varepsilon'(\omega) \leftrightarrow \pi\delta(\omega - \omega_{n0}) \text{ in } \varepsilon''(\omega).$$

For our particular case, this correspondence yields the following result (for  $\omega > 0$ ):

$$\varepsilon''(\omega) = nZ \frac{\pi q^2}{2m} \sum_{n>0} \frac{f_n}{\omega_{n0}} \delta(\omega - \omega_{n0}), \quad \text{(***)}$$

describing a series of infinitely narrow resonance peaks of the media's absorption at each quantum transition frequency.

This result may look mysterious because at our current description of the system by a Hamiltonian, it should not, apparently, have any energy loss. Indeed, this result, of the same class as the Golden Rule discussed in Secs. 6.6-6.7 of the lecture notes,<sup>112</sup> is one of the non-trivial (and hence most beautiful :-)) results of quantum mechanics, which essentially preempts the analysis of open quantum systems. Such analysis, to be discussed in Chapter 7, describes the system's energy loss by its coupling to the environment, and in particular, shows that as the coupling tends to zero, the finite-width peaks of the dissipative functions similar to  $\varepsilon''(\omega)$  become infinitely narrow but retain their "areas", i.e. the delta functions' weights given by Eq. (\*\*\*)).

<sup>110</sup> See, e.g., EM Sec. 7.2.

<sup>111</sup> See, e.g., EM Eqs. (7.55)-(7.56)

<sup>112</sup> Actually, all the essential physics of the relation between the reversible and irreversible quantum dynamics is described already by the simple metastable state model discussed at the end of Sec. 2.5, and the reader having conceptual issues with this relation may be referred there for an additional thoughtful review.

The result (\*\*\*) may be readily re-calculated into the absorption cross-section  $\sigma$  of one atom, which may be defined by the following (hopefully, self-explanatory) relation for the time-averaged power of the incident wave per unit area of its front:<sup>113</sup>

$$\frac{d\overline{\mathcal{P}}}{dz} = -n\sigma\overline{\mathcal{P}},$$

where  $z$  is the direction of the wave propagation. Namely, basic macroscopic electrodynamics tells us that the same power gradient of a monochromatic wave of frequency  $\omega$  may be calculated as<sup>114</sup>

$$\frac{d\overline{\mathcal{P}}}{\overline{\mathcal{P}}} = -2k''(\omega)dz,$$

where  $k''(\omega)$  is the imaginary part of the complex wave number  $k(\omega) = \omega[\epsilon(\omega)\mu(\omega)]^{1/2}$ . For a non-magnetic medium (with  $\mu(\omega) = \mu_0$ ), with relatively weak absorption ( $\epsilon''(\omega) \ll \epsilon'(\omega) = \epsilon_0$ ), we may Taylor-expand this expression for  $k$ :

$$k \equiv k' + ik'' = \omega[(\epsilon_0 + i\epsilon'')\mu_0]^{1/2} \equiv \omega \left[ \epsilon_0 \left( 1 + i \frac{\epsilon''}{\epsilon_0} \right) \mu_0 \right]^{1/2} \approx \omega(\epsilon_0\mu_0)^{1/2} \left( 1 + i \frac{\epsilon''}{2\epsilon_0} \right),$$

thus getting

$$2k''(\omega) = \omega \left( \frac{\mu_0}{\epsilon_0} \right)^{1/2} \epsilon''(\omega) \equiv \frac{\omega}{\epsilon_0 c} \epsilon''(\omega).$$

Now comparing the two above expressions for the power loss per unit length, we get

$$\sigma = \frac{1}{n} \frac{\omega}{\epsilon_0 c} \epsilon''(\omega),$$

so by using Eq. (\*\*\*), with  $q = -e$ , we finally get<sup>115</sup>

$$\sigma = Z \frac{\pi e^2}{2m\epsilon_0 c} \sum_{n>0} f_n \delta(\omega - \omega_{n0}) \equiv 4\pi^2 Z\alpha\omega \sum_{n>0} |x_{n0}|^2 \delta(\omega - \omega_{n0}),$$

where  $\alpha \equiv (e^2/4\pi\epsilon_0)/\hbar c \approx 1/137$  is the fine-structure constant.

Since the square of the coordinate matrix element is typically of the order of the “physical” cross-section  $\sigma_0$  of the atom, this result shows that the frequency-averaged cross-section,

$$\sigma_{\text{ave}} \equiv \frac{1}{\omega_{n0}} \int_{\Delta\omega \sim \omega_{n0}} \sigma d\omega,$$

is of the order of  $\alpha Z\sigma_0$ , i.e. is much smaller than  $\sigma_0$  for not-too-heavy atoms. This relation gives one more illustration of the fine-structure constant  $\alpha$  as a measure of the electromagnetic interaction weakness on the quantum-mechanical energy scale.

<sup>113</sup> This expression implies incoherent addition of the energies absorbed by each atom, which is a good approximation for gases, with random interatomic distances.

<sup>114</sup> See, e.g., EM Sec. 7.9, in particular, Eqs. (7.215)-(7.216).

<sup>115</sup> In a slightly different form, this result was first obtained by H. Kramers and W. Heisenberg as early as 1925.

**Problem 6.19.** Use the solution of the previous problem to generalize the expression for the London dispersion force between two atoms (whose calculation in the harmonic oscillator model was the subject of Problems 3.20 and 5.20) to the single-particle model with an arbitrary energy spectrum.

*Solution:* The result obtained in Problem 5.20 for a spherically symmetric harmonic oscillator model of each atom,

$$U = -\frac{3q^4\hbar}{2(4\pi\epsilon_0)^2 m^2 r^6} \frac{1}{\omega_1\omega_2(\omega_1 + \omega_2)},$$

may be readily generalized to modeling each atom by a set of such oscillators, with eigenfrequencies  $\omega_n$  and relative numbers  $f_n$ :

$$U = -\frac{3q^4\hbar}{2(4\pi\epsilon_0)^2 m^2 r^6} \sum_{n,n'} \frac{f_n f_{n'}}{\omega_n \omega_{n'} (\omega_n + \omega_{n'})}.$$

Now using the fact that according to the model solution of Problem 5.20, this formula is based on the same resonance response as was discussed in the solution of the previous problem, we may generalize it further to describe the long-range interaction between two arbitrary (but still isotropic) single-particle systems:

$$U = -\frac{3q^4\hbar}{2(4\pi\epsilon_0)^2 m^2 r^6} \sum_{n,n'>0} \frac{f_n f_{n'}}{\omega_{n0} \omega_{n'0} (\omega_{n0} + \omega_{n'0})}, \quad (*)$$

where the frequency sets  $\omega_{n0} \equiv (E_n - E_0)/\hbar$  and  $\omega_{n'0} \equiv (E_{n'} - E_0)/\hbar$  describe the excitation spectra of the counterpart atoms, and  $f_n$  and  $f_{n'}$  are the oscillator strengths of the corresponding transitions:

$$f_n \equiv \frac{2m}{\hbar} \omega_{n0} |x_{n0}|^2.$$

(Due to the assumed isotropy, the matrix elements  $x_{n0}$  are the same for all coordinates.)

For a typical atom, the lowest energy differences  $(E_n - E_0)$  and  $(E_{n'} - E_0)$ , giving the largest contributions to the sum in Eq. (\*), are of the order of the Hartree energy  $E_H$  – see Eq. (1.13). Plugging such values into Eq. (\*), and also taking  $m = m_e$  and ignoring numerical factors of the order of 1, we get the following crude estimate of the London dispersion force's potential:

$$|U| \sim E_H \left( \frac{r_B}{r} \right)^6.$$

Formula (\*) was the main result obtained in 1930 by F. London. Its main restriction is that it assumes the instant propagation of the dipole's electric field by the inter-atomic distance  $r$ . This assumption (which was clearly made in the model solutions of Problems 3.20 and 5.20) is valid only if  $k_{n0}r \ll 1$ , where the wave number  $k_{n0}$  equals  $\omega_{n0}/c$  in vacuum, and may be moderately higher in a dense medium. Since the typical frequencies  $\omega_{n0}$  for atoms and molecules are rather high ( $\sim 10^{16} \text{ s}^{-1}$ ), noticeable deviations from London's result may start already from  $r \sim 1 \mu\text{m}$ . The later extensions of this theory to arbitrary values of  $k_{n0}r$ , notably by H. Casimir and D. Polder in 1948, and by E. Lifshitz in 1956,<sup>116</sup> have shown a remarkable (and rather counter-intuitive!) connection between the London dispersion force and the fundamental *Casimir effect* – for its discussion, see Sec. 9.1 of the lecture notes.

<sup>116</sup> For a comprehensive review of this topic see, e.g., I. Dzyaloshinskii *et al.*, *Sov. Phys. Uspekhi* **4**, 153 (1961).

**Problem 6.20.** Use the solution of the previous problem to calculate the potential energy of the interaction of two hydrogen atoms, both in their ground state, separated by distance  $r \gg r_B$ .

*Solution:* For the effective potential energy of the far-range interaction of two similar atoms, we may use the solution of the previous problem, with  $f_n = f_n'$  and  $\omega_{n0} = \omega_{n'0}$ :

$$U = -\frac{3}{4} \left( \frac{q^2}{4\pi\epsilon_0} \right)^2 \frac{\hbar}{m^2 r^6} \sum_{n>0} \frac{f_n^2}{\omega_{n0}^3} \equiv -3 \left( \frac{q^2}{4\pi\epsilon_0} \right)^2 \frac{1}{\hbar r^6} \sum_{n>0} \frac{|x_{n0}|^4}{\omega_{n0}}.$$

For a hydrogen atom,  $q = -e$ , and  $m = m_e$ , so according to the Eq. (1.9) of the lecture notes,  $(q^2/4\pi\epsilon_0)^2 = (e^2/4\pi\epsilon_0)^2 = (\hbar^2/m_e)E_H$ , where  $E_H \approx 27.2$  eV is the Hartree energy unit, and we may rewrite  $U$  in a form more convenient for our purposes:

$$U = -3E_H \frac{\hbar}{m_e r^6} \sum_{n>0} \frac{|x_{n0}|^4}{\omega_{n0}}. \quad (*)$$

Due to the ground state's isotropy, we may replace<sup>117</sup> the matrix elements  $x_{n0}$  with the elements<sup>118</sup>

$$z_{n1} \equiv \langle n, l, m | \hat{z} | 1, 0, 0 \rangle = \langle n, l, m | r \cos \theta | 1, 0, 0 \rangle = I_\Omega I_n,$$

with the same moduli, where

$$I_\Omega \equiv \oint d\Omega [Y_l^m(\theta, \varphi)]^* \cos \theta Y_0^0(\theta, \varphi), \quad \text{and} \quad I_n \equiv \int_0^\infty r^2 dr \mathcal{R}_{nl}^*(r) r \mathcal{R}_{1,0}(r).$$

Since  $\cos \theta \equiv P_1(\cos \theta)$ , Eq. (3.170) of the lecture notes shows<sup>119</sup> that all integrals  $I_\Omega$  vanish beside one, with  $l = 1$  and  $m = 0$ :<sup>120</sup>

$$I_\Omega = 2\pi \int_0^\pi \sin \theta d\theta \left[ \left( \frac{3}{4\pi} \right)^{1/2} \cos \theta \right] \cos \theta \left( \frac{1}{4\pi} \right)^{1/2} = \frac{\sqrt{3}}{2} \int_{-1}^{+1} \cos^2 \theta d(\cos \theta) = \frac{1}{\sqrt{3}}.$$

As a result, Eq. (\*) is reduced to

$$U = -\frac{1}{3} E_H \frac{\hbar^2}{m_e r^6} \sum_{n>1} \frac{|I_n|^4}{\hbar \omega_{n0}},$$

where, according to Eq. (1.8),<sup>43</sup>

<sup>117</sup> One has to resist the possible temptation to *add*, to Eq. (\*), similar contributions from other Cartesian components. Indeed, that relation *already* takes their contributions into account – see the solutions of Problems 3.20 and 5.20.

<sup>118</sup> Note that due to the traditional choice of the principal quantum numbers  $n$ , taken equal to 1 rather than 0 for the ground state, in atom-related problems, the index “0” in the general formulas of the perturbation theory has to be understood as the set  $\{n = 1, l = 0, m = 0\}$ .

<sup>119</sup> This fact may be even more obvious from the explicit form of the lowest-order spherical harmonics – see Eqs. (3.174)-(3.176).

<sup>120</sup> This is just one more manifestation of the selection rules for the orbital electric-dipole transitions,  $\Delta l = 1$ ,  $\Delta m = 0, \pm 1$ , which were repeatedly discussed in this course – see in particular Problem 5.35.

<sup>43</sup> Alternatively, see Eq. (3.201) with  $C = e^2/4\pi\epsilon_0$ .

$$\hbar\omega_{n,0} = E_H \left[ -\frac{1}{2n^2} - \left( -\frac{1}{2 \cdot 1^2} \right) \right] \equiv \frac{\hbar^2}{2m_e r_B^2} \left( 1 - \frac{1}{n^2} \right),$$

so, finally

$$U = -\frac{2}{3} E_H \left( \frac{r_B}{r} \right)^6 \sum_{n>1} \frac{(|I_n|/r_B)^4}{1-1/n^2}. \quad (**)$$

For the first (and the largest) term of the sum, with  $n = 2$ ,  $I_n$  may be readily calculated by using Eqs. (3.208)-(3.209) with  $r_0 = r_B$  and a well-known integral<sup>121</sup>:

$$\begin{aligned} I_2 &= \int_0^\infty r^2 dr \frac{1}{(2r_B)^{3/2}} \frac{r}{3^{1/2} r_B} \exp\left\{-\frac{r}{2r_B}\right\} r \frac{2}{r_B^{3/2}} \exp\left\{-\frac{r}{r_B}\right\} \\ &\equiv \frac{r_B^2}{6^{1/2}} \left(\frac{2}{3}\right)^5 \int_0^\infty \xi^4 e^{-\xi} d\xi = \frac{r_B^2}{6^{1/2}} \left(\frac{2}{3}\right)^5 4! \equiv \frac{2^{15/2}}{3^{9/2}} r_B, \end{aligned}$$

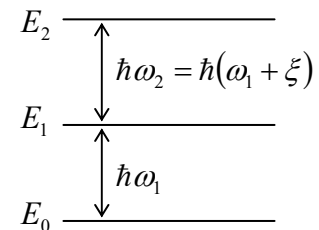
so the first term of the sum in Eq. (\*\*) equals  $(2^{15/2}/3^{9/2})^4/(1-1/2^2) = 2^{32}/3^{20} \approx 3.69$ .

In order to calculate  $I_n$  for higher values of  $n$ , we would need to use the heavy artillery of Eqs. (3.195)-(3.197), but since the radial wavefunctions  $\mathcal{R}_{n,l}$  in the integrals  $I_n$  are normalized in the sense of Eq. (3.194), and the scale of the spatial extension of the product  $\mathcal{R}_{n,1}\mathcal{R}_{1,0}$  is  $[n/(n+1)]r_B$ , all these integrals are proportional to  $r_B$ , while decreasing fast with  $n$  – compare, for example, the blue-line plots for  $\mathcal{R}_{n,1}$  with  $n = 2$  and  $n = 3$  in Fig. 3.22. As a result, the whole sum in Eq. (\*\*) is not much larger than its first term, and hence, taking into account the front coefficient  $(2/3)$ , the interaction energy may be fairly estimated as

$$U \approx -3E_H \left( \frac{r_B}{r} \right)^6.$$

Since our calculations are based on a perturbative approach, this result is only valid if  $|U| \ll E_H$ , i.e. if  $r \gg r_B$ . (On shorter distances between the atoms, the much stronger covalent bonding takes over – see its discussion in Sec. 2.6 of the lecture notes.)

**Problem 6.21.** In a certain quantum system, distances between the three lowest energy levels are slightly different – see the figure on the right ( $|\xi| \ll \omega_{1,2}$ ). Assuming that the involved matrix elements of the perturbation Hamiltonian are known and are all proportional to the external ac field's amplitude, find the time necessary to populate the first excited level almost completely (with a given precision  $\varepsilon \ll 1$ ), by using the Rabi oscillation effect, if at  $t = 0$ , the system is in its ground state. Spell out your result for a weakly anharmonic 1D oscillator.



**Solution:** Since  $\varepsilon \equiv 1 - (W_1)_{\max} \ll 1$ , the undesirable population of the second excited level,  $W_2 < \varepsilon$ , is small, so we may first calculate  $W_1$  ignoring the probability amplitude  $a_2$ , i.e. exactly as it was done in the two-level approximation in Sec. 6.5 of the lecture notes. For the precise tuning of the external

<sup>121</sup> See, e.g., MA (6.7d) with  $n = 4$ .

excitation frequency,  $\omega = \omega_1$  (which is necessary to approach  $(W_1)_{\max} = 1$ ), i.e. for  $\Delta \rightarrow \Delta_{10} = 0$ , Eq. (6.99) with  $A = A_{10}$  gives  $\Omega = |A_{10}|/\hbar$ , and we may use Eq. (6.100) of the lecture notes to write

$$b_1(t) = -i \sin \frac{|A_{10}|t}{\hbar} \equiv -i \sin \zeta t, \quad \text{where } \zeta \equiv \frac{|A_{10}|}{\hbar},$$

so from the first of Eqs. (6.96), also with  $\Delta = 0$ , we get

$$a_1(t) = -i \sin \zeta t. \quad (*)$$

Now, neglecting the effect of the small amplitude  $a_2(t)$  of the second excited state on the function  $a_1(t)$ , we may plug Eq. (\*) into the first of Eqs. (6.94) written for  $n = 2$ ,  $n' = 1$ , and hence with  $\Delta = \Delta_{21} \equiv \omega - \omega_2 = -\xi$ , and  $A = A_{21}$ ;<sup>122</sup>

$$i\hbar \dot{a}_2 = a_1(t) A_{21} e^{i\xi t} = -i A_{21} \sin \zeta t e^{i\xi t} \equiv -\frac{A_{21}}{2} [\exp\{i(\xi + \zeta)t\} - \exp\{i(\xi - \zeta)t\}].$$

Its integration is elementary, and (with the initial condition  $a_2(0) = 0$ ) yields

$$a_2(t) = \frac{A_{21}}{2\hbar} \left[ \frac{\exp\{i(\xi + \zeta)t\} - 1}{\xi + \zeta} - \frac{\exp\{i(\xi - \zeta)t\} - 1}{\xi - \zeta} \right].$$

According to Eq. (\*), the occupation  $W_1(t) = |a_1(t)|^2 = |\sin \zeta t|^2$  of the 1<sup>st</sup> excited state reaches its maximum periodically, at the moments

$$t_m = \frac{\pi(m + 1/2)}{\zeta}, \quad \text{when } \exp\{i\zeta t_m\} = \pm i, \quad (**)$$

where the sign depends on whether the integer  $m$  is even (+) or odd (-). At these moments,

$$a_2(t_m) = \frac{A_{21}}{\hbar} \frac{\pm i\xi - \zeta \exp\{i\xi t_m\}}{\xi^2 - \zeta^2},$$

From here, the 2<sup>nd</sup> level's occupation at these moments is

$$W_2(t_m) = |a_2(t_m)|^2 = \frac{|A_{21}|^2}{\hbar^2} \frac{\xi^2 \mp 2\xi\zeta \sin \xi t_m + \zeta^2}{|\xi^2 - \zeta^2|^2}.$$

Generally, the frequencies  $\xi$  and  $\zeta$  are incommensurate, so the sine function in this result may take any values between  $-1$  and  $+1$ . We are interested in the *smallest possible*  $W_2$ , which is achieved in the latter case:

$$W_2(t_m) \rightarrow \frac{|A_{21}|^2}{\hbar^2} \frac{\xi^2 - 2\xi\zeta + \zeta^2}{(\xi^2 - \zeta^2)^2} \equiv \frac{|A_{21}|^2}{\hbar^2} \frac{1}{(\xi + \zeta)^2}.$$

From the requirement for this expression to be not larger than the given  $\varepsilon \ll 1$ , and the assumed proportionality of both  $|A_{10}|$  and  $|A_{21}|$  to the same ac excitation amplitude, the smallest (in that amplitude) occupancy inversion time is achieved at  $|\zeta| \ll \xi$ :

<sup>122</sup> At  $\xi \rightarrow 0$ , the direct excitation of the second-level state from the initial one is negligible in comparison with the nearly resonant excitation of that level from the first excited state, which we are calculating.

$$(t_m)_{\min} = \frac{\pi}{2\zeta_{\max}} = \frac{\pi\hbar}{2|A_{10}|_{\max}} = \frac{\pi\hbar}{2} \frac{|A_{21}|}{|A_{10}|} \frac{1}{|A_{21}|_{\max}} = \frac{\pi}{2} \frac{|A_{21}|}{|A_{10}|} \frac{1}{\varepsilon^{1/2}|\xi|}. \quad (***)$$

This time tends to infinity at  $\varepsilon \rightarrow 0$  (the perfect inversion requirement) and/or  $\xi \rightarrow 0$  (equidistant energy levels, such as in a harmonic oscillator). For a slightly anharmonic 1D oscillator, excited by an external classical force  $F(t)$ , the perturbation Hamiltonian is

$$\hat{H}^{(1)}(t) = -F(t)\hat{x},$$

and the matrix element ratio that participates in Eq. (\*\*\*) may be readily calculated from Eq. (5.92):

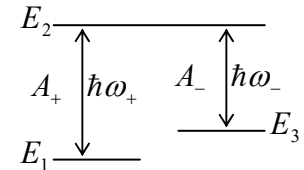
$$\frac{|A_{21}|}{|A_{10}|} = \frac{|x_{21}|}{|x_{10}|} = \frac{|\langle 2|\hat{x}|1\rangle|}{|\langle 1|\hat{x}|0\rangle|} = \sqrt{2},$$

while the detuning  $\xi$  may be evaluated using Eqs. (6.16) and (6.23):

$$\xi \equiv \omega_2 - \omega_1 = \frac{(E_2 - E_1) - (E_1 - E_0)}{\hbar} = 3 \frac{\beta x_0^4}{\hbar} - \frac{15}{2} \frac{\alpha x_0^6}{\hbar^2 \omega_0} \equiv 3 \frac{\beta\hbar}{m^2 \omega_0^2} - \frac{15}{2} \frac{\alpha\hbar}{m^3 \omega_0^4},$$

where  $\alpha$  and  $\beta$  are the anharmonicity coefficients defined by Eq. (6.2). Evidently, the smaller the coefficients (or rather the magnitude of their combination on the right-hand side of the last expression) the larger the shortest population inversion time (\*\*\*). This trend will be used in Sec. 8.5 of the lecture notes to explain why adding external (linear) circuit elements to Josephson-junction qubits, while having a beneficial effect of decreasing their relative coupling to the environment and hence increasing the dephasing time, creates a problem of the quantum computing speed reduction.

**Problem 6.22.** \* Analyze the possibility of a slow transfer of a system from one of its energy levels to another one (in the figure on the right, from level 1 to level 3), by using the scheme shown in that figure, in which the monochromatic external excitation amplitudes  $A_+$  and  $A_-$  may be slowly changed at will.



*Solution:* Assuming, for the sake of simplicity, the exact tuning of the excitation frequencies,<sup>123</sup>

$$\hbar\omega_+ = E_2 - E_1, \quad \hbar\omega_- = E_2 - E_3,$$

and ignoring, for now, the slow change of the amplitudes  $A_+$  and  $A_-$  with time, we may write the following obvious generalization of Eqs. (6.97), with  $\Delta = 0$ , for this system:

$$i\hbar\dot{b}_1 = A_+ b_2, \quad i\hbar\dot{b}_2 = A_+^* b_1 + A_-^* b_3, \quad i\hbar\dot{b}_3 = A_- b_2. \quad (*)$$

Looking for the partial solution of this system of three homogeneous linear differential equations in the usual form  $\exp\{\lambda t\}$ , we get the following characteristic equation:

<sup>123</sup> A more detailed analysis shows that the procedure discussed below is more tolerant to the common detuning  $\Delta \equiv E_2 - (E_1 + \hbar\omega_+) = E_2 - (E_3 + \hbar\omega_-)$  than to the relative detuning  $\delta \equiv (E_1 + \hbar\omega_+) - (E_3 + \hbar\omega_-)$  – see, e.g., Fig. 10 in the review by N. Vitanov *et al.*, *Rev. Mod. Phys.* **89**, 015006 (2017).



$$\begin{vmatrix} -i\hbar\lambda & A_+ & 0 \\ A_+^* & -i\hbar\lambda & A_-^* \\ 0 & A_- & -i\hbar\lambda \end{vmatrix} = 0, \quad \text{i.e. } -i\hbar\lambda \left[ (-i\hbar\lambda)^2 - A_+ A_+^* - A_- A_-^* \right] = 0.$$

This equation has 3 roots: two of them corresponding to the Rabi oscillation's half-frequency:<sup>124</sup>

$$\lambda_{\pm} = \pm i\Omega, \quad \text{where } \Omega = \frac{1}{\hbar} \left( A_+ A_+^* + A_- A_-^* \right)^{1/2} \quad (**)$$

and one more root  $\lambda_0 = 0$ . The mathematical origin of the last result is clearly visible from the comparison of the first and the last equations (\*): it shows that if  $b_2 \neq 0$ , then

$$\frac{\dot{b}_1}{A_+} = \frac{\dot{b}_3}{A_-},$$

i.e. that the system of equations has the following integral of motion:

$$A_- b_1 - A_+ b_3 = C = \text{const.} \quad (***)$$

Physically, the origin of this relation is that in this three-level system, the probability amplitudes  $b_1$  and  $b_3$  may change only due to  $b_2$ , and at fixed  $A_{\pm}$ , these changes are proportional.

It is intuitively clear that Eqs. (\*)-(\*\*\*) hold even if the excitation amplitudes  $A_+$  and  $A_-$  are changed in time sufficiently slowly (“adiabatically”) – much slower than the Rabi frequency  $\Omega$ . As a result, they may be used to describe the following counter-intuitive operation. First, starting with one of the energy levels being fully populated (say,  $b_1 = 1$ ) but two other energy levels 2 and 3 empty ( $b_2 = b_3 = 0$ ), let us turn on the external field of the frequency  $\omega_+$ , i.e. make  $A_-^*$  equal to some  $A_0 \neq 0$ , thus making the last two of Eqs. (\*) valid – so far, with  $A_+ = 0$ . (Such Rabi-connected, but unoccupied states are frequently called *dark*.) However, since  $b_2 = 0$ , Eq. (\*\*\*) is still *not* valid. Indeed, as the first of Eqs. (\*) shows, the state corresponding to the energy level  $E_1$  is still fully uncoupled from the (now, Rabi-coupled) “dark” quantum states of the levels  $E_2$  and  $E_3$ .

Now let us slowly increase the amplitude  $A_+$  of the external field of the frequency  $\omega_+$ , simultaneously decreasing  $A_-$ , so the Rabi frequency (\*\*) would stay constant, equal to  $A_0/\hbar$ ; in this case, Eq. (\*\*\*) , now valid, may be conveniently rewritten as

$$b_1 \cos \theta - b_3 \sin \theta = c = \text{const}, \quad \text{where } \cos \theta = \frac{A_-}{A_0}, \quad \sin \theta = \frac{A_+}{A_0}. \quad (***)$$

At some, rather small, value of  $A_+$  (which depends on the rate of its increase), the Rabi effect makes the probability amplitude  $b_2$  sufficiently different from zero to make Eq. (\*\*\*) valid, thus establishing the integration constant  $c$ . Since at this moment,  $b_1$  is still very close to 1, and  $A_-$  to  $A_0$ , i.e. the angle  $\theta$  to 0, this constant  $c$  is close to 1. According to Eq. (\*\*\*) , as this slow process is continued, with the parameter  $\theta$  being changed from 0 to  $\pi/2$ , the variable  $|b_3|$ , and hence the occupancy  $W_3 = |b_3|^2$  of the level  $E_3$  gradually increases, while  $W_1 = |b_1|^2$  decreases. Finally, at some small value  $A_- \ll A_0$ , i.e. at  $\theta \approx \pi/2$ , when Eq. (\*\*\*) is still valid, it yields  $b_3 \approx -1$ , and  $b_1 \approx 0$ , i.e.  $W_3 \approx 1$ , while  $W_1 \approx 0$ . At this

<sup>124</sup> This expression for  $\Omega$  is an obvious generalization of Eq. (6.99) of the lecture notes, with  $\Delta = 0$ .

point, a full turn-off of the field of the frequency  $\omega_-$  completely isolates the now-occupied state on level  $E_3$  from the other two states (which now form another pair of Rabi-coupled “dark” states, with  $W_{1,2} \ll 1$ ). After that, the excitation of frequency  $\omega_+$  may be turned off without any effect on these (zero) occupancies.

So, using the Rabi coupling of two initially empty (“dark”) states *first*, and only *then* turning on the coupling of this pair with the initially occupied state, we may perform a virtually complete adiabatic transfer of the system from one energy level to another one.<sup>125</sup> In contrast to the direct  $\pi$ -pulse of Rabi-oscillations between the initial and final levels, this procedure does not require exact timing. Due to this advantage, the STIRAP process, initially just a quantum curiosity, is now finding more and more applications in atomic, molecular, and solid-state physics and chemistry – see, e.g., the already cited review by Vitanov *et al.*

**Problem 6.23.** A weak external force pulse  $F(t)$ , of a finite time duration, is applied to the particle in a system with a discrete energy spectrum, which initially was in its ground state.

(i) Derive, in the lowest nonvanishing order of the perturbation theory, a formula for the probability that the pulse drives the particle into its  $n^{\text{th}}$  excited state.

(ii) Specify this formula for a 1D harmonic oscillator and compare the result with the exact solution of the problem.

(iii) Spell out the perturbative result for the Gaussian-shaped waveform  $F(t) = F_0 \exp\{-t^2/\tau^2\}$  and analyze its dependence on the scale  $\tau$  of the pulse duration.

*Solutions:*

(i) The general approach to such problems is given by the set of (exact!) Eqs. (6.84) of the lecture notes. As was argued at the derivation of Eq. (6.90) (for a specific time dependence of the perturbation), in the lowest order of the perturbation theory we may leave, on the right-hand sides of these equations, only the terms whose probability amplitudes  $a_{n'}$  are initially different from zero. In our current problem, this is only the ground-state amplitude  $a_0 = 1$ , so the right-hand side of each Eq. (6.84), with  $n' = 0$ , is reduced to just one term:

$$i\hbar\dot{a}_n = H_{n0}^{(1)}(t)e^{i\omega_{n0}t}. \quad (*)$$

As was repeatedly discussed in this course, a weak, coordinate-independent force  $F(t)$  may be described by the following perturbation:

$$\hat{H}^{(1)}(t) = -F(t)\hat{x},$$

so Eq. (\*) takes the form

$$i\hbar\dot{a}_n = -F(t)x_{n0}e^{i\omega_{n0}t},$$

where  $x_{n0}$  are the matrix elements of the coordinate operator in the unperturbed brackets – see Eq. (6.8). This equation may be readily integrated, with zero initial conditions  $a_n(-\infty) = 0$ , to give

<sup>125</sup> Because of its counter-intuitive nature, this *STIRAP* (*Stimulated Raman Adiabatic Passage*) procedure was invented, by U. Gaubatz *et al.*, only in 1988, i.e. only after four decades of studies of various Rabi-oscillation effects by many research groups. It is even more curious that the opposite, more apparent time sequence of the external ac field changes gives worse transfer results, in particular because of its higher sensitivity to unintentional (but unavoidable) coupling to the environment – to be discussed in Chapter 7.

$$a_n(t) = -\frac{x_{n0}}{i\hbar} \int_{-\infty}^t F(t') \exp\{i\omega_{n0}t'\} dt', \quad \text{for } n > 0.$$

Hence the probability of finding the system, at a moment  $t > 0$ , in its  $n^{\text{th}}$  excited state is

$$W_n(t) = \frac{|x_{n0}|^2}{\hbar^2} \left| \int_{-\infty}^t F(t') \exp\{i\omega_{n0}t'\} dt' \right|^2. \quad (**)$$

If the pulse has a finite duration, the final value of  $W_n$  is described by this formula with the upper limit taken at any time after the pulse's end.<sup>126</sup>

(ii) As Eq. (5.92) of the lecture notes shows, for a 1D harmonic oscillator, all  $x_{n0}$  equal zero, with just one exception:

$$x_{n0} = \left( \frac{\hbar}{2m\omega_0} \right)^{1/2} \times \begin{cases} 1, & \text{for } n = 1, \\ 0, & \text{otherwise,} \end{cases}$$

so Eq. (\*\*) yields the result that was already obtained in the model solution of Problem 17 (by somewhat different means):

$$W_1(+\infty) = \frac{|I|^2}{2m\hbar\omega_0}, \quad \text{where } I \equiv \int_{-\infty}^{+\infty} F(t) e^{i\omega_0 t} dt. \quad (***)$$

Just as in that solution, due to our initial assumptions, Eq. (\*\*\*) is only valid if  $W_1(+\infty) \ll 1$ , i.e. if

$$|I|^2 \ll 2m\hbar\omega_0. \quad (***)$$

As was discussed in the model solution of the same Problem 17, for this particular system (the harmonic oscillator, initially in the ground state), the exact solution valid for *any*  $W_1$  is also possible:

$$W_1 = \frac{|I|^2}{2m\hbar\omega_0} \exp\left\{ -\frac{|I|^2}{2m\hbar\omega_0} \right\};$$

if the condition (\*\*\*\*) is satisfied, this formula duly reduces to the perturbative result (\*\*\*)

(iii) For the particular pulse shape given in the assignment,  $I$  is a standard Gaussian integral, which may be readily worked out as was discussed in Sec. 2.2 of the lecture notes – see Eqs. (2.21)–(2.23):

$$\begin{aligned} I &= F_0 \int_{-\infty}^{+\infty} \exp\left\{ -\frac{t^2}{\tau^2} + i\omega_0 t \right\} dt \equiv F_0 \exp\left\{ \left( \frac{-i\omega_0\tau}{2} \right)^2 \right\} \int_{-\infty}^{+\infty} \exp\left\{ -\left[ \left( \frac{t}{\tau} \right)^2 + 2\left( \frac{t}{\tau} \right) \left( \frac{-i\omega_0\tau}{2} \right) + \left( \frac{-i\omega_0\tau}{2} \right)^2 \right] \right\} dt \\ &\equiv F_0 \exp\left\{ -\frac{\omega_0^2\tau^2}{4} \right\} \int_{-\infty}^{+\infty} \exp\left\{ -\left( \frac{t}{\tau} + \frac{-i\omega_0\tau}{2} \right)^2 \right\} dt = \pi^{1/2} F_0 \tau \exp\left\{ -\frac{\omega_0^2\tau^2}{4} \right\}, \end{aligned}$$

so, finally, the probability (\*\*\*) of the oscillator's excitation is

<sup>126</sup> The integral converges for any pulse of finite duration, i.e. if  $F(t) \rightarrow 0$  at  $t \rightarrow \pm\infty$ .

$$W_1(+\infty) = \frac{|I|^2}{2m\hbar\omega_0} = \frac{\pi F_0^2 \tau^2}{2m\hbar\omega_0} \exp\left\{-\frac{\omega_0^2 \tau^2}{2}\right\}.$$

According to this formula, at fixed other parameters, the excitation is most effective at  $\tau_{\text{opt}} = \sqrt{2}/\omega_0$ , i.e. if the pulse's duration is of the order of the oscillator's period. This is natural because a much shorter pulse does not give the system enough time to accomplish the interstate quantum transition, while a very long pulse is just an adiabatic change of an oscillator's parameter (namely, of its equilibrium position  $X_0(t) = F(t)/m\omega_0^2$ ) and, according to the discussion at the beginning of Sec. 6.5 of the lecture notes (and in the solution of Problem 17), leaves the system in its initial quantum state with a nearly 100% probability.

**Problem 6.24.** A spatially uniform but time-dependent external electric field  $\mathcal{E}(t)$  is applied, starting from  $t = 0$ , to a charged planar rotor, initially in its ground state.

(i) Calculate, in the lowest nonvanishing order in the field's strength, the probability that by a certain time  $t > 0$ , the rotor is in its  $m^{\text{th}}$  excited state.

(ii) Spell out and analyze your results for a constant-magnitude field rotating, with a constant angular velocity  $\omega$ , within the rotor's plane.

(iii) Do the same for a monochromatic field of frequency  $\omega$ , with a fixed direction.

*Solutions:*

(i) Acting exactly as in Sec. 6.5 of the lecture notes (see also the model solution of the previous problem), let us solve Eq. (6.84) of the lecture notes, with the appropriate notation replacement  $n \rightarrow m$ , in the first perturbation order by taking, on its right-hand side, all probability amplitudes  $a_m(t)$  equal zero except for that of the ground state:  $a_0(t) = 1$  for all  $t$ . The resulting (approximate) equation of motion is

$$i\hbar \dot{a}_m = H_{m0}^{(1)}(t) \exp\{i\omega_{m0}t\}, \quad \text{with } \omega_{m0} = \frac{E_m - E_0}{\hbar}, \quad \text{for } m \neq 0, \quad (*)$$

where  $H_{m0}^{(1)}$  are the matrix elements of the perturbation created by the field, in the unperturbed-state basis of the rotor.

Now let us specify these matrix elements. The perturbation Hamiltonian created by a uniform electric plane is a natural generalization of Eq. (6.29):

$$\hat{H}^{(1)}(t) = -q\mathbf{p} \cdot \mathcal{E}(t) = -q[x\mathcal{E}_x(t) + y\mathcal{E}_y(t)] = -qR[\cos\varphi\mathcal{E}_x(t) + \sin\varphi\mathcal{E}_y(t)],$$

where  $[x, y]$  is the rotor's plane, and  $\varphi$  is the polar angle within it.<sup>127</sup> In the basis of the stationary states of the rotor, with the wavefunctions given by Eq. (3.129) with the evident normalization  $|C_m|^2 = 1/2\pi$ .

$$\psi_m = \frac{1}{(2\pi)^{1/2}} e^{im\varphi}, \quad \text{with } m = 0, \pm 1, \pm 2, \dots, \quad (**)$$

the matrix elements participating in Eq. (\*) are

<sup>127</sup> For the 2D model of the rotor, the field's component normal to this plane, does not have any effect on its dynamics. (Formally, you may say that its contribution to the perturbation Hamiltonian is  $z\mathcal{E}_z(t)$ , where  $z = 0$ .)

$$\begin{aligned}
H_{m0}^{(1)}(t) &= -qR \int_0^{2\pi} \psi_m^* [\cos \varphi \mathcal{E}_x(t) + \sin \varphi \mathcal{E}_y(t)] \psi_0 d\varphi \\
&\equiv -\frac{qR}{2\pi} \int_0^{2\pi} e^{-im\varphi} \left[ \frac{e^{i\varphi} + e^{-i\varphi}}{2} \mathcal{E}_x(t) + \frac{e^{i\varphi} - e^{-i\varphi}}{2i} \mathcal{E}_y(t) \right] d\varphi \\
&\equiv -\frac{qR}{4\pi} \left\{ [\mathcal{E}_x(t) - i\mathcal{E}_y(t)] \int_0^{2\pi} e^{i(1-m)\varphi} d\varphi + [\mathcal{E}_x(t) + i\mathcal{E}_y(t)] \int_0^{2\pi} e^{i(-1-m)\varphi} d\varphi \right\}.
\end{aligned}$$

Per this expression, only the matrix elements with  $m = \pm 1$  are different from zero:<sup>128</sup>

$$H_{\pm 1,0}^{(1)}(t) = -\frac{qR}{2} [\mathcal{E}_x(t) \mp i\mathcal{E}_y(t)].$$

so, solving the simple Eq. (\*), we see that the weak pulse may drive the system only into its two lowest excited states, with the same energy  $E_{+1} = E_{-1} = \hbar^2/2mR^2$ :

$$W_{\pm 1}(t) = \frac{q^2 R^2}{4\hbar^2} \left| \int_0^t [\mathcal{E}_x(t') \mp i\mathcal{E}_y(t')] \exp\{i\omega_{10}t'\} dt' \right|^2, \quad \text{with } \omega_{10} = \frac{E_{\pm 1}}{\hbar} = \frac{\hbar}{2mR^2}. \quad (***)$$

(ii) This result shows that the probabilities of excitation of these two degenerate states are not always equal. The best example is that of a field rapidly rotating within the rotor's plane – for example, in the positive direction (counterclockwise):

$$\mathcal{E}_x(t) = \mathcal{E}_0 \cos(\omega t + \alpha), \quad \mathcal{E}_y(t) = \mathcal{E}_0 \sin(\omega t + \alpha), \quad \text{for } t > 0,$$

where  $\mathcal{E}_0$ ,  $\omega$ , and  $\alpha$  are constants, so

$$\mathcal{E}_x(t) \mp i\mathcal{E}_y(t) = \mathcal{E}_0 [\cos(\omega t + \alpha) \mp i \sin(\omega t + \alpha)] \equiv \mathcal{E}_0 \exp\{\mp i(\omega t + \alpha)\}.$$

Plugging this expression into Eq. (\*\*\*), we get

$$\begin{aligned}
W_{\pm 1}(t) &= \frac{q^2 R^2 \mathcal{E}_0^2}{4\hbar^2} \left| \int_0^t \exp\{i[(\omega_{10} \mp \omega)t' - \alpha]\} dt' \right|^2 = \frac{q^2 R^2 \mathcal{E}_0^2}{4\hbar^2} \left| \frac{\exp\{i[(\omega_{10} \mp \omega)t]\} - 1}{i(\omega_{10} \mp \omega)} e^{-i\alpha} \right|^2 \\
&\equiv \frac{q^2 R^2 \mathcal{E}_0^2}{2\hbar^2} \frac{1 - \cos(\omega_{10} \mp \omega)t}{(\omega_{10} \mp \omega)^2} \equiv \frac{q^2 R^2 \mathcal{E}_0^2}{\hbar^2 (\omega_{10} \mp \omega)^2} \sin^2 \frac{(\omega_{10} \mp \omega)t}{2}.
\end{aligned}$$

This expression shows that, as might be expected from the discussion in Sec. 6.5 of the lecture notes and in particular Eq. (6.90), both probabilities oscillate in time, generally with comparable if quantitatively different amplitudes. However, if the external field frequency  $\omega$  is very close to that ( $\omega_{10}$ ) of the potential interlevel transitions, the oscillations of the probability  $W_{+1}$  are much larger than those

<sup>128</sup> This is again one of the manifestations of the selection rules in quantum transitions. Note that according to our calculation, in axially symmetric 2D systems the rules require a change of the *magnetic* quantum number  $m$  by  $\pm 1$ , while in the spherically-symmetric 3D systems, they require a similar change of the *orbital* quantum number  $l$ , while the magnetic number may either change by  $\pm 1$  or stay constant – see the footnote at the end of Sec. 5.6, and also Problem 5.41.

of its counterpart,  $W_{-1}$ .<sup>129</sup> This is very natural because the time-dependent wavefunction corresponding to Eq. (\*\*) with  $m = +1$ ,

$$\Psi_{+1}(\varphi, t) \propto \psi_{+1}(\varphi) \exp\left\{-\frac{iE_{+1}t}{\hbar}\right\} \propto \exp\{i(\varphi - \omega_{10}t)\},$$

describes a de Broglie wave propagating in the same (counterclockwise) direction as the field. (In the case of the opposite, clockwise direction of the field's rotation, the probability of the opposite state, with  $m = -1$ , is similarly enhanced.)

This effect may be partly interpreted classically, by saying that the rotor's angular momentum  $L_z$  picks up a part of the angular momentum of the rotating field.

(iii) For an ac field with a fixed direction,

$$\mathcal{E}_x(t) = \mathcal{E}_0 \cos \varphi_0 \cos(\omega t + \alpha), \quad \mathcal{E}_y(t) = \mathcal{E}_0 \sin \varphi_0 \cos(\omega t + \alpha), \quad \text{for } t > 0,$$

where  $\varphi_0$  is the angle between the field's direction and the  $x$ -axis, the result is different:

$$\mathcal{E}_x(t) \mp i\mathcal{E}_y(t) = \mathcal{E}_0 [\cos \varphi_0 \mp i \sin \varphi_0] \cos(\omega t + \alpha) = \mathcal{E}_0 \exp\{\mp i\varphi_0\} \frac{\exp\{i(\omega t + \alpha)\} + \exp\{-i(\omega t + \alpha)\}}{2},$$

so Eq. (\*\*\*) yields

$$\begin{aligned} W_{\pm 1}(t) &= \frac{q^2 R^2 \mathcal{E}_0^2}{4\hbar^2} \left| \int_0^t \exp\{i[(\omega_{10} + \omega)t' + \alpha]\} dt' + \int_0^t \exp\{i[(\omega_{10} - \omega)t' - \alpha]\} dt' \right|^2 \\ &= \frac{q^2 R^2 \mathcal{E}_0^2}{4\hbar^2} \left| \frac{\exp\{i[(\omega_{10} + \omega)t]\} - 1}{i(\omega_{10} + \omega)} e^{i\alpha} + \frac{\exp\{i[(\omega_{10} - \omega)t]\} - 1}{i(\omega_{10} - \omega)} e^{-i\alpha} \right|^2. \end{aligned}$$

This bulky result (which does not benefit much from its further processing) shows that the probabilities of the excitation of both states are equal, and do not depend on the field's inclination angle  $\varphi_0$ . Both these features may be explained by the fact that the "linearly-polarized" field of a fixed direction may be always represented as the sum of two rotating fields (if we speak about waves, by two circularly-polarized waves) with equal amplitudes, regardless of the angle  $\varphi_0$ . In particular, at  $\omega \rightarrow \omega_{10}$ , both probabilities exhibit the same resonant behavior as in the rotating field case.

**Problem 6.25.** A heavy relativistic particle, with electric charge  $q = Ze$ , flies by a hydrogen atom, initially in its ground state, with an impact parameter  $b$  within the range  $r_B \ll b \ll r_B/\alpha$ , where  $\alpha$  is the fine structure constant (6.62). Calculate the total probability of the atom's transition into one of its lowest excited states.

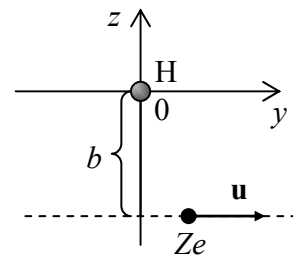
*Solution:* Due to the large mass of the flying-by particle, we may neglect the effects of its Coulomb interaction with the atom, as well as quantum-mechanical uncertainty, on its motion. In the

<sup>129</sup> In exploring this resonance behavior, we should not forget that our perturbative result is only valid if both probabilities  $W_{\pm 1}$  are much smaller than 1.

absence of these effects, the motion is classical and uniform (acceleration-free), so the electric and magnetic fields felt by the atom may be readily calculated. Such calculation yields<sup>130</sup>

$$\begin{aligned} \mathcal{E}_x(t) &= 0, & \mathcal{E}_y(t) &= -\frac{q}{4\pi\epsilon_0} \frac{u\gamma t}{(u^2\gamma^2 t^2 + b^2)^{3/2}}, & \mathcal{E}_z(t) &= \frac{q}{4\pi\epsilon_0} \frac{\gamma b}{(u^2\gamma^2 t^2 + b^2)^{3/2}}, \\ \mathcal{B}_x(t) &= \frac{u}{c^2} \mathcal{E}_z(t), & \mathcal{B}_y(t) &= 0, & \mathcal{B}_z(t) &= 0. \end{aligned} \quad (*)$$

Here the  $y$ -axis is directed along the particle's velocity  $\mathbf{u}$ ,  $z$  is the direction from the nearest-approach point toward the atom (see the figure on the right), time  $t$  (as measured in the reference frame of the hydrogen atom) is referred to the instant of the nearest approach, and  $\gamma \equiv (1 - u^2/c^2)^{-1/2} \geq 1$  is the relativistic Lorentz parameter. Note that Eqs. (\*) are exactly valid only at the center of the atom (from which the impact parameter is measured), but given the condition  $r_B \ll b$ , we may use them at all essential distances  $r \sim r_B$  of the electron from the center.



Since, according to Eqs. (1.13) of the lecture notes, the effective speed  $v \sim \omega_0 r_B$  (where  $\omega_0 \equiv E_H/\hbar$ ) of the electron inside the atom is of the order of  $\alpha c \ll c$ , Eqs. (\*) show that the magnetic component  $-e\mathbf{v} \times \mathcal{B}$  of the Lorentz force acting on the atom's electron is much smaller than its electric component  $-e\mathcal{E}$ . Hence we may include only the latter force into the Hamiltonian of the particle-electron interaction:

$$\hat{H}_{\text{int}}(t) = e\mathcal{E}(t) \cdot \mathbf{r} = e[\mathcal{E}_y(t)y + \mathcal{E}_z(t)z] \equiv e r [\mathcal{E}_y(t)\sin\theta\sin\varphi + \mathcal{E}_z(t)\cos\theta],$$

where  $\theta$  and  $\varphi$  are the spherical angles of the atom's electron.

Now acting exactly as in the solutions of the two previous problems, in the 1<sup>st</sup> order of the perturbation theory, we get the following total probability (reached at  $t \gg b/u\gamma$ ) of the transition from the ground state (with the quantum numbers  $n = 1$ ,  $l = 0$ , and  $m = 0$ ) into the lowest excited states (with  $n = 2$ , and either  $l = 0$  and  $m = 0$ , or  $l = 1$  and  $m = -1, 0$ , or  $+1$ ):

$$W = \sum_{l,m} W_{l,m}, \quad \text{where } W_{l,m} = \frac{1}{\hbar^2} \left| \int_{-\infty}^{+\infty} \langle 1,0,0 | \hat{H}_{\text{int}}(t) | 2,l,m \rangle \exp\{i\omega_{21}t\} dt \right|^2, \quad (**)$$

where  $n = 2$ ,  $l$ , and  $m$  are the quantum numbers of the final state, while

$$\omega_{21} \equiv \frac{E_2 - E_1}{\hbar} = \frac{E_H}{\hbar} \left[ -\frac{1}{2 \cdot 2^2} - \left( -\frac{1}{2 \cdot 1^2} \right) \right] \equiv \frac{3E_H}{8\hbar}.$$

As Eqs. (\*) show, for a relativistic particle with  $u \sim c$ , the field's pulse it induces at the atom's location, and hence the interaction Hamiltonian as the function of time, have the duration  $\Delta t$  of the order of  $b/\gamma u$ , i.e. either of the order or even shorter than  $b/c$ . The second of the conditions given in the assignment,  $b \ll r_B/\alpha$ , means that this  $\Delta t$  is much smaller than  $r_B/\alpha c$ . On the other hand, the exponent in Eq. (\*\*) changes with frequency  $\omega_{12} \sim E_H/\hbar$ , so their product satisfies the condition

<sup>130</sup> See, e.g., EM Sec. 9.5, in particular, Eqs. (9.139)-(9.140), with the axis notation replacement  $x \rightarrow y \rightarrow z \rightarrow x$ .

$$\omega_{12}\Delta t \ll \frac{E_H}{\hbar} \frac{r_B}{\alpha c} \equiv 1.$$

Hence the exponent in Eq. (\*\*) cannot change significantly during the particle's passage, and we may take it from under the integral over time, getting

$$W_{l,m} = \frac{1}{\hbar^2} \left| \int_{-\infty}^{+\infty} \langle 1,0,0 | \hat{H}_{\text{int}}(t) | 2,l,m \rangle dt \right|^2 \equiv \frac{e^2}{\hbar^2} \left| \int_{-\infty}^{+\infty} \langle 1,0,0 | r [\mathcal{E}_y(t) \sin \theta \sin \varphi + \mathcal{E}_z(t) \cos \theta] | 2,l,m \rangle dt \right|^2.$$

Since, according to Eq. (\*),  $\mathcal{E}_y(t)$  is an odd function of time, the integral of the first term in its symmetric (infinite) limits vanishes, and we are left with

$$W_{l,m} = \frac{e^2}{\hbar^2} |I|^2 |\langle 1,0,0 | r \cos \theta | 2,l,m \rangle|^2, \quad \text{where } I \equiv \int_{-\infty}^{+\infty} \mathcal{E}_z(t) dt.$$

The integral  $I$  is readily reduced to a table one:<sup>131</sup>

$$I \equiv \int_{-\infty}^{+\infty} \mathcal{E}_z(t) dt = \frac{q}{4\pi\epsilon_0} \gamma b \int_{-\infty}^{+\infty} \frac{dt}{(u^2 \gamma^2 t^2 + b^2)^{3/2}} = \frac{q}{4\pi\epsilon_0} \frac{2}{ub} \int_0^{+\infty} \frac{d\xi}{(\xi^2 + 1)^{3/2}} = \frac{q}{4\pi\epsilon_0} \frac{2}{ub}.$$

Now we can make use of Eq. (3.200) of the lecture notes to spell out the needed matrix elements:

$$\langle 1,0,0 | r \cos \theta | 2,l,m \rangle = \int_0^{2\pi} d\varphi \int_0^\pi \sin \theta d\theta Y_0^0(\theta, \varphi) \cos \theta Y_l^m(\theta, \varphi) \int_0^\infty r^2 dr \mathcal{R}_{1,0}(r) r \mathcal{R}_{2,l}(r).$$

Together with Eqs. (3.174)-(3.175), this expression shows, first of all, that the matrix element for the final  $2s$  state (with  $l = 0$ ,  $m = 0$ ) vanishes because of the integral over the polar angle  $\theta$ :

$$\int_0^\pi \sin \theta d\theta Y_0^0(\theta, \varphi) \cos \theta Y_0^0(\theta, \varphi) = \frac{1}{4\pi} \int_{-1}^{+1} \cos \theta d(\cos \theta) = 0.$$

For two of the three  $2p$  states (with  $l = 1$ , and  $m = \pm 1$ ), whose spherical harmonics are proportional to  $e^{\pm i\varphi}$ , the matrix elements vanish because of the integral over the azimuthal angle, and only for the  $2p$  state with  $m = 0$ , the matrix element is different from zero:

$$\langle 1,0,0 | r \cos \theta | 2,1,0 \rangle = I_\Omega I_2, \quad \text{with } I_\Omega \equiv \oint d\Omega [Y_l^m(\theta, \varphi)]^* \cos \theta Y_0^0(\theta, \varphi), \quad \text{and } I_2 \equiv \int_0^\infty r^2 dr \mathcal{R}_{1,0}^*(r) r \mathcal{R}_{2,1}(r).$$

Both these integrals were (easily :- ) calculated in the solution of Problem 20:

$$I_\Omega = \frac{1}{\sqrt{3}}, \quad I_2 = \frac{2^5 r_B}{3^5 \sqrt{6}} 4!,$$

so, finally (for  $q = Ze$ ):

$$W = \frac{e^2}{\hbar^2} \left( \frac{q}{4\pi\epsilon_0} \frac{2}{ub} \right)^2 \left( \frac{1}{\sqrt{3}} \frac{2^5 r_B}{3^5 \sqrt{6}} 4! \right)^2 = \frac{2^{17}}{3^{10}} \left( \frac{Ze^2}{4\pi\epsilon_0} \frac{r_B}{\hbar u b} \right)^2 \equiv \frac{2^{17}}{3^{10}} \left( \frac{Z\omega_0 r_B^2}{ub} \right)^2 \approx 2.22 \left( Z\gamma \frac{\omega_0 b}{u\gamma} \frac{r_B^2}{b^2} \right)^2,$$

<sup>131</sup> See, e.g., MA Eq. (6.5c).



where  $\omega_0 \equiv E_H/\hbar$ .

As was discussed above, this result was derived for  $\omega_{12}\Delta t \sim \omega_0 b/u\gamma \ll 1$  and  $r_B \ll b$ , so the two last fractions inside the last parentheses are much smaller than 1, meaning that for not extremely high values of  $Z$  and  $\gamma$ , the excitation probability is very low. (If the product  $Z\gamma$  is so high that our result yields  $W$  of the order of 1 or higher, it should be revised, because the approximation leading to Eq. (\*\*\*) is only valid if it yields  $W \ll 1$  – see Eq. (6.89) of the lecture notes.)

**Problem 6.26.** Develop a general theory of quantum excitations of the higher levels of a discrete-spectrum system, initially in the ground state, by a weak time-dependent perturbation, up to the 2<sup>nd</sup> order. Spell out and discuss the result for the case of monochromatic excitation, at a nearly perfect tuning of its frequency  $\omega$  to *the half* of a certain quantum transition frequency  $\omega_{n0} \equiv (E_n - E_0)/\hbar$ .

*Solution:* Let us start from the general system of (exact) equations (6.84) for the state probability amplitudes  $a_n$ :

$$i\hbar\dot{a}_n = \sum_{n'} a_{n'} H_{nn'}^{(1)}(t) \exp\{i\omega_{nn'}t\}, \quad \text{with } \omega_{nn'} \equiv \frac{E_n - E_{n'}}{\hbar}, \quad (*)$$

where  $E_n$  are the energy levels of the system in the absence of perturbation, and look for its solution in the form of an expansion similar to Eqs. (6.9)-(6.10) of the lecture notes:

$$a_n(t) = a_n^{(0)}(t) + a_n^{(1)}(t) + a_n^{(2)}(t) + \dots, \quad \text{with } a_n^{(k)}(t) \propto \mu^k,$$

where the small parameter  $\mu$  is the scale of the perturbation Hamiltonian  $\hat{H}^{(1)}(t)$ . If by the beginning of the perturbation (the instant that we may take for  $t = 0$ ), the system was definitely in its ground state ( $n = 0$ ), then we may take  $a_n^{(0)}(0) = \delta_{n,0}$ . Plugging these values into the right-hand side of Eqs. (\*) with  $n \neq 0$ , in the 1<sup>st</sup> order of the theory, we get the simplified equation

$$i\hbar\dot{a}_n^{(1)} = H_{n0}^{(1)}(t) \exp\{i\omega_{n0}t\},$$

with an easy solution:<sup>132</sup>

$$a_n^{(1)}(t) = \frac{1}{i\hbar} \int_0^t H_{n0}^{(1)}(t') \exp\{i\omega_{n0}t'\} dt', \quad \text{for } n \neq 0. \quad (**)$$

The resulting occupancy of the  $n^{\text{th}}$  energy level is

$$W_n^{(1)}(t) = |a_n^{(1)}(t)|^2$$

If for some reason we need a more exact result (say, if the resulting  $W_n^{(1)}$  vanishes for a certain state we are interested in), we may pursue the 2<sup>nd</sup>-order approximation by plugging Eq. (\*\*), rewritten for index  $n'$ , into the right-hand side of Eqs. (\*). This gives us the equation,

$$i\hbar\dot{a}_n^{(2)} = \sum_{n' \neq 0} a_{n'}^{(1)} H_{nn'}^{(1)}(t) \exp\{i\omega_{nn'}t\} = \sum_{n' \neq 0} \frac{1}{i\hbar} H_{nn'}^{(1)}(t) \exp\{i\omega_{nn'}t\} \int_0^t H_{n'0}^{(1)}(t') \exp\{i\omega_{n'0}t'\} dt',$$

whose solution may be also expressed in the integral form:

<sup>132</sup> Note that this approximation was already used in the model solutions of the three previous problems.

$$a_n^{(2)}(t) = -\frac{1}{\hbar^2} \sum_{n' \neq 0} \int_0^t dt' H_{nn'}^{(1)}(t') \exp\{i\omega_{nn'} t'\} \int_0^{t'} dt'' H_{n'0}^{(1)}(t'') \exp\{i\omega_{n'0} t''\}. \quad (***)$$

This probability amplitude determines the occupation of the levels whose excitation is not described in the 1<sup>st</sup> order:

$$W_n^{(2)}(t) = |a_n^{(2)}(t)|^2.$$

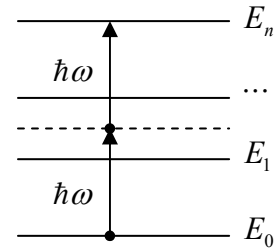
In the particular case of the monochromatic (sinusoidal) excitation described by Eq. (6.86) of the lecture notes,

$$\hat{H}^{(1)}(t) = \begin{cases} 0, & \text{for } t < 0, \\ \hat{A}e^{-i\omega t} + \hat{A}^\dagger e^{+i\omega t}, & \text{for } t \geq 0, \end{cases}$$

both integrals in Eq. (\*\*\*) may be readily worked out. The result is bulky but becomes compact in the case of a nearly perfect tuning mentioned in the assignment, i.e. when  $\xi \equiv 2\omega - \omega_{n0} \rightarrow 0$ :

$$a_n^{(2)} \approx \frac{1}{\hbar^2 \xi} \sum_{n' \neq 0} \frac{A_{nn'} A_{n'0}}{\omega_{n'0} - \omega} \left( e^{i\xi t} - 1 \right), \quad \text{so } W_n^{(2)} \approx \frac{4}{\hbar^4 \xi^2} \left| \sum_{n' \neq 0} \frac{A_{nn'} A_{n'0}}{\omega_{n'0} - \omega} \right|^2 \sin^2 \frac{\xi t}{2}.$$

This expression (strictly valid only if  $W_n^{(2)} \ll 1$ ) formally diverges at  $\xi \rightarrow 0$ , i.e. describes a resonant excitation of the  $n^{\text{th}}$  state, which is possible even if the “direct” matrix element  $A_{n0}$  vanishes, and even if the excitation frequency  $\omega$  itself is not in resonance with any of the quantum transition frequencies  $\omega_{n'0}$ , so as a result, no other states are strongly excited – see the sketch in the figure on the right.<sup>133</sup> This is an example of what is usually, especially in quantum optics, called the *two-photon excitation*.



Another possible case of the two-photon (and more generally, *multi-photon*) excitation takes place when the perturbation Hamiltonian  $\hat{H}^{(1)}$  is a nonlinear function of the applied field. (At the perturbative treatment of this case, it may be unnecessary to go beyond the 1<sup>st</sup>-order result (\*\*\*) because the time dependence of the perturbation may contain higher harmonics of the field’s frequency.)

**Problem 6.27.** A particle of mass  $m$  is initially in a localized ground state, with energy  $E_g < 0$ , of a very-short-range, spherically symmetric potential well. Calculate the rate of its delocalization by an applied classical force  $\mathbf{F}(t) = \mathbf{n}F_0 \cos \omega t$  with a time-independent direction  $\mathbf{n}$ .

**Solution:** This is essentially a generalization of the 1D problem solved in Sec. 6.6 of the lecture notes, and may be solved similarly, with due respect to its 3D aspects. First, the wavefunction of the initial (ground) state is different – see the solution of Problem 9:

$$\psi_0 = \left( \frac{\kappa}{2\pi} \right)^{1/2} \frac{\exp\{-\kappa r\}}{r}, \quad \text{where } \frac{\hbar^2 \kappa^2}{2m} = -E_g > 0.$$

<sup>133</sup> Note that this situation differs from that considered in Problem 21, where the involved energy levels are nearly equidistant, and the excitation of the second of them is conditioned by a high occupation of the first one.

Second, the perturbative Hamiltonian now includes a scalar product:

$$\hat{H}^{(1)} = -\mathbf{F}(t) \cdot \hat{\mathbf{r}} = -\mathbf{n} \cdot \hat{\mathbf{r}} F_0 \cos \omega t.$$

Since the state is spherically symmetric, it is beneficial to direct the  $z$ -axis along the (time-independent) direction  $\mathbf{n}$  of the force, and thus reduce the perturbation Hamiltonian to the simple form (6.86):

$$\hat{H}^{(1)} = -F_0 \hat{z} \cos \omega t \equiv \hat{A} e^{-i\omega t} + \hat{A}^\dagger e^{i\omega t}, \quad \text{with } \hat{A} = -\frac{F_0 z}{2} \equiv -\frac{F_0 r \cos \theta}{2}, \quad \text{for } t \geq 0,$$

where  $\theta$  is the usual polar angle. Finally, we need to find the extended final-state wavefunctions  $\psi_n$  describing the escaped (delocalized) particle,<sup>134</sup> that would have non-zero values of the matrix elements

$$A_{n0} = \int \psi_n^*(\mathbf{r}) \hat{A} \psi_0(\mathbf{r}) d^3 r = -\frac{F_0}{2} \left( \frac{\kappa}{2\pi} \right)^{1/2} \int_0^\infty r e^{-\kappa r} dr \int d\Omega \cos \theta \psi_n(\mathbf{r})$$

that determine the Golden Rule rate (6.111) of transitions from the ground state with  $n' = 0$ . Since  $\cos \theta$  is proportional to only one of the spherical harmonics (namely,  $Y_1^0(\theta, \varphi)$  – see Eq. (3.175) of the lecture notes), and all such harmonics are orthogonal, this integral does not vanish only for the final-state wavefunctions proportional to  $\cos \theta$  and independent of  $\varphi$ .

There are two natural ways to construct such wavefunctions. One is to use the solution of the problem solved at the end of Sec. 3.6, giving such functions in the form Eq. (3.187) with  $l = 1$ :

$$\psi_n(\mathbf{r}) = C_n j_1(k_n r) \cos \theta,$$

where  $j_1(\xi)$  is a spherical Bessel function, and  $k_n$  is related to the final-state energy as

$$E_n = \frac{\hbar^2 k_n^2}{2m}. \quad (*)$$

However, let me leave using this approach for the next, similar problem, and use this occasion to illustrate an alternative approach based on *plane* de Broglie waves  $\psi_n(\mathbf{r}) \propto \exp\{i\mathbf{k}_n \cdot \mathbf{r}\}$ , where the magnitude of vector  $\mathbf{k}_n$  satisfies the same Eq. (\*). Indeed, since the localizing potential  $U(\mathbf{r})$  differs from zero only at the origin, such wavefunctions are legitimate solutions of the Schrödinger equation at  $r \neq 0$ . Moreover, the spherically symmetric potential  $U(\mathbf{r})$ , proportional to  $Y_0^0(\theta, \varphi) = \text{const}$ , does not alter those of the waves that give nonvanishing contributions to  $A_{n0}$ . The normalization coefficient may be found, as usual (see, e.g., Sec. 1.7), by requiring the particle to be confined within an artificial, very large volume  $V \gg 1/k_n^3, 1/\kappa^3$ . Then the normalized wavefunctions are

$$\psi_n(r) = \frac{1}{V^{1/2}} \exp\{i\mathbf{k}_n \cdot \mathbf{r}\} \equiv \frac{1}{V^{1/2}} \exp\{i(k_x x + k_y y + k_z z)\},$$

and our matrix elements may be rewritten as

$$A_{n0} = -\frac{F_0}{2} \left( \frac{\kappa}{2\pi V} \right)^{1/2} \int_V z \exp\{i(k_x x + k_y y + k_z z)\} \frac{\exp\{-\kappa r\}}{r} d^3 r.$$

<sup>134</sup> Of course, such states exist only for energies  $E_n > 0$ , and hence the “ionization” is an effect with a low-frequency threshold:  $\Gamma = 0$  if  $\omega < \omega_{\min} \equiv |E_g|/\hbar$ .

Perhaps the easiest way to calculate the integral in this expression is to notice that it is equal to  $\partial I/\partial(ik_z)$ , where  $I$  is a similar integral but without the factor  $z$  before the exponent:

$$I \equiv \int_V \exp\{i(k_x x + k_y y + k_z z)\} \frac{\exp\{-\kappa r\}}{r} d^3 r \equiv \int_V \exp\{i\mathbf{k}_n \cdot \mathbf{r}\} \frac{\exp\{-\kappa r\}}{r} d^3 r.$$

Indeed, the integral  $I$  is evidently independent of the direction of the vector  $\mathbf{k}_n$ , and we may take this direction for a new axis  $z'$  (independent of the direction  $z$  of the applied force!), and calculate it in these new spherical coordinates  $\{r, \theta', \varphi'\}$ :<sup>135</sup>

$$\begin{aligned} I &= \int_V \exp\{ik_n r \cos \theta'\} \frac{\exp\{-\kappa r\}}{r} d^3 r \equiv \int_0^\infty r^2 dr \int_0^\pi \sin \theta' d\theta' \int_0^{2\pi} d\varphi' \exp\{ik_n r \cos \theta'\} \frac{\exp\{-\kappa r\}}{r} \\ &= 2\pi \int_0^\infty r e^{-\kappa r} dr \int_{-1}^{+1} \exp\{ik_n r \xi\} d\xi = -2\pi \int_0^\infty r e^{-\kappa r} dr \frac{\exp\{-ik_n r\} - \exp\{+ik_n r\}}{ik_n r} \\ &\equiv \frac{4\pi}{k_n} \int_0^\infty e^{-\kappa r} \sin k_n r dr = \frac{4\pi}{k_n} \operatorname{Im} \int_0^\infty \exp\{(-\kappa + ik_n)r\} dr = -\frac{4\pi}{k_n} \operatorname{Im} \frac{1}{-\kappa + ik_n} \equiv \frac{4\pi}{\kappa^2 + k_n^2}, \end{aligned}$$

where  $k_n^2 = k_x^2 + k_y^2 + k_z^2$ . From here,

$$A_{n0} = -\frac{F_0}{2} \left( \frac{\kappa}{2\pi V} \right)^{1/2} \frac{\partial I}{\partial(ik_z)} = -iF_0 \left( \frac{2\pi\kappa}{V} \right)^{1/2} \frac{2k_z}{(\kappa^2 + k_x^2 + k_y^2 + k_z^2)^2} = -iF_0 \left( \frac{8\pi\kappa}{V} \right)^{1/2} \frac{k_n \cos \theta}{(\kappa^2 + k_n^2)^2}.$$

Since this matrix element depends not only on the magnitude but also on the direction of the vector  $\mathbf{k}_n$ , we should use the state number counting rule (1.90) with caution, first applying it to the states with vectors  $\mathbf{k}_n$  within a small solid angle  $d\Omega \ll 4\pi$ , with a virtually constant angle  $\theta$ .

$$dN_n = \frac{V}{(2\pi)^3} k_n^2 dk_n d\Omega.$$

Combined with the derivative of Eq. (\*),  $dE_n = (\hbar^2/m)k_n dk_n$ , this relation gives the following “directional” (angle-differential) density of states:

$$d\rho_n \equiv \frac{dN_n}{dE_n} \equiv \frac{dN}{dk_n} \bigg/ \frac{dE_n}{dk_n} = \frac{V}{(2\pi)^3} k_n^2 dk_n d\Omega \bigg/ \frac{\hbar^2}{m} k_n dk_n = \frac{Vm k_n}{(2\pi)^3 \hbar^2} d\Omega,$$

so the Golden Rule (6.111) yields<sup>136</sup>

$$d\Gamma = \frac{2\pi}{\hbar} |A_{n0}|^2 d\rho_n = \frac{2\pi}{\hbar} \times F_0^2 \frac{8\pi\kappa}{V} \frac{k_n^2 \cos^2 \theta}{(\kappa^2 + k_n^2)^4} \times \frac{Vm k_n}{(2\pi)^3 \hbar^2} d\Omega \equiv \frac{2}{\pi} \frac{F_0^2 m}{\hbar^3} \frac{\kappa k_n^3}{(\kappa^2 + k_n^2)^4} \cos^2 \theta d\Omega.$$

This partial rate is the probability of the particle’s delocalization in unit time, with the condition that its final wave vector  $\mathbf{k}_n$  is within the elementary solid angle  $d\Omega$ . Note that the angular distribution of

<sup>135</sup> Since the function under integral decays at distances  $r \sim \kappa^{-1} \ll V^{1/3}$ , the integration volume restriction may be ignored here.

<sup>136</sup> Note that the artificial binding volume  $V$  has canceled – the condition necessary for the legitimacy of this normalization procedure.

the delocalized particles vanishes in all directions normal to that of the applied force (with  $\theta = \pi/2$ ). The total rate may now be calculated by the summation of such partial rates over the whole solid angle:

$$\Gamma = \oint d\Gamma = \frac{2 F_0^2 m}{\pi \hbar^3} \frac{\kappa \kappa_n^3}{(\kappa^2 + k_n^2)^4} \times 2\pi \int_0^\pi \cos^2 \theta \sin \theta d\theta = \frac{8 F_0^2 m}{3 \hbar^3} \frac{\kappa \kappa_n^3}{(\kappa^2 + k_n^2)^4}.$$

In order to discuss the frequency dependence of this rate, it is useful to notice that due to the energy conservation (formally expressed by Eq. (6.93) of the lecture notes – see also Fig. 6.10),

$$\hbar \omega = E_n - E_g \equiv \frac{\hbar^2 k_n^2}{2m} - \left( -\frac{\hbar^2 \kappa^2}{2m} \right) \equiv \frac{\hbar^2 (k_n^2 + \kappa^2)}{2m},$$

our result may be rewritten in a simpler form:

$$\Gamma = \frac{8 F_0^2 m}{3 \hbar^3} \frac{\kappa \kappa_n^3}{(2m\omega/\hbar)^4} \equiv \frac{1 F_0^2 \hbar}{6 m^3} \frac{\kappa \kappa_n^3}{\omega^4} \propto \frac{(\omega - \omega_{\min})^{3/2}}{\omega^4}.$$

Per this formula, the rate first increases when  $\omega$  exceeds its threshold value  $\omega_{\min} \equiv |E_g|/\hbar$ , and then (beyond  $\omega = (8/5)\omega_{\min}$ ) decreases again, vanishing at  $\omega \rightarrow \infty$ . This behavior is qualitatively similar to, but quantitatively different from that in the 1D case – cf. Eq. (6.133) of the lecture notes.

**Problem 6.28.** Calculate the rate of ionization of a hydrogen atom, initially in its ground state, by a classical, linearly polarized electromagnetic wave with a frequency  $\omega$  within the range

$$\frac{\hbar}{m_e r_B^2} \ll \omega \ll \frac{c}{r_B}.$$

Recast your result in terms of the cross-section of electromagnetic wave absorption. Discuss briefly what changes of the theory would be necessary if each of the above two conditions had been violated.

*Solution:* Due to the second of the conditions specified in the assignment, the electromagnetic wavelength,  $\lambda = 2\pi c/\omega$ , is much larger than the Bohr radius  $r_B$ , i.e. the linear scale of the atom's wavefunction extension. In this limit, the spatial variation of the field may be ignored, so following Eq. (6.29) of the lecture notes, with  $q = -e$ , the perturbation Hamiltonian may be taken in the form

$$\hat{H}^{(1)} = e \mathcal{E}_0 \hat{z} \cos \omega t = \hat{A} e^{-i\omega t} + \hat{A}^\dagger e^{+i\omega t}, \quad \text{with } \hat{A} = \hat{A}^\dagger = \frac{1}{2} e \mathcal{E}_0 \hat{z},$$

where  $\mathcal{E}_0$  is the wave field's amplitude, and the  $z$ -axis is directed along the electric field's polarization.

The first of the given conditions ensures that the electron's final state energy,

$$E_n = E_{n'} + \hbar \omega = -\frac{E_H}{2} + \hbar \omega,$$

is much higher than the Hartree energy  $E_H \approx 27$  eV. This condition allows us to neglect the atom's effect on the final state's wavefunctions, and take them in the form of free-particle de Broglie waves.<sup>137</sup> It is

<sup>137</sup> Note that the previous, conceptually very similar problem could be solved analytically without imposing such a condition because the very short-range binding potential  $U(\mathbf{r})$ , considered in it, does not disturb the relevant final states, corresponding to  $l = 1$ , with any energy  $E_n > 0$ .

possible to take these wavefunctions in the form of plane waves,  $\psi_n(\mathbf{r}) \propto \exp\{i\mathbf{k}_n \cdot \mathbf{r}\}$ , with the magnitude of wave vector  $\mathbf{k}_n$  related to the final state energy  $E_n > 0$  as

$$\frac{\hbar^2 k_n^2}{2m_e} = E_n, \quad (*)$$

but then the matrix elements  $A_{n0}$  that participate in the Golden Rule (6.111) would depend not only on the magnitude of vector  $\mathbf{k}_n$  (i.e., on the final state energy  $E_n$ ) but also on the direction of this vector, making that formula directly applicable only to each subset of final states within a small solid angle  $d\Omega$ , with a definite angle  $\theta$  between the vectors  $\mathbf{k}_n$  and  $\mathbf{n}_z$ . Though this technical difficulty may be readily overcome (see the solution of the previous problem), let me use here an alternative approach, which was only mentioned in that solution.

Let us look at the angular structure of the matrix elements, in the coordinate representation:

$$A_{n0} = \int \psi_n^* \hat{A} \psi_0 d^3 r.$$

While according to Eqs. (3.174), (3.200), and (3.208) of the lecture note (with  $r_0 = r_B$ ), the initial, ground-state wavefunction  $\psi_0$  is spherically symmetric,

$$\psi_0 = Y_0^0(\theta, \varphi) \mathcal{R}_{1,0}(r) = \frac{1}{\pi^{1/2} r_B^{3/2}} \exp\left\{-\frac{r}{r_B}\right\},$$

the perturbation operator does have an angular dependence, and according to Eq. (3.175), may be represented as

$$\hat{A} = \frac{1}{2} e \mathcal{E}_0 z \equiv \frac{1}{2} e \mathcal{E}_0 r \cos \theta \equiv \left(\frac{\pi}{3}\right)^{1/2} e \mathcal{E}_0 r Y_1^0(\theta, \varphi).$$

Since the spherical harmonics are orthogonal, the angular factor of the matrix element integral does not vanish only if the final state is also proportional to the same spherical harmonic – with the quantum numbers  $l = 1$  and  $m = 0$ . As we know from the problem solved in the end of Sec. 3.6 of the lecture notes, for a free particle with energy  $E_n$ , such a function is

$$\psi_n = C_n j_1(k_n r) Y_1^0(\theta, \varphi),$$

where the wave number  $k_n$  satisfies the same Eq. (\*), and the spherical Bessel function  $j_1$  is rather simple – see Eq. (3.186):

$$j_1(\xi) = \frac{\sin \xi}{\xi^2} - \frac{\cos \xi}{\xi}.$$

The normalization coefficient  $C_n$  may be readily calculated by introducing an auxiliary confining sphere of a sufficiently large radius  $R \gg 1/k_n$ , and imposing some boundary condition, say  $\psi_n(R) = 0$ , on its surface. In this case, the second term in the expression for  $j_1(\xi)$  dominates the normalization integral:

$$\int \psi_n \psi_n^* d^3 r = \oint |Y_{10}(\theta, \varphi)|^2 d\Omega \int_0^R |j_1(k_n r)|^2 r^2 dr = |C_n|^2 \int_0^R \left(\frac{\cos k_n r}{k_n r}\right)^2 r^2 dr = |C_n|^2 \frac{R}{2k_n^2} = 1$$

(where at the second step, the spherical harmonics' orthonormality was used), so we may take

$$C_n = \left(\frac{2}{R}\right)^{1/2} k_n.$$

Now, by assuming that this  $R$  is much larger than  $r_B$  as well (as we certainly may, due to the artificial character of  $R$ ), we can calculate the required matrix element by ignoring that upper bound:

$$A_{n0} = \left(\frac{\pi}{3}\right)^{1/2} e\mathcal{E}_0 \left(\frac{2}{R}\right)^{1/2} k_n \frac{1}{\pi^{1/2} r_B^{3/2}} \oint |Y_1^0(\theta, \varphi)|^2 d\Omega \times I, \quad \text{with } I \equiv \int_0^\infty \exp\left\{-\frac{r}{r_B}\right\} r j_1(k_n r) r^2 dr,$$

where the angular integral equals 1 again. It may look like that due to the first of the conditions given in the assignment,  $k_n \gg 1/r_B$ , in the radial integral  $I$ , we can again keep only the second, more slowly decaying part of  $j_1(k_n r)$ . However, due to the exponential cut-off at  $r \sim r_B$ , this is not so; indeed:

$$\begin{aligned} I &= \int_0^\infty \exp\left\{-\frac{r}{r_B}\right\} r \left(\frac{\sin k_n r}{k_n^2 r^2} - \frac{\cos k_n r}{k_n r}\right) r^2 dr \\ &\equiv \frac{1}{k_n^2} \text{Im} \int_0^\infty \exp\{-\lambda r\} r dr - \frac{1}{k_n} \text{Re} \int_0^\infty \exp\{-\lambda r\} r^2 dr, \quad \text{with } \lambda \equiv r_B^{-1} - ik_n r. \end{aligned}$$

These are two well-known integrals,<sup>138</sup> equal to  $1/\lambda^2$  and  $2/\lambda^3$ , correspondingly, so

$$I = \frac{1}{k_n^2} \text{Im} \frac{1}{(r_B^{-1} - ik_n)^2} - \frac{2}{k_n} \text{Re} \frac{1}{(r_B^{-1} - ik_n)^3} = \frac{1}{k_n^2} \frac{2r_B^{-1} k_n}{(r_B^{-2} + k_n^2)^2} - \frac{2}{k_n} \frac{r_B^{-3} - 3r_B^{-1} k_n^2}{(r_B^{-2} + k_n^2)^3} \rightarrow \frac{2r_B^{-1}}{k_n^5} + \frac{6r_B^{-1}}{k_n^5}.$$

We see that the contributions from both terms are comparable even in the limit  $k_n \gg r_B^{-1}$  pursued at the last step. As a result, we get

$$A_{n0} = \left(\frac{\pi}{3}\right)^{1/2} e\mathcal{E}_0 \left(\frac{2}{R}\right)^{1/2} k_n \frac{1}{\pi^{1/2} r_B^{3/2}} \times \frac{8}{k_n^5 r_B} \equiv \left(\frac{128}{3}\right)^{1/2} \frac{e\mathcal{E}_0}{k_n^4 r_B^{5/2} R^{1/2}}.$$

What remains is to calculate the density of the final states. For  $k_n R \gg 1$ , the boundary condition  $j_1(k_n R) = 0$  yields  $k_n R \approx \pi n + \text{const}$ , so  $dn/dk_n = R/\pi$ . Combining this relation with the derivative of Eq. (\*),  $dE_n = (\hbar^2/m_e)k_n dk_n$ , we get

$$\rho_n \equiv \frac{dn}{dE_n} \equiv \frac{dn}{dk_n} \Big/ \frac{dE_n}{dk_n} = \frac{R}{\pi} \Big/ \frac{\hbar^2 k_n}{m_e} \equiv \frac{R m_e}{\pi \hbar^2 k_n}.$$

With that, the Golden Rule (6.111) yields<sup>139</sup>

$$\Gamma = \frac{2\pi}{\hbar} \left[ \left(\frac{128}{3}\right)^{1/2} \frac{e\mathcal{E}_0}{k_n^4 r_B^{5/2} R^{1/2}} \right]^2 \frac{R m_e}{\pi \hbar^2 k_n} \equiv \frac{256}{3} \frac{e^2 \mathcal{E}_0^2 m_e}{\hbar^3 k_n^9 r_B^5}.$$

(Notice that the artificial confinement radius  $R$  has canceled, as it had to.)

<sup>138</sup> See, e.g., MA Eq. (6.7d) with  $n = 1$  and  $n = 2$ . Since the functions under the integrals are analytical, these formulas are valid even for complex  $\lambda$ , provided that  $\text{Re}\lambda > 0$ , so the integrals converge at their upper limits.

<sup>139</sup> The reader is highly encouraged to re-derive this result by using the alternative plane-wave approach employed in the previous problem, as an additional exercise.

In order to get a better feeling of the intensity of the ionization process, it is useful to consider it as the electromagnetic wave's absorption (with the corresponding emission of one photoelectron per each absorbed photon) and borrow the notion of its total cross-section  $\sigma$  from the scattering theory. Creatively adjusting Eq. (3.59) of the lecture notes, we may define this notion as

$$\sigma \equiv \frac{\text{average number of photons absorbed by atom per second}}{\text{incident flux of photons per unit area}} = \frac{\Gamma}{S/\hbar\omega},$$

where  $S$  is the Poynting vector's magnitude, i.e. the plane electromagnetic wave's power per unit area of its front. For plane waves in vacuum:<sup>140</sup>

$$S = \frac{\mathcal{E}_0^2}{2Z_0}, \quad \text{where } Z_0 \equiv \left( \frac{\mu_0}{\epsilon_0} \right)^{1/2} \equiv \frac{1}{\epsilon_0 c}.$$

Using our result for  $\Gamma$ , the cross-section may be represented in the form

$$\sigma = \frac{256 e^2 \mathcal{E}_0^2 m_e}{3 \hbar^3 k_n^9 r_B^5} \bigg/ \frac{\epsilon_0 c \mathcal{E}_0^2}{2\hbar\omega} \equiv \frac{512 k_{EM} e^2 m_e}{3 \epsilon_0 \hbar^2 k_n^9 r_B^5} \equiv \frac{2,048\pi}{3} \sigma_B \frac{k_{EM} r_B}{(k_n r_B)^9},$$

where  $k_{EM} = \omega/c$  is the electromagnetic wave's wave number, and

$$\sigma_B \equiv \pi r_B^2 \approx 0.88 \times 10^{-20} \text{ m}^2$$

is the effective "Bohr" cross-section area of the hydrogen atom. (As a reminder,  $r_B \equiv 4\pi\epsilon_0\hbar^2/e^2m_e$ .)

Since the strong conditions given in the assignment (and used in the solution) may be recast as

$$k_{EM} r_B \ll 1 \ll k_n r_B,$$

we see that within our frequency range, the cross-section of the ionization process is much smaller than  $\sigma_B$ . By the way, it is useful to estimate how broad this frequency range is. The ratio of the upper and lower bounds for  $\omega$ , by the order of magnitude, is

$$\frac{c/r_B}{\hbar/m_e r_B^2} = \frac{4\pi\epsilon_0 c \hbar}{e^2} \equiv \frac{1}{\alpha} \approx 137,$$

where  $\alpha$  is the fine structure constant (6.62). So, the specified frequency range is broad, but not too broad: if we want to keep both inequalities strong indeed, it is about one order of magnitude – in the electromagnetic wavelength, from  $\sim 10$  nm to  $\sim 100$  nm.<sup>141</sup> In the middle of the range (at  $k_{EM} r_B \sim 0.1$ ,  $k_n r_B \sim 10$ ), we get  $\sigma \sim 2 \times 10^{-5} \sigma_B \sim 2 \times 10^{-25} \text{ m}^2$ .<sup>142</sup> This number means that if a sample has  $n \sim 0.5 \times 10^{28}$  hydrogen atoms per  $\text{m}^3$  (the number typical for the organic condensed matter), the penetration length  $\delta = 1/n\sigma$  of such radiation,<sup>143</sup> limited by the hydrogen photo-ionization, is about  $10^{-3}$  m, i.e. 1 mm.

<sup>140</sup> See, e.g., EM Sec. 7.1.

<sup>141</sup> Electromagnetic waves in this range are usually called *extreme ultraviolet* radiation – EUV (or XUV).

<sup>142</sup> Note that this  $\sigma$  of the *inelastic* photoionization process is still much larger than the electron's cross-section  $\sigma_T = (8/3)\sigma_B\alpha^4 \approx 0.67 \times 10^{-29} \text{ m}^2$  of the *elastic* ("Thomson") scattering of electromagnetic waves – see, e.g., EM Sec. 8.3, in particular Eq. (8.41).

<sup>143</sup> Let me hope that the reader has met the used expression,  $\delta = 1/n\sigma$ , earlier. If not: it may be readily obtained from the requirement that the expression for the decay  $-dS$  of the incident radiation in a layer of thickness  $dx \ll$



Moreover, as may be readily proved by reviewing the above calculations, for hydrogen-like atoms/ions with an atomic number  $Z > 1$ , our result is valid with the replacement  $\sigma \rightarrow Z^5 \sigma$ . Though this model is rather crude for other atoms, such scaling still hints that the EUV penetration length into any condensed matter is very small. This is true indeed, causing many problems with practical applications of such radiation, including high-resolution photolithography – the main process used for integrated circuit patterning. (For one, no refractive optics is available for the EUV, due to such high absorption.)<sup>144</sup>

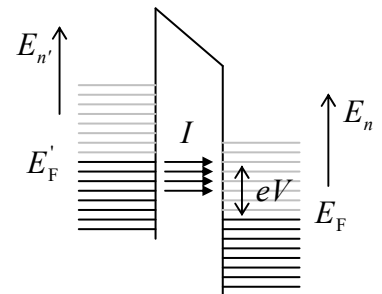
Returning to the last assignment of the problem, in order to overcome the given lower frequency bound, we would need to modify the final-state wavefunctions to account for their interaction with the  $1/r$ -type potential profile of the hydrogen nuclei. (This may be done by studying the solutions of Eq. (3.193) of the lecture notes, with  $l = 1$ , for  $\varepsilon > 0$ .) On the other hand, at frequencies higher than the specified upper bound of the frequency range, we would need to take into account the spatial dependence of the electromagnetic field. Any of the changes would make the calculations rather involved.

**Problem 6.29.\*** Use the quantum-mechanical Golden Rule to derive the general expression for the electric current  $I$  through a weak tunnel junction between two conductors, biased with dc voltage  $V$ , via the matrix elements that describe the tunneling, by treating the conductors as degenerate Fermi gases of electrons with negligible direct interaction. Simplify the result in the low-voltage limit.

*Hint:* The electric current flowing through a weak tunnel junction is so low that it does not substantially perturb the electron states inside each conductor.

*Solution:* In thermal equilibrium (which is not perturbed by weak tunnel current), the Fermi gas of non-interacting electrons in each conductor may be described by a dense (quasi-continuous) set of energy levels  $E_n$ , occupied by electrons in accordance with the Fermi distribution  $f(E_n)$ , which drops from 1 to 0 on the scale  $\sim k_B T$  as soon as the energy is increased above some value  $E_F$ , called the *Fermi energy*.<sup>145</sup>

The figure on the right shows (very schematically) the energy diagram of a tunnel junction biased by a time-independent (dc) voltage  $V$ , which creates the Fermi levels' difference  $E_F - E'_F = -eV$ . Hence each energy level  $E_{n'}$  in one conductor (referred to its Fermi level) becomes aligned with the level  $E_n = E_{n'} + eV$  of another conductor. If level  $E_{n'}$  is fully occupied, and level  $E_n$  is completely empty, the Golden Rule (6.137) for the rate of electron tunneling from left to right reads



$$\Gamma(E_{n'}) = \frac{2\pi}{\hbar} |T_{nn'}|^2 \rho_R(E_{n'} + eV),$$

$\delta$ , calculated from the definition of the cross-section,  $-dS = \sigma S dN = S \sigma n dx$ , coincides with the one,  $-dS = S dx / \delta$ , following from the exponential decay law,  $S \propto \exp\{-x/\delta\}$ , where  $x$  is the direction of radiation's propagation. Note that similar (though not always identical) expressions are valid for the particle's mean free path – see, e.g., SM Chapter 6.

<sup>144</sup> See, e.g., V. Bakshi, *EUV Lithography*, 2<sup>nd</sup> ed., SPIE (2018).

<sup>145</sup> For a detailed discussion of the Fermi distribution and the Fermi gas see, e.g., SM Secs. 2.8 and 3.3; for our current purposes, the particular form of the function  $f(E)$  is not important.

where  $T_{nn'}$  is the matrix element of the electrode interaction, describing the tunneling barrier's transparency, and  $\rho_R$  is the density of states in the right electrode (which should take into account the two-fold spin degeneracy of each orbital energy level). The electric current due to this rate would be just  $-e\Gamma(E_{n'})$ . However, to account for an incomplete occupancy of the initial and final states of the electron, this expression has to be multiplied by  $f(E_{n'})[1 - f(E_{n'} + eV)]$ . (The second multiplier reflects the Pauli principle for Fermi particles: if a state is already occupied by an electron, tunneling of an additional electron into the same state is forbidden.) Thus the electric current from the left (L) conductor into the right (R) one may be calculated as a sum over a quasi-continuous set of the levels  $E_{n'}$ , with the density  $\rho_L(E_{n'})$ :

$$\begin{aligned} I_{\rightarrow} &= -e \frac{2\pi}{\hbar} \sum_{n'} |T_{nn'}|^2 \rho_R(E_{n'} + eV) f(E_{n'}) [1 - f(E_{n'} + eV)] \\ &\approx -\frac{2\pi e}{\hbar} \int \rho_L(E_{n'}) dE_{n'} |T_{nn'}|^2 \rho_R(E_{n'} + eV) f(E_{n'}) [1 - f(E_{n'} + eV)]. \end{aligned}$$

We should also take into account the back current  $I_{\leftarrow}$  due to the reciprocal tunneling from the right into the left conductor, which differs from  $I_{\rightarrow}$  only by the occupancy factors. As a result, for the net current we get

$$\begin{aligned} I(V) &\equiv I_{\rightarrow} - I_{\leftarrow} = -\frac{2\pi e}{\hbar} \int \rho_L(E_{n'}) dE_{n'} |T_{nn'}|^2 \rho_R(E_{n'} + eV) \times \left\{ \begin{array}{l} f(E_{n'}) [1 - f(E_{n'} + eV)] \\ - f(E_{n'} + eV) [1 - f(E_{n'})] \end{array} \right\} \\ &\equiv -\frac{2\pi e}{\hbar} \int |T_{nn'}|^2 \rho_L(E_{n'}) \rho_R(E_{n'} + eV) [f(E_{n'}) - f(E_{n'} + eV)] dE_{n'}. \end{aligned}$$

This expression is broadly used in the theory of tunnel junctions. It may be readily simplified in the limit when  $eV$  is small in comparison with the scale of the energy dependence of the matrix elements  $T_{nn'}$  and the densities of states (but not necessarily with the thermal excitation scale  $k_B T$ ), so  $[f(E_{n'}) - f(E_{n'} + eV)] \approx -df/dE|_{E_{n'}=E_F} eV$ , and

$$I(V) \rightarrow GV, \quad \text{with } G = \frac{2\pi e^2}{\hbar} \left\langle |T_{nn'}|^2 \right\rangle_{E=E_F} \rho_L(E_F) \rho_R(E_F),$$

where the averaging is over all states on the Fermi surface (which is dominated by the states with the group velocity virtually normal to the junction plane).

In tunnel junctions between most conductors (say, semiconductors or normal metals), this Ohm's law works very well at applied voltages up to several hundred mV. However, in some cases, this is not so. For example, in superconductors, the effective density of single-electron states is strongly suppressed within the so-called *superconducting energy gap*  $\Delta \sim k_B T_c$ , where  $T_c$  is the critical temperature, near the Fermi energy. As a result, the  $I$ - $V$  curves of tunnel junctions between superconductors may be strongly nonlinear on the scale of just a few meV, with the current rising sharply as the voltage reaches the threshold value  $V_t = (\Delta_L + \Delta_R)/e$ .<sup>146</sup>

<sup>146</sup> Historically, the experimental observation of this threshold in 1960 by I. Giaever (which brought him a Nobel Prize in Physics) was a key confirmation of the BCS theory of superconductivity developed in 1956-57 by J. Bardeen, L. Cooper, and R. Schrieffer.

**Problem 6.30.\*** Generalize the result of the previous problem to the case when a weak tunnel junction is biased with voltage  $V(t) = V_0 + A\cos\omega t$ , with  $\hbar\omega$  generally comparable with  $eV_0$  and  $eA$ .

*Solution:* Since weak tunneling does not perturb the electron states inside conductors, they remain stationary, i.e. their time dependence is reduced to  $\exp\{-iE_n t/\hbar\}$ , if the energy  $E_n$  of each state is referred to a fixed level inside the same conductor. However, if the voltage  $V(t)$  between two conductors is changed in time, we should count their energies from the same reference level, for example, the Fermi level of one of the conductors – say the “left” one (see the figure in the previous problem). Then for the states in that electrode, we may still use the same time dependence,  $\exp\{-iE'_n t/\hbar\}$ , but that in the “right” conductor should be appropriately generalized.

To do that, let us recall that the simple complex-exponential (i.e. sinusoidal) dependence results from applying the Schrödinger equation (1.25)<sup>147</sup> to the situation when the wavefunction may be factored into its spatial and temporal parts – see Eq. (1.57):

$$\Psi_n(\mathbf{r}, t) = a_n(t)\psi_n(\mathbf{r}).$$

We can perform such a partition in our current case as well because the stationary eigenfunctions  $\psi_n(\mathbf{r})$  do not depend on the energy reference level. However, the Hamiltonian of the right electrode now acquires a time-dependent component:

$$\hat{H}_R(t) = \hat{H}_R|_{V=0} - eV(t),$$

so the equation for the complex amplitudes  $a_n(t)$  is now more general than Eq. (1.61a):

$$i\hbar\dot{a}_n = [E_n - eV(t)]a_n, \quad \text{i.e. } d(\ln a_n) = -i\frac{E_n - eV(t)}{\hbar}dt,$$

This simple equation may be easily integrated for an arbitrary time dependence  $V(t)$ , giving

$$a_n(t) = a_n(0) \exp\left\{-i\frac{E_n t}{\hbar} + i\frac{e}{\hbar}\int_0^t V(t')dt'\right\}. \quad (*)$$

If the voltage is constant in time (say,  $A = 0$ ), this result is reduced to the usual exponential dependence:

$$a_n(t)|_{A=0} = a_n(0) \exp\left\{-i\frac{E_n t}{\hbar} + i\frac{e}{\hbar}V_0 t\right\} \equiv a_n(0) \exp\left\{-i\frac{(E_n - eV_0)t}{\hbar}\right\}.$$

In this case, the requirement for the matrix element  $T_{nn'} \propto a_n^*(t)a_n(t)$  to be time-independent leads to the level-alignment condition  $E_n - eV = E_{n'}$  that was already used in the solution of the previous problem. However, for the voltage  $V(t) = V_0 + A\cos\omega t$ , Eq. (\*) yields a more general result:

$$a_n(t) = a_n(0) \exp\left\{-i\frac{(E_n - eV_0)t}{\hbar} + i\frac{eA}{\hbar}\int_0^t \cos\omega t' dt'\right\} = a_n(0) \exp\left\{-i\frac{(E_n - eV_0)t}{\hbar}\right\} \exp\left\{i\frac{eA}{\hbar\omega} \sin\omega t\right\}.$$

Using the integral representation of the Bessel functions  $J_k(\xi)$  of the first kind with integer indices,<sup>148</sup> the last exponent may be represented as a simple Fourier series:<sup>149</sup>

<sup>147</sup> The absolutely similar separation follows from the bra-ket form, Eq. (4.158), of the Schrödinger equation.

$$\exp\left\{i\frac{eA}{\hbar\omega}\sin\omega t\right\} = \sum_{k=-\infty}^{+\infty} J_k\left(\frac{eA}{\hbar\omega}\right)e^{ik\omega t}.$$

Let us use this representation to rewrite the above result for  $a_n(t)$  as

$$a_n(t) = a_n(0) \sum_{k=-\infty}^{+\infty} J_k\left(\frac{eA}{\hbar\omega}\right) \exp\left\{-\frac{i(E_n - eV_k)t}{\hbar}\right\}, \quad \text{with } V_k \equiv V_0 + k\frac{\hbar\omega}{e}.$$

Translated into plain English, this formula tells us that from the point of view of the left conductor (where our energy reference is now located), each eigenstate of the right conductor is reproduced at an infinite set of energies separated by equal intervals  $\Delta E = \hbar\omega$ , each with an amplitude multiplier of  $J_k(eA/\hbar\omega)$ . Since within the region of validity of the Golden Rule, these states may be treated as independent (incoherent) ones, the tunneling currents into/from each state of this set just add up. Hence, repeating all calculations of the previous problem, and taking into account that the component of  $|T_{m'}|^2 \propto a_n^*(t)a_n(t)$  corresponding to the  $k^{\text{th}}$  term of the sum is now proportional to  $J_k^2(eA/\hbar\omega)$ , we may express the final result via that in the dc case (at  $A = 0$ ):

$$I(\bar{V}, A) = \sum_{k=-\infty}^{\infty} J_k^2\left(\frac{eA}{\hbar\omega}\right) I(V_k, 0) \equiv \sum_{k=-\infty}^{\infty} J_k^2\left(\frac{eA}{\hbar\omega}\right) I\left(V_0 + k\frac{\hbar\omega}{e}, 0\right). \quad (**)$$

This famous *Tien-Gordon formula*<sup>150</sup> shows that in the presence of an ac signal of amplitude  $A$ , the dc  $I$ - $V$  curve may be represented as a sum of the original  $I$ - $V$  curves (measured at  $A = 0$ ), shifted along the dc voltage by intervals  $k\hbar\omega/e$ , with their currents weight by  $J_k^2(eA/\hbar\omega)$ . (Since at large  $k$ , these factors decrease faster than  $1/k$ , the sum is always finite.) This result is especially spectacular if the original current (in the absence of ac voltage) is negligible until a certain threshold  $V_t$  where it makes a finite jump, as it does in the case of tunnel junctions between two superconductors – see the discussion in the end of the previous problem’s solution. In this case, the external electromagnetic radiation creates similar jumps (“current steps”) at lower voltages  $V_t - k\hbar\omega/e$ . This effect, called *photon-assisted tunneling*, may be interpreted as follows: the  $k^{\text{th}}$  term of the sum (\*\*) describes either absorption or emission of  $k$  quanta of the external radiation responsible for the ac part of the voltage  $V(t)$ . Let me hope that the reader appreciates how smartly quantum mechanics manages to smuggle in the notion of electromagnetic field quanta even when we try to describe the field in a completely classical way.

Let me finish by offering the reader two additional tasks:

(i) Use the properties of the Bessel functions to show that if the frequency  $\omega$  is reduced so much that the voltage interval  $\hbar\omega/e$  becomes much smaller than the voltage scale of the original  $I$ - $V$  curve’s nonlinearity, the Tien-Gordon formula (\*\*) is reduced to the classical result

$$I(V_0, A) = \overline{I(V_0 + A\cos\omega t, 0)},$$

<sup>148</sup> See, e.g., MA Eq. (6.15a).

<sup>149</sup> Such an expansion is of course possible for any periodic function of time, but for the exponent of a sinusoidal argument, it has especially simple coefficients.

<sup>150</sup> It was derived in 1963 by P. Tien and J. Gordon to explain the spectacular (and initially very surprising) effects of microwave irradiation on tunnel junctions between two superconductors, observed a year earlier by A. Dayem and R. Martin.

where the top bar means, as usual, time averaging – in our case, over the ac signal’s period.

(ii) Explain why the Tien-Gordon formula differs from the solution of a similar problem for a Josephson junction – see Problem 1.8.

**Problem 6.31.\*** Use the quantum-mechanical Golden Rule to derive the Landau-Zener formula (2.257).

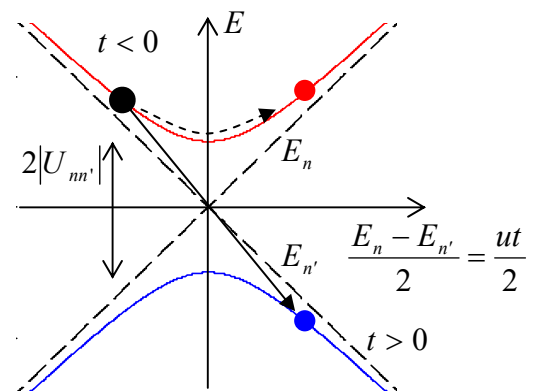
*Solution:*<sup>151</sup> As was discussed in Sec. 2.8 of the lecture notes, the Landau-Zener formula, which may be conveniently rewritten in the form (2.259),

$$W_{n'} = \exp\left\{-\frac{2\pi|U_{nn'}|^2}{\hbar u}\right\},$$

may be interpreted as the expression for the probability of the system’s transfer to another branch of the anticrossing diagram (reproduced in the figure on the right), provided that it is dragged through the anticrossing with a constant “energy speed”

$$u \equiv \frac{d}{dt}(E_n - E_{n'}),$$

where  $E_n$  and  $E_{n'}$  are the unperturbed energies of the two states in the absence of their coupling described by the matrix coefficient  $U_{nn'}$ . Note again that the Landau-Zener tunneling (indicated schematically with the solid straight arrow in the figure on the right) corresponds to the *conservation* of the initial unperturbed state  $n'$ , while its *change*,  $n' \rightarrow n$  (shown with the dashed, curved arrow) corresponds to an adiabatic motion of the system along the same branch of the anticrossing.



Of course, there is no explicit continuum of final states in this situation; however, from the point of view of the initial state (with the energy  $E_{n'}$ ), the second energy level  $E_n$  passes by the reference level with the “velocity”  $u$ , and on average may be considered as forming a pseudo-continuum of states. As was briefly discussed in Sec. 6.6, a formal way to describe this fact is to replace the density of states  $\rho_n$  with the Dirac delta function  $\delta(E_n - E_{n'})$ . In our current case, it is equal to  $\delta(ut)$ , so the Golden Rule gives a time-dependent transition rate

$$\Gamma(t) = \frac{2\pi}{\hbar} |U_{nn'}|^2 \delta(ut). \quad (*)$$

Now let us write the probability decay equation (6.113) (essentially the definition of the rate  $\Gamma$ ):

$$\dot{W}_{n'} = -\Gamma(t)W_{n'}, \quad \text{i.e.} \quad \frac{dW_{n'}}{W_{n'}} = -\Gamma(t)dt,$$

where  $W_{n'}$  is the probability of the particle to remain in the initial state  $n'$ , i.e. in our case, the probability of the Landau-Zener tunneling – see the figure above. This equation may be readily solved for an arbitrary function  $\Gamma(t)$ , provided that its difference from zero has a limited time duration:

<sup>151</sup> See, e.g., M. Amin *et al.*, *Phys. Rev. A* **79**, 022107 (2009) and references therein.

$$W_{n'}(t) = W_{n'}(-\infty) \exp \left\{ - \int_{-\infty}^t \Gamma(t') dt' \right\}.$$

For our particular case (\*), and  $W_{n'}(t < 0) = 1$ , the integration immediately yields

$$W_{n'}(t > 0) = \exp \left\{ - \frac{2\pi}{\hbar} |U_{nn'}|^2 \int_{t < 0}^{t > 0} \delta(ut') dt' \right\} = \exp \left\{ - \frac{2\pi}{\hbar u} |U_{nn'}|^2 \int_{\xi < 0}^{\xi > 0} \delta(\xi) d\xi \right\} = \exp \left\{ - \frac{2\pi}{\hbar u} |U_{nn'}|^2 \right\},$$

thus giving us the Landau-Zener formula.

Actually, this result is highly nontrivial. Indeed, the standard derivation of the Golden Rule (see Sec. 6.6) is based on ignoring the coherence of the partial final states with close but different energies  $E_n$ . At the Landau-Zener transition, the role of all these fixed-energy states is played by a single state  $n$  at different moments of time, with the coherence of its increments effectively destroyed by the linear change of its eigenenergy in time. So, this is a spectacular example of a powerful theory working beyond its anticipated limits.

## Chapter 7. Open Quantum Systems

**Problem 7.1.** Calculate the density matrix of a two-level system whose Hamiltonian is described, in a certain basis, by the following matrix:

$$\mathbf{H} = \mathbf{c} \cdot \boldsymbol{\sigma} \equiv c_x \sigma_x + c_y \sigma_y + c_z \sigma_z,$$

where  $\sigma_k$  are the Pauli matrices and  $c_j$  are  $c$ -numbers, in thermodynamic equilibrium at temperature  $T$ .

*Solution:* According to Eq. (7.24) of the lecture notes, in thermodynamic equilibrium, the density operator is diagonal in the energy eigenstate basis:

$$w_{nn'} = W_n \delta_{nn'}, \quad \text{with } W_n = \frac{1}{Z} \exp\left\{-\frac{E_n}{k_B T}\right\}, \quad Z = \sum_n \exp\left\{-\frac{E_n}{k_B T}\right\}.$$

The eigenenergies of a two-level system are given by Eq. (5.6):

$$E_{\pm} = b \pm c, \quad \text{where } c \equiv (c_x^2 + c_y^2 + c_z^2)^{1/2} \geq 0.$$

As a result, the statistical sum is

$$Z = \exp\left\{\frac{b+c}{k_B T}\right\} + \exp\left\{\frac{b-c}{k_B T}\right\},$$

so the state probabilities are

$$W_{\pm} = \frac{\exp\{(b \mp c)/k_B T\}}{\exp\{(b+c)/k_B T\} + \exp\{(b-c)/k_B T\}} \equiv \frac{1}{\exp\{\pm 2c/k_B T\} + 1}, \quad (*)$$

and in particular, do not depend on the average energy  $b$ .

Now we have to transfer the density operator from the basis of the energy eigenstates (let us call them  $+$  and  $-$ ) to the  $z$ -basis of the states (say,  $\uparrow$  and  $\downarrow$ ), in which the Hamiltonian matrix is given. This may be done by using Eq. (4.93) valid for any operator and any two bases  $\{a\}$  and  $\{u\}$ . For the case when in the  $\{a\}$  basis,  $w_{nn'}$  is diagonal ( $w_{nn'}|_{in a} = W_n \delta_{n,n'}$ ), that general expression is reduced to

$$w_{jj'}|_{in u} = \sum_{n=1,2} U_{jn} W_n U_{nj'}^{\dagger} \equiv U_{j1} W_1 U_{1j'}^{\dagger} + U_{j2} W_2 U_{2j'}^{\dagger},$$

where  $U$  is the unitary matrix of transform between the bases, with its elements given by Eqs. (4.83)-(4.84):

$$U_{jn} = \langle u_j | a_n \rangle, \quad U_{nj'}^{\dagger} = \langle a_{n'} | u_{j'} \rangle = \langle u_{j'} | a_{n'} \rangle^*,$$

so

$$w_{jj'}|_{in u} = \langle u_j | a_1 \rangle W_1 \langle u_{j'} | a_1 \rangle^* + \langle u_j | a_2 \rangle W_2 \langle u_{j'} | a_2 \rangle^*.$$

With the stationary basis states  $a_{1,2}$  denoted as  $\{+, -\}$ , and the  $z$ -basis states  $u_{1,2}$ , as  $\{\uparrow, \downarrow\}$ , the last relation gives the density matrix

$$w = \begin{pmatrix} \langle \uparrow|+\rangle W_+ \langle \uparrow|+\rangle^* + \langle \uparrow|-\rangle W_- \langle \uparrow|-\rangle^* & \langle \uparrow|+\rangle W_+ \langle \downarrow|+\rangle^* + \langle \uparrow|-\rangle W_- \langle \downarrow|-\rangle^* \\ \langle \downarrow|+\rangle W_+ \langle \downarrow|+\rangle^* + \langle \downarrow|-\rangle W_- \langle \downarrow|-\rangle^* & \langle \downarrow|+\rangle W_+ \langle \downarrow|+\rangle^* + \langle \downarrow|-\rangle W_- \langle \downarrow|-\rangle^* \end{pmatrix},$$

while the transfer matrix coefficients are given by Eqs. (7.207):

$$\langle \uparrow|+\rangle = \langle \downarrow|-\rangle = \cos \frac{\theta}{2} \equiv \frac{c + c_z}{[2c(c + c_z)]^{1/2}}, \quad \langle \downarrow|+\rangle = -\langle \uparrow|-\rangle = \sin \frac{\theta}{2} e^{i\varphi} \equiv \frac{c_+}{[2c(c + c_z)]^{1/2}},$$

where  $\theta$  and  $\varphi$  are the angular variables discussed in Sec. 5.1,<sup>152</sup> in which the c-number vector  $\mathbf{c}$  is represented in the usual spherical-coordinate form

$$\mathbf{c} \equiv c(\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta),$$

while  $c_{\pm} \equiv c_x \pm ic_y$ , so we get<sup>153</sup>

$$w = \begin{pmatrix} W_+ \cos^2 \frac{\theta}{2} + W_- \sin^2 \frac{\theta}{2} & (W_+ - W_-) \cos \frac{\theta}{2} \sin \frac{\theta}{2} e^{+i\varphi} \\ (W_+ - W_-) \sin \frac{\theta}{2} \cos \frac{\theta}{2} e^{-i\varphi} & W_+ \sin^2 \frac{\theta}{2} + W_- \cos^2 \frac{\theta}{2} \end{pmatrix} \\ \equiv \frac{1}{2c} \begin{pmatrix} (c + c_z)W_+ + (c - c_z)W_- & c_+(W_+ - W_-) \\ c_-(W_+ - W_-) & (c - c_z)W_+ + (c + c_z)W_- \end{pmatrix},$$

with  $W_{\pm}$  given by Eq. (\*). (As a sanity check, if  $c_x = c_y = 0$ , i.e.  $c = c_z$  and  $c_{\pm} = 0$ , the matrix becomes diagonal, as it should.)

This result emphasizes once again that even in thermal equilibrium, the density matrix is diagonal only in a certain (stationary) basis, but not in others.

**Problem 7.2.** In the usual  $z$ -basis, spell out the density matrix of a spin- $\frac{1}{2}$  with gyromagnetic ratio  $\gamma$ :

- (i) in a pure state with the spin definitely directed along the  $z$ -axis,
- (ii) in a pure state with the spin definitely directed along the  $x$ -axis,
- (iii) in thermal equilibrium at temperature  $T$ , in a magnetic field directed along the  $z$ -axis, and
- (iv) in thermal equilibrium at temperature  $T$ , in a magnetic field directed along the  $x$ -axis.

*Solutions:*

(i) In this case, the probability of the  $\uparrow$ -state is 100%, so the basis of the states  $w_j$  in which the density matrix is diagonal coincides with the  $z$ -basis. Hence we may use Eq. (7.18a) of the lecture notes to write

<sup>152</sup> See also the model solutions of Problems 4.27 and 5.4.

<sup>153</sup> As a reminder, the unitary matrix elements  $U_{jj}$ , and hence the off-diagonal elements of the  $w$ -matrix, are defined to an arbitrary phase multiplier  $\exp\{i\varphi_j\}$ .



$$w = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}.$$

(ii) In this case, the density matrix is diagonal in a different ( $x$ -) basis, so we need to use Eq. (7.18b),

$$w_{jj'} = U_{1j}^* U_{1j'}, \quad (*)$$

where  $U_{jj'} \equiv \langle x_j | z_{j'} \rangle$  is the unitary matrix of the transform from the  $x$ -basis to the  $z$ -basis, and the  $x$ -basis'  $w_{1,1}$  is taken for 1,<sup>154</sup> with all other matrix elements equal to zero. As we know from Sec. 4.4 of the lecture notes, this matrix may be taken in the form

$$U = U^\dagger = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad (**)$$

As a result, in the  $z$ -basis we get

$$w = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}.$$

(iii) In thermal equilibrium, the density matrix is diagonal in the basis of the stationary states  $n$  of the system, i.e. in the eigenbasis of its Hamiltonian – see Eq. (7.23)-(7.24) of the lecture notes:

$$w_{nn'} = W_n \delta_{nn'}, \quad \text{with } W_n = \frac{1}{Z} \exp\left\{-\frac{E_n}{k_B T}\right\}, \quad \text{and } Z \equiv \sum_n \exp\left\{-\frac{E_n}{k_B T}\right\},$$

where  $E_n$  are the eigenvalues of the system's energy. As was discussed in Sec. 4.4 of the lecture notes, for a spin- $\frac{1}{2}$  particle with the gyromagnetic ratio  $\gamma$  in the magnetic field  $\mathcal{B}$ , the energy (referred to its field-free value) has two eigenvalues,

$$E_{1,2} = \mp \gamma \frac{\hbar}{2} \mathcal{B},$$

so the two-term statistical sum and the  $2 \times 2$  density matrix may be readily spelled out:

$$Z = e^+ + e^- \equiv 2 \cosh \frac{\gamma \hbar \mathcal{B}}{2k_B T}, \quad \text{where } e^\pm \equiv \exp\left\{\pm \frac{\gamma \hbar \mathcal{B}}{2k_B T}\right\},$$

$$w = \frac{1}{e^+ + e^-} \begin{pmatrix} e^+ & 0 \\ 0 & e^- \end{pmatrix}. \quad (***)$$

In our current case of the field directed along axis  $z$ , the stationary states basis coincides with the  $z$ -basis, i.e. the last formula gives the final answer to the posed question. In the limit of low temperatures,  $k_B T / \gamma \hbar \mathcal{B} \rightarrow 0$ , we have  $e^- / e^+ \rightarrow 0$ , and Eq. (\*\*\*) is reduced to the result of Task (i), showing that the system is definitely in the pure  $\uparrow$ -state.

(iv) In the case of the magnetic field directed along axis  $x$ , Eq. (\*\*\*) is valid in the  $x$ -basis, and we may apply the general rule (4.93), with the unitary matrix (\*\*), to the statistical operator, to calculate each element of the density matrix in the  $z$ -basis:

<sup>154</sup> In the original Eq. (7.18b), describing a general quantum system, this state had the number  $j$ '

$$w_{jj'} = \sum_{n,n'=1}^2 U_{jn} w_{nn'} |_{\text{in } x} U_{nj'}^\dagger = \sum_{n=1}^2 U_{jn} W_n U_{nj'}^\dagger.$$

A straightforward calculation yields

$$w = \frac{1}{2(e^+ + e^-)} \begin{pmatrix} e^+ + e^- & e^+ - e^- \\ e^+ - e^- & e^+ + e^- \end{pmatrix} \equiv \frac{1}{2} \begin{pmatrix} 1 & \tanh(\gamma \hbar \mathcal{B} / 2k_B T) \\ \tanh(\gamma \hbar \mathcal{B} / 2k_B T) & 1 \end{pmatrix}.$$

This result shows that the diagonal elements of the density matrix, i.e., the probabilities of finding the spin oriented in both directions of axis  $z$ , are equal to 50% each. This is exactly what we could expect for the particle in an  $x$ -oriented field, with a zero-average  $z$ -component. The result for the off-diagonal elements is somewhat less trivial. It shows that these elements, equal to each other, are always smaller than the diagonal ones, approaching them only in the low-temperature limit  $k_B T / \gamma \hbar \mathcal{B} \rightarrow 0$ , when the density matrix is reduced to the one calculated in Task (ii).

Note that all these results may be obtained, in the corresponding limits, from the solution of Problem 1, with the vector  $\mathbf{c}$  equal to  $-\gamma \hbar \mathcal{B} / 2$ .

**Problem 7.3.** Calculate the Wigner function of a harmonic oscillator, with mass  $m$  and frequency  $\omega_0$ , in thermodynamic equilibrium at temperature  $T$ . Discuss the relation between the result and the Gibbs distribution.

*Solution:* In Sec. 7.2 of the lecture notes, the following result for the density matrix of the system was derived – see Eq. (7.44),

$$w(x, x') = \frac{1}{Z} \left( \frac{m\omega_0}{2\pi\hbar \sinh(\hbar\omega_0 / k_B T)} \right)^{1/2} \exp \left\{ - \frac{m\omega_0 [(x^2 + x'^2) \cosh(\hbar\omega_0 / k_B T) - 2xx']}{2\hbar \sinh(\hbar\omega_0 / k_B T)} \right\}, \quad (*)$$

where the statistical sum  $Z$  is given by Eq. (7.25):

$$Z = \frac{\exp\{-\hbar\omega_0 / 2k_B T\}}{1 - \exp\{-\hbar\omega_0 / k_B T\}}.$$

Let us use Eq. (7.50) to recalculate this matrix into the Wigner function

$$W(X, P) \equiv \frac{1}{2\pi\hbar} \int w \left( X + \frac{\tilde{X}}{2}, X - \frac{\tilde{X}}{2} \right) \exp \left\{ - \frac{iP\tilde{X}}{\hbar} \right\} d\tilde{X}.$$

Leaving the normalization coefficient alone for a while, let us spell out the exponent in Eq. (\*) as a function of the new variables:

$$x^2 + x'^2 = \left( X + \frac{\tilde{X}}{2} \right)^2 + \left( X - \frac{\tilde{X}}{2} \right)^2 = 2 \left( X^2 + \frac{\tilde{X}^2}{4} \right), \quad 2xx' = 2 \left( X + \frac{\tilde{X}}{2} \right) \left( X - \frac{\tilde{X}}{2} \right) = 2 \left( X^2 - \frac{\tilde{X}^2}{4} \right),$$

so

$$\exp \left\{ - \frac{m\omega_0 [(x^2 + x'^2) \cosh(\hbar\omega_0 / k_B T) - 2xx']}{2\hbar \sinh(\hbar\omega_0 / k_B T)} \right\}$$

$$\begin{aligned}
&= \exp \left\{ -\frac{m\omega_0}{\hbar} \left( X^2 \frac{\cosh(\hbar\omega_0/k_B T) - 1}{\sinh(\hbar\omega_0/k_B T)} + \frac{\tilde{X}^2}{4} \frac{\cosh(\hbar\omega_0/k_B T) + 1}{\sinh(\hbar\omega_0/k_B T)} \right) \right\} \\
&\equiv \exp \left\{ -X^2 \frac{m\omega_0}{\hbar} \tanh \frac{\hbar\omega_0}{2k_B T} \right\} \exp \left\{ -\frac{\tilde{X}^2}{4} \frac{m\omega_0}{\hbar} \coth \frac{\hbar\omega_0}{2k_B T} \right\}.
\end{aligned}$$

The Fourier transform in the Wigner function's definition affects only the second exponent in the last expression and is a standard Gaussian integral:

$$\int_{-\infty}^{+\infty} \exp \left\{ -\frac{\tilde{X}^2}{4} \frac{m\omega_0}{\hbar} \coth \frac{\hbar\omega_0}{2k_B T} \right\} \exp \left\{ -\frac{iP\tilde{X}}{\hbar} \right\} d\tilde{X} \equiv \int_{-\infty}^{+\infty} \exp \left\{ -\frac{\tilde{X}^2}{2x_c^2} - \frac{iP\tilde{X}}{\hbar} \right\} d\tilde{X},$$

where<sup>155</sup>

$$x_c^2 = \frac{2\hbar}{m\omega_0} \tanh \frac{\hbar\omega_0}{2k_B T}.$$

This integral may be worked out either as usual, by complementing the exponent to a full square, or just reusing the results of an absolutely similar integration performed in Sec. 2.2. The final result is proportional to

$$\exp \left\{ -\frac{x_c^2 P^2}{2\hbar^2} \right\} \equiv \exp \left\{ -\frac{P^2}{\hbar m\omega_0} \tanh \frac{\hbar\omega_0}{2k_B T} \right\},$$

so the Wigner function as a whole is

$$W(X, P) = A \exp \left\{ -\left[ \frac{P^2}{\hbar m\omega_0} + \frac{m\omega_0 X^2}{\hbar} \right] \tanh \frac{\hbar\omega_0}{2k_B T} \right\} \equiv A \exp \left\{ -\frac{H(X, P)}{\langle E \rangle} \right\}, \quad (***)$$

where  $H(X, P)$  is the classical Hamiltonian function of the oscillator, of the arguments  $X$  and  $P$ :

$$H(X, P) \equiv \frac{P^2}{2m} + \frac{m\omega_0^2 X^2}{2},$$

and  $\langle E \rangle$  is its average energy – see Eq. (7.26) of the lecture notes:

$$\langle E \rangle = \frac{\hbar\omega_0}{2} \coth \frac{\hbar\omega_0}{2k_B T}.$$

So, we have proved Eq. (7.62) and simultaneously found the coefficient  $C$  participating in it. What remains is to calculate the normalization coefficient  $A$ . The easiest way to do this is to require that the integration of  $W$  over  $X$  and  $P$  gives 1. This procedure readily yields

$$A = \frac{\omega_0}{2\pi\langle E \rangle} = \frac{1}{\pi\hbar} \tanh \frac{\hbar\omega_0}{2k_B T},$$

so, finally,

<sup>155</sup> Note that this parameter (essentially the correlation length of the oscillator) has a temperature dependence opposite to  $\langle x^2 \rangle$  (the coordinate's variance – see Eq. (7.48) of the lecture notes): it *decreases* with the growth of temperature, at  $k_B T \gg \hbar\omega_0$  approaching its value (7.37) for a free particle, with the qualitatively similar temperature behavior. Its discussion may be found in Sec. 7.2 of the lecture notes, just after Eq. (7.37).

$$W(X, P) = \frac{\omega_0}{2\pi\langle E \rangle} \exp\left\{-\frac{H(X, P)}{\langle E \rangle}\right\}.$$

We see that the Wigner function looks much simpler than the corresponding density matrix (\*) per se while carrying all the information contained in the latter. A very interesting feature of this result is that it's the functional dependence on  $H(X, P)$  coincides with that of the Gibbs distribution (7.25), but with the energy normalized to  $\langle E \rangle$  rather than  $k_B T$ . (The two coincide only in the high-temperature limit  $k_B T \gg \hbar\omega_0$ .)

**Problem 7.4.** Calculate the Wigner function of a harmonic oscillator, with mass  $m$  and frequency  $\omega_0$ :

- (i) in the ground state,
- (ii) in the first excited stationary state ( $n = 1$ ),
- (iii) in the Glauber state with an arbitrary dimensionless complex amplitude  $\alpha$ , and
- (iv) in the so-called *cat state*:<sup>156</sup> a linear superposition of two Glauber states with equal and opposite values of  $\alpha$ .

In the last case, explore and interpret the behavior of the function near the origin at  $|\alpha| \gg 1$ .

*Solutions:*

(i) With the solution of the previous problem on hand, the easiest way to calculate the Wigner function in the ground state is to use that solution in the low-temperature limit ( $k_B T \ll \hbar\omega_0$ ,  $\langle E \rangle \approx E_0 \equiv \hbar\omega_0/2$ ):

$$W_0(X, P) = \frac{1}{\pi\hbar} \exp\left\{-\left(\frac{m\omega_0^2 X^2}{2} + \frac{P^2}{2m}\right) / \frac{\hbar\omega_0}{2}\right\} \equiv \frac{1}{\pi\hbar} \exp\left\{-\frac{H(X, P)}{E_0}\right\}. \quad (*)$$

This is the function plotted on panel (a) of Fig. 7.3 in the lecture notes.

Alternatively, this result may be readily obtained by the direct integration of the factorable density matrix of this pure quantum state – see Eq. (7.63) of the lecture notes:

$$W(X, P) = \frac{1}{2\pi\hbar} \int \psi_0\left(X + \frac{\tilde{X}}{2}\right) \psi_0^*\left(X - \frac{\tilde{X}}{2}\right) \exp\left\{-\frac{iP\tilde{X}}{\hbar}\right\} d\tilde{X},$$

with the function  $\psi_0$  given by Eq. (2.275):

$$\psi_0 = \left(\frac{m\omega_0}{\pi\hbar}\right)^{1/4} \exp\left\{-\frac{m\omega_0 x^2}{2\hbar}\right\}.$$

(ii) Since here we are also discussing a pure state, we may also use Eq. (7.63), now in the form

$$W(X, P) = \frac{1}{2\pi\hbar} \int \psi_1\left(X + \frac{\tilde{X}}{2}\right) \psi_1^*\left(X - \frac{\tilde{X}}{2}\right) \exp\left\{-\frac{iP\tilde{X}}{\hbar}\right\} d\tilde{X},$$

<sup>156</sup> This state is frequently used to discuss the well-known *Schrödinger cat paradox* – see Sec. 10.1 of the lecture notes.

where  $\psi_1(x)$  is the wavefunction of the oscillator in its first excited stationary (Fock) state. This function is given by Eqs. (2.282) and (2.284) with  $n = 1$ :

$$\psi_1(x) = \frac{1}{(2^1 \cdot 1!)^{1/2} \pi^{1/4} x_0^{1/2}} \exp\left\{-\frac{x^2}{2x_0^2}\right\} H_1\left(\frac{x}{x_0}\right) \equiv \frac{2^{1/2} x}{\pi^{1/4} x_0^{3/2}} \exp\left\{-\frac{x^2}{2x_0^2}\right\},$$

where  $x_0 \equiv (\hbar/m\omega)^{1/2}$ , so

$$\begin{aligned} \psi_1\left(X + \frac{\tilde{X}}{2}\right) \psi_1^*\left(X - \frac{\tilde{X}}{2}\right) &= 2 \frac{(X + \tilde{X}/2)(X - \tilde{X}/2)}{\pi^{1/2} x_0^3} \exp\left\{-\frac{(X + \tilde{X}/2)^2 + (X - \tilde{X}/2)^2}{2x_0^2}\right\} \\ &\equiv 2 \frac{X^2 - \tilde{X}^2/4}{\pi^{1/2} x_0^3} \exp\left\{-\frac{X^2 + \tilde{X}^2/4}{x_0^2}\right\}, \end{aligned}$$

giving

$$\begin{aligned} W(X, P) &= \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} 2 \frac{X^2 - \tilde{X}^2/4}{\pi^{1/2} x_0^3} \exp\left\{-\frac{X^2 + \tilde{X}^2/4}{x_0^2}\right\} \exp\left\{-\frac{iP\tilde{X}}{\hbar}\right\} d\tilde{X} \\ &\equiv \frac{1}{\pi^{3/2} \hbar x_0^3} \exp\left\{-\frac{X^2}{x_0^2}\right\} \int_{-\infty}^{+\infty} \left(X^2 - \frac{\tilde{X}^2}{4}\right) \exp\left\{-\frac{\tilde{X}^2}{4x_0^2} - \frac{iP\tilde{X}}{\hbar}\right\} d\tilde{X}. \end{aligned}$$

After the usual completion of the expression under the exponent to the full square,

$$-\frac{\tilde{X}^2}{4x_0^2} - \frac{iP\tilde{X}}{\hbar} \equiv -\frac{(\tilde{X} + 2iPx_0^2/\hbar)^2}{4x_0^2} - \frac{P^2 x_0^2}{\hbar^2} \equiv -\frac{Z^2}{4x_0^2} - \frac{P^2 x_0^2}{\hbar^2},$$

where  $Z \equiv \tilde{X} + 2iPx_0^2/\hbar$ , so  $\tilde{X} = Z - 2iPx_0^2/\hbar$ , we get

$$W(X, P) = \frac{1}{\pi^{3/2} \hbar x_0} \exp\left\{-\frac{X^2}{x_0^2} - \frac{P^2 x_0^2}{\hbar^2}\right\} I,$$

where

$$\begin{aligned} I &\equiv \int_{-\infty}^{+\infty} \left[\frac{X^2}{x_0^2} - \frac{(Z - 2iPx_0^2/\hbar)^2}{4x_0^2}\right] \exp\left\{-\frac{Z^2}{4x_0^2}\right\} d\tilde{X} \\ &= \left(\frac{X^2}{x_0^2} + \frac{P^2 x_0^2}{\hbar^2}\right) \int_{-\infty}^{+\infty} \exp\left\{-\frac{Z^2}{4x_0^2}\right\} d\tilde{X} + \frac{iP}{\hbar} \int_{-\infty}^{+\infty} Z \exp\left\{-\frac{Z^2}{4x_0^2}\right\} d\tilde{X} - \frac{1}{4x_0^2} \int_{-\infty}^{+\infty} Z^2 \exp\left\{-\frac{Z^2}{4x_0^2}\right\} d\tilde{X}. \end{aligned}$$

As was discussed in Sec. 2.2 of the lecture notes, since the functions under these integrals are analytical, and tend to zero at  $\tilde{X} \rightarrow \pm\infty$ , the purely imaginary shift between  $Z$  and  $\tilde{X}$  does not affect them, so the second integral vanishes (because the function under it is antisymmetric), while the first and the third ones are reduced, by substitution  $\xi \equiv \tilde{X}/2x_0$ , to the table integrals<sup>157</sup>

$$\int_{-\infty}^{+\infty} e^{-\xi^2} d\xi = \pi^{1/2}, \quad \int_{-\infty}^{+\infty} \xi^2 e^{-\xi^2} d\xi = \frac{\pi^{1/2}}{2}.$$

As a result, we finally get

<sup>157</sup> See, e.g., MA Eq. (6.9c).

$$W(X, P) = \frac{2}{\pi\hbar} \left( \frac{X^2}{x_0^2} + \frac{P^2 x_0^2}{\hbar^2} - \frac{1}{2} \right) \exp \left\{ -\frac{X^2}{x_0^2} - \frac{P^2 x_0^2}{\hbar^2} \right\} \equiv \frac{2}{\pi\hbar} \left( \rho^2 - \frac{1}{2} \right) \exp \{ -\rho^2 \},$$

where

$$\rho \equiv \left( \frac{X^2}{x_0^2} + \frac{P^2 x_0^2}{\hbar^2} \right)^{1/2} \equiv \frac{H(X, P)}{E_0}, \quad \text{with } H = \frac{P^2}{2m} + \frac{m\omega_0^2 X^2}{2} \text{ and } E_0 = \frac{\hbar\omega_0}{2},$$

is the normalized distance from the center of the  $[X, P]$  plane. This function, whose plot is shown on panel (b) of Fig. 7.3 of the lecture notes, is negative at  $\rho < 1/\sqrt{2}$ , illustrating the impossibility of interpreting the Wigner function as the probability density – see the conclusion of Sec. 7.2.

(iii) According to Eqs. (5.107) of the lecture notes, the wavefunction of the Glauber state with a dimensionless complex amplitude  $\alpha$  (5.102) may be obtained from the ground-state wavefunction  $\psi_0(x)$  by the shift of its argument by  $\sqrt{2}x_0 \operatorname{Re}\alpha$ , and its multiplication by a phase exponent corresponding to a monochromatic wave with the momentum  $\sqrt{2} m\omega_0 x_0 \operatorname{Im}\alpha$ . These changes result in similar shifts of the arguments of the ground-state Wigner function by the listed amounts, so it becomes

$$W(X, P) = \frac{1}{\pi\hbar} \exp \left\{ - \left[ \frac{m\omega_0^2 (X - \sqrt{2}x_0 \operatorname{Re}\alpha)^2}{2} + \frac{(P - \sqrt{2}x_0 m\omega_0 \operatorname{Im}\alpha)^2}{2m} \right] / \frac{\hbar\omega_0}{2} \right\},$$

where  $x_0 \equiv (\hbar/m\omega_0)^{1/2}$ . According to this formula, the Wigner function is just a Gaussian function of both  $X$  and  $P$ , similar to that of the ground state (see Fig. 7.3a of the lecture notes) but with its center shifted to the point (5.102):

$$\left\{ X_c, \frac{P_c}{m\omega_0} \right\} = \sqrt{2}x_0 \{ \operatorname{Re}\alpha, \operatorname{Im}\alpha \} \equiv \sqrt{2}x_0 \alpha.$$

(iv) By definition, the cat state's vector is

$$|\text{cat}\rangle = C (|+\alpha\rangle + |-\alpha\rangle),$$

where  $C$  is the normalization coefficient that may be calculated, for example, by using the Fock-state expansion (5.134). Assuming that each of the component Glauber-state vectors is already normalized, we get

$$\begin{aligned} |C|^{-2} &= (\langle +\alpha| + \langle -\alpha|)(|+\alpha\rangle + |-\alpha\rangle) = \langle +\alpha|+\alpha\rangle + \langle +\alpha|-\alpha\rangle + \langle -\alpha|+\alpha\rangle + \langle -\alpha|-\alpha\rangle \\ &= 2 + 2\langle +\alpha|-\alpha\rangle = 2 + 2 \exp\{-|\alpha|^2\} \sum_{n, n'=0}^{\infty} \langle n| \frac{(\alpha^*)^n}{(n!)^{1/2}} \frac{(-\alpha)^{n'}}{(n'!)^{1/2}} |n'\rangle \\ &= 2 + 2 \exp\{-|\alpha|^2\} \sum_{n=0}^{\infty} \frac{(-|\alpha|^2)^n}{n!} = 2 \left( 1 + \exp\{-2|\alpha|^2\} \right), \end{aligned}$$

because the last sum is just the Taylor expansion of the function  $\exp\{-|\alpha|^2\}$ . Since the cat state is pure, we may again use Eq. (7.63), with

$$\psi = \psi_{\text{cat}}(x) = C [\psi_{+\alpha}(x) + \psi_{-\alpha}(x)] = C [\Psi_{+\alpha}(x, 0) + \Psi_{-\alpha}(x, 0)],$$

where the function  $\Psi_{\alpha}(x, t)$  is given by Eq. (5.107) with  $X$  and  $P$  from Eq. (5.102):

$$\begin{aligned}\psi_\alpha(x) &= \left(\frac{m\omega_0}{\pi\hbar}\right)^{1/4} \exp\left\{-\frac{m\omega_0}{2\hbar}(x-X)^2 + i\frac{Px}{\hbar}\right\} \\ &\equiv \left(\frac{m\omega_0}{\pi\hbar}\right)^{1/4} \exp\left\{-\frac{m\omega_0}{2\hbar}(x-\sqrt{2}x_0 \operatorname{Re}\alpha)^2 - i\frac{\sqrt{2}x_0 m\omega_0 \operatorname{Im}\alpha x}{\hbar}\right\}.\end{aligned}$$

The remaining calculation is conceptually straightforward but, in the general case, somewhat bulky. To make it more transparent, let us, first, assume that the parameter  $\alpha$  is real:

$$\alpha = \frac{a}{\sqrt{2}} \equiv \frac{A}{\sqrt{2}x_0},$$

where  $A$  is the amplitude of the classical oscillations best mimicking the Glauber state (see Fig. 5.8 in the lecture notes). Now let us use normalized variables defined similarly to Eqs. (5.63):

$$\xi \equiv \frac{x}{x_0}, \quad \zeta \equiv \frac{p}{m\omega_0 x_0}, \quad \text{where } x_0 \equiv \left(\frac{\hbar}{m\omega_0}\right)^{1/2}.$$

In these variables, Eq. (7.63), for our case of real  $\alpha$ , may be recast as

$$w_{\text{cat}}(\xi, \zeta) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \psi_{\text{cat}}\left(\xi + \frac{\tilde{\xi}}{2}\right) \psi_{\text{cat}}^*\left(\xi - \frac{\tilde{\xi}}{2}\right) \exp\{-i\zeta\tilde{\xi}\} d\tilde{\xi}, \quad (**)$$

where

$$\psi_{\text{cat}}(\xi) = C[\psi_0(\xi - a) + \psi_0(\xi + a)], \quad \text{with } \psi_0(\xi) = \frac{1}{\pi^{1/4}} \exp\left\{-\frac{\xi^2}{2}\right\}, \quad |C|^2 = \frac{1}{2(1 + \exp\{-a^2\})}.$$

(Note that in the most interesting case when  $a \gg 1$ , the normalization factor  $|C|^2$  is just  $1/2$ .)

Let us spell out the wavefunction product participating in Eq. (\*\*):

$$\begin{aligned}\psi_{\text{cat}}(\xi_+) \psi_{\text{cat}}^*(\xi_-) &= |C|^2 [\psi_0(\xi_+ - a) + \psi_0(\xi_+ + a)][\psi_0(\xi_- - a) + \psi_0(\xi_- + a)] \\ &\equiv |C|^2 \left[ \begin{array}{l} \psi_0(\xi_+ - a)\psi_0(\xi_- - a) + \psi_0(\xi_+ + a)\psi_0(\xi_- + a) \\ + \psi_0(\xi_+ + a)\psi_0(\xi_- - a) + \psi_0(\xi_- + a)\psi_0(\xi_+ - a) \end{array} \right], \quad \text{where } \xi_\pm \equiv \xi \pm \frac{\tilde{\xi}}{2}.\end{aligned}$$

The integral (\*\*) of the first two terms in the square brackets gives the sum of two Wigner functions of the Glauber states, such as the one that was already calculated in Task (iii), but with their centers at the points  $\xi = \pm a$ , i.e.  $x_\pm = \pm x_0 a \equiv \pm A$ , and of a renormalized magnitude:

$$w_\pm(\xi, \zeta) = \frac{|C|^2}{\pi} \exp\left\{-\left[(\xi \pm a)^2 + \zeta^2\right]\right\} \propto \exp\left\{-\frac{H(X \pm A, P)}{E_0}\right\}. \quad (***)$$

This expression describes two uneventful Gaussian peaks, which are well separated if  $a \gg 1$ . The sum of the remaining two terms, describing the quantum interference of these states,

$$w_{\text{int}}(\xi, \zeta) = |C|^2 \int_{-\infty}^{+\infty} \left[ \psi_0\left(\xi + \frac{\tilde{\xi}}{2} + a\right) \psi_0\left(\xi - \frac{\tilde{\xi}}{2} - a\right) + \psi_0\left(\xi - \frac{\tilde{\xi}}{2} + a\right) \psi_0\left(\xi + \frac{\tilde{\xi}}{2} - a\right) \right] \exp\{-i\zeta\tilde{\xi}\} d\tilde{\xi},$$

is much more interesting. Indeed, after plugging in the explicit expression for  $\psi_0$  and spelling out the squares of the parentheses, the contents of the square brackets in the last expression are reduced to

$$[\dots] = \frac{1}{\pi^{1/2}} \exp\{-\xi^2\} \left[ \exp\left\{-\left(\frac{\xi}{2} + a\right)^2\right\} + \exp\left\{-\left(\frac{\xi}{2} - a\right)^2\right\} \right].$$

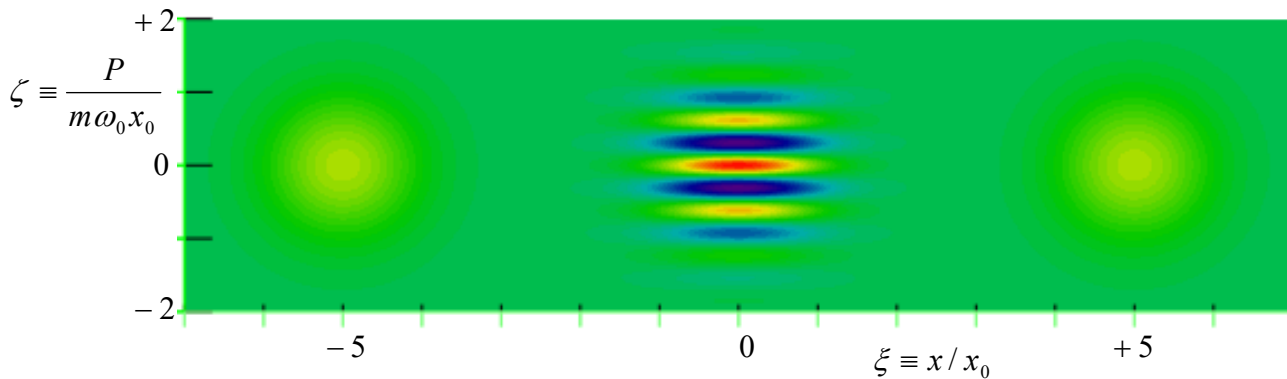
Already from here, we may see that the interference term of the Wigner function is noticeable only at  $\xi \sim 1$ , i.e. at  $x \sim x_0$ , i.e., in the case  $a \gg 1$ , in the region well separated from the two Glauber-state peaks (\*\*\*)). By working out two similar Gaussian integrals, we get

$$w_{\text{int}}(\xi, \zeta) = \frac{2|C|^2}{\pi} \exp\{-(\xi^2 + \zeta^2)\} \cos 2\zeta a.$$

Here, the origin-centered Gaussian peak, of a height twice larger than that of the Glauber-state peaks (\*\*\*)), serves as the envelope for the oscillating function

$$\cos 2\zeta a \equiv \cos\left(2 \frac{P}{m\omega_0 x_0} \frac{A}{x_0}\right) \equiv \cos\left(\frac{2AP}{\hbar}\right),$$

which describes the mutual interference of the two Glauber components forming the cat state. The figure below shows the color-coded contour plot of the full Wigner function for the particular case  $a = 5$ .



The reader should agree that this pattern is rather spectacular; this is why the Wigner function, even with its drawback discussed in Sec. 7.2 of the lecture notes, remains a popular way of visualization (and hence comprehension) of elaborate quantum states.

To complete our solution, we should consider the case when the complex parameter  $\alpha$  is complex:  $\alpha = |\alpha| e^{i\varphi}$ , with  $\varphi \neq 0$ . Since, as was discussed in Sec. 5.5 (see especially Fig. 5.8), the phase shift  $\varphi$  just rotates the Glauber state by the same angle on the phase plane, it is clear that this shift causes only a similar rigid rotation of the whole Wigner function's pattern (see, e.g., the figure above), without any change of its structure.

One more popular modification of the cat state is the relative phase shift of its Glauber components, for example:

$$|\text{cat}_\phi\rangle \equiv C(|+\alpha\rangle + |-\alpha\rangle e^{i\phi})$$



Reviewing the above calculation, we can see that this modification just shifts the interference pattern inside the Wigner function's central peak:

$$\cos 2\zeta a \rightarrow \cos(2\zeta a + \phi),$$

without changing its envelope.

**Problem 7.5.\*** A harmonic oscillator is weakly coupled to an Ohmic environment that is in thermal equilibrium at temperature  $T$ .

(i) Use the rotating-wave approximation to write the reduced equations of motion for the Heisenberg operators of the complex amplitude of oscillations.

(ii) Calculate the expectation values of the correlators of the fluctuation force operators participating in these equations, and express them via the average number  $n_e$  of thermally-induced excitations in equilibrium, given by Eq. (7.225) of the lecture notes.

*Solutions:*

(i) Differentiating the definitions (5.65) of the creation-annihilation operators over time, then using the Heisenberg equations (7.144) of motion of an oscillator with Ohmic damping, and then applying the reciprocal relations (5.66), we get the following equations of motion of these operators:

$$\begin{aligned}\dot{\hat{a}} &= -i\omega_0\hat{a} - \delta(\hat{a} - \hat{a}^\dagger) + \frac{i}{(2\hbar m\omega_0)^{1/2}}\hat{\tilde{F}}(t), \\ \dot{\hat{a}}^\dagger &= i\omega_0\hat{a}^\dagger + \delta(\hat{a} - \hat{a}^\dagger) - \frac{i}{(2\hbar m\omega_0)^{1/2}}\hat{\tilde{F}}(t),\end{aligned}\tag{*}$$

where  $\delta \equiv \eta/2m$  is the damping constant. At negligible coupling to the environment (i.e., at  $\delta = 0$ ), these equations are reduced to Eqs. (5.140) with just the first terms on their right-hand sides, and hence have the oscillating solutions (5.141). In this case, the following operators:

$$\hat{\alpha} \equiv \hat{a}e^{i\omega_0 t}, \quad \hat{\alpha}^\dagger \equiv \hat{a}^\dagger e^{-i\omega_0 t},\tag{**}$$

remain constant in time. Obviously, in the classical limit (e.g., for the Glauber states with  $|\alpha| \gg 1$ ), these operators correspond to the complex amplitude of the oscillations and its complex conjugate, so even in the quantum case, they may be interpreted as the Heisenberg operators of these amplitudes.

Coupling with the environment results in the amplitudes changing in time. The exact equations of this motion, which may be obtained by plugging Eqs. (\*) into Eqs. (\*\*) differentiated over time,

$$\begin{aligned}\dot{\hat{\alpha}} &= (\dot{\hat{a}} + i\omega_0\hat{a})e^{i\omega_0 t} = -\delta(\hat{\alpha}e^{-i\omega_0 t} - \hat{\alpha}^\dagger e^{i\omega_0 t})e^{i\omega_0 t} + \frac{i}{(2\hbar m\omega_0)^{1/2}}\hat{\tilde{F}}(t)e^{i\omega_0 t}, \\ \dot{\hat{\alpha}}^\dagger &= (\dot{\hat{a}}^\dagger - i\omega_0\hat{a}^\dagger)e^{-i\omega_0 t} = \delta(\hat{\alpha}e^{-i\omega_0 t} - \hat{\alpha}^\dagger e^{i\omega_0 t})e^{-i\omega_0 t} - \frac{i}{(2\hbar m\omega_0)^{1/2}}\hat{\tilde{F}}(t)e^{-i\omega_0 t},\end{aligned}$$

are coupled and their analytical solution is rather cumbersome.

However, we may notice that all right-hand-side terms of these equations are proportional to the coupling to the environment, i.e. if the coupling is weak, the time evolution of the operators (\*\*) is slow.

Hence, using the basic idea of the rotating-wave approximation (RWA) discussed in Sec. 6.5,<sup>158</sup> we may average these right-hand sides over a relatively long time interval  $\Delta t$ , thus eliminating the rapidly oscillating terms because they have a small effect on the amplitude evolution. This first-order approximation yields the following “reduced” (or “RWA”) Heisenberg-Langevin equations:<sup>159</sup>

$$\dot{\hat{\alpha}} = -\delta\hat{\alpha} + \hat{f}(t), \quad \dot{\hat{\alpha}}^\dagger = -\delta\hat{\alpha}^\dagger + \hat{f}^\dagger(t), \quad (***)$$

where the reduced force operator is defined as

$$\hat{f}(t) \equiv \frac{i}{(2\hbar m\omega_0)^{1/2}} \overline{\hat{F}(t)e^{i\omega_0 t}} \equiv \frac{i}{(2\hbar m\omega_0)^{1/2}} \frac{1}{\Delta t} \int_{t-\Delta t/2}^{t+\Delta t/2} \hat{F}(t)e^{i\omega_0 t} dt,$$

and  $\hat{f}^\dagger(t)$  is its Hermitian adjoint. Evidently, the first terms on the right-hand sides of Eqs. (\*\*\*), which dominate if  $\langle\alpha\rangle$  is large enough to neglect fluctuations, try to decrease the amplitudes exponentially, as  $\exp\{-\delta t\}$ , while the second terms, representing the fluctuation force, disturb such deterministic decay. In particular, these terms do not allow the operators  $\hat{\alpha}$  and  $\hat{\alpha}^\dagger$  to approach zero, because that would violate their commutation relation

$$\left[ \hat{\alpha}, \hat{\alpha}^\dagger \right] = \hat{I},$$

which follows from the combination of Eq. (\*\*\*) above and Eq. (5.68) of the lecture notes.

Note that since the Langevin operator  $\hat{F}(t)$  is a random function of time, i.e. is not periodic, the averaging interval  $\Delta t$  should be chosen more carefully than in the deterministic case.<sup>160</sup> On one hand, it should be *much longer* than  $2\pi/\omega_0$ , to suppress the high-frequency components of the product under the integral. On the other hand, to describe the amplitude evolution correctly,  $\Delta t$  should be *much shorter* than the decay time constant  $1/\delta$ :

$$\frac{2\pi}{\omega_0} \ll \Delta t \ll \frac{1}{\delta}.$$

Such choice is of course possible only if the  $Q$ -factor  $Q \equiv \omega_0/2\delta$  of the oscillator is much higher than 1, which is therefore a necessary condition of applicability of the rotating-wave approximation.

(ii) Let us calculate the statistical properties of the effective low-frequency forces  $\hat{f}(t)$  and  $\hat{f}^\dagger(t)$ . Their statistical averages (in the language of mathematical statistics, their *first moments*), are proportional to those of the “parent force”  $\hat{F}(t)$  and hence are equal to zero – see the discussion of Eq.

<sup>158</sup> See also a detailed discussion of the van der Pol method (i.e. the RWA’s classical version) in CM Sec. 5.3.

<sup>159</sup> Actually, such equations are also valid in more general situations when the operator  $\hat{F}(t)$  describes not only the fluctuations but also external forces with frequencies close enough to the frequency  $\omega_0$  of the oscillator. Quantum-mechanical solutions of several other problems (such as parametric excitation, see CM Sec. 5.6) may be also obtained using straightforward generalizations of these equations.

<sup>160</sup> If the right-hand side is  $2\pi/\omega$  – periodic (where  $\omega$  is close to, but not necessarily exactly equal to  $\omega_0$  – see CM Secs. 5.3-5.6), then a perfect averaging out of fast components may be achieved by taking  $\Delta t$  equal to that period.

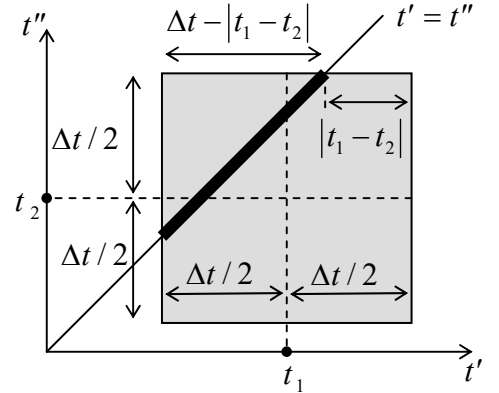
(7.92) in the lecture notes. Thus, let us start from the calculation of the following *second moment* of the forces, based on their *anticommutator*:

$$\left\langle \left\{ \hat{f}(t_1), \hat{f}^\dagger(t_2) \right\} \right\rangle = \frac{1}{2\hbar m \omega_0} \frac{1}{(\Delta t)^2} \int_{t_1 - \Delta t/2}^{t_1 + \Delta t/2} dt' \int_{t_2 - \Delta t/2}^{t_2 + \Delta t/2} dt'' \left\langle \left\{ \hat{F}(t'), \hat{F}(t'') \right\} \right\rangle \exp\{i\omega_0(t' - t'')\}.$$

With the account of Eqs. (7.110)-(7.111), the double integral in this relation is

$$\int_{t_1 - \Delta t/2}^{t_1 + \Delta t/2} dt' \int_{t_2 - \Delta t/2}^{t_2 + \Delta t/2} dt'' 2K_F(t' - t'') \exp\{i\omega_0(t' - t'')\}.$$

The averaging time  $\Delta t$  that satisfies the above strong conditions is much longer than the correlation time  $\tau_c$  of the environment force fluctuations (i.e. the characteristic time of decay of its correlation function  $K_F$ ), so only a relatively narrow area on the  $[t', t'']$  plane, shown schematically by the bold line segment in the figure on the right, gives a noticeable contribution into this double integral. (Note that at  $|t_1 - t_2| > \Delta t$ , the segment disappears, i.e. the integral vanishes.) Hence the internal integral may be formally taken in the infinite limits of the difference  $t'' - t'$ , and we may use the first form of Eq. (7.112) to get



$$\left\langle \left\{ \hat{f}(t_1), \hat{f}^\dagger(t_2) \right\} \right\rangle = \frac{2\pi S_F(\omega_0)}{\hbar m \omega_0} D(t_1 - t_2),$$

$$\text{with } D(\tau) \equiv \frac{1}{(\Delta t)^2} \times \begin{cases} \Delta t - |\tau|, & \text{if } |\tau| < \Delta t, \\ 0, & \text{otherwise.} \end{cases}$$

On the amplitude evolution's time scale  $\sim 1/\delta$ , the function  $D(\tau)$  may be well approximated with a delta function  $C\delta(\tau)$  with the "weight"

$$C = \frac{1}{(\Delta t)^2} \int_{-\Delta t}^{+\Delta t} (\Delta t - |\tau|) d\tau = \int_{-1}^1 (1 - |\xi|) d\xi = 1,$$

so we may write

$$\left\langle \left\{ \hat{f}(t_1), \hat{f}^\dagger(t_2) \right\} \right\rangle = \frac{2\pi S_F(\omega_0)}{\hbar m \omega_0} \delta(t_1 - t_2).$$

Now the fluctuation-dissipation theorem (7.134) may be used to recast this result as

$$\left\langle \left\{ \hat{f}(t_1), \hat{f}^\dagger(t_2) \right\} \right\rangle = \frac{\chi''(\omega_0)}{m\omega_0} \coth \frac{\hbar\omega_0}{2k_B T} \delta(t_1 - t_2),$$

so at the Ohmic dissipation (7.138),

$$\left\langle \left\{ \hat{f}(t_1), \hat{f}^\dagger(t_2) \right\} \right\rangle = \frac{\eta}{m} \coth \frac{\hbar\omega_0}{2k_B T} \delta(t_1 - t_2) \equiv 2\delta \coth \frac{\hbar\omega_0}{2k_B T} \delta(t_1 - t_2).$$

Performing an absolutely similar calculation for the *commutator* of the two fluctuating force operators, with the only difference of using the Green-Kubo formula Eq. (7.109) rather than the fluctuation-dissipation theorem (7.134), we get

$$\left\langle \left[ \hat{f}(t_1), \hat{f}^\dagger(t_2) \right] \right\rangle = 2\delta \times \delta(t_1 - t_2).$$

Now we may combine these two results to calculate the required correlation functions:

$$\begin{aligned} \left\langle \hat{f}(t_1) \hat{f}^\dagger(t_2) \right\rangle &\equiv \frac{1}{2} \left( \left\langle \left\{ \hat{f}(t_1), \hat{f}^\dagger(t_2) \right\} \right\rangle + \left\langle \left[ \hat{f}(t_1), \hat{f}^\dagger(t_2) \right] \right\rangle \right) = \delta \left( \coth \frac{\hbar\omega_0}{2k_B T} + 1 \right) \delta(t_1 - t_2), \\ \left\langle \hat{f}(t_1)^\dagger \hat{f}(t_2) \right\rangle &\equiv \frac{1}{2} \left( \left\langle \left\{ \hat{f}(t_1), \hat{f}^\dagger(t_2) \right\} \right\rangle - \left\langle \left[ \hat{f}(t_1), \hat{f}^\dagger(t_2) \right] \right\rangle \right) = \delta \left( \coth \frac{\hbar\omega_0}{2k_B T} - 1 \right) \delta(t_1 - t_2). \end{aligned}$$

Comparing these formulas with Eq. (7.225),

$$n_e = \frac{1}{\exp\{\hbar\omega_0/k_B T\} - 1} \equiv \frac{1}{2} \left( \coth \frac{\hbar\omega_0}{2k_B T} - 1 \right),$$

we, finally, get a very elegant couple of relations,<sup>161</sup>

$$\begin{aligned} \left\langle \hat{f}(t_1) \hat{f}^\dagger(t_2) \right\rangle &= 2\delta(n_e + 1) \delta(t_1 - t_2), \\ \left\langle \hat{f}^\dagger(t_1) \hat{f}(t_2) \right\rangle &= 2\delta n_e \delta(t_1 - t_2). \end{aligned} \tag{****}$$

The equations expressed by Eqs. (\*\*\*) and (\*\*\*\*), frequently with the addition of other terms describing other forces acting upon the oscillator, is broadly used in quantum optics and electronics.

The physical reason why the noise source approximation by the delta-correlated functions in the RWA equations gives a sufficient accuracy (i.e. the equations correct to the first order in  $H_{\text{int}}$ ) is very simple. As was discussed in Sec. 7.5, of the whole broad spectrum of the fluctuations (in our case, coming from a thermally-equilibrium environment), a high- $Q$  oscillator is substantially affected only by the Fourier components very close to its resonance frequency, and we make no substantial error when we replace the genuine spectral density  $S_F(\omega)$  with a frequency-independent value equal to  $S_F(\omega_0)$ . But, as was discussed in Sec. 7.4, a random process with a constant spectral density is delta-correlated. This argumentation may be used for a faster calculation of the average *anticommutator* of the “values” of the fluctuation force operators at different times; however, for the calculation of their *commutator*, we still need an integration similar to the one described above, by using the (more subtle) Green-Kubo formula.

**Problem 7.6.** Calculate the average potential energy of the long-range electrostatic interaction between two similar isotropic 3D harmonic oscillators, each with the electric dipole moment  $\mathbf{d} = q\mathbf{s}$ , where  $\mathbf{s}$  is the oscillator’s displacement from its equilibrium position, at arbitrary temperature  $T$ .

*Solution:* For  $T = 0$ , this interaction (in the zero-temperature limit, called the London dispersion force) was calculated by two different methods (both due to F. London) in the solutions of Problems

<sup>161</sup> To the best of my knowledge, they were first derived by M. Lax in 1966.

3.20 and 5.20. Reviewing the latter solution,<sup>162</sup> we see that the calculations are completely valid for  $T \neq 0$  as well, up to the following result,

$$\left\langle \hat{\mathcal{E}}_1 \cdot \hat{\mathbf{d}}_2 \right\rangle = \frac{3q^2}{m^2} \left( \frac{q}{4\pi\epsilon_0 r^3} \right)^2 \frac{\hbar}{\omega_1(\omega_2^2 - \omega_1^2)} \left\langle \hat{a} \hat{a}^\dagger + \text{h.c.} \right\rangle_1, \quad (*)$$

and the similar result, with swapped indices 1 and 2, for the second component,

$$\left\langle \hat{\mathcal{E}}_2 \cdot \hat{\mathbf{d}}_1 \right\rangle = \frac{3q^2}{m^2} \left( \frac{q}{4\pi\epsilon_0 r^3} \right)^2 \frac{\hbar}{\omega_2(\omega_1^2 - \omega_2^2)} \left\langle \hat{a} \hat{a}^\dagger + \text{h.c.} \right\rangle_2, \quad (**)$$

of the average interaction between the oscillators,

$$\langle U \rangle = -\frac{1}{2} \left\langle \hat{\mathcal{E}}_1 \cdot \hat{\mathbf{d}}_2 \right\rangle - \frac{1}{2} \left\langle \hat{\mathcal{E}}_2 \cdot \hat{\mathbf{d}}_1 \right\rangle,$$

provided that the averaging on the right-hand sides of Eqs. (\*) and (\*\*) (where the creation-annihilation operators are in the Schrödinger picture) is understood not only in the quantum-mechanical but also in the statistical ensemble sense. According to Eq. (5.70) of the lecture notes, each of these averages is just that of the Hamiltonian of the corresponding oscillator, i.e. its average energy  $\langle E \rangle$ , divided by its ground-state energy  $\hbar\omega_k/2$ , so for the system in thermal equilibrium at temperature  $T$ , we may use Eq. (7.26) to immediately obtain the required answer:

$$\langle U \rangle = -\frac{3q^2}{2m^2} \left( \frac{q}{4\pi\epsilon_0 r^3} \right)^2 \left[ \frac{\hbar}{\omega_1(\omega_2^2 - \omega_1^2)} \coth \frac{\hbar\omega_1}{2k_B T} + \frac{\hbar}{\omega_2(\omega_1^2 - \omega_2^2)} \coth \frac{\hbar\omega_2}{2k_B T} \right]. \quad (***)$$

At low temperatures,  $\coth(\hbar\omega_{1,2}/2k_B T) \rightarrow 1$ , so this result naturally tends to that spelled out in the solution of Problem 5.20; in the most important case of two similar oscillators of frequency  $\omega_0 \equiv \omega_1 = \omega_2$ ,

$$\langle U \rangle = -\frac{3q^2}{4m^2\omega_0^4} \left( \frac{q}{4\pi\epsilon_0 r^3} \right)^2 \hbar\omega_0 \equiv -\frac{3}{4} \mu^2 \hbar\omega_0, \quad \text{where } \mu \equiv \frac{q^2}{4\pi\epsilon_0 r^3 m \omega_0^2} \ll 1. \quad (***)$$

On the other hand, in the classical limit ( $k_B T \gg \hbar\omega_{1,2}$ ), when  $\coth(\hbar\omega_{1,2}/2k_B T) \approx 2k_B T/\hbar\omega_{1,2}$ , Eq. (\*\*\*) reduces to

$$\langle U \rangle = -\frac{3q^2}{m^2} \left( \frac{q}{4\pi\epsilon_0 r^3} \right)^2 \left[ \frac{1}{\omega_1^2(\omega_2^2 - \omega_1^2)} + \frac{1}{\omega_2^2(\omega_1^2 - \omega_2^2)} \right] k_B T \equiv -\frac{3q^2}{m^2} \left( \frac{q}{4\pi\epsilon_0 r^3} \right)^2 \frac{1}{\omega_1^2 \omega_2^2} k_B T,$$

so for similar oscillators,

$$\langle U \rangle = -\frac{3q^2}{m^2} \left( \frac{q}{4\pi\epsilon_0 r^3} \right)^2 \frac{1}{\omega_0^4} k_B T \equiv -3\mu^2 k_B T.$$

Note that the last expression differs from Eq. (\*\*\*) by a not-quite-trivial replacement  $\hbar\omega_0/4 \rightarrow k_B T$  (instead of the more usual  $\hbar\omega_0/2 \rightarrow k_B T$ ), because of the resonant behavior of both terms in the

<sup>162</sup> The reader is challenged to generalize the solution of Problem 3.20 to the case  $T > 0$  as well.

general result (\*\*). One more remark: this solution neglects the oscillator damping, apparently requiring  $\delta_{1,2} \ll |\omega_1 - \omega_2|$ , but the direct solution of the same problem for nonvanishing  $\delta$  (see, e.g., SM Problem 5.19) shows that the above results are much more robust, requiring only  $\delta_{1,2} \ll \omega_{1,2}$ .

**Problem 7.7.** A semi-infinite string with mass  $\mu$  per unit length is attached to a wall and stretched with a constant force (tension)  $\mathcal{F}$ . Calculate the spectral density of the transverse force exerted on the wall, in thermal equilibrium at temperature  $T$ .

*Solution:* Classical mechanics says that the string may support transverse waves with two independent polarizations – for example, two mutually perpendicular linear polarizations.<sup>163</sup> If the waves are small, their dynamics are independent, so to calculate one Cartesian coordinate of the transverse force (say, along the  $x$ -axis, normal to the string's direction  $z$ ), we may analyze waves  $x(z, t)$  of the string's displacements within the  $[x, z]$  plane.

According to the discussion in Sec. 7.4 of the lecture notes, in order to use Eq. (7.134) of the lecture notes for the spectral density of the transverse force,

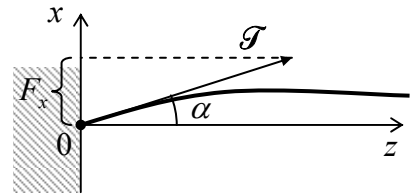
$$S_F(\omega) = \frac{\hbar}{2\pi} \text{Im} \chi(\omega) \coth \frac{\hbar\omega}{2k_B T}, \quad (*)$$

it is sufficient to calculate the generalized susceptibility  $\chi(\omega)$  defined by Eq. (7.124),

$$F_\omega = \chi(\omega)x_\omega,$$

i.e. the ratio of complex amplitudes of two *classical* processes: externally imposed classical 1D oscillations  $x(0, t)$  of the string's support point, and the resulting transverse force  $F_x$  exerted on the point by the string.

From the system's geometry (see the figure on the right), with the wall's position taken for  $z = 0$ , in the small oscillation limit ( $dx/dz \rightarrow 0$ ), this component of the force is



$$F_x = \mathcal{F} \sin \alpha \approx \mathcal{F} \tan \alpha \equiv \mathcal{F} \left. \frac{\partial x}{\partial z} \right|_{z=+0}. \quad (**)$$

Very similarly, the net force exerted on a small internal segment  $[z - dz/2, z + dz/2]$  of the string by its adjacent (right and left) segments is

$$dF_x \approx \mathcal{F} \left( \left. \frac{\partial x}{\partial z} \right|_{z+dz/2} - \left. \frac{\partial x}{\partial z} \right|_{z-dz/2} \right) \approx \mathcal{F} \left[ \left. \frac{\partial^2 x}{\partial z^2} \right|_z \left( + \frac{dz}{2} \right) - \left. \frac{\partial^2 x}{\partial z^2} \right|_z \left( - \frac{dz}{2} \right) \right] = \mathcal{F} \frac{\partial^2 x}{\partial z^2} dz.$$

Since the mass of the segment is  $\mu dz$ , the 2<sup>nd</sup> Newton law for its motion in the  $x$ -direction gives us the following equation:

$$\mu dz \frac{\partial^2 x}{\partial t^2} = dF_x, \quad \text{i.e.} \quad \mu \frac{\partial^2 x}{\partial t^2} = \mathcal{F} \frac{\partial^2 x}{\partial z^2}.$$

<sup>163</sup> See, e.g., CM Sec. 6.4. Note that (thanks to the fluctuation-dissipation theorem!) much of this solution just reproduces the classical analysis discussed in that part of the series.

This is the well-known 1D wave equation, with the general solution

$$x(z, t) = f_{\rightarrow}\left(t - \frac{z}{v}\right) + f_{\leftarrow}\left(t + \frac{z}{v}\right),$$

where  $v \equiv (\mathcal{F}/\mu)^{1/2} > 0$  is the wave velocity, and  $f_{\rightarrow}$  and  $f_{\leftarrow}$  are some functions of a single argument, which are determined by the initial and boundary conditions. If the wave on the string is excited, as in our case, only by the motion of its end located at  $z = 0$ , the wave may travel only to the right:

$$x(z, t) = f_{\rightarrow}\left(t - \frac{z}{v}\right), \quad \text{so } \frac{\partial x}{\partial z}(z, t) = -\frac{1}{v} \frac{\partial f_{\rightarrow}}{\partial t}\left(t - \frac{z}{v}\right), \quad \text{at } z \geq 0. \quad (***)$$

Plugging these expressions, for  $z = +0$ , into Eq. (\*\*), we get

$$F_x(t) = \mathcal{F} \frac{\partial x}{\partial z}(0, t) = -\frac{\mathcal{F}}{v} \frac{\partial f_{\rightarrow}}{\partial t}(t) \equiv -\frac{\mathcal{F}}{v} \frac{\partial x}{\partial t}(0, t).$$

Comparing this relation with Eq. (7.137) of the lecture notes, we see that the effect of the string (which carries the induced wave (\*\*\*) , together with the associated energy, away from the wall) is equivalent to kinematic friction, with the drag coefficient<sup>164</sup>

$$\eta = \frac{\mathcal{F}}{v} = (\mathcal{F}\mu)^{1/2}.$$

This means that we may immediately use Eq. (7.138),

$$\text{Im } \chi(\omega) = \eta \omega = (\mathcal{F}\mu)^{1/2} \omega,$$

in Eq. (\*), which yields the required answer:

$$S_F(\omega) = \frac{\hbar \omega}{2\pi} (\mathcal{F}\mu)^{1/2} \coth \frac{\hbar \omega}{2k_B T}.$$

Note that this is one more good example of a dissipative environment that may be described by a time-independent Hamiltonian. (Another example is the two-tunnel-barrier system discussed in Sec. 2.5 of the lecture notes.) Such models give a good opportunity to explore some challenging issues of the theory of open systems, by using reliable theoretical methods developed for Hamiltonian systems.

**Problem 7.8.**\* Calculate the low-frequency spectral density of small fluctuations of the voltage  $V$  across a Josephson junction shunted with an Ohmic conductor and biased with a dc external current  $\bar{I} > I_c$ .

*Hint:* You may use Eqs. (1.73)-(1.74) of the lecture notes to describe the junction's dynamics, and assume that the shunting conductor remains in thermal equilibrium.

*Solution:* In the Heisenberg-Langevin approach, we may use Eqs. (1.73)-(1.74) for the Heisenberg operators of the corresponding observables:

<sup>164</sup> Note that in our case, this coefficient is just the *wave impedance*  $Z$  of the string – see, e.g., CM Eq. (6.48).

$$\hat{I}(t) = I_c \sin \hat{\varphi}, \quad \hat{V} = \frac{\hbar}{2e} \frac{d\hat{\varphi}}{dt},$$

while taking

$$\hat{I}(t) = \bar{I} - \hat{I}_G(t),$$

where  $I_G$  is the current flowing through the shunt – see the figure on the right. As we know from Sec. 7.4 (see in particular Eq. (7.92) and its discussion), we may represent this current as the sum of its average component and the fluctuations that may be calculated in the absence of the voltage:<sup>165</sup>

$$\hat{I}_G(t) = \langle \hat{I}_G \rangle - \tilde{I}(t) = G\hat{V} - \tilde{I}(t),$$

where  $G$  is the Ohmic conductance of the shunt, so the resulting Heisenberg equation of motion of the Josephson phase  $\varphi$  is

$$I_c \sin \hat{\varphi} + \frac{\hbar G}{2e} \frac{d\hat{\varphi}}{dt} = \bar{I} + \tilde{I}(t). \quad (*)$$

Since we have been asked to analyze only small fluctuations, we may look for the solution of this equation in the form  $\hat{\varphi} = \varphi_0 + \hat{\tilde{\varphi}}$ , where  $\varphi_0$  is the solution of the fluctuation-free classical equation

$$I_c \sin \varphi + \frac{\hbar G}{2e} \frac{d\varphi}{dt} = \bar{I},$$

while the operator  $\hat{\tilde{\varphi}}$  describes small fluctuations of the phase, obeying the linearized version of Eq. (\*):

$$I_c \cos \varphi \hat{\tilde{\varphi}} + \frac{\hbar G}{2e} \frac{d\hat{\tilde{\varphi}}}{dt} = \hat{\tilde{I}}(t).$$

The solutions of these two differential equations may be made less bulky by introducing normalized variables: current  $i \equiv I/I_c$  and time  $\tau \equiv t/(\hbar G/2eI_c)$ .<sup>166</sup> In these dimensionless variables,

$$\dot{\varphi}_0 + \sin \varphi_0 = \bar{i}, \quad \dot{\hat{\tilde{\varphi}}} + \cos \varphi_0 \hat{\tilde{\varphi}} = \hat{\tilde{i}}(\tau), \quad (**)$$

where (in this solution only!) the dot means the differentiation over  $\tau$  rather than  $t$ .

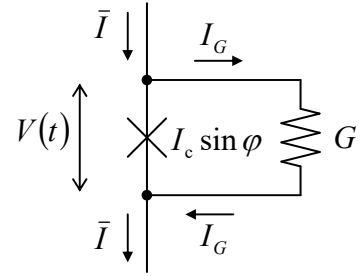
The first (classical but nonlinear) equation<sup>167</sup> may be readily solved analytically, because the separation of variables leads to a table integral:<sup>168</sup>

<sup>165</sup> Note that the statistical averaging in the first form of this relation is only over the degrees of freedom of the environment (i.e. the shunting conductor), so from the point of view of the Josephson junction as such, the voltage in its second form is still an operator. Also, the sign before the fluctuating term is a matter of convention and is taken negative here just for the compactness of the following calculations.

<sup>166</sup> Let me hope that the use of different fonts makes the difference between the normalized current ( $i$ ) and the imaginary unity ( $i$ ) sufficiently clear.

<sup>167</sup> This well-known equation (see, e.g., CM Sec. 5.4) at  $\bar{i} < 1$  has the stationary solution  $\varphi_0 = \sin^{-1} \bar{i}$ . The calculation of the phase and voltage fluctuations, in this case, is recommended to the reader as a (simple) additional exercise. The answers are: at  $\omega \rightarrow 0$ ,  $S_\varphi(\omega) \rightarrow S_I(\omega)/I_c^2 \cos^2 \varphi_0$ ;  $S_V(\omega) \rightarrow (\hbar\omega/2e)^2 S_\varphi(\omega) \rightarrow 0$ .

<sup>168</sup> See, e.g., MA Eq. (6.3c).





$$\frac{d\varphi_0}{\bar{i} - \cos\varphi_0} = d\tau, \quad \text{so that } \tau = \int \frac{d\varphi_0}{\bar{i} - \cos\varphi_0}.$$

However, for our purposes, the explicit form of the function  $\varphi_0(t)$  is less important than the following expression for its time derivative, and hence for the unperturbed part of the voltage  $V \propto d\varphi/dt \propto d\varphi/d\tau$  across the junction (see the figure above):

$$\dot{\varphi}_0 = \frac{\bar{v}^2}{\bar{i} - \cos(\bar{v}\tau + \text{const})}, \quad \text{where } \bar{v} \equiv (\bar{i}^2 - 1)^{1/2} > 0, \quad \text{for } \bar{i} > 1, \text{ i.e. } \bar{I} > I_c,$$

where the inconsequential constant depends on the selected origin of time; for what follows, it is convenient to take it equal to zero. This result shows that  $\dot{\varphi}_0$  is a periodic (but, generally, not a sinusoidal!) function of  $\tau$ , with the normalized frequency  $\bar{v}$  approaching zero at  $\bar{i} \rightarrow 1$ . (This is just the same Josephson oscillations of frequency (1.75) that were briefly discussed at the end of Sec. 1.6 of the lecture notes, besides that in our current case of a constant external current, they are the simultaneous, self-consistent oscillations of the supercurrent  $I_c \sin\varphi$  and the voltage  $V$ .) For our calculation, we will need the Fourier expansion of this periodic function and its time derivative,

$$\dot{\varphi}_0 = \sum_{k=-\infty}^{+\infty} v_k e^{-ik\bar{v}\tau}, \quad \ddot{\varphi}_0 = \sum_{k=-\infty}^{+\infty} v_k (-ik\bar{v}) e^{-ik\bar{v}\tau}, \quad \text{with } v_k = \frac{1}{2\pi} \int_{-\pi}^{\pi} \dot{\varphi}_0 e^{ik\bar{v}\tau} d(\bar{v}\tau) \equiv \frac{\bar{v}^2}{\pi} \int_0^{\pi} \frac{\cos k\xi d\xi}{\bar{i} - \cos\xi}.$$

This is also a table integral,<sup>169</sup> giving

$$v_k = \bar{v} (\bar{i} - \bar{v})^{|k|},$$

so, in particular,  $v_0 = \bar{v}$  – hence the notation.

Now solving the second of Eqs. (\*\*) by the standard method of variable coefficients (fully applicable to linear equations for operators), we readily get

$$\hat{\varphi}(\tau) = f(\tau) \int \frac{\hat{i}(\tau')}{f(\tau')} d\tau', \quad \text{where } f(\tau) \equiv \exp\left\{-\int \cos\varphi_0(\tau'') d\tau''\right\}.$$

This result may be recast in a form more convenient for calculations. Indeed, differentiating the first of Eqs. (\*\*) over  $\tau$ , we get

$$\ddot{\varphi}_0 + \cos\varphi_0 \dot{\varphi}_0 = 0, \quad \text{i.e. } \frac{d\dot{\varphi}_0}{d\tau} + \cos\varphi_0 \dot{\varphi}_0 = 0, \quad \text{so } \frac{d\dot{\varphi}_0}{\dot{\varphi}_0} = -\cos\varphi_0 d\tau.$$

Integrating this elementary differential equation, we see that the above function  $f(\tau)$  is just  $\dot{\varphi}(\tau)$ , give or take a time-independent multiplier – which is not important for the final result. As a result, we get,

$$\hat{\varphi}(\tau) = \dot{\varphi}_0(\tau) \int \frac{\hat{i}(\tau')}{\dot{\varphi}_0(\tau')} d\tau', \quad \text{so } \dot{\hat{\varphi}}(\tau) = \hat{i}(\tau) + \ddot{\varphi}_0(\tau) \int \frac{\hat{i}(\tau')}{\dot{\varphi}_0(\tau')} d\tau'.$$

The last formula describes the (normalized) fluctuations of the voltage  $V$ , i.e. exactly the subject of our interest. With the above explicit forms of  $\dot{\varphi}_0$  and the Fourier expansion of  $\ddot{\varphi}_0$ , it becomes

<sup>169</sup> See, e.g., Eq. 2.5.16-22 in the manual by A. Prudnikov *et al.*, cited in MA Sec. 16.

$$\dot{\hat{\varphi}}(\tau) = \hat{i}(\tau) - i \sum_{k=-\infty}^{\infty} k\bar{v} (\bar{i} - \bar{v})^{|k|} e^{-ik\bar{v}\tau} \int \left( \bar{i} - \frac{e^{i\bar{v}\tau'} + e^{-i\bar{v}\tau'}}{2} \right) \hat{i}(\tau') d\tau'. \quad (***)$$

Now introducing the Fourier expansions of the (normalized) voltage and current fluctuations, similar to Eq. (7.115) of the lecture notes,

$$\dot{\hat{\varphi}}(\tau) = \int_{-\infty}^{+\infty} \hat{v}_{\omega} e^{-i\omega\tau} d\omega, \quad \hat{i}(\tau) = \int_{-\infty}^{+\infty} \hat{i}_{\omega} e^{-i\omega\tau} d\omega,$$

we may readily perform the integration in Eq. (\*\*\*) explicitly. Requiring the complex amplitudes of all harmonics in both parts of the resulting equation to be equal, we get

$$\hat{v}_{\omega} = \sum_{k=-\infty}^{+\infty} z_k(\omega) \hat{i}_{\omega - k\bar{v}}, \quad \text{with } z_k(\omega) = \delta_{k,0} + \frac{k(\bar{i} - \bar{v})^{|k|} \bar{i}}{\omega - k\bar{v}} - \frac{1}{2} \sum_{\pm} \frac{(k \pm 1)(\bar{i} - \bar{v})^{|k \pm 1|}}{\omega - (k \pm 1)\bar{v}}.$$

The first of these expressions describes the so-called *mixing* of the current fluctuations with harmonics of the Josephson oscillations, due to the nonlinearity of the Josephson supercurrent.<sup>170</sup> According to Eq. (7.114) of the lecture notes, it means that the symmetrized spectral densities of the voltage and current fluctuations are related as follows:

$$S_v(\omega) = \sum_{k=-\infty}^{+\infty} |z_k|^2 S_i(\omega - k\bar{v}).$$

This is a very informative result, in particular (at  $\omega \approx n\bar{v}$ ) describing the fluctuation-induced broadening of the Josephson oscillation harmonics. For our purposes, however, we need only its low-frequency limit,  $\omega \rightarrow 0$ . In this limit, thanks to the identity  $(\bar{i} - \bar{v})^{-1} = (\bar{i} + \bar{v})$  following from the above formula for  $\bar{v}$ , the result simplifies and includes only three (essentially, two) terms:

$$S_v(0) = \frac{1}{\bar{v}^2} \left[ \bar{i}^2 S_i(0) + \frac{1}{4} S_i(\bar{v}) + \frac{1}{4} S_i(-\bar{v}) \right] = \frac{\bar{i}^2}{\bar{v}^2} \left[ S_i(0) + \frac{1}{2\bar{i}^2} S_i(\bar{v}) \right].$$

The front factor in the last expression is just the square of the dc differential (“dynamic”) resistance  $R_d \equiv d\bar{V} / d\bar{I}$  of the system, in our normalized units:

$$r_d = \frac{d\bar{v}}{d\bar{i}} = \frac{d(\bar{i}^2 - 1)^{1/2}}{d\bar{i}} = \frac{\bar{i}}{(\bar{i}^2 - 1)^{1/2}} = \frac{\bar{i}}{\bar{v}},$$

so returning to the initial dimensional units, we finally get

$$S_v(0) = R_d^2 \left[ S_I(0) + \frac{I_c^2}{2\bar{I}^2} S_I(\omega_J) \right], \quad (****)$$

where

$$\omega_J = \frac{2eI_c}{\hbar G} \bar{v} \equiv \frac{2e}{\hbar} \bar{V}$$

<sup>170</sup> For a brief discussion of this (essentially, classical, or rather mathematical) effect see, e.g., CM Sec. 6.7.

is the dimensional frequency of the Josephson oscillations – see Eq. (1.75). The first term inside the square brackets of Eq. (\*\*\*\*) describes the simple and very natural transform of low-frequency fluctuations of the current in the shunt into voltage fluctuations at the same frequency, at the differential resistance of the system:  $\tilde{V} = R_d \tilde{I}$ . The second term is much less trivial: it describes the intensity of the fluctuations induced by high-frequency ( $\omega \approx \omega_J$ ) current fluctuations and transformed to nearly zero frequencies due to their mixing with the Josephson self-oscillations.

Since the current fluctuations of the conductance  $G$ , remaining in thermal equilibrium with temperature  $T$ , obey the fluctuation-dissipation theorem (7.134) with  $\text{Im}\chi(\omega)/\omega = G$ :<sup>171</sup>

$$S_I(\omega) = \frac{\hbar\omega}{2\pi} G \coth \frac{\hbar\omega}{2k_B T},$$

their spectral density at frequency  $\omega_J$  does not vanish even at low temperatures:

$$S_I(\omega_J) \approx \frac{\hbar\omega_J}{2\pi} G, \quad \text{at } k_B T \ll \hbar\omega_J,$$

and represents purely quantum fluctuations – see the discussion following Eq. (7.152) of the lecture notes. Eq. (\*\*\*\*) is exactly the theoretical formula (derived in 1972) that was later used by R. Koch *et al.* for comparison with their experimental results.<sup>172</sup> The good agreement of the data with this theory gave firm evidence of the reality of the quantum fluctuations in an Ohmic environment, without any explicit oscillator at their frequency  $\sim \omega_J$ .

**Problem 7.9.** Prove that in the interaction picture of quantum dynamics, the expectation value of an arbitrary observable  $A$  may be indeed calculated using Eq. (7.167) of the lecture notes.

*Solution:* The basic Eq. (7.5) may be represented as

$$\langle A \rangle(t) = \text{Tr} \left[ \hat{A} \hat{u} \hat{w}(0) \hat{u}^\dagger \right],$$

where  $\hat{u}$  is the full evolution operator that obeys Eq. (4.157b). By using Eqs. (4.209)-(4.210) of the interaction picture, we may express this expectation value via products of the partial evolution operators  $\hat{u}_0$  and  $\hat{u}_1$ , and their Hermitian conjugates, and then group the operands as follows:

$$\langle A \rangle(t) = \text{Tr} \left[ \hat{A} \hat{u}_0 \hat{u}_1 \hat{w}(0) \hat{u}_1^\dagger \hat{u}_0^\dagger \right] = \text{Tr} \left[ \left( \hat{A} \hat{u}_0 \hat{u}_1 \hat{w}(0) \hat{u}_1^\dagger \right) \left( \hat{u}_0^\dagger \right) \right].$$

From Chapter 4, we know that the trace of a product of two operators does not depend on their order, so in the last relation, we may swap the parentheses and then regroup the terms as follows:

$$\langle A \rangle(t) = \text{Tr} \left[ \left( \hat{u}_0^\dagger \right) \left( \hat{A} \hat{u}_0 \hat{u}_1 \hat{w}(0) \hat{u}_1^\dagger \right) \right] = \text{Tr} \left[ \left( \hat{u}_0^\dagger \hat{A} \hat{u}_0 \right) \left( \hat{u}_1 \hat{w}(0) \hat{u}_1^\dagger \right) \right].$$

But according to Eqs. (4.214) and (7.166), this relation is nothing other but Eq. (7.167):

<sup>171</sup> See the footnote just before Eq. (7.139) of the lecture notes.

<sup>172</sup> For the reference, see Chapter 7 of the lecture notes.

$$\langle A \rangle(t) = \text{Tr}[A_1(t)\hat{w}_1(t)].$$

**Problem 7.10.** Show that the quantum-mechanical Golden Rule (6.149) and the master equation (7.196) give the same results for the rate of spontaneous quantum transitions  $n' \rightarrow n$  in a system with a discrete energy spectrum, which is weakly coupled to a low-temperature heat bath (with  $k_B T \ll \hbar \omega_{nn'}$ ).

*Hint:* You may establish the relation between the function  $\chi''(\omega_{nn'})$  that participates in Eq. (7.196) and the density of states  $\rho_n$  that participates in the Golden Rule, by considering the particular case of sinusoidal classical oscillations in the system of interest.

*Solution:* Let us consider a system coupled with the environment via the interaction Hamiltonian (7.90), in the particular case when its variable  $x$  performs sinusoidal classical oscillations,  $x = x_0 \cos \omega t \equiv (x_0/2)(\exp\{-i\omega t\} + \exp\{i\omega t\})$ , with a frequency  $\omega \approx \omega_{nn'} \gg k_B T/\hbar$ . In this low-temperature limit, the occupation of the corresponding excited levels ( $n$ ) of the environment is negligible, and we may apply to the induced quantum transitions in it the Golden Rule in the form of Eq. (6.111), with  $A_{nn'} = (x_0/2)F_{nn'}$ :

$$\Gamma = \frac{2\pi}{\hbar} \left| \frac{x_0 F_{nn'}}{2} \right|^2 \rho_n = \frac{\pi}{2\hbar} x_0^2 |F_{nn'}|^2 \rho_n.$$

The quantum transitions at this rate, transferring to the environment the energy  $\hbar\omega$  each, result in the average power flow from the system:

$$\langle \overline{\mathcal{P}} \rangle = \Gamma \hbar \omega = \frac{\pi}{2} \omega x_0^2 |F_{nn'}|^2 \rho_n.$$

On the other hand, the same power may be expressed by Eq. (7.127):

$$\langle \overline{\mathcal{P}} \rangle = \frac{\omega x_0^2}{2} \chi''(\omega).$$

Comparing these two expressions, we find the connection we have been looking for:

$$\chi''(\omega_{nn'}) = \pi |F_{nn'}|^2 \rho_n.$$

Since this expression includes only the characteristics of the environment, it should be valid for any process in the system of our interest – either classical or quantum. With this substitution, Eq. (7.196) applied to the spontaneous energy-reducing transition, i.e. to the case  $E_{n'} > E_n$ , and taken in the low-temperature limit,

$$\Gamma_{n' \rightarrow n} = \frac{2}{\hbar} |x_{nn'}|^2 \chi''(\omega_{nn'}),$$

reads

$$\Gamma_{n' \rightarrow n} = \frac{2\pi}{\hbar} |x_{nn'}|^2 |F_{nn'}|^2 \rho_n.$$

However, this is exactly Eq. (6.149), taking into account the notation replacements  $A \rightarrow \pm x$  and  $B \rightarrow \mp F$ , which follow from the comparison of the interaction Hamiltonians (6.145) and (7.90).

**Problem 7.11.** A spin- $1/2$  with gyromagnetic ratio  $\gamma$  had been placed into a constant magnetic field with magnitude  $\mathcal{B} \gg k_B T / \hbar \gamma$ , and let relax into its ground state. Then the direction of the field was suddenly changed by  $\pi/2$  and kept constant after that. Taking into account the spin's weak coupling to a dissipative environment:

- (i) calculate the time evolution of the spin's density matrix (in any basis you like), and
- (ii) calculate the time evolution of the spin vector's expectation value  $\langle \mathbf{S} \rangle$  and sketch its trajectory.

*Solutions:*

(i) Let us direct the  $x$ -axis along the initial direction of the field, the  $z$ -axis, along its direction after the change, and work in the usual  $z$ -basis. Then the initial state of the system is described by the ket  $|\rightarrow\rangle$  given (to an arbitrary and inconsequential common phase factor) by the first of Eqs. (4.122) of the lecture notes:

$$|\rightarrow\rangle \equiv \frac{1}{\sqrt{2}} (|\uparrow\rangle + |\downarrow\rangle),$$

so in the usual expansion (5.1),

$$|\alpha\rangle \equiv \alpha_\uparrow |\uparrow\rangle + \alpha_\downarrow |\downarrow\rangle,$$

we have  $\alpha_\uparrow = \alpha_\downarrow = 1/\sqrt{2}$ . Hence, according to Eq. (7.20), each element of the initial  $2 \times 2$  density matrix of the spin is equal to  $1/2$ . The further evolution of the matrix is described by Eqs. (7.212) and (7.214), where (due to the given condition  $k_B T \ll \hbar \gamma \mathcal{B}$ ) we may take  $w_{\uparrow\uparrow}(\infty) \equiv W_+(\infty) = 1$ ,  $w_{\downarrow\downarrow}(\infty) \equiv W_-(\infty) = 0$ :

$$w(t) = \begin{pmatrix} 1 - \frac{1}{2} \exp\{-t/T_1\} & \frac{1}{2} \exp\{-t/T_2 + i\Omega t\} \\ \frac{1}{2} \exp\{-t/T_2 - i\Omega t\} & \frac{1}{2} \exp\{-t/T_1\} \end{pmatrix},$$

the moment of the field change it taken for  $t = 0$ , and  $\Omega \equiv 2c/\hbar = -\gamma \mathcal{B}$  – see Eq. (5.13).

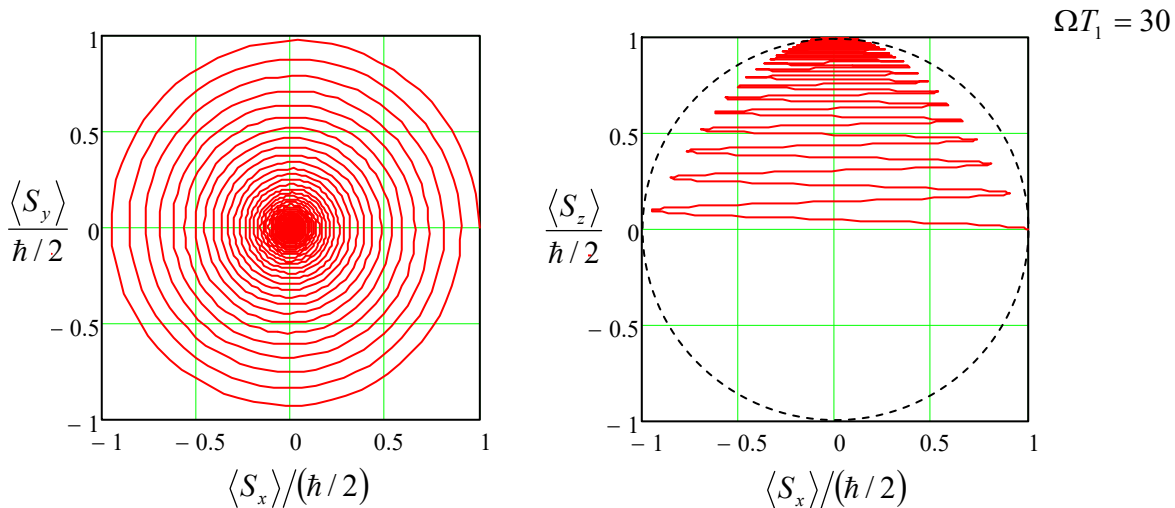
(ii) The Cartesian components of the vector  $\langle \mathbf{S} \rangle$  may be expressed via this density matrix by using the basic Eq. (7.5):<sup>173</sup>

$$\begin{aligned} \langle S_x \rangle(t) &= \text{Tr} [\hat{S}_x \hat{w}(t)] = \text{Tr} \left[ \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} w(t) \right] = \frac{\hbar}{2} \cos \Omega t \exp\left\{-\frac{t}{T_2}\right\}, \\ \langle S_y \rangle(t) &= \text{Tr} [\hat{S}_y \hat{w}(t)] = \text{Tr} \left[ \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} w(t) \right] = \frac{\hbar}{2} \sin \Omega t \exp\left\{-\frac{t}{T_2}\right\}, \\ \langle S_z \rangle(t) &= \text{Tr} [\hat{S}_z \hat{w}(t)] = \text{Tr} \left[ \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} w(t) \right] = \frac{\hbar}{2} \left( 1 - \exp\left\{-\frac{t}{T_1}\right\} \right). \end{aligned}$$

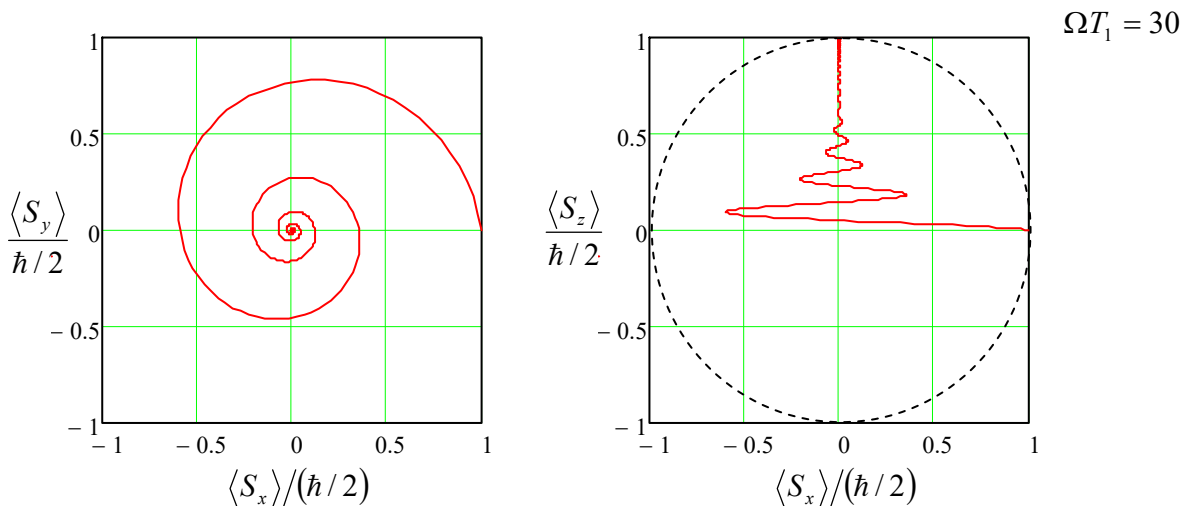
(As a sanity check, at  $T_2 \rightarrow \infty$ , i.e. at vanishing dephasing, the first two formulas tend to Eqs. (4.173)-(4.174) with the corresponding initial conditions:  $\langle S_x \rangle(0) = \hbar/2$ ,  $\langle S_y \rangle(0) = 0$ .)

<sup>173</sup> See also Eq. (7.75).

These formulas describe an exponentially decaying spin precession about the  $z$ -axis, with a simultaneous relaxation of its  $z$ -component to its equilibrium value  $\langle S_z \rangle(\infty) = \hbar/2$  – generally with a different relaxation time. This means that the trajectory of the vector  $\langle \mathbf{S} \rangle$  in the angular momentum space is spiral-like. The figure below shows two projections of this trajectory for the ratio  $T_2/T_1 = 2$  typical for optical two-level systems (where the second, low-frequency term on the right-hand side of Eq. (7.210) is usually negligible), and for a particular value of the product  $\Omega T_1$ .<sup>174</sup>



Perhaps the only surprise for the reader may be that the end of the vector deviates from the Bloch sphere (where it always remains in closed, i.e. Hamiltonian two-level quantum systems).<sup>175</sup> This fact is even more clearly visible in the figure below where the trajectory of  $\langle \mathbf{S} \rangle$  is plotted for the lower ratio  $T_2/T_1 = 0.2$ . (This value is typical for nuclear spins in condensed matter, where the random “tumbling” motion of the surrounding molecules suppresses  $T_2$  more than  $T_1$ .)



An alternative way to obtain the same results is to use the *Bloch equations* whose derivation is the task of the next problem.

<sup>174</sup> Admittedly, in most practical systems, the product  $\Omega T_1$  is much higher than the value of 30, which is used here just for the plot clarity.

<sup>175</sup> Actually, attracting the reader’s attention to this fact was the main goal of assigning this simple problem.

**Problem 7.12.** A spin- $1/2$  with gyromagnetic ratio  $\gamma$  is placed into the magnetic field  $\mathcal{B}(t) = \mathcal{B}_0 + \widetilde{\mathcal{B}}(t)$  with an arbitrary but small time-dependent component, and is also weakly coupled to a dissipative environment in thermal equilibrium at temperature  $T$ . Derive differential equations describing the time evolution of the expectation values of the spin's Cartesian components.

*Solution:* At the specified conditions, the Hamiltonians of the spin's interaction with its environment and with the time-dependent component of the magnetic field may be both considered as small perturbations of the basic Pauli Hamiltonian given by Eq. (4.163) of the lecture notes:

$$\hat{H}^{(0)} = -\hat{\mathbf{m}} \cdot \mathcal{B}_0 = -\gamma \hat{S}_z \mathcal{B}_0$$

(where the  $z$ -axis is directed along the dc magnetic field), so the contributions by these perturbations to the right-hand sides of the differential equation of motion of the vector  $\langle \mathbf{S} \rangle$  may be calculated independently.

The contribution due to the environment coupling for such two-level systems as ours was discussed in Sec. 7.7 of the lecture notes. For the diagonal elements of the density matrix in the stationary-state basis  $\pm$  of the unperturbed Hamiltonian, they are described by the master equations (7.211):

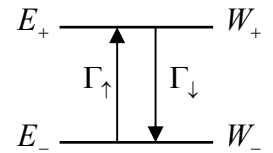
$$\begin{aligned} \dot{w}_{++} &= \Gamma_{\uparrow} w_{--} - \Gamma_{\downarrow} w_{++}, \\ \dot{w}_{--} &= -\Gamma_{\uparrow} w_{--} + \Gamma_{\downarrow} w_{++}, \end{aligned} \quad (*)$$

where  $w_{++} \equiv W_+$  and  $w_{--} \equiv W_-$  have the physical sense of occupations of the corresponding energy levels

$$E_{\pm} = \pm \frac{\Delta}{2} \equiv \pm \gamma \frac{\hbar}{2} \mathcal{B}_0,$$

and  $\Gamma_{\pm}$  are the interlevel transition rates – see the figure on the right. In thermal equilibrium at temperature  $T$ , these rates are related by Eq. (7.197):

$$\frac{\Gamma_{\uparrow}}{\Gamma_{\downarrow}} = \exp\left\{-\frac{\Delta}{k_B T}\right\}.$$



The differential equations (\*) are sufficient to derive one for the expectation value of the spin's  $z$ -component, i.e. its component along the direction of the base field  $\mathcal{B}_0$ .<sup>176</sup> Indeed, let us use the fundamental relation (7.5) between the expectation value of any observable and the density matrix, in the Schrödinger picture of quantum dynamics – in that all time evolution is delegated to the matrix:

$$\langle S_z(t) \rangle = \frac{\hbar}{2} \text{Tr}\{\sigma_z \mathbf{w}(t)\} = \frac{\hbar}{2} \text{Tr}\left\{\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} w_{++}(t) & w_{+-}(t) \\ w_{-+}(t) & w_{--}(t) \end{pmatrix}\right\} = \frac{\hbar}{2} \{w_{++}(t) - w_{--}(t)\}. \quad (**)$$

<sup>176</sup> Please note that this choice of the  $z$ -axis (which is common for discussions of spin dynamics) differs from that used in Sec. 7.7 of the lecture notes, where that axis described the system's coupling (7.70) with the environment. As a result, in Eqs. (7.209) and (7.210) for the time constants  $T_1 \equiv 1/(\Gamma_{\uparrow} + \Gamma_{\downarrow})$  and  $T_2$ , we cannot take  $\theta = 0$ . In this solution, these constants are treated as certain known parameters. (In most practical applications, they are taken from experiment.)

(See also Eq. (7.75) of the lecture notes.) Solving this equation together with the normalization condition  $w_{++} + w_{--} = 1$  for these two probabilities, we get

$$w_{++} = \frac{1}{2} \left( 1 + \frac{\langle S_z \rangle}{\hbar/2} \right), \quad w_{--} = \frac{1}{2} \left( 1 - \frac{\langle S_z \rangle}{\hbar/2} \right).$$

Now differentiating both sides of Eq. (\*\*) over time, and using Eqs. (\*) and the above expressions for  $w_{++}$  and  $w_{--}$ , we get the differential equation

$$\langle \dot{S}_z \rangle_{\text{env}} = (\Gamma_{\uparrow} - \Gamma_{\downarrow}) \frac{\hbar}{2} - (\Gamma_{\uparrow} + \Gamma_{\downarrow}) \langle S_z \rangle,$$

which is usually recast in the following equivalent form:

$$\langle \dot{S}_z \rangle_{\text{env}} = -\frac{\langle S_z \rangle - S_e}{T_1},$$

where  $1/T_1$  is the effective spin relaxation rate:

$$\frac{1}{T_1} \equiv \Gamma_{\Sigma} \equiv \Gamma_{\uparrow} + \Gamma_{\downarrow},$$

while the constant

$$S_e \equiv \frac{\hbar}{2} \frac{\Gamma_{\uparrow} - \Gamma_{\downarrow}}{\Gamma_{\uparrow} + \Gamma_{\downarrow}} \equiv \frac{\hbar}{2} \frac{\Gamma_{\uparrow}/\Gamma_{\downarrow} - 1}{\Gamma_{\uparrow}/\Gamma_{\downarrow} + 1} = \frac{\hbar \exp\{-\Delta/k_B T\} - 1}{2 \exp\{-\Delta/k_B T\} + 1} \equiv \frac{\hbar}{2} \tanh \frac{\Delta}{2k_B T}$$

has the physical sense of the thermal-equilibrium value of  $\langle S_z \rangle$ . Note that at high temperatures,  $k_B T \gg \Delta$ , this value tends to zero because both energy levels of the system, in equilibrium, are equally occupied.

Making calculation similar to Eq. (\*\*) for the  $S_x$ -component of spin,

$$\langle S_x(t) \rangle = \text{Tr}\{S_x w(t)\} = \frac{\hbar}{2} \text{Tr}\{\sigma_x w(t)\} = \frac{\hbar}{2} \text{Tr} \left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} w_{++}(t) & w_{+-}(t) \\ w_{-+}(t) & w_{--}(t) \end{pmatrix} \right\} = \frac{\hbar}{2} \{w_{+-}(t) + w_{-+}(t)\}, \quad (***)$$

we see that its dynamics is determined by the off-diagonal elements of the density matrix. For these elements, we may use the environment-related part of Eq. (7.214):

$$(\dot{w}_{+-})_{\text{env}} = -\frac{1}{T_2} w_{+-}, \quad (\dot{w}_{-+})_{\text{env}} = -\frac{1}{T_2} w_{-+}. \quad (***)$$

Differentiating both parts of Eq. (\*\*\*) over time, and then using Eq. (\*\*\*), we get the following expression for the environment's contribution to the spin's derivative:

$$\langle \dot{S}_x \rangle_{\text{env}} = \frac{\hbar}{2} (\dot{w}_{+-} + \dot{w}_{-+}) = -\frac{\hbar}{2} \frac{1}{T_2} (w_{+-} + w_{-+}).$$

Now using Eq. (\*\*\*) again (backward), we get a very simple equation describing spin's dephasing:

$$\langle \dot{S}_x \rangle_{\text{env}} = -\frac{1}{T_2} \langle S_x \rangle.$$

An absolutely similar calculation for the  $y$ -component of spin gives a similar result:



$$\langle \dot{S}_y \rangle_{\text{env}} = -\frac{1}{T_2} \langle S_y \rangle.$$

On the other hand, as was discussed in Sec. 5.1 of the lecture notes, the contribution of the time-dependent magnetic field into the spin dynamics may be merged with that of the base field  $\mathcal{B}_0$ , into one vector equation (5.22):

$$\langle \dot{\mathbf{S}} \rangle_{\text{field}} = \gamma \langle \mathbf{S} \rangle \times \mathcal{B}(t).$$

Now merging all right-hand sides of the equations for the spin component derivatives, we finally get the so-called *Bloch equations*

$$\langle \dot{S}_x \rangle = \gamma [\langle \mathbf{S} \rangle \times \mathcal{B}(t)]_x - \frac{\langle S_x \rangle}{T_2}, \quad \langle \dot{S}_y \rangle = \gamma [\langle \mathbf{S} \rangle \times \mathcal{B}(t)]_y - \frac{\langle S_y \rangle}{T_2}, \quad \langle \dot{S}_z \rangle = \gamma [\langle \mathbf{S} \rangle \times \mathcal{B}(t)]_z - \frac{\langle S_z \rangle - S_e}{T_1},$$

whose dissipation-free form (5.23) was discussed at the end of Sec. 5.1 of the lecture notes.

These equations are especially popular for the description of experiments with the sets of  $N \gg 1$  similar (practically, non-interacting) nuclear spins in condensed matter samples, where they are commonly rewritten for the Cartesian components of the nuclear magnetization  $\mathbf{M} = n\gamma\langle \mathbf{S} \rangle$  of the sample (where  $n \equiv N/V$  is the spin density):

$$\dot{M}_x = \gamma [\mathbf{M} \times \mathcal{B}(t)]_x - \frac{M_x}{T_2}, \quad \dot{M}_y = \gamma [\mathbf{M} \times \mathcal{B}(t)]_y - \frac{M_y}{T_2}, \quad \dot{M}_z = \gamma [\mathbf{M} \times \mathcal{B}(t)]_z - \frac{M_z - M_e}{T_1}.$$

Since at  $N \gg 1$ , the quantum fluctuations of individual spins are effectively averaged out, in many cases, these equations may be treated as classical equations of motion of  $c$ -number variables – somewhat similar to those describing the classical torque-induced precession of a symmetric top,<sup>177</sup> but with a very specific damping – different for the longitudinal and transverse spin components.

Perhaps the most important application of these equations is the description of the environment-induced broadening of the magnetic resonance, which was briefly discussed in Chapters 5 and 6 – see also the model solution of Problem 5.5. As was shown in that solution, in the simplest case when  $\tilde{\mathcal{B}}(t)$  is a field with a constant magnitude  $\mathcal{B}_1$ , rotating in the plane perpendicular to the time-independent field  $\mathcal{B}_0$  with the angular velocity  $\omega$ ,<sup>178</sup> this effect obeys Eqs. (6.94) of the lecture notes, with  $|A| = \gamma\mathcal{B}_1/2$ , which describe the Rabi oscillations of the level occupancy, with an oscillation amplitude exhibiting a resonance at  $\omega \approx \Delta/\hbar \equiv \gamma\mathcal{B}_1/2\hbar$ . At negligible coupling of the spin to its dissipative environment, the FWHM bandwidth  $\Delta\omega$  of this resonance is equal to  $2\gamma\mathcal{B}_1$ , but as the above Bloch equations imply, the environment provides an additional broadening of the resonance by  $\Delta\omega \sim 1/T_{1,2}$  – see the next problem.

For the most important variety of this effect, the *nuclear magnetic resonance* (NMR), the nuclear spin interaction with the environment is typically very weak, with the times  $T_{1,2}$ , in practical magnetic fields  $\mathcal{B}_0$  of a few teslas, in some cases exceeding a second, while the resonance frequency  $\Delta/2\pi\hbar$  may be of the order 100 MHz. As a result, the resonance may have a very small relative bandwidth, of the

<sup>177</sup> See, e.g., CM Sec. 4.5.

<sup>178</sup> Actually, the resonance takes place for any sinusoidal field of frequency  $\omega \approx \Delta/\hbar$ ; just the quantitative description of its effect far from the resonance may be somewhat different.

order of  $10^{-8}$ , so its detection allows experimental measurements of tiny local variations of  $\mathcal{B}_0$ . This effect has many important applications in condensed matter physics, chemistry, and biomedicine.<sup>179</sup>

**Problem 7.13.** Use the Bloch equations derived in the previous problem to analyze the magnetic resonance<sup>180</sup> in a spin- $1/2$  which is weakly connected to a dissipative environment in thermal equilibrium. Use the result for a semi-quantitative discussion of the environmental broadening of arbitrary quantum transitions in systems with discrete energy spectra.

*Hint:* You may use the same rotating field model as in Problem 5.5.

*Solution:* With the magnetic field taken in the same form as in Problem 5.5,

$$\mathcal{B} = \mathcal{B}_1(\mathbf{n}_x \cos \omega t + \mathbf{n}_y \sin \omega t) + \mathcal{B}_0 \mathbf{n}_z,$$

the Bloch equations take the form

$$\begin{aligned} \langle \dot{S}_x \rangle &= -\Omega_0 \langle S_y \rangle + \Omega_1 \langle S_z \rangle \sin \omega t - \frac{\langle S_x \rangle}{T_2}, & \langle \dot{S}_y \rangle &= \Omega_0 \langle S_x \rangle - \Omega_1 \langle S_z \rangle \cos \omega t - \frac{\langle S_y \rangle}{T_2}, \\ \langle \dot{S}_z \rangle &= \Omega_1 \left( \langle S_y \rangle \cos \omega t - \langle S_x \rangle \sin \omega t \right) - \frac{\langle S_z \rangle - S_e}{T_1}, \end{aligned}$$

where  $\Omega_{0,1} \equiv -\gamma \mathcal{B}_{0,1}$ , and  $S_e$  is the thermally-equilibrium value of  $\langle S_z \rangle$  in the absence of the rotating field – see the solution of the previous problem:

$$S_e = \frac{\hbar}{2} \tanh \frac{\hbar \gamma \mathcal{B}_0}{2k_B T} \equiv -\frac{\hbar}{2} \tanh \frac{\hbar \Omega_0}{2k_B T}.$$

These equations look simpler in the complex variables  $\langle S_{\pm} \rangle \equiv \langle S_x \rangle \pm i \langle S_y \rangle$ :<sup>181</sup>

$$\begin{aligned} \langle \dot{S}_{\pm} \rangle &= \pm i \left( \Omega_0 \langle S_{\pm} \rangle - \Omega_1 \langle S_z \rangle \right) e^{\pm i \omega t} - \frac{\langle S_{\pm} \rangle}{T_2}, \\ \langle \dot{S}_z \rangle &= i \frac{\Omega_1}{2} \left( \langle S_- \rangle e^{+i \omega t} - \langle S_+ \rangle e^{-i \omega t} \right) - \frac{\langle S_z \rangle - S_e}{T_1}. \end{aligned} \quad (*)$$

From their structure, and the model solution of Problem 5.5, we may guess that the equations may be further simplified by the transfer into a reference frame rotating with the field  $\mathcal{B}_1$ , which may be accomplished by taking  $\langle S_{\pm} \rangle \equiv \langle S'_{\pm} \rangle \exp\{\pm i \omega t\}$ . Indeed, when rewritten for these new variables, Eqs. (\*) lose the explicit time dependence of their right-hand sides:

$$\begin{aligned} \langle \dot{S}'_{\pm} \rangle &= \pm i \left( -\xi \langle S'_{\pm} \rangle - \Omega_1 \langle S_z \rangle \right) - \frac{\langle S'_{\pm} \rangle}{T_2}, \quad \text{where } \xi \equiv \omega - \Omega_0, \\ \langle \dot{S}'_z \rangle &= i \frac{\Omega_1}{2} \left( \langle S'_- \rangle - \langle S'_+ \rangle \right) - \frac{\langle S'_z \rangle - S_e}{T_1}, \end{aligned} \quad (**)$$

<sup>179</sup> See, e.g., the monograph by J. Keeler, cited in Sec. 6.5 of the lecture notes.

<sup>180</sup> See the discussion in Sec. 5.2 and the solution of Problem 5.5.

<sup>181</sup> As a reminder, they are the expectation values of the spin-ladder operators and were already used in Eqs. (4.172)-(4.173) of the lecture notes and in the model solution of the (very similar) Problem 5.2.

and have a stationary solution<sup>182</sup> satisfying a simple system of three linear algebraic equations for three spin components:

$$\begin{aligned} \left(-i\xi + \frac{1}{T_2}\right)\langle S_+' \rangle - i\Omega_1\langle S_z \rangle &= 0, & \left(i\xi + \frac{1}{T_2}\right)\langle S_-' \rangle + i\Omega_1\langle S_z \rangle &= 0, \\ -i\frac{\Omega_1}{2}\langle S_+' \rangle + i\frac{\Omega_1}{2}\langle S_-' \rangle - \frac{1}{T_1}\langle S_z \rangle &= -\frac{S_e}{T_1}. \end{aligned}$$

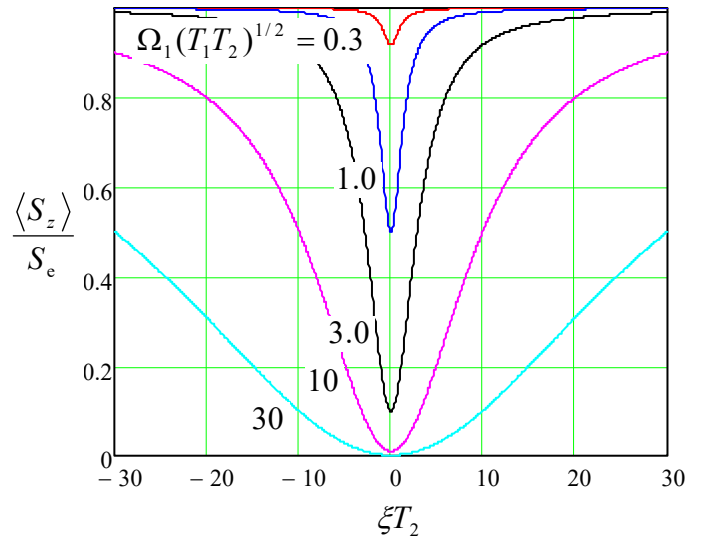
Solving it, we readily get

$$\langle S_z \rangle = \left(1 + \frac{\Omega_1^2 T_1 T_2}{1 + \xi^2 T_2^2}\right)^{-1} S_e \equiv \frac{1 + \xi^2 T_2^2}{1 + \xi^2 T_2^2 + \Omega_1^2 T_1 T_2} S_e. \quad (***)$$

Let us analyze this result. (See the figure on the right.) If the rotating field is weak in the sense  $\Omega_1^2 \equiv (\gamma\mathcal{B}_1)^2 \ll 1/T_1 T_2$ , the magnetic resonance leads to a relatively small suppression of the spin's  $z$ -component:

$$\Delta\langle S_z \rangle \equiv \langle S_z \rangle - S_e = -\frac{\Omega_1^2 T_1 T_2}{1 + \xi^2 T_2^2} S_e,$$

which peaks at the resonance frequency  $\omega = \Omega_0$ , and has a FWHM<sup>183</sup> of  $\Delta\xi = \Delta\omega = 2/T_2$ , independent of the field's amplitude. However, as the rotating field becomes stronger, it causes additional broadening of the resonance curve: in the opposite limit  $\Omega_1^2 \gg 1/T_1 T_2$ , to  $\Delta\omega = 2\Omega_1(T_1 T_2)^{1/2}$ . Such additional broadening is typical for all Rabi oscillations (whose particular case the magnetic resonance is) – see, e.g., Eq. (6.101).



This resonance broadening is detrimental for most practical applications of the resonance (especially NMR) because their goal is the detection of small local variations of the field  $\mathcal{B}_0 \propto \Omega_0$ , i.e. of the resonance's position on the frequency axis. On the other hand, the larger  $\Omega_1$  the larger all possible signals used for resonance monitoring. (Conceptually, the simplest of them is the change of the spin's average magnetic moment  $m_z = \gamma\langle S_z \rangle$  along the dc field's direction, illustrated with Eq. (\*\*\*) and the picture above.) As a result, for such “continuous-wave” (CW) methods, compromise values  $\Omega_1 \sim 1/(T_1 T_2)^{1/2}$  are used. However, some refined field-pulsing techniques (see the literature recommended in Sec. 5.1 of the lecture notes) enable operation with higher rotating fields and hence higher output signals.

<sup>182</sup> It is straightforward to use Eqs. (\*\*) to verify that at  $T_{1,2} > 0$ , this stationary solution is stable. Note also that the existence of such a stationary state in the rotating reference frame is by no means surprising: as was discussed in Sec. 7.7 of the lecture notes, in the absence of the ac field ( $\Omega_1 = 0$ ), the spin precession decays ( $\langle S_{x,y} \rangle \rightarrow 0$ ) at times  $\sim T_2$ , while  $\langle S_z \rangle$  relaxes to the stationary value  $S_e$  at times  $\sim T_1$ . The rotating magnetic field, perceived constant in the rotating reference frame, just displaces these stationary values. This means that in the initial (“lab”) reference frame, the vector  $\langle \mathbf{S} \rangle$  rotates with the angular velocity  $\omega$ , being “dragged” by the rotating field.

<sup>183</sup> As a reminder: FWHM = Full Width at Half-Maximum – see, e.g., Sec. 2.5.

The analyzed effect of resonance broadening due to environment is much more general than the considered model. First of all, the external field's rotation ("circular polarization") assumed in this model is needed only to make the result (\*\*\*) exact for an arbitrary frequency of the field. Indeed, a linearly-polarized ac field may be always represented as a sum of two fields that are circularly polarized in opposite directions, i.e. described by our model with equal but opposite values of  $\omega$ . If the field amplitude and the environmental coupling are sufficiently small ( $\Omega_1, 1/T_{1,2} \ll \Omega_0$ ), the effects of these two rotating fields just add up, and at small detuning of one of them,  $\xi \equiv \omega - \Omega_0 \rightarrow 0$ , leading to the sharp resonance (\*\*\*), the effect of its counterpart is negligible.

Second, as was discussed in Sec. 6.5 of the lecture notes, even if a quantum system has many discrete energy levels, its weak monochromatic perturbation with a frequency  $\omega$  close to one of the quantum transition frequencies  $\omega_{nn'}$  causes substantial Rabi oscillations of occupations of only two involved energy levels, just as in a genuine two-level system as the spin  $1/2$ . In the presence of weak coupling to the environment, the equations describing this effect, and hence their solutions are similar to those discussed above. This means, in particular, that the environment coupling modifies Eq. (\*\*) in the solution of Problem 6.18 as

$$\varepsilon(\omega) - \varepsilon_0 = nZ \frac{q^2}{\hbar} \sum_{n>0} \frac{|x_{n0}|^2}{\omega_{n0} - \omega} \equiv nZ \frac{q^2}{2m} \sum_{n>0} \frac{f_n}{\omega_{n0}(\omega_{n0} - \omega)} \rightarrow nZ \frac{q^2}{2m} \sum_{n>0} \frac{f_n}{\omega_{n0}[(\omega_{n0} - \omega) - i\delta_n]}, \quad (****)$$

i.e. broadens each resonance just as it does in classical systems,<sup>184</sup> even though the resonance's half-widths  $\delta_n$  depend on the strength and the type of environmental coupling. (For the case of electromagnetic coupling, such spectral linewidth will be calculated in Sec. 9.3.) From general electrodynamics, the electromagnetic energy's dissipation, in particular the EM wave absorption, is described by the imaginary part of the complex dielectric constant  $\varepsilon(\omega)$ . As Eq. (\*\*\*\*) shows,

$$\varepsilon''(\omega) \equiv \text{Im} \varepsilon(\omega) = nZ \frac{q^2}{2m} \sum_{n>0} \frac{f_n \delta_n}{\omega_{n0} [(\omega_{n0} - \omega)^2 + \delta_n^2]},$$

i.e. the dissipation peaks near each quantum transition frequency  $\omega_{nn'}$ . (In Problem 6.18, only transitions from the ground state, with  $n' = 0$ , were considered.) Note that in the limit  $\delta_n \rightarrow 0$ , the last expression tends to Eq. (\*\*\*\*) of that problem's solution, making the appeal to the Kramers-Kronig formula unnecessary.

**Problem 7.14.** Use the Bloch equations (see the solution of Problem 12) to analyze the dynamics of spin- $1/2$  with gyromagnetic ratio  $\gamma$  under the effect of an external ac magnetic field with a relatively low frequency  $\omega$  and/or large amplitude  $\mathcal{B}_{\max}$  (so that  $|\gamma \mathcal{B}_{\max}| \gg \omega, 1/T_{1,2}$ ), assuming that the constants  $T_{1,2}$  are field-independent.

*Solution:* With the direction of the applied field taken for the  $z$ -axis, the Bloch equations, rewritten for the complex lateral components

$$\langle S_{\pm} \rangle \equiv \langle S_x \rangle \pm i \langle S_y \rangle,$$

read

<sup>184</sup> See, e.g., CM Eq. (5.17) and EM (7.32).

$$\langle \dot{S}_{\pm} \rangle = \pm i\Omega(t)\langle S_{\mp} \rangle - \frac{\langle S_{\pm} \rangle}{T_2}, \quad \langle \dot{S}_z \rangle = -\frac{\langle S_z \rangle - S_e(t)}{T_1}, \quad (*)$$

where, in our current case, the spin precession frequency (4.163) is a sinusoidal function of time:

$$\Omega(t) = -\gamma\mathcal{B}(t) = \Omega_{\max} \sin \omega t,$$

so the quasi-equilibrium value of  $S_z$  (see the solution of Problem 12) changes in time as

$$S_e(t) = \frac{\hbar}{2} \tanh \frac{\hbar\Omega(t)}{k_B T} = \frac{\hbar}{2} \tanh \left( \frac{\hbar\Omega_{\max}}{k_B T} \sin \omega t \right). \quad (**)$$

The two equations (\*) are decoupled and thus may be analyzed separately.

Due to our problem's strong condition, during the dominating part of the field oscillation period, the frequency  $\Omega(t)$  is much higher than  $\omega$  and than the spin relaxation rates  $1/T_1$  and  $1/T_2$ . In this case, the only effect of the relatively small dephasing term in the first of Eqs. (\*) is limiting the depth of the system's memory of its initial conditions, making it possible to use the so-modified solution of Problem 5.2 to write

$$\langle S_{\pm} \rangle(t) = \frac{\hbar}{2} \exp\{\pm i\varphi(t)\}, \quad \text{with } \varphi(t) = \int_{-\infty}^t \Omega(t') dt' + \tilde{\varphi}(t),$$

where the term  $\tilde{\varphi}(t)$  describes a relatively slow phase diffusion due to the dephasing effect of the environment.<sup>185</sup>

The second of Eqs. (\*) is a linear ordinary differential equation, and its solution may be expressed in a direct *Duhamel integral* form. Just for the benefit of the readers who have not yet encountered this general and very useful *method of variable coefficients*,<sup>186</sup> we look for the solution in the form

$$\langle S_z \rangle(t) = C(t) \exp\left\{-\frac{t}{T_1}\right\},$$

because this exponent gives the solution of the corresponding homogeneous equation (with  $S_e = 0$ ). Plugging this solution into the full (inhomogeneous) Bloch equation for  $\langle S_z \rangle$ , we get a simple equation

$$\dot{C} \exp\left\{-\frac{t}{T_1}\right\} = \frac{S_e(t)}{T_1}, \quad \text{i.e. } \dot{C} = \exp\left\{\frac{t}{T_1}\right\} \frac{S_e(t)}{T_1},$$

which may be readily integrated, giving

$$C(t) = \frac{1}{T_1} \int_{-\infty}^t \exp\left\{\frac{t'}{T_1}\right\} S_e(t') dt', \quad \text{so } \langle S_z \rangle(t) = \frac{1}{T_1} \int_{-\infty}^t \exp\left\{-\frac{t-t'}{T_1}\right\} S_e(t') dt'.$$

Solid lines on the two panels of the figure below show this result, with the account of Eq. (\*\*), for small and large values of the ratio  $\hbar\Omega_{\max}/k_B T$ , both for several representative values of the product

<sup>185</sup> The Bloch equations are insufficient for the full characterization of this diffusion but from the analysis in Secs. 7.3-7.4, we may conclude that it obeys the diffusion equation (7.85) and that for the case of thermal fluctuations ( $k_B T \gg \hbar\Omega_{\max}$ ), the corresponding diffusion coefficient is given by Eq. (7.142).

<sup>186</sup> Admittedly, this approach was already used in the model solution of Problem 8, without much explanation.

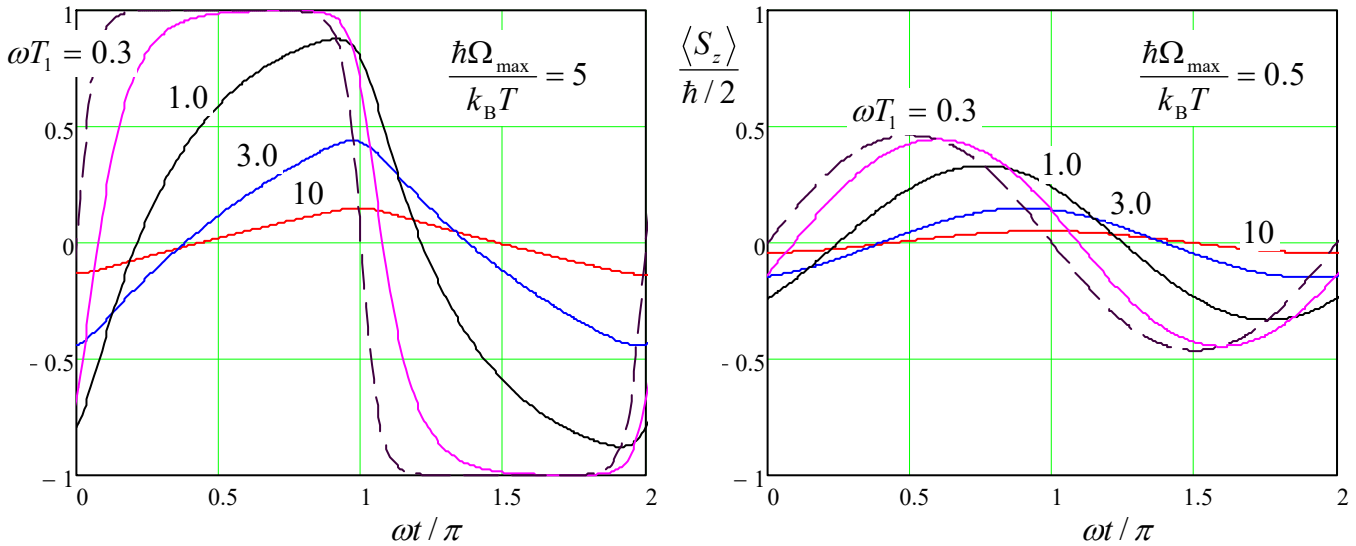
$\omega T_1$ , while the dashed lines show the function  $S_e(t)$ . The plots demonstrate that at relatively low frequencies,  $\omega \ll 1/T_1$ , the expectation value of  $S_z$  faithfully follows its quasi-equilibrium value  $S_e(t)$  (which is a square-wave-like function of time at  $\hbar\Omega_{\max} \gg k_B T$  and sinusoidal in the opposite limit), while at high frequencies, it substantially lags behind the field variations. For example, in the low-field limit,  $\hbar\Omega_{\max} \ll k_B T$ , when  $S_e(t)$  changes sinusoidally,

$$S_e(t) \approx \frac{\hbar \hbar\Omega_{\max}}{2 k_B T} \sin \omega t,$$

the above Duhamel integral for  $\langle S_z \rangle$  may be readily worked out for an arbitrary  $\omega T_1$ :

$$\begin{aligned} \langle S_z \rangle(t) &\approx \frac{\hbar \hbar\Omega_{\max}}{2 k_B T} \frac{1}{T_1} \int_{-\infty}^t \exp\left\{-\frac{t-t'}{T_1}\right\} \sin \omega t' dt' = \frac{\hbar \hbar\Omega_{\max}}{2 k_B T} \frac{1}{T_1} \text{Im} \int_{-\infty}^t \exp\left\{-\frac{t-t'}{T_1} + i\omega t'\right\} dt' \\ &= \frac{\hbar \hbar\Omega_{\max}}{2 k_B T} \frac{1}{T_1} \text{Im} \frac{\exp\{i\omega t\}}{-1/T_1 + i\omega} \equiv \frac{\hbar \hbar\Omega_{\max}}{2 k_B T} \frac{\sin \omega t - \omega T_1 \cos \omega t}{(\omega T_1)^2 + 1}, \end{aligned}$$

showing that at  $\omega T_1 \rightarrow \infty$ , the lag of the function  $\langle S_z \rangle(t)$  behind  $S_e(t)$  reaches a quarter of the field period, and its amplitude drops as  $1/\omega T_1$ . (The last conclusion is valid for any  $\hbar\Omega_{\max}/k_B T$  ratio.)



**Problem 7.15.** Derive Eq. (7.220) of the lecture notes from Eq. (7.222).

*Solution:* Spelling out both anticommutators in Eq. (7.222), we get

$$\dot{\hat{w}} = -\delta \left[ (n_e + 1) \left( \hat{a}^\dagger \hat{a} \hat{w} + \hat{w} \hat{a}^\dagger \hat{a} - 2 \hat{a} \hat{w} \hat{a}^\dagger \right) + n_e \left( \hat{a} \hat{a}^\dagger \hat{w} + \hat{w} \hat{a} \hat{a}^\dagger - 2 \hat{a}^\dagger \hat{w} \hat{a} \right) \right].$$

For the matrix elements in the (time-independent) basis of the Fock states  $n$ , this equation yields:

$$\dot{w}_{mm'} \equiv \langle n | \dot{\hat{w}} | n' \rangle = -\delta \times \left[ \begin{aligned} &(n_e + 1) \left( \langle n | \hat{a}^\dagger \hat{a} \hat{w} | n' \rangle + \langle n | \hat{w} \hat{a}^\dagger \hat{a} | n' \rangle - 2 \langle n | \hat{a} \hat{w} \hat{a}^\dagger | n' \rangle \right) \\ &+ n_e \left( \langle n | \hat{a} \hat{a}^\dagger \hat{w} | n' \rangle + \langle n | \hat{w} \hat{a} \hat{a}^\dagger | n' \rangle - 2 \langle n | \hat{a}^\dagger \hat{w} \hat{a} | n' \rangle \right) \end{aligned} \right]. \quad (*)$$

Let us simplify all bra-kets on the right-hand side of this equation by using Eqs. (5.89) and their Hermitian conjugates:

$$\hat{a}|n'\rangle = n'^{1/2}|n'-1\rangle, \quad \hat{a}^\dagger|n'\rangle = (n'+1)^{1/2}|n'+1\rangle, \quad \langle n|\hat{a} = (n+1)^{1/2}\langle n+1|, \quad \langle n|\hat{a}^\dagger = n^{1/2}\langle n-1|.$$

For the first term on the right-hand side of Eq. (\*), acting by the creation and annihilation operators sequentially upon the immediately adjacent state vectors, we get

$$\langle n|\hat{a}^\dagger\hat{a}\hat{w}|n'\rangle = n^{1/2}\langle n-1|\hat{a}\hat{w}|n'\rangle = n^{1/2}n^{1/2}\langle n|\hat{w}|n'\rangle \equiv nw_{nn'}.$$

Similarly, the second term,

$$\langle n|\hat{w}\hat{a}^\dagger\hat{a}|n'\rangle = n'^{1/2}\langle n-1|\hat{w}\hat{a}^\dagger|n'-1\rangle = n'^{1/2}n'^{1/2}\langle n|\hat{w}|n'\rangle \equiv n'w_{nn'},$$

is proportional to the same matrix element. However, the third term, with the density operator sandwiched between two creation and annihilation operators, is different, and may be calculated in a single shot:

$$\langle n|\hat{a}\hat{w}\hat{a}^\dagger|n'\rangle = (n+1)^{1/2}(n'+1)^{1/2}\langle n+1|\hat{w}|n'+1\rangle \equiv (n+1)^{1/2}(n'+1)^{1/2}w_{n+1,n'+1}.$$

Performing absolutely similar transformations of the remaining three bra-kets, we arrive at the equation

$$\dot{w}_{nn'} = -\delta \times \left\{ \begin{array}{l} (n_e + 1) \left[ nw_{nn'} + n'w_{nn'} - 2(n+1)^{1/2}(n'+1)^{1/2}w_{n+1,n'+1} \right] \\ + n_e \left[ (n+1)w_{nn'} + (n'+1)w_{nn'} - 2n^{1/2}n'^{1/2}w_{n-1,n'-1} \right] \end{array} \right\},$$

which differs from Eq. (7.220) only by a different grouping of the terms on its right-hand side.

**Problem 7.16.** For a harmonic oscillator with weak Ohmic dissipation, use Eq. (7.220) of the lecture notes to find the time evolution of the expectation value  $\langle E \rangle$  of the oscillator's energy for an arbitrary initial state, and compare the result with that following from the Heisenberg-Langevin approach.

*Solution:* Writing Eq. (7.220) for the diagonal elements  $W_n \equiv w_{nn}$  of the density matrix, i.e. for the probabilities to find the oscillator on its  $n^{\text{th}}$  energy level,

$$\dot{W}_n = 2\delta \left\{ (n+1)(n_e + 1)W_{n+1} + nn_e W_{n-1} - [(n+1)n_e + n(n_e + 1)]W_n \right\},$$

and plugging it into the expression for the expectation value of the oscillator's energy (referred, for calculation convenience, to its ground-state level  $\hbar\omega_0/2$ ),

$$\langle E \rangle = \hbar\omega_0 \sum_{n=1}^{\infty} nW_n, \quad \text{so} \quad \frac{d}{dt}\langle E \rangle = \hbar\omega_0 \sum_{n=1}^{\infty} n\dot{W}_n.$$

we get

$$\frac{d}{dt}\langle E \rangle = 2\delta \hbar\omega_0 \sum_{n=1}^{\infty} n \left\{ (n+1)(n_e + 1)W_{n+1} + nn_e W_{n-1} - [(n+1)n_e + n(n_e + 1)]W_n \right\}.$$

$$\equiv 2\delta\hbar\omega_0 \left\{ \sum_{n=1}^{\infty} n(n+1)(n_e+1)W_{n+1} + \sum_{n=1}^{\infty} n^2 n_e W_{n-1} - \sum_{n=1}^{\infty} n[(n+1)n_e + n(n_e+1)]W_n \right\}.$$

Let us replace the summation index  $n$  with  $(n-1)$  in the first sum, and with  $(n+1)$  in the second sum. This gives us

$$\begin{aligned} \frac{d}{dt}\langle E \rangle &= 2\delta\hbar\omega_0 \left\{ \sum_{n=2}^{\infty} (n-1)n(n_e+1)W_n + \sum_{n=0}^{\infty} (n+1)^2 n_e W_n - \sum_{n=1}^{\infty} n[(n+1)n_e + n(n_e+1)]W_n \right\} \\ &\equiv 2\delta\hbar\omega_0 \sum_{n=0}^{\infty} (n_e - n)W_n \equiv 2\delta(E_e - \langle E \rangle), \end{aligned} \quad (*)$$

where  $E_e$  is the energy's equilibrium value:

$$E_e \equiv \hbar\omega_0 \sum_{n=0}^{\infty} n_e W_n = \hbar\omega_0 n_e \sum_{n=0}^{\infty} W_n = \hbar\omega_0 n_e.$$

Since this value is time-independent, Eq. (\*) may be rewritten as

$$\frac{d}{dt}\tilde{E} = -2\delta\tilde{E}, \quad \text{where } \tilde{E} \equiv \langle E \rangle - E_e,$$

and has a simple solution,

$$\tilde{E}(t) = \tilde{E}(0)\exp\{-2\delta t\}, \quad \text{i.e. } \langle E \rangle(t) = E_e + [\langle E \rangle(0) - E_e]\exp\{-2\delta t\}, \quad (**)$$

describing the exponential-law transient of the energy from its initial value to the equilibrium one.

It is remarkable that this very simple result<sup>187</sup> is valid for an arbitrary initial distribution of the probabilities  $W_n$  (even though their time evolution may be rather involved – see Fig. 7.8 of the lecture notes), and for arbitrary phase shifts between the initial Fock states (because, according to Eq. (7.220) the off-diagonal elements of the density matrix of the oscillator do not affect the evolution of its diagonal elements.)

Now proceeding to the Heisenberg-Langevin approach to the same problem, we may start from Eq. (7.145) of the lecture notes:

$$m\ddot{\hat{x}} + \eta\dot{\hat{x}} + m\omega_0^2\hat{x} = \hat{F}(t). \quad (***)$$

Looking for a solution of the corresponding homogeneous equation in the usual form  $\exp\{\lambda t\}$ , we get the following well-known<sup>188</sup> characteristic equation

$$\lambda^2 + \frac{\eta}{m}\lambda + \omega_0^2 = 0,$$

whose roots may be simplified in the low-damping limit:

$$\lambda_{\pm} \approx \pm i\omega_0 - \frac{\eta}{2m} \equiv \pm i\omega_0 - \delta.$$

<sup>187</sup> This is the same law as given by classical mechanics – see, e.g., CM Sec. 5.1, besides that in this limit,  $E_e = 0$ .

<sup>188</sup> See, e.g., the same CM Sec. 5.1.



This means that in the absence of the external force  $F(t)$ , all linear operators ( $\hat{x}, \hat{p}, \hat{a}, \hat{a}^\dagger$ , etc.) of the system depend on time as  $\exp\{(\pm i\omega_0 - \delta)t\}$ , so their Hermitian quadratic forms (such as the energy) are proportional to the modulus square of this function, i.e. to  $\exp\{-2\delta t\}$ .

Due to the linearity of Eq. (\*\*), its solution may be represented as the sum of stationary fluctuations induced by the force described by its right-hand side, and the exponentially decaying oscillations due to the initial conditions. Since these two processes are independent of each other (mutually incoherent), their energies may be just added up:

$$\langle E \rangle(t) = E_e + C \exp\{-2\delta t\}.$$

Selecting the constant  $C$  in this expression so that at  $t = 0$ , it coincides with the initial energy  $\langle E \rangle(0)$ , we get

$$\langle E \rangle(t) = \langle E \rangle(0) \exp\{-2\delta t\} + E_e (1 - \exp\{-2\delta t\}),$$

i.e. the same result as follows from the density matrix approach – cf. Eq. (\*\*). We see that calculations using the Heisenberg-Langevin formalism are indeed much simpler – as is usual when it works, i.e. for linear systems.

**Problem 7.17.** Derive Eq. (7.234) of the lecture notes in an alternative way – by using an expression dual to Eq. (4.244).

*Solution:* We need to calculate the diagonal matrix element of the operator  $[\hat{x}, [\hat{x}, \hat{w}]]$  in the momentum representation. First, let us rewrite each component of this element by using (twice in each product) the closure condition (4.220) written for the eigenstates  $p$  of the momentum operator:

$$\begin{aligned} \langle p | [\hat{x}, [\hat{x}, \hat{w}]] | p \rangle &= \langle p | [\hat{x}(\hat{x}\hat{w} - \hat{w}\hat{x}) - (\hat{x}\hat{w} - \hat{w}\hat{x})\hat{x}] | p \rangle \equiv \langle p | [\hat{x}\hat{I}(\hat{x}\hat{I}\hat{w} - \hat{w}\hat{I}\hat{x}) - (\hat{x}\hat{I}\hat{w} - \hat{w}\hat{I}\hat{x})\hat{I}\hat{x}] | p \rangle \\ &= \int dp' \langle p | \hat{x} | p' \rangle \int dp'' [\langle p' | \hat{x} | p'' \rangle w(p'', p) - w(p', p'') \langle p'' | \hat{x} | p \rangle] \\ &\quad - \int dp'' \langle p'' | \hat{x} | p \rangle \int dp' [\langle p | \hat{x} | p' \rangle w(p', p'') - w(p, p') \langle p' | \hat{x} | p'' \rangle], \end{aligned} \quad (*)$$

thus expressing it via the matrix elements of the coordinate operator in this representation. On the other hand, reproducing, for the momentum representation, the discussion that has led us from Eq. (4.240) to Eq. (4.245), we may readily get a formula dual to Eq. (4.244):

$$\int dp' \langle \hat{p} | \hat{x} | \hat{p}' \rangle \varphi(p') = i\hbar \frac{\partial}{\partial p} \varphi(p), \quad (**)$$

where  $\varphi(p)$  is an arbitrary wavefunction in the momentum representation. In order to make calculations more compact, we may use the definition of the delta function to represent Eq. (\*\*) in a shorthand form

$$\langle \hat{p} | \hat{x} | \hat{p}' \rangle = i\hbar \frac{\partial}{\partial p} \delta(p - p'). \quad (***)$$

This relation may look a bit intimidating because it apparently requires one to differentiate the delta function explicitly. However, the symmetric nature of the commutators to be evaluated eliminates

the need to do that.<sup>189</sup> Indeed, let us start by using Eq. (\*\*\*) to spell out the inner integral (over  $p''$ ) in the first term on the right-hand side of the last form of Eq. (\*):

$$\begin{aligned} & \int dp'' \left[ \langle p' | \hat{x} | p'' \rangle w(p'', p) - w(p', p'') \langle p'' | \hat{x} | p \rangle \right] \\ &= i\hbar \int dp'' \left[ \frac{\partial}{\partial p'} \delta(p' - p'') w(p'', p) - w(p', p'') \frac{\partial}{\partial p''} \delta(p'' - p) \right]. \end{aligned}$$

Differentiating the product  $\delta(p' - p'') w(p'' - p)$  by parts, and noticing that the derivative of the delta function  $\delta(p' - p'')$  is nonvanishing only at  $p' \rightarrow p''$ , we see that, after the forthcoming integration over  $p''$ , the terms with such derivatives cancel, so in this sense, the inner integral reduces to

$$i\hbar \int dp'' \delta(p' - p'') \frac{\partial}{\partial p''} w(p'', p) = i\hbar \frac{\partial}{\partial p'} w(p', p).$$

The inner integral (over  $p'$ ) in the second term of Eq. (\*) is similar, with the replacements  $p' \rightarrow p$ , and  $p \rightarrow p''$ , giving (also, in the sense of the forthcoming integration over  $p''$ ):

$$\int dp' \left[ \langle p | \hat{x} | p' \rangle w(p', p'') - w(p, p') \langle p' | \hat{x} | p'' \rangle \right] \rightarrow i\hbar \frac{\partial}{\partial p} w(p, p'').$$

Now let us change the notation from  $p''$  to  $p'$  in the second term of Eq. (\*) and then merge both terms on its right-hand side:

$$\begin{aligned} \langle p | [\hat{x}, [\hat{x}, \hat{w}]] | p \rangle &= \int dp' \left[ \langle p | \hat{x} | p' \rangle i\hbar \frac{\partial}{\partial p'} w(p', p) - i\hbar \frac{\partial}{\partial p} w(p, p') \langle p' | \hat{x} | p \rangle \right] \\ &= -\hbar^2 \int dp' \left[ \frac{\partial}{\partial p} \delta(p - p') \frac{\partial}{\partial p'} w(p', p) - \frac{\partial}{\partial p} w(p, p') \frac{\partial}{\partial p'} \delta(p - p') \right], \end{aligned}$$

so by repeating the same arguments as were used for the inner integrals, we get a simple result,

$$\langle p | [\hat{x}, [\hat{x}, \hat{w}]] | p \rangle = -\hbar^2 \int dp' \delta(p - p') \frac{\partial}{\partial p} \frac{\partial}{\partial p'} w(p', p) = -\hbar^2 \frac{\partial^2}{\partial p^2} w(p),$$

which is equivalent to Eq. (7.234). (Its derivation described in Sec. 7.6 of the lecture notes is arguably more elegant.)

<sup>189</sup> The reader who is reluctant to trust such high-riding is encouraged to reproduce the following calculation in a (longer) integral form, by using Eq. (\*\*).

## Chapter 8. Multiparticle Systems

**Problem 8.1.** Prove that Eq. (8.30) of the lecture notes indeed yields  $E_g^{(1)} = (5/4)E_H$ .

*Solution:* According to Eq. (8.30), we need to calculate

$$E_g^{(1)} = \frac{1}{(\pi r_0^3)^2} \int \exp\left\{-\frac{2r_1}{r_0}\right\} d^3 r_1 \int \exp\left\{-\frac{2r_2}{r_0}\right\} d^3 r_2 \frac{e^2}{4\pi\epsilon_0 |\mathbf{r}_1 - \mathbf{r}_2|}.$$

Instead of calculating this 6D integral directly, we may notice that this is just the classical energy of the Coulomb interaction<sup>1</sup> of two independent distributed electrostatic charges with similar spherically symmetric densities:

$$\rho(r) = \frac{e}{\pi r_0^3} \exp\left\{-\frac{2r}{r_0}\right\}.$$

The (radially directed) electric field  $\mathcal{E}$  induced by any one of these charges may be readily calculated by applying the Gauss law<sup>2</sup> to a sphere of radius  $r$  :

$$4\pi r^2 \mathcal{E}(r) = \frac{Q}{\epsilon_0} \equiv \frac{1}{\epsilon_0} \int_{r' < r} \rho(r') d^3 r' \equiv \frac{1}{\epsilon_0} \frac{e}{\pi r_0^3} 4\pi \int_0^r \exp\left\{-\frac{2r'}{r_0}\right\} r'^2 dr' \equiv \frac{e}{2\epsilon_0} \int_0^{2r/r_0} \exp\{-\xi\} \xi^2 d\xi,$$

where  $\xi \equiv 2r'/r_0$ . The last (dimensionless) integral may be readily worked out by parts; its indefinite form is  $\exp\{-\xi\}(-\xi^2 - 2\xi - 2)$ , so after the limit substitution, we get

$$\mathcal{E}(r) = \frac{e}{4\pi\epsilon_0 r^2} \left[ \exp\left\{-\frac{2r}{r_0}\right\} \left( -\frac{2r^2}{r_0^2} - \frac{2r}{r_0} - 1 \right) + 1 \right].$$

The second charge creates an absolutely similar field, so  $\mathcal{E}_{\text{total}} = 2\mathcal{E}(r)$ , and using the well-known expression for the electric field energy,<sup>3</sup> the Coulomb energy of interaction of these two distributed charges may be calculated as

$$\begin{aligned} E_{\text{int}} &\equiv E_{\text{total}} - 2E_{\text{partial}} = \frac{\epsilon_0}{2} \int [2\mathcal{E}(r)]^2 d^3 r - 2 \frac{\epsilon_0}{2} \int [\mathcal{E}(r)]^2 d^3 r \equiv \epsilon_0 \int [\mathcal{E}(r)]^2 d^3 r = 4\pi\epsilon_0 \int_0^\infty [\mathcal{E}(r)]^2 r^2 dr \\ &= \frac{e^2}{4\pi\epsilon_0} \int_0^\infty \left[ \exp\left\{-\frac{2r}{r_0}\right\} \left( -\frac{2r}{r_0^2} - \frac{2}{r_0} - \frac{1}{r} \right) + \frac{1}{r} \right]^2 dr \equiv \frac{e^2}{4\pi\epsilon_0} \frac{1}{2r_0} \int_0^\infty \left[ \exp\{-\xi\} \left( \xi + 2 + \frac{2}{\xi} \right) - \frac{2}{\xi} \right]^2 d\xi, \end{aligned}$$

where  $\xi \equiv 2r/r_0$  again. The last integral may be readily calculated by squaring the brackets and integrating each of the resulting terms by parts.<sup>4</sup> The result equals 5/4, so using the fact that for helium ( $Z = 2$ ),  $r_0 \equiv r_B/Z = r_B/2$ , we finally get

<sup>1</sup> See, e.g., EM Eqs. (1.38) and (1.55).

<sup>2</sup> See, e.g., EM Eq. (1.16).

<sup>3</sup> See, e.g., EM Eq. (1.65).

<sup>4</sup> Alternatively, we may use, for most of them, the table integral MA (6.7d) with the corresponding values of  $n$ .

$$E_g^{(1)} = E_{\text{int}} = \frac{e^2}{4\pi\epsilon_0} \frac{1}{2r_0} \frac{5}{4} \equiv \frac{5}{4} \frac{e^2}{4\pi\epsilon_0 r_B} \equiv \frac{5}{4} E_H,$$

i.e. the result used in Sec. 8.2 of the lecture notes.

**Problem 8.2.** For a dilute gas of helium atoms in their ground state, with  $n$  atoms per unit volume, calculate its weak-field

- (i) electric susceptibility  $\chi_e$ , and
- (ii) magnetic susceptibility  $\chi_m$ ,

and compare the results.

*Hint:* You may use the results of the variational description of the helium atom's ground state in Sec. 8.2 of the lecture notes, and the model solutions of Problems 6.8 and 6.15.

*Solutions:*

(i) As was discussed in the model solution of Problem 6.8, the atomic polarizability of the hydrogen atom, in its ground state, is

$$\alpha = 4\pi\epsilon_0 \frac{9}{2} r_B^3, \quad (*)$$

where  $r_B$  is the Bohr radius (1.13). Rescaling this result for a hydrogen-like “atom” (or rather a positive ion) with the nuclear charge  $Q = Ze$  and one bound electron, we get

$$\alpha = 4\pi\epsilon_0 \frac{9}{2} \frac{r_B^3}{Z^4}. \quad (**)$$

Indeed, Eq. (\*) is just a representation of the following result of the solution of Problem 6.8: the ion's energy change due to the applied electric field  $\mathcal{E}$  is

$$\Delta E = -\frac{9}{2} \frac{r_B^2}{E_H} \frac{e^2 \mathcal{E}^2}{2}, \quad (***)$$

where  $E_H$  is the Hartree energy unit (1.9). As was discussed in Sec. 3.6 of the lecture notes, for the Bohr-like atom/ion with  $Q = Ze$ ,  $r_B$  should be replaced with  $r_0 = r_B/Z$ , and  $E_H$ , with  $E_0 = E_H Z^2$ , so instead of Eq. (\*\*\*) we get

$$\Delta E = -\frac{9}{2} \frac{(r_B/Z)^2}{(E_H Z^2)} \frac{e^2 \mathcal{E}^2}{2} \equiv -\frac{9}{2Z^4} \frac{r_B^2}{E_H} \frac{e^2 \mathcal{E}^2}{2},$$

immediately giving Eq. (\*\*).

Now taking  $Z$  equal to its variational-optimized value (8.34),  $Z_{\text{ef}} = 2 - 5/16 \equiv 27/16$ ,<sup>5</sup> adding the contributions from two electrons of the helium atom, and using the general formulas for the atomic susceptibility,<sup>6</sup>  $\alpha = -\Delta E/(\mathcal{E}^2/2)$ , and for the Hartree energy,  $E_H = e^2/4\pi\epsilon_0 r_B$ , we get

<sup>5</sup> As was mentioned in Sec. 8.2 of the lecture notes, this variational approach describes experimental results with an accuracy better than 1%.

<sup>6</sup> See, e.g., the model solution of Problem 6.8(iii).

$$\frac{\alpha_{\text{He}}}{4\pi\epsilon_0} = 2 \cdot \frac{9}{2} \frac{r_{\text{B}}^3}{(27/16)^4} \approx 1.11 r_{\text{B}}^3.$$

In a diluted gas (with a volumic density  $n \ll r_{\text{B}}^{-3}$ ), the atom interactions are negligible, so their induced electric dipole moments  $\mathbf{d} = \alpha\mathcal{E}$  just add up. As a result, according to the basic electrostatics,<sup>7</sup> such a linear isotropic polarization may be readily recalculated into the electric susceptibility:

$$(\chi_e)_{\text{He}} = \frac{n\alpha_{\text{He}}}{\epsilon_0} \approx 1.11 \times 4\pi n r_{\text{B}}^3 \ll 1.$$

(ii) As was discussed in Sec. 8.2 of the lecture notes, the ground state of the helium atom is a spin singlet, with a zero net spin:  $S = M_S = 0$ . As a result, the atom does not have electron-spin paramagnetism, and its magnetic susceptibility is due to the orbital diamagnetism of the electrons.<sup>8</sup> Since, according to the discussion in Sec. 8.2 of the lecture notes, the orbital ground state of each electron is very close to that of a hydrogen-like atom, with the effective nuclear charge  $Z_{\text{ef}} = 2 - 5/16 \equiv 27/16$ , we may use the solution of Problem 6.15 for an arbitrary single-electron system,

$$(\chi_m)_{\text{single}} = -\frac{2\pi}{3} n \alpha^2 r_{\text{B}} \langle r^2 \rangle,$$

(where  $\alpha \approx 1/137$  is the fine structure constant), by adding equal contributions to  $\chi_m$  from two electrons, to write

$$(\chi_m)_{\text{He}} = -2 \cdot \frac{2\pi}{3} n \alpha^2 r_{\text{B}} \langle r_1^2 \rangle_{\text{H with } Z \rightarrow Z_{\text{ef}}}.$$

This expectation value of  $r^2$ , for a hydrogen-like atom/ion in its ground state, may be readily calculated by using Eq. (3.208):<sup>9</sup>

$$\langle r_1^2 \rangle = \oint_{4\pi} |Y_0^0(\theta, \varphi)|^2 d\Omega \int_0^\infty r^2 |\mathcal{R}_{1,0}(r)|^2 r^2 dr = \frac{4}{r_0^3} \int_0^\infty r^4 e^{-2r/r_0} dr \equiv \frac{r_0^2}{8} \int_0^\infty \xi^4 e^{-\xi} d\xi,$$

with  $\xi \equiv 2r/r_0$ . This is a well-known integral,<sup>10</sup> equal to  $4! \equiv 24$ , so

$$\langle r_1^2 \rangle = 3r_0^2,$$

where, according to Eqs. (1.13) and (3.192),  $r_0 = r_{\text{B}}/Z$ . Now making the replacement  $Z \rightarrow Z_{\text{ef}} = 27/16$ , we get

$$(\chi_m)_{\text{He}} = -2 \frac{2\pi}{3} n \alpha^2 r_{\text{B}} \frac{3r_{\text{B}}^2}{Z_{\text{ef}}^2} = -4\pi \left( \frac{16}{27} \right)^2 \alpha^2 n r_{\text{B}}^3.$$

<sup>7</sup> See, e.g., EM Sec. 3.3, in particular, Eqs. (3.44) and (3.50).

<sup>8</sup> Strictly speaking, we also should consider the (very weak) nuclear spin paramagnetism of the atom, but since protons are also spin- $1/2$  fermions, the ground state of the helium nucleus may be also considered as a spin singlet (despite the strong interaction of its protons), making its net spin equal to zero as well.

<sup>9</sup> As a reminder, the spherical harmonics and the radial wavefunctions (including  $\mathcal{R}_{1,0}$ ) listed in Chapter 3 are already normalized – see Eqs. (3.173) and (3.194).

<sup>10</sup> See, e.g., MA Eq. (6.7d) with  $n = 4$ .

Now comparing the results for  $\chi_e$  and  $\chi_m$ , we see that of these two dimensionless parameters (for the same  $n$ ), the magnitude of the latter one is much (by a factor of  $\sim \alpha^{-2} \sim 10^4$ ) smaller. This is very natural, since (as was repeatedly discussed in the EM part of this series) the orbital magnetism is a relativistic effect, which is very small for the effective velocities  $v \sim c/\alpha \sim 10^{-2} c$  of the quantum motion of electrons inside atoms and molecules.

**Problem 8.3.** Calculate the expectation values of the observables  $\mathbf{s}_1 \cdot \mathbf{s}_2$ ,  $S^2 \equiv (\mathbf{s}_1 + \mathbf{s}_2)^2$ , and  $S_z \equiv s_{1z} + s_{2z}$ , for the singlet and triplet states of the system of two spins- $1/2$ , directly – without using the general Eq. (8.48). Compare the results with those for the system of two classical geometric vectors of length  $\hbar/2$  each.

*Solution:* Let us calculate the action of the scalar product operator on the ket-vectors of all states of the uncoupled-representation basis of the system, by first spelling them out and then returning to the shorthand notation. Starting from the state with both spins up:

$$\begin{aligned} \hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2 |\uparrow\uparrow\rangle &= (\hat{s}_{1x}\hat{s}_{2x} + \hat{s}_{1y}\hat{s}_{2y} + \hat{s}_{1z}\hat{s}_{2z}) |\uparrow\uparrow\rangle \equiv (\hat{s}_{1x}\hat{s}_{2x} + \hat{s}_{1y}\hat{s}_{2y} + \hat{s}_{1z}\hat{s}_{2z}) |\uparrow\rangle \otimes |\uparrow\rangle \\ &= \hat{s}_{1x} |\uparrow\rangle \otimes \hat{s}_{2x} |\uparrow\rangle + \hat{s}_{1y} |\uparrow\rangle \otimes \hat{s}_{2y} |\uparrow\rangle + \hat{s}_{1z} |\uparrow\rangle \otimes \hat{s}_{2z} |\uparrow\rangle. \end{aligned}$$

As the reader should know quite well by now (see, e.g., Eq. (4.128) of the lecture notes), for each of the particles:

$$\hat{s}_x |\uparrow\rangle = \frac{\hbar}{2} |\downarrow\rangle, \quad \hat{s}_y |\uparrow\rangle = i \frac{\hbar}{2} |\downarrow\rangle, \quad \hat{s}_z |\uparrow\rangle = \frac{\hbar}{2} |\uparrow\rangle.$$

Since the operators of one spin do not affect the ket-vectors of its counterpart, we get

$$\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2 |\uparrow\uparrow\rangle = \left(\frac{\hbar}{2}\right)^2 (|\downarrow\rangle \otimes |\downarrow\rangle - |\downarrow\rangle \otimes |\downarrow\rangle + |\uparrow\rangle \otimes |\uparrow\rangle) \equiv \left(\frac{\hbar}{2}\right)^2 |\uparrow\rangle \otimes |\uparrow\rangle \equiv \left(\frac{\hbar}{2}\right)^2 |\uparrow\uparrow\rangle. \quad (*)$$

So, the simple (factorable) triplet state  $\uparrow\uparrow$  is indeed an eigenstate of the scalar product's operator, with the eigenvalue  $(\hbar/2)^2$ . An absolutely similar calculation for the opposite simple triplet state,  $\downarrow\downarrow$ , by taking into account that

$$\hat{s}_x |\downarrow\rangle = \frac{\hbar}{2} |\uparrow\rangle, \quad \hat{s}_y |\downarrow\rangle = -i \frac{\hbar}{2} |\uparrow\rangle, \quad \hat{s}_z |\downarrow\rangle = -\frac{\hbar}{2} |\downarrow\rangle,$$

yields a similar result:

$$\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2 |\downarrow\downarrow\rangle = \left(\frac{\hbar}{2}\right)^2 |\downarrow\downarrow\rangle, \quad (**)$$

also corresponding to the initial state. These two results are in agreement with the classical picture of two aligned vectors of length  $\hbar/2$  each.

However, similar calculations for the oppositely directed spin states give quite different results:

$$\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2 |\uparrow\downarrow\rangle = \left(\frac{\hbar}{2}\right)^2 (2|\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle), \quad \hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2 |\downarrow\uparrow\rangle = \left(\frac{\hbar}{2}\right)^2 (2|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle),$$

showing that these states are *not* eigenstates of the scalar product's operator. However, their two linear superpositions: the entangled triplet state (sign +) and the singlet state (sign -), defined by Eqs. (8.18) and (8.20),

$$|s_{\pm}\rangle = \frac{1}{\sqrt{2}} \left( |\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle \right),$$

are eigenstates of this operator:

$$\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2 |s_{\pm}\rangle = \left(\frac{\hbar}{2}\right)^2 \frac{1}{\sqrt{2}} \times \begin{cases} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \\ (-3|\uparrow\downarrow\rangle - 3|\downarrow\uparrow\rangle) \end{cases} \equiv \left(\frac{\hbar}{2}\right)^2 \times \begin{cases} |s_+\rangle, \\ -3|s_-\rangle, \end{cases}$$

though with rather different eigenvalues:

$$\langle \hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2 \rangle_{\pm} = \left(\frac{\hbar}{2}\right)^2 \times \begin{cases} (+1), & \text{for the triplet state } (s_+), \\ (-3), & \text{for the singlet state } (s_-). \end{cases} \quad (***)$$

Note that according to Eqs. (\*)-(\*\*\*), the product's eigenvalue for the entangled triplet state is the same as for both factorable triplet states – the fact rather counter-intuitive for a linear superposition of two states with *oppositely* directed spins as  $s_+$ . The same may be said about the result (\*\*\*) for the singlet state, with its “unnaturally” high modulus; it is obviously in a sharp contradiction with the classical prediction  $\mathbf{s}_1 \cdot \mathbf{s}_2 = -(\hbar/2)^2$  for two equal and antiparallel vectors of magnitude  $\hbar/2$  each.

Let us now consider the total spin operator (8.47),

$$\hat{\mathbf{S}} \equiv \hat{\mathbf{s}}_1 + \hat{\mathbf{s}}_2.$$

By using the fact that the operators of the two partial spins are defined in different Hilbert spaces, and hence commute, we may readily calculate the operator of its square:

$$\hat{S}^2 \equiv \hat{\mathbf{S}} \cdot \hat{\mathbf{S}} \equiv (\hat{\mathbf{s}}_1 + \hat{\mathbf{s}}_2) \cdot (\hat{\mathbf{s}}_1 + \hat{\mathbf{s}}_2) = \hat{\mathbf{s}}_1^2 + \hat{\mathbf{s}}_2^2 + 2\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2. \quad (***)$$

As we know from Chapter 4, squares of all single-particle spin- $1/2$  operators are proportional to the identity operator:

$$\hat{s}_{1,2}^2 \equiv (\hat{s}_x^2 + \hat{s}_y^2 + \hat{s}_z^2)_{1,2} = 3\left(\frac{\hbar}{2}\right)^2 \hat{I}.$$

Hence in any state of the system, the expectation value of the operator (\*\*\*) is

$$\langle S^2 \rangle = 6\left(\frac{\hbar}{2}\right)^2 + 2\langle \mathbf{s}_1 \cdot \mathbf{s}_2 \rangle,$$

so by using Eqs. (\*)-(\*\*\*), we get the same Eq. (8.52),

$$\langle S^2 \rangle = \left(\frac{\hbar}{2}\right)^2 \times \begin{cases} 8, & \text{for all triplet states,} \\ 0, & \text{for the singlet state,} \end{cases}$$

which was obtained in Sec. 8.2 from the general relations (8.48) (valid for any spin), with the quantum number  $S = 1$  for the triplet states and  $S = 0$  for the singlet state – see also the “rectangular diagram” in

Fig. 8.2. (The counter-intuitive nature of this result for the entangled triplet state was already noted at its discussion in the lecture notes.)

However, for the z-component of the vector sum (8.47), the quantum-mechanical result coincides with what we could expect for classical geometric vectors. Indeed, for example,

$$\hat{S}_z |\uparrow\downarrow\rangle \equiv (\hat{s}_{1z} + \hat{s}_{2z}) |\uparrow\rangle \otimes |\downarrow\rangle = \hat{s}_{1z} |\uparrow\rangle \otimes |\downarrow\rangle + |\uparrow\rangle \otimes \hat{s}_{2z} |\downarrow\rangle = |\uparrow\rangle \otimes |\downarrow\rangle - |\uparrow\rangle \otimes |\downarrow\rangle = 0,$$

and similarly for the second component state,  $|\downarrow\uparrow\rangle$ ; hence for both entangled states:

$$\hat{S}_z |s_{\pm}\rangle = 0.$$

This result is again in full agreement with the general theory of the spin addition because, as shown in Fig. 8.2, for both these states, the “magnetic” quantum number  $M_S = (m_s)_1 + (m_s)_2$  is equal to zero. An absolutely similar calculation shows that the factorable states  $|\uparrow\uparrow\rangle$  and  $|\downarrow\downarrow\rangle$  are also eigenstates of the operator  $\hat{S}_z$ , with the eigenvalues, respectively,  $+\hbar$  and  $-\hbar$ , corresponding to  $M_S = \pm 1$  – also in concord with the second of Eqs. (8.48) for the net spin  $S = 1$ , and also with classical expectations.

**Problem 8.4.** Discuss the factors  $\pm 1/\sqrt{2}$  that participate in Eqs. (8.18) and (8.20) of the lecture notes for the entangled states of the system of two spins- $1/2$ , in terms of Clebsh-Gordan coefficients similar to those discussed in Sec. 5.7.

*Solution:* As was discussed in Sec. 8.2 of the lecture notes, the sum (8.47) of two spins has the same properties (8.48) as the sum (5.170) of the orbital and spin angular momenta of a single particle. Hence, for a system of two spins- $1/2$ , we may repeat all the discussion of Sec. 5.7 with the following replacements:

$$\begin{aligned} \hat{\mathbf{L}} &\rightarrow \hat{\mathbf{s}}_1, & \hat{\mathbf{S}} &\rightarrow \hat{\mathbf{s}}_2, & \hat{\mathbf{J}} \equiv \hat{\mathbf{L}} + \hat{\mathbf{S}} &\rightarrow \hat{\mathbf{S}} = \hat{\mathbf{s}}_1 + \hat{\mathbf{s}}_2, \\ l &\rightarrow s_1 = 1/2, & s &\rightarrow s_2 = 1/2, & j \rightarrow S = s_1 \pm s_2 &= \begin{cases} 1 \\ 0 \end{cases}, \\ m_l &\rightarrow m_1 = \pm 1/2, & m_s &\rightarrow m_2 = \pm 1/2, & m_j \rightarrow M &= \begin{cases} 0, & \text{for } S = 0, \\ 0, \pm 1, & \text{for } S = 1, \end{cases} \end{aligned} \quad (*)$$

where the index  $s$  in the magnetic quantum numbers  $m$  and  $M$  are just implied, to avoid an unnecessarily cluttered notation.

With these replacements, instead of the two state groups listed in Eq. (5.182), we get the following two possible bases, of four states each, available for the representation of an arbitrary state of the composite system of two spins- $1/2$ :

- the uncoupled-representation basis: states  $|m_1, m_2\rangle$ , and
- the coupled-representation basis: states  $|S, M\rangle$ .

In particular, as was discussed in Sec. 8.2, and confirmed by the direct calculation in the solution of the previous problem, the entangled states (8.18) and (8.20) belong to the coupled-representation basis, both with  $M_S = 0$ , but with  $S = 1$  for the triplet state, and  $S = 0$  for the singlet state.



Now we may use the replacements (\*) to write the following analogs of Eqs. (5.190) for the Clebsh-Gordan coefficients of the two-particle system:

$$\begin{aligned}\langle m_1 = M - 1/2, m_2 = +1/2 | S = 1/2 \pm 1/2, M \rangle &= \pm \left( \frac{1/2 \pm M + 1/2}{2 \cdot 1/2 + 1} \right)^{1/2} \equiv \pm \frac{1}{\sqrt{2}} (1 \pm M)^{1/2}, \\ \langle m_1 = M + 1/2, m_2 = -1/2 | S = 1/2 \pm 1/2, M \rangle &= \pm \left( \frac{1/2 \mp M + 1/2}{2 \cdot 1/2 + 1} \right)^{1/2} \equiv \pm \frac{1}{\sqrt{2}} (1 \mp M)^{1/2}.\end{aligned}\quad (**)$$

These results are valid for states with any  $S$  and  $M$  of our list. In particular, for the factorable triplet state  $\uparrow\uparrow$ , with  $S = 1$  and  $M = +1$ , these formulas are reduced to

$$\langle m_1 = +1/2, m_2 = +1/2 | S = 1, M = +1 \rangle = 1, \quad \langle m_1 = +3/2, m_2 = -1/2 | S = 1, M = +1 \rangle = 0,$$

while for the factorable triplet state  $\downarrow\downarrow$ , with  $S = 1$  and  $M = -1$ ,

$$\langle m_1 = -3/2, m_2 = +1/2 | S = 1, M = -1 \rangle = 0, \quad \langle m_1 = +1/2, m_2 = -1/2 | S = 1, M = -1 \rangle = 1$$

– both very expectable results. Indeed, for the spins- $1/2$ , states with  $m = \pm 3/2$  simply do not exist, while the two non-zero results mean simply that the factorable triplet states belong to both the coupled- and uncoupled representations:

$$\begin{aligned}|\uparrow\uparrow\rangle &\equiv |m_1 = +1/2, m_2 = +1/2\rangle = |S = 1, M = +1\rangle, \\ |\downarrow\downarrow\rangle &\equiv |m_1 = -1/2, m_2 = -1/2\rangle = |S = 1, M = -1\rangle,\end{aligned}$$

as was already discussed in Sec. 8.2 of the lecture notes – see the top-right and bottom-left points in the “rectangular diagram” shown in Fig. 8.2. On the other hand, for the entangled states, both with  $M = 0$ , Eqs. (\*\*) are reduced to

$$\begin{aligned}\langle m_1 = -1/2, m_2 = +1/2 | S = 1/2 \pm 1/2, M = 0 \rangle &\equiv \langle \downarrow\uparrow | S = 1/2 \pm 1/2, M = 0 \rangle = \pm 1/\sqrt{2}, \\ \langle m_1 = +1/2, m_2 = -1/2 | S = 1/2 \pm 1/2, M = 0 \rangle &\equiv \langle \uparrow\downarrow | S = 1/2 \pm 1/2, M = 0 \rangle = \pm 1/\sqrt{2}.\end{aligned}$$

According to these relations, we may write

$$|S = 1, M = 0\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \equiv |s_+\rangle, \quad |S = 0, M = 0\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \equiv |s_-\rangle,$$

confirming once again the fact that the entangled states  $s_{\pm}$  belong to the coupled-representation basis, with the listed quantum numbers of the net spin.

Thus the factors  $\pm 1/\sqrt{2}$  that participate in the definitions (8.18) and (8.20) of these states may be considered just as particular cases of the Clebsh-Gordan coefficients.

**Problem 8.5.\*** Use the perturbation theory to calculate the so-called *hyperfine splitting* of the ground energy of the hydrogen atom,<sup>11</sup> due to the interaction between the spins of its nucleus (proton) and electron.

<sup>11</sup> This effect was discovered by A. Michelson in 1881 and explained theoretically by W. Pauli in 1924, with the first quantitative calculation made in 1930 by E. Fermi.

*Hint:* The proton's magnetic moment operator is described by the same Eq. (4.115) of the lecture notes as the electron, but with a positive gyromagnetic ratio  $\gamma_p = g_p e / 2m_p \approx 2.675 \times 10^8 \text{ s}^{-1} \text{ T}^{-1}$ , whose magnitude is much smaller than that of the electron ( $|\gamma_e| \approx 1.761 \times 10^{11} \text{ s}^{-1} \text{ T}^{-1}$ ), due to the much higher mass,  $m_p \approx 1.673 \times 10^{-27} \text{ kg} \approx 1,835 m_e$ . (The  $g$ -factor of the proton is also different,  $g_p \approx 5.586$ .<sup>12</sup>)

*Solution:* The perturbation Hamiltonian of the interaction between the magnetic dipole  $\mathbf{m}_e$  of the electron and the magnetic field  $\mathcal{B}_p$  induced by the proton's magnetic moment,

$$\hat{\mathbf{m}}_p = \gamma_p \hat{\mathbf{s}}_p = g_p \frac{e}{2m_p} \hat{\mathbf{s}}_p,$$

may be taken in the usual Pauli form – see Eq. (4.163) of the lecture notes):

$$\hat{H}_{ss} = -\hat{\mathbf{m}}_e \cdot \hat{\mathcal{B}}_p, \quad \text{with } \hat{\mathbf{m}}_e = \gamma_e \hat{\mathbf{s}}_e = -g_e \frac{e}{2m_e} \hat{\mathbf{s}}_e, \quad g_e \approx 2.0023.$$

Due to the proton's relatively large mass, its position's uncertainty (very small in comparison with the scale of the electron's wavefunction spread, the Bohr radius  $r_B$ ) may be disregarded, so the relation between the operators of  $\mathcal{B}_p$  and  $\mathbf{m}_p$  may be borrowed from the classical electrodynamics' result for the field of an immobile point dipole:<sup>13</sup>

$$\hat{\mathcal{B}}_p(\mathbf{r}) = \frac{\mu_0}{4\pi} \left( \frac{3\mathbf{r}(\mathbf{r} \cdot \hat{\mathbf{m}}_p) - r^2 \hat{\mathbf{m}}_p}{r^5} + \frac{8\pi}{3} \hat{\mathbf{m}}_p \delta(\mathbf{r}) \right).$$

As a reminder, the delta-functional term in this expression provides a “coarse-grain” description of the field source – in our case, the proton. In our case, its use is legitimate due to the (very) strong relation  $r_B \gg a_p$ , where  $a_p \sim 10^{-15} \text{ m}$  is the effective spread of the proton's electric charge.

Combining these formulas, we may use Eq. (6.14) of the lecture notes to write the following 1<sup>st</sup>-order correction to the energy of the ground (and hence non-degenerate) state of the atom, denoted as 0:

$$\begin{aligned} E_0^{(1)} &= \langle 0 | \hat{H}_{ss} | 0 \rangle \\ &= \frac{\mu_0}{4\pi} \frac{g_e g_p e^2}{4m_e m_p} \left[ \langle 0 | \frac{3(\mathbf{r} \cdot \hat{\mathbf{s}}_e)(\mathbf{r} \cdot \hat{\mathbf{s}}_p)}{r^5} | 0 \rangle - \langle 0 | \frac{r^2 \hat{\mathbf{s}}_e \cdot \hat{\mathbf{s}}_p}{r^5} | 0 \rangle + \frac{8\pi}{3} \langle 0 | \hat{\mathbf{s}}_e \cdot \hat{\mathbf{s}}_p \delta(\mathbf{r}) | 0 \rangle \right]. \end{aligned} \quad (*)$$

Since the vectors of this state are spin-orbit factorable in the sense of Eq. (8.12), each average inside the square brackets of the last expression may be calculated separately for its orbital and spin components. For example, the first average is

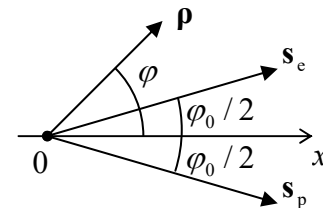
$$\langle s_{ep} | \otimes \langle o_0 | \frac{3(\mathbf{r} \cdot \hat{\mathbf{s}}_e)(\mathbf{r} \cdot \hat{\mathbf{s}}_p)}{r^5} | o_0 \rangle \otimes | s_{ep} \rangle = \langle s_{ep} | \int \psi_{100}^*(\mathbf{r}) \frac{3(\mathbf{r} \cdot \hat{\mathbf{s}}_e)(\mathbf{r} \cdot \hat{\mathbf{s}}_p)}{r^5} \psi_{100}(\mathbf{r}) d^3 r | s_{ep} \rangle$$

(with the ground-state wavefunctions calculated in Sec. 3.6), where the integral over the orbital motion's space may be taken by temporarily treating the electron and proton spin operators as  $c$ -number geometric 3D vectors  $\mathbf{s}_e$  and  $\mathbf{s}_p$  – because such treatment is valid for any matrix element of these operators.

<sup>12</sup> The relatively large value of the proton's  $g$ -factor results from the quark-gluon structure of this particle. (An exact calculation of  $g_p$  remains a challenge for quantum chromodynamics.)

<sup>13</sup> See, e.g., EM Sec. 5.4.

By selecting the  $x$ -axis, within the common plane of these two vectors, to bisect the angle  $\varphi_0$  between them (see the figure on the right), and the  $z$ -axis normal to this plane, in the usual polar coordinates (in which the 2D component  $\boldsymbol{\rho}$  of the radius vector  $\mathbf{r}$  in the  $[x, y]$ -plane has the length  $\rho = r \sin \theta$ ), we get



$$3(\mathbf{r} \cdot \hat{\mathbf{s}}_e)(\mathbf{r} \cdot \hat{\mathbf{s}}_p) = 3(\boldsymbol{\rho} \cdot \mathbf{s}_e)(\boldsymbol{\rho} \cdot \mathbf{s}_p)$$

$$= 3 \left[ \hat{s}_e r \sin \theta \cos \left( \varphi - \frac{\varphi_0}{2} \right) \right] \left[ \hat{s}_p r \sin \theta \cos \left( \varphi + \frac{\varphi_0}{2} \right) \right] \equiv \frac{3}{2} r^2 \hat{s}_e \hat{s}_p \sin^2 \theta (\cos \varphi_0 + \cos 2\varphi);$$

$$r^2 (\hat{\mathbf{s}}_e \cdot \hat{\mathbf{s}}_p) = r^2 \hat{s}_e \hat{s}_p \cos \varphi_0.$$

The wavefunction  $\psi_{100}(\mathbf{r})$  (describing the ground  $1s$  electronic state of the atom) is spherically symmetric. With the account of this fact and the above expressions, the integration over the full solid angle of these terms gives exactly similar results, so their difference, on the right-hand side of Eq. (\*), vanishes. As a result, the only contribution to the energy correction comes from the third, delta-functional term:

$$E_0^{(1)} = \frac{\mu_0 g_e g_p e^2}{4\pi 4m_e m_p} \frac{8\pi}{3} \langle s_{ep} | \int \psi_{100}^*(\mathbf{r}) \hat{\mathbf{s}}_e \cdot \hat{\mathbf{s}}_p \delta(\mathbf{r}) \psi_{100}(\mathbf{r}) d^3 r | s_{ep} \rangle$$

$$\equiv \frac{\mu_0 g_e g_p e^2}{6 m_e m_p} |\psi_{100}(0)|^2 \langle s_{ep} | \hat{\mathbf{s}}_e \cdot \hat{\mathbf{s}}_p | s_{ep} \rangle.$$

(According to Eqs. (3.174) and (3.208),  $|\psi_{100}(0)|^2 = 1/\pi r_B^3$ .)

Now proceeding to the spin factor in this result: since the proton is also a Fermi-particle with spin  $1/2$ , the spin average in the above expression may be calculated exactly as in the solution of Problem 3, giving  $(\hbar/2)^2$  for any triplet state, and  $-3(\hbar/2)^2$  for the singlet state, with the difference equal to  $\hbar^2$ . As a result, the ground state energy splits into two hyperfine sublevels,<sup>14</sup> with the triplet states' energy higher than that of the singlet state by

$$\Delta E_{ss} = \frac{\mu_0 g_e g_p e^2 \hbar^2}{6\pi m_e m_p r_B^3}. \quad (**)$$

Plugging in the values of the involved constants, we get  $\Delta E_{ss} \approx 5.884 \times 10^{-6}$  eV, almost seven orders of magnitude smaller than the Hartree energy  $E_0 \approx 27$  eV, thus giving *a posteriori* justification of our perturbative treatment. Moreover, this splitting is much smaller than the *fine* structure of the energy due to the spin-orbit interaction (see Sec. 6.3 of the lecture notes) – hence the term *hyperfine*.<sup>15</sup>

<sup>14</sup> Note that according to the solution of the same Problem 8.3, all triplet states have the net spin  $S = 1$ , while the singlet state,  $S = 0$ . The change of  $S$  at a spontaneous quantum transition between the hyperfine sublevels may be interpreted by saying that the spin balance is carried away by the emitted circularly polarized photon with spin 1 – the notion to be discussed in Chapter 9.

<sup>15</sup> The splitting (\*\*) affects each sub-level of the ground state's fine structure. Note also that in more complex atoms and molecules, several other mechanisms, most notably including the interaction between the quadrupole electric moment of the nucleus (see, e.g., EM Sec. 8.9) with the electrons' electric field gradient, make comparable contributions to the hyperfine structure of their energy levels.

The hyperfine splitting of hydrogen levels is very important for astronomy because due to the cosmic microwave background radiation, the effective temperature of the hydrogen gas in space is at least  $\sim 3\text{K}$ , i.e. substantially higher than the minimum ( $T_{\text{ss}} \sim \Delta E_{\text{ss}}/k_{\text{B}} \sim 0.1\text{ K}$ ) necessary for the spontaneous thermal excitation of the higher (triplet) states. After such a thermal excitation, the hydrogen atom eventually returns to the genuine ground (singlet) state, emitting a microwave photon with the frequency  $\omega_{\text{ss}} = \Delta E_{\text{ss}}/\hbar \approx 0.8924 \times 10^{10}\text{ s}^{-1}$  ( $f_{\text{ss}} \equiv \omega_{\text{ss}}/2\pi \approx 1,420.4\text{ MHz}$ )<sup>16</sup> corresponding to the wavelength  $\lambda_{\text{ss}} = c/f_{\text{ss}} \approx 21.11\text{ cm}$ . This famous *21-cm line*, first observed in 1951 by E. Purcell and H. Ewen, gives radioastronomy one of the most important tools for measurements of the spatial distribution of the Universe's most abundant atoms. (In particular, it was used to discover the spiral structure of our galaxy.)

Note also that the legal unit of time, the second, is currently defined in terms of the hyperfine splitting of the ground state of the cesium-133 atom, because of a high stability of the frequency of the corresponding transitions and its technically convenient value of 9.192 631 770 GHz.

**Problem 8.6.** In the simple case of just two similar spin-interacting particles, distinguishable by their spatial location, the famous *Heisenberg model* of ferromagnetism<sup>17</sup> is reduced to the following Hamiltonian:

$$\hat{H} = -J \hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2 - \gamma \mathcal{B} \cdot (\hat{\mathbf{s}}_1 + \hat{\mathbf{s}}_2),$$

where  $J$  is the spin interaction constant,  $\gamma$  is the gyromagnetic ratio of each particle, and  $\mathcal{B}$  is the external magnetic field. Find the stationary states and energies of this system for spin- $1/2$  particles.

*Solution:* According to the solution of Problem 3, all three triplet states (8.21), and the singlet state (8.18) are eigenstates of both terms of this Hamiltonian, and hence are stationary states of this system, with the following energies:

$$E = \begin{cases} -J(\hbar/2)^2 - \hbar\gamma\mathcal{B}, & \text{for the simple triplet state } \uparrow\uparrow, \\ -J(\hbar/2)^2 + \hbar\gamma\mathcal{B}, & \text{for the simple triplet state } \downarrow\downarrow, \\ -J(\hbar/2)^2, & \text{for the entangled triplet state,} \\ +3J(\hbar/2)^2, & \text{for the (entangled) singlet state.} \end{cases}$$

If the magnetic field effect is negligibly small, this energy spectrum is reduced to just two levels: the triple-degenerate level  $E_{\text{triplet}} \equiv -J(\hbar/2)^2$  and the singlet level  $E_{\text{singlet}} \equiv 3J(\hbar/2)^2$ . So, the singlet and triplet spin states may naturally form even if two similar particles are distinguishable (in our current case, by their fixed spatial positions), due to their explicit interaction.

On the other hand, a substantial magnetic field, with  $\gamma\mathcal{B} \sim \hbar J$ , lifts the triplet level's degeneracy. (Note a substantial similarity of this effect with that for the excited states of the  $^4\text{He}$  atom, discussed at the end of Sec. 8.2 of the lecture notes.)

<sup>16</sup> These experimental values (measured to the 13<sup>th</sup> decimal place!) differ from the above theoretical value by  $\sim 0.2\%$ , due to quantum-electrodynamics effects ignored in the above treatment.

<sup>17</sup> It was suggested in 1926 independently by W. Heisenberg and P. Dirac. A discussion of thermal effects in this and other similar systems (especially the Ising model of ferromagnetism) may be found in SM Chapter 4.

**Problem 8.7.** Two spins- $\frac{1}{2}$ , with different gyromagnetic ratios  $\gamma_1$  and  $\gamma_2$ , are placed in an external magnetic field  $\mathcal{B}$ . In addition, the spins interact as in the Heisenberg model:

$$\hat{H}_{\text{int}} = -J \hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2.$$

Find the stationary states and energies of the system.

*Solution:* In the usual  $z$ -basis for each spin, with the  $z$ -axis directed along the applied magnetic field, the total Hamiltonian of the system has the following matrix:

$$H = -J \left( \frac{\hbar}{2} \right)^2 (\sigma_{1x} \sigma_{2x} + \sigma_{1y} \sigma_{2y} + \sigma_{1z} \sigma_{2z}) - \gamma_1 \mathcal{B} \frac{\hbar}{2} \sigma_{1z} - \gamma_2 \mathcal{B} \frac{\hbar}{2} \sigma_{2z}.$$

By using this expression and the solution of Problem 3, we may readily calculate the effects of the Hamiltonian on each of the four states of the uncoupled-representation basis of the system:

$$\begin{aligned} \hat{H}|\uparrow\uparrow\rangle &= \left( -J \frac{\hbar^2}{4} - \gamma_1 \mathcal{B} \frac{\hbar}{2} - \gamma_2 \mathcal{B} \frac{\hbar}{2} \right) |\uparrow\uparrow\rangle, & \hat{H}|\downarrow\downarrow\rangle &= \left( -J \frac{\hbar^2}{4} + \gamma_1 \mathcal{B} \frac{\hbar}{2} + \gamma_2 \mathcal{B} \frac{\hbar}{2} \right) |\downarrow\downarrow\rangle, \\ \hat{H}|\uparrow\downarrow\rangle &= \left( J \frac{\hbar^2}{4} - \gamma_1 \mathcal{B} \frac{\hbar}{2} + \gamma_2 \mathcal{B} \frac{\hbar}{2} \right) |\uparrow\downarrow\rangle - 2J \frac{\hbar^2}{4} |\downarrow\uparrow\rangle, \\ \hat{H}|\downarrow\uparrow\rangle &= \left( J \frac{\hbar^2}{4} + \gamma_1 \mathcal{B} \frac{\hbar}{2} - \gamma_2 \mathcal{B} \frac{\hbar}{2} \right) |\downarrow\uparrow\rangle - 2J \frac{\hbar^2}{4} |\uparrow\downarrow\rangle. \end{aligned} \quad (*)$$

The first two of these formulas show that the factorable triplet states  $\uparrow\uparrow$  and  $\downarrow\downarrow$  are always stationary states of this system, with energies, respectively,

$$E_{\uparrow\uparrow} = -J \frac{\hbar^2}{4} - (\gamma_1 + \gamma_2) \mathcal{B} \frac{\hbar}{2}, \quad \text{and} \quad E_{\downarrow\downarrow} = -J \frac{\hbar^2}{4} + (\gamma_1 + \gamma_2) \mathcal{B} \frac{\hbar}{2}. \quad (**)$$

On the other hand, Eqs. (\*) mean that the two remaining stationary states, which will be denoted  $(\pm)$ , generally are neither the factorable states  $\uparrow\downarrow$  and  $\downarrow\uparrow$ , nor the simple entangled singlet and triplet states described by Eqs. (8.18) and (8.20), but rather different linear superpositions:

$$|+\rangle = a_+ |\uparrow\downarrow\rangle + b_+ |\downarrow\uparrow\rangle, \quad |-\rangle = a_- |\uparrow\downarrow\rangle + b_- |\downarrow\uparrow\rangle.$$

The coefficient pairs  $\{a_{\pm}, b_{\pm}\}$  in these relations may be found (to a common multiplier, which should be calculated from the normalization condition) as the eigenvectors of the following partial  $(2 \times 2)$  matrix of the Hamiltonian, written in the basis of two uncoupled-representation states  $\uparrow\downarrow$  and  $\downarrow\uparrow$ :

$$\begin{pmatrix} J \frac{\hbar^2}{4} - (\gamma_1 - \gamma_2) \mathcal{B} \frac{\hbar}{2} & -2J \frac{\hbar^2}{4} \\ -2J \frac{\hbar^2}{4} & J \frac{\hbar^2}{4} + (\gamma_1 - \gamma_2) \mathcal{B} \frac{\hbar}{2} \end{pmatrix}. \quad (***)$$

As usual, we should find the corresponding eigenvalues (i.e. the energy levels) first, as the roots  $E_{\pm}$  of the consistency equation (4.103); in our current case, it reads

$$\begin{vmatrix} J\frac{\hbar^2}{4} - (\gamma_1 - \gamma_2)\mathcal{B}\frac{\hbar}{2} - E & -2J\frac{\hbar^2}{4} \\ -2J\frac{\hbar^2}{4} & J\frac{\hbar^2}{4} + (\gamma_1 - \gamma_2)\mathcal{B}\frac{\hbar}{2} - E \end{vmatrix} = 0.$$

A straightforward calculation yields:

$$E_{\mp} = J\frac{\hbar^2}{4} \pm \left\{ \left[ 2J\frac{\hbar^2}{4} \right]^2 + \left[ (\gamma_1 - \gamma_2)\mathcal{B}\frac{\hbar}{2} \right]^2 \right\}^{1/2}. \quad (****)$$

According to Eqs. (\*\*\*) and (\*\*\*\*), at very low magnetic fields ( $\gamma_{1,2}\mathcal{B} \ll \hbar J$ ), the energy spectrum of the system is reduced to just two levels: a triplet level:  $E_{\uparrow\uparrow} \approx E_{\downarrow\downarrow} \approx E_+ \approx E_{\text{triplet}} \equiv -J\hbar^2/4$ , and a singlet level,  $E_- \approx E_{\text{singlet}} \equiv 3J\hbar^2/4$ . However, the field makes all four energies different. In particular, in the limit of very high fields, when  $(\gamma_1 \pm \gamma_2)\mathcal{B} \gg \hbar J$ , these energies are

$$E_{\uparrow\uparrow} \approx (-\gamma_1 - \gamma_2)\mathcal{B}\frac{\hbar}{2}, \quad E_{\downarrow\downarrow} \approx (\gamma_1 + \gamma_2)\mathcal{B}\frac{\hbar}{2}, \quad E_- \approx (\gamma_1 - \gamma_2)\mathcal{B}\frac{\hbar}{2}, \quad E_+ \approx (-\gamma_1 + \gamma_2)\mathcal{B}\frac{\hbar}{2},$$

and may be interpreted as algebraic sums of individual spin energies in the magnetic field. Thus, at very high fields, the spin coupling is unimportant and the spins behave independently – as could be expected.

Returning to arbitrary field values: plugging the results (\*\*\*\*), one by one, into the system of equations for the coefficients  $\{a_{\pm}, b_{\pm}\}$  that corresponds to the matrix (\*\*\*), we get similar expressions for their ratios:

$$\frac{b_+}{a_+} = -\frac{a_-}{b_-} = \frac{(\gamma_1 - \gamma_2)\mathcal{B}}{\hbar J} + \left\{ 1 + \left[ \frac{(\gamma_1 - \gamma_2)\mathcal{B}}{\hbar J} \right]^2 \right\}^{1/2}.$$

For either similar particles, i.e. for  $\gamma_1 - \gamma_2 = 0$ , or for any  $\gamma_{1,2}$  but in the field's absence, these formulas yield  $b_+ = a_+$  and  $b_- = -a_-$ , so the eigenstate (+) is the simple mixed triplet state  $s_+$  (see, e.g., Eq. (8.20) of the lecture notes), while the eigenstate (–) is the singlet state (8.18), in agreement with the previous problem's solution. However, at  $\gamma_1 \neq \gamma_2$ , the magnetic field lifts the triplet's degeneracy and makes the linear superpositions ( $\pm$ ) different from the entangled states of the coupled-representation basis. In the limit of very large fields,  $(\gamma_1 - \gamma_2)\mathcal{B} \gg \hbar J$ , the coefficient  $a_+$  becomes much smaller than  $b_+$ , and the coefficient  $b_-$  much smaller than  $a_-$ , meaning that the eigenstate (+) tends to the state  $\uparrow\downarrow$  of the uncoupled-representation basis, while the eigenstate (–) tends to the opposite state  $\downarrow\uparrow$  of this basis.

**Problem 8.8.** Two similar spins- $1/2$  with a gyromagnetic ratio  $\gamma$ , localized at two points separated by distance  $a$ , interact via the field of their magnetic dipole moments. Calculate the stationary states and energies of the system.

*Solution:* In classical electrodynamics, the energy of interaction of two magnetic dipoles  $\mathbf{m}_1$  and  $\mathbf{m}_2$ , separated by distance  $a$ , is<sup>18</sup>

<sup>18</sup> See, e.g., EM Eqs. (5.99)-(5.100).

$$U = -\frac{\mu_0}{4\pi a^3} \frac{3\mathbf{a}(\mathbf{a} \cdot \mathbf{m}_1) - a^2 \mathbf{m}_1}{a^5} \cdot \mathbf{m}_2 \equiv \frac{\mu_0}{4\pi a^3} (m_{1x} m_{2x} + m_{1y} m_{2y} - 2m_{1z} m_{2z}),$$

where the  $z$ -axis is directed along the vector  $\mathbf{a}$  connecting the dipole positions. In accordance with the correspondence principle, in quantum mechanics, the interaction is described by the Hamiltonian that is similarly expressed via the Cartesian components of the magnetic moment operators given by Eq. (4.115) of the lecture notes:

$$\hat{H} = \frac{\mu_0}{4\pi a^3} (\hat{m}_{1x} \hat{m}_{2x} + \hat{m}_{1y} \hat{m}_{2y} - 2\hat{m}_{1z} \hat{m}_{2z}), \quad \text{where } \hat{\mathbf{m}}_k = \gamma \hat{\mathbf{s}}_k,$$

and  $\hat{\mathbf{s}}_k$  is the spin vector operator of the  $k^{\text{th}}$  particle. For spins- $1/2$ , in the standard  $z$ -basis, the operator is described by Eqs. (4.116)-(4.117), so the Hamiltonian matrix of the system is

$$H = E_0 (\sigma_{1x} \sigma_{2x} + \sigma_{1y} \sigma_{2y} - 2\sigma_{1z} \sigma_{2z}), \quad \text{with } E_0 \equiv \frac{\mu_0}{4\pi a^3} \left( \gamma \frac{\hbar}{2} \right)^2 \geq 0,$$

where  $\sigma_{1,2}$  are the Pauli matrices (4.105) acting on spin vectors of the corresponding particles. (Note that this Hamiltonian is substantially different from the Heisenberg model discussed in two previous problems.)

Using this expression and acting just as in Problem 3, we may readily calculate the result of this Hamiltonian's action on each of the four states of the uncoupled-representation basis of the two-spin system. The result is

$$\begin{aligned} \hat{H}|\uparrow\uparrow\rangle &= -2E_0|\uparrow\uparrow\rangle, & \hat{H}|\downarrow\downarrow\rangle &= -2E_0|\downarrow\downarrow\rangle, \\ \hat{H}|\uparrow\downarrow\rangle &= 2E_0(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle), & \hat{H}|\downarrow\uparrow\rangle &= 2E_0(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle). \end{aligned}$$

This means that the spin-aligned states  $\uparrow\uparrow$  and  $\downarrow\downarrow$  are stationary states of the system, with the same energy,

$$E_{\uparrow\uparrow} = E_{\downarrow\downarrow} = -2E_0.$$

On the other hand, the spin-opposite states  $\uparrow\downarrow$  and  $\downarrow\uparrow$ , while not mixing with the spin-aligned states, mix with each other as described by the following partial (2x2) matrix

$$H = 2E_0 \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}. \quad (*)$$

Solving the characteristic equation (4.103) for this matrix,

$$\begin{vmatrix} 1 - \lambda_{\pm} & 1 \\ 1 & 1 - \lambda_{\pm} \end{vmatrix} = 0, \quad \text{i.e. } \lambda_{\pm}^2 - 2\lambda_{\pm} = 0,$$

we get  $\lambda_+ = 2$ ,  $\lambda_- = 0$ , giving us two more (non-degenerate) energy levels:

$$E_+ = 2E_0\lambda_+ = 4E_0, \quad E_- = 2E_0\lambda_- = 0.$$

Now plugging these values, one by one, into any equation (4.102) used for the diagonalization of the matrix (\*),

$$(1 - \lambda_{\pm})U_{1\pm} + U_{2\pm} = 0, \quad U_{1\pm} + (1 - \lambda_{\pm})U_{2\pm} = 0,$$

we get  $U_{1+} = U_{2+}$ ,  $U_{1-} = -U_{2-}$ , meaning that the eigenstates corresponding to the energy levels  $E_{\pm}$  are, respectively, the familiar entangled triplet and singlet – see Eqs. (8.18) and (8.20):

$$|s_{\pm}\rangle \equiv \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle).$$

Hence, in this system, the energies of the triplet states are different even in the absence of the external magnetic field: the spin-aligned (factorable) triplet states have the energy  $(-2E_0)$ , which is lower than that  $(+4E_0)$  of the entangled triplet state – and even than that  $(0)$  of the singlet state. This difference is in qualitative agreement with the classical trend of electric and magnetic moments to align due to their dipole interaction.<sup>19</sup>

**Problem 8.9.** Consider the permutation of two identical particles, each of spin  $s$ . How many different symmetric and antisymmetric spin states can the system have?

*Solution:* As was discussed in Section 5.7 of the lecture notes, each of the particles of spin  $s$  may have  $(2s + 1)$  different, linearly-independent spin states – for example, the states with definite and different “magnetic” quantum numbers  $m_s$  on the interval  $-s \leq m_s \leq +s$  – see, e.g., Eq. (5.169) of the lecture notes. Thus, generally, for two such particles, there are  $(2s + 1)^2$  different direct products,

$$|m_s\rangle \otimes |m_s'\rangle, \quad (*)$$

with arbitrary  $m_s$  and  $m_s'$  of the above list. Of them,  $(2s + 1)$  products have  $m_s = m_s'$ , and hence are symmetric with respect to the particle permutations, while

$$(2s + 1)^2 - (2s + 1) \equiv 2s(2s + 1)$$

other states have  $m_s \neq m_s'$ . Of the latter states, we can form  $s(2s + 1)$  symmetric and the same number of antisymmetric combinations of the type

$$|m_s\rangle \otimes |m_s'\rangle \pm |m_s'\rangle \otimes |m_s\rangle. \quad (**)$$

Since all these states are linearly-independent, they form a full system of  $(2s + 1)^2$  spin states, because the formation of the symmetric and antisymmetric independent linear combinations does not change that number. Hence, the total number of different symmetric states is

$$N_s = (2s + 1) + s(2s + 1) \equiv (s + 1)(2s + 1),$$

while the number of different antisymmetric states is only

$$N_a = s(2s + 1) < N_s.$$

As the simplest example, for two spin-free particles ( $s = 0$ ) we get  $N_s = 1$ ,  $N_a = 0$  – fine because the only possible spin(-free) state of this system is symmetric with respect to the particle permutation. As the next simplest example,  $s = 1/2$ , our results yield  $N_s = (1/2 + 1) \cdot (2 \cdot 1/2 + 1) = 3$  and  $N_a = 1/2 \cdot (2 \cdot 1/2 + 1) = 1$ , corresponding to the three triplet states (8.21) and the only singlet state (8.18).

<sup>19</sup> See, e.g., the solutions of EM Problems 3.7 and 6.15.



Note, however, that for systems of two particles with  $s > \frac{1}{2}$ , not all basis vectors of the coupled representation, i.e. not all simultaneous eigenkets of the operators  $\hat{S}^2$  and  $\hat{S}_z$  have the simple forms (\*) or (\*\*), so more complex linear superpositions may be needed – see, for example, the next problem.

**Problem 8.10.** For a system of two identical particles with  $s = 1$ :

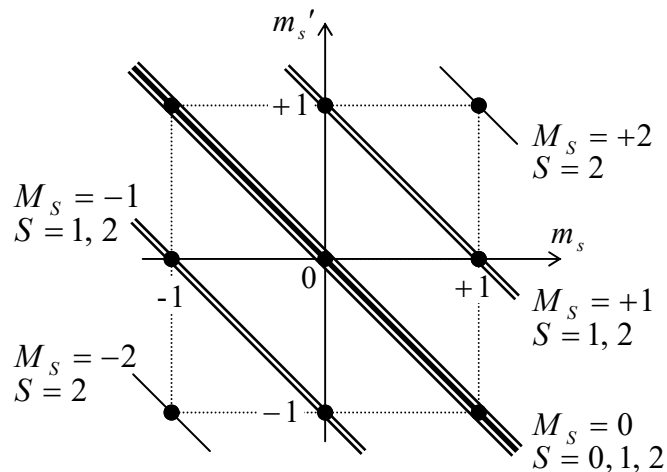
- (i) List all spin states forming the uncoupled-representation basis.
- (ii) List all possible pairs  $\{S, M_S\}$  of the quantum numbers describing the states of the coupled-representation basis – see Eq. (8.48) of the lecture notes.
- (iii) Which of the  $\{S, M_S\}$  pairs describe the states symmetric, and which the states antisymmetric, with respect to the particle permutation?

*Solutions:*

(i) The state vectors of the uncoupled representation are given by Eq. (\*) of the solution of the previous problem. In our current case, each of quantum numbers  $m_s$  and  $m_s'$  may take one of the three values of the set  $\{-1, 0, +1\}$ . In the shorthand notation used in Secs. 8.1 and 8.2 of the lecture notes, their ket-vectors are

$$|+1,+1\rangle, |+1,0\rangle, |+1,-1\rangle, |0,+1\rangle, |0,0\rangle, |0,-1\rangle, |-1,+1\rangle, |-1,0\rangle, |-1,-1\rangle.$$

For what follows, it is helpful to represent these states as the points at the “rectangular diagram” shown in the figure below. (Its structure is similar to that for  $s = \frac{1}{2}$ , shown in Fig. 8.2 of the lecture notes.)



(ii) As was discussed in Sec. 5.7 of the lecture notes for the addition of the angular momentum operators  $\hat{L}$  and  $\hat{S}$ , and reproduced in Sec. 8.2 for the addition of two spin operators  $\hat{s}_1$  and  $\hat{s}_2$ , the kets of the coupled-representation basis, i.e. the common eigenkets of the operators  $\hat{S}^2 \equiv (\hat{s}_1 + \hat{s}_2)^2$  and  $\hat{S}_z = \hat{s}_{1z} + \hat{s}_{2z}$ , are linear combinations of the uncoupled-representation kets with the fixed sum

$$m_s + m_s' = M_S,$$

and hence may be represented, on the rectangular diagram, by the straight lines of the slope  $(-1)$ , that connect the corresponding  $\{m_s, m_s'\}$  points – see the figure above. Hence, the assignment of the numbers  $M_S$  is elementary – see the labels in that figure.

For several coupled-representation states, the assignment of the quantum number  $S$  is also straightforward. For example, let us consider the top-right and bottom-left points of the rectangular diagram, representing the states with  $m_s = m_s' = +1$  and  $m_s = m_s' = -1$ . Since each of the lines representing a coupled-representation state, which passes through one of these points, does not pass through any other point, the corresponding states belong also to the coupled-representation basis, with  $M_S = \pm 2$ . They, evidently have the largest possible value of  $M_S$ , namely  $|M_S|_{\max} = 2$ . According to Eq. (8.48), this value serves as the corresponding number  $S$ , so we may write

$$|S = 2, M_S = +2\rangle = |m_s = +1, m_s' = +1\rangle, \quad |S = 2, M_S = -2\rangle = |m_s = -1, m_s' = -1\rangle. \quad (*)$$

Now going, from the corners, one step toward the center of the diagram, i.e. to the states with  $M_S = \pm 1$ , we may notice, first of all, that since there are two uncoupled-representation states for each of these values, there should be also two their linear superpositions giving different coupled-representation states, and they cannot have the same number  $S$  – otherwise they would not be linearly-independent. Next, as was discussed in Sec. 5.7 for the addition of  $\mathbf{L}$  and  $\mathbf{S}$  of a single particle, the quantum number characterizing the square of their sum (there,  $j$ , while in our current case,  $S$ ) can change, at such step, only by  $\pm 1$ . Hence the two coupled-representation states, for each of these  $M_S$ , should have  $S = 1$  and  $S = 2$ . Since, due to the symmetry of the rectangular diagram with respect to the axis  $m_s = m_s'$ , the moduli of the weights of the two uncoupled-representation kets participating in each of such superpositions have to be equal, the only possible superpositions have (to an arbitrary phase multiplier) the familiar form:

$$\begin{aligned} \left| S = \begin{Bmatrix} 2 \\ 1 \end{Bmatrix}, M_S = +1 \right\rangle &= \frac{1}{\sqrt{2}} \left( |m_s = +1, m_s' = 0\rangle \pm |m_s = 0, m_s' = +1\rangle \right), \\ \left| S = \begin{Bmatrix} 2 \\ 1 \end{Bmatrix}, M_S = -1 \right\rangle &= \frac{1}{\sqrt{2}} \left( |m_s = -1, m_s' = 0\rangle \pm |m_s = 0, m_s' = -1\rangle \right), \end{aligned} \quad (**)$$

– cf. Eqs. (8.18) and (8.20) of the lecture notes.

Finding the similarly explicit forms for the three remaining coupled-representation states with  $M_S = 0$ , corresponding to the three lines passing through the origin of the rectangular diagram, in a bit more complex,<sup>20</sup> but this is not necessary to fulfill our task. Indeed, since all these kets have the same  $M_S$ , they all should have different  $S$ , to be linearly independent. However, according to Eq. (8.50),

<sup>20</sup> This may be done, for example, using the Clebsh-Gordan coefficients for  $s_1 = s_2 = 1$  – which, in turn, may be derived from the recurrence relations that were derived (for the  $\mathbf{L} + \mathbf{S} = \mathbf{J}$  addition) in the solution of Problem 5.41. Just for the reader's reference:

$$\begin{aligned} |S = 2, M_S = 0\rangle &= \left( |m_s = +1, m_s' = -1\rangle + |m_s = -1, m_s' = +1\rangle + 2|m_s = 0, m_s' = 0\rangle \right) / \sqrt{6}, \\ |S = 1, M_S = 0\rangle &= \left( |m_s = +1, m_s' = -1\rangle - |m_s = -1, m_s' = +1\rangle \right) / \sqrt{2}, \\ |S = 0, M_S = 0\rangle &= \left( |m_s = +1, m_s' = -1\rangle + |m_s = -1, m_s' = +1\rangle - |m_s = 0, m_s' = 0\rangle \right) / \sqrt{3}. \end{aligned}$$

These expressions may be readily verified, for example, by combining Eq. (5.164) of the lecture notes, with  $l = 1$ , duly translated to the spin language, and Eq. (\*\*\*) of the solution of Problem 8.3. This verification is highly recommended to the reader as an additional task.

spelled out for our case  $S_{\max} = s_1 + s_2 = 2$ , the list of possible values of  $S$  is limited to  $S = 0, 1$ , and  $2$ , thus giving us the final answer – see the labels in the figure above.

(iii) The two states (\*) are evidently symmetric with respect to the particles' permutation, and so are two of the four states (\*\*), corresponding to  $S = 2$ . So, besides the three states with  $M_S = 0$ , four states are symmetric, and two are antisymmetric. But according to the solution of the previous problem, for  $s = 1$ , we must have six symmetric and three antisymmetric states, so of the three states with  $M_S = 0$ , two have to be symmetric and one antisymmetric. Since the net-spin-free state with  $S = 0$  and  $M_S = 0$  has to be symmetric for any  $s$ , this means that the state with  $S = 1$  and  $M_S = 0$  has to be antisymmetric, while the state with  $S = 2$  and  $M_S = 0$ , symmetric. This is indeed true – see the last footnote.

**Problem 8.11.** Represent the operators of the total kinetic energy and the total orbital angular momentum of a system of two particles, with masses  $m_1$  and  $m_2$ , as combinations of the terms describing the center-of-mass motion and the relative motion. Use the results to calculate the energy spectrum of the so-called *positronium* – a metastable “atom”<sup>21</sup> consisting of one electron and its positively charged antiparticle, the positron.

*Solution:* The operators in question are the sums of the single-particle operators defined by Eqs. (1.27) and (5.147) of the lecture notes:

$$\hat{T} = \hat{T}_1 + \hat{T}_2 \equiv \frac{\hat{p}_1^2}{2m_1} + \frac{\hat{p}_2^2}{2m_2}, \quad \hat{\mathbf{L}} = \hat{\mathbf{L}}_1 + \hat{\mathbf{L}}_2 \equiv [\hat{\mathbf{r}}_1 \times \hat{\mathbf{p}}_1] + [\hat{\mathbf{r}}_2 \times \hat{\mathbf{p}}_2].$$

Following a clue from classical mechanics,<sup>22</sup> let us introduce two new radius vector operators:

$$\hat{\mathbf{R}} \equiv \frac{m_1 \hat{\mathbf{r}}_1 + m_2 \hat{\mathbf{r}}_2}{M} \quad \text{and} \quad \hat{\mathbf{r}} \equiv \hat{\mathbf{r}}_1 - \hat{\mathbf{r}}_2, \quad (*)$$

where  $M \equiv m_1 + m_2$  is the total mass of the system. Considering these definitions as a system of two linear equations for the initial radius vector operators, we may readily solve it to get the following reciprocal relations:

$$\hat{\mathbf{r}}_1 = \hat{\mathbf{R}} + \frac{m_2}{M} \hat{\mathbf{r}}, \quad \hat{\mathbf{r}}_2 = \hat{\mathbf{R}} - \frac{m_1}{M} \hat{\mathbf{r}}. \quad (**)$$

Now let us define two new momentum operators as

$$\hat{\mathbf{P}} \equiv \hat{\mathbf{p}}_1 + \hat{\mathbf{p}}_2, \quad \hat{\mathbf{p}} \equiv \frac{m_2 \hat{\mathbf{p}}_1 - m_1 \hat{\mathbf{p}}_2}{M}, \quad (***)$$

with the reciprocal relations

$$\hat{\mathbf{p}}_1 = \frac{m_1}{M} \hat{\mathbf{P}} + \hat{\mathbf{p}}, \quad \hat{\mathbf{p}}_2 = \frac{m_2}{M} \hat{\mathbf{P}} - \hat{\mathbf{p}}. \quad (****)$$

By using the fact that the operators of different particles are defined in their own Hilbert spaces and hence commute, we may verify that the Cartesian components of the new operators satisfy the

<sup>21</sup> Its lifetime (either 0.124 ns or 138 ns, depending on the spin state) is limited by the weak interaction of the components, which leads to their mutual annihilation with the emission of several gamma-ray photons.

<sup>22</sup> See, e.g., CM Eq. (3.32).

Heisenberg commutation relations (2.14), while commuting with each other. For example (with the index  $x$  of the particle momentum operators just implied):

$$[\hat{X}, \hat{P}_x] = \left[ \left( \frac{m_1}{M} \hat{x}_1 + \frac{m_2}{M} \hat{x}_2 \right), (\hat{p}_1 + \hat{p}_2) \right] = \frac{m_1}{M} [\hat{x}_1, \hat{p}_1] + \frac{m_2}{M} [\hat{x}_2, \hat{p}_2] = \frac{m_1}{M} i\hbar + \frac{m_2}{M} i\hbar = i\hbar,$$

$$[\hat{x}, \hat{p}_x] = \left[ (\hat{x}_1 - \hat{x}_2), \left( \frac{m_2}{M} \hat{p}_1 - \frac{m_1}{M} \hat{p}_2 \right) \right] = \frac{m_2}{M} [\hat{x}_1, \hat{p}_1] + \frac{m_1}{M} [\hat{x}_2, \hat{p}_2] = \frac{m_2}{M} i\hbar + \frac{m_1}{M} i\hbar = i\hbar,$$

$$[\hat{X}, \hat{p}_x] = \left[ \left( \frac{m_1}{M} \hat{x}_1 + \frac{m_2}{M} \hat{x}_2 \right), \left( \frac{m_2}{M} \hat{p}_1 - \frac{m_1}{M} \hat{p}_2 \right) \right] = \frac{m_1 m_2}{M^2} [\hat{x}_1, \hat{p}_1] - \frac{m_2 m_1}{M^2} [\hat{x}_2, \hat{p}_2] = 0,$$

$$[\hat{x}, \hat{P}_x] = [(\hat{x}_1 - \hat{x}_2), (\hat{p}_1 - \hat{p}_2)] = [\hat{x}_1, \hat{p}_1] - [\hat{x}_2, \hat{p}_2] = 0,$$

with similar relations for two other Cartesian components. Hence, the operators (\*\*\*) are the legitimate operators of the momenta corresponding to the radius vector operators (\*).<sup>23</sup>

Now plugging Eqs. (\*\*) and (\*\*\*\*) into the operators of our current interest, we readily get

$$\hat{T} = \frac{\hat{P}^2}{2M} + \frac{\hat{p}^2}{2m}, \quad \hat{\mathbf{L}} = [\hat{\mathbf{R}} \times \hat{\mathbf{P}}] + [\hat{\mathbf{r}} \times \hat{\mathbf{p}}],$$

where  $m$  is the same *reduced mass* that participates in classical dynamics of two-particle systems:

$$m = \frac{m_1 m_2}{M}, \quad \text{i.e. } \frac{1}{m} = \frac{1}{m_1} + \frac{1}{m_2}, \quad \text{so } m \leq m_1, m_2.$$

Evidently, the uppercase operators (and the total mass  $M$ ) describe the motion of the center of mass of the system of two particles, while the lowercase operators (and the reduced mass  $m$ ) describe their mutual motion. If we are not interested in the motion of the atom as the whole, in the case of a purely Coulomb interaction of the electron and positron with equal and opposite charges  $\pm e$ , i.e. neglecting the very small fine-structure effects discussed in Sec. 6.3, we may take the Hamiltonian of the system in the form

$$\hat{H} = \hat{T} + \hat{U} = \frac{\hat{\mathbf{p}}^2}{2m} - \frac{e^2}{4\pi\epsilon_0 r},$$

where  $m$  is the reduced mass (in this particular case, equal to  $m_e/2$ ), so the energy spectrum is similar to that of the hydrogen atom, but with twice smaller mass. This change leaves the functional form of Bohr's theory result (1.12) intact, but according to Eq. (1.13), reduces the effective value of the Hartree energy  $E_H$  (and hence of all eigenenergies) by a factor of two:

$$E_n = -\frac{(E_H/2)}{2n^2} \equiv -\frac{E_H}{4n^2}, \quad \text{with } E_H \equiv \left( \frac{e^2}{4\pi\epsilon_0 \hbar c} \right)^2 m_e c^2 \equiv \alpha^2 m_e c^2 \approx 27.2 \text{ eV},$$

so the ground-state energy of the positronium, i.e. its ionization energy, is  $-E_H/4 \approx -6.8 \text{ eV}$ .

<sup>23</sup> Another, perhaps less convincing way to prove this fact is to plug Eqs. (\*\*) into the coordinate-representation form of the particle momentum operators,  $\hat{\mathbf{p}}_{1,2} = -i\hbar \nabla_{1,2}$  to get Eqs. (\*\*\*\*) with  $\hat{\mathbf{P}} = -i\hbar \nabla_{\mathbf{R}}$ ,  $\hat{\mathbf{p}} = -i\hbar \nabla_{\mathbf{r}}$ , and then argue that the relation between the operators should not depend on their particular representation.

**Problem 8.12.** Calculate the energy spectrum of the system of two identical spin- $1/2$  particles moving along the  $x$ -axis, which is described by the following Hamiltonian:

$$\hat{H} = \frac{\hat{p}_1^2}{2m_0} + \frac{\hat{p}_2^2}{2m_0} + \frac{m_0\omega_0^2}{2}(x_1^2 + x_2^2 + \varepsilon x_1 x_2),$$

and the degeneracy of each energy level.

*Solution:* Acting just as in the previous problem and using the Hamiltonian's symmetry with respect to particle permutation, let us introduce the following two linear combinations of their coordinates  $x_1$  and  $x_2$ : the distance  $x \equiv x_1 - x_2$  between the particles, and the coordinate  $X \equiv (x_1 + x_2)/2$  of their center of mass. Plugging the reciprocal relations,

$$x_1 = X + \frac{x}{2}, \quad x_2 = X - \frac{x}{2},$$

into the given Hamiltonian, we see that it separates into two independent parts:

$$\hat{H} = \left( \frac{\hat{P}^2}{2M} + \frac{M\Omega^2 X^2}{2} \right) + \left( \frac{\hat{p}^2}{2m} + \frac{m\omega^2 x^2}{2} \right), \quad (*)$$

where

$$\Omega \equiv \omega_0 \left( 1 + \frac{\varepsilon}{2} \right)^{1/2}, \quad \omega \equiv \omega_0 \left( 1 - \frac{\varepsilon}{2} \right)^{1/2}, \quad (**)$$

$M \equiv 2m_0$  is the total mass of the system,  $m \equiv m_0/2$  is the "reduced" mass of the relative motion, and

$$\hat{P} \equiv \hat{p}_1 + \hat{p}_2, \quad \hat{p} \equiv \frac{\hat{p}_1 - \hat{p}_2}{2}.$$

(As we know from the solution of the previous problem, the operators so defined are the legitimate generalized momenta corresponding to the generalized coordinates  $X$  and  $x$ , respectively.)

So, the total Hamiltonian is the sum of the usual Hamiltonians of two independent 1D harmonic oscillators with frequencies given by Eq. (\*\*). Hence the total energy of the system is just the sum of the oscillator energies:

$$E_{N,n} = \hbar\Omega \left( N + \frac{1}{2} \right) + \hbar\omega \left( n + \frac{1}{2} \right), \quad \text{with } N, n = 0, 1, 2, \dots \quad (***)$$

Besides certain exact values of the parameter  $\varepsilon$  (such as  $\varepsilon = 6/5$ , when  $\Omega = 2\omega$ ), the frequencies  $\Omega$  and  $\omega$  are incommensurate, so the energy levels (\*\*\*) are orbitally non-degenerate. In order to analyze their spin degeneracy, let us spell out the orbital wavefunction corresponding to a certain pair of the quantum numbers  $N$  and  $n$ :

$$\Psi_{N,n}(x_1, x_2) = \psi_N(X)\psi_n(x) \equiv \psi_N\left(\frac{x_1 + x_2}{2}\right)\psi_n(x_1 - x_2), \quad (***)$$

where  $\psi_N$  and  $\psi_n$  are the single-oscillator's eigenfunctions. According to Eqs. (2.281) and (2.284) of the lecture notes (see also Fig. 2.35), these functions are symmetric if their index is even, and antisymmetric if it is odd. Since the first operand of the product in Eq. (\*\*\*) is symmetric with respect to the particle permutation ( $x_1 \leftrightarrow x_2$ ) for any  $N$ , the total orbital wavefunction's parity depends only on  $n$ :

$$\Psi_{N,n}(x_2, x_1) = (-1)^n \Psi_{N,n}(x_1, x_2) \equiv \begin{cases} +\Psi_{N,n}(x_1, x_2), & \text{for } n \text{ even,} \\ -\Psi_{N,n}(x_1, x_2), & \text{for } n \text{ odd.} \end{cases}$$

Since the total (orbital plus spin) state vector of the system of two indistinguishable fermions has to be antisymmetric with respect to particle permutation, each energy level (\*\*\*) with an even  $n$  may only house the spin singlet state (8.18), and hence is non-degenerate. On the other hand, each level with an odd  $n$  may correspond to any of the three triplet states (8.21) and hence is triple-degenerate.

**Problem 8.13.** Two particles with similar masses  $m$  and charges  $q$  are free to move along a planar circle of radius  $R$ . In the limit of very strong Coulomb interaction of the particles, find the lowest eigenenergies of the system, and sketch the system of its energy levels. Discuss possible effects of particle indistinguishability.

*Solution:* Per the discussion of single-particle rotation in Secs. 3.5 and 5.6 of the lecture notes, we may write the system's Hamiltonian as follows:

$$\hat{H} = \hat{T} + \hat{U}, \quad \hat{T} = -\frac{1}{2mR^2} \frac{\partial^2}{\partial \varphi_1^2} - \frac{1}{2mR^2} \frac{\partial^2}{\partial \varphi_2^2}, \quad \hat{U} = \frac{q^2}{4\pi\epsilon_0 r_{12}}.$$

Here  $r_{12}$  is the distance between the particles, which may be readily expressed via the difference,

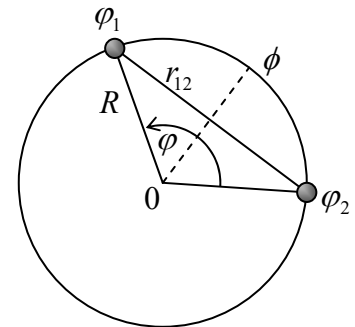
$$\varphi \equiv \varphi_1 - \varphi_2, \quad (*)$$

of their angular coordinates  $\varphi_{1,2}$  – see the figure on the right:

$$r_{12} = 2R \sin \left| \frac{\varphi}{2} \right|.$$

Despite the apparent simplicity of the Hamiltonian, its general analysis is rather involved. However, in the strong interaction limit,

$$\frac{q^2}{4\pi\epsilon_0 R} \gg \frac{\hbar^2}{2mR^2},$$



the lowest energy levels may be readily found analytically, using clues from the classical properties of the system. Indeed, classically, the lowest energy of the system corresponds to the particles pushed, by their Coulomb repulsion, to the opposite ends of the same diameter  $D = 2R$ , so the potential energy  $U$  of the system equals  $U_0 \equiv q^2/4\pi\epsilon_0 D = q^2/8\pi\epsilon_0 R$ . This interaction, however, does not prevent the pair from its free joint rotation around the circle with an arbitrary angular velocity  $\Omega$ . If  $U_0$  is finite, one more contribution to the system's energy may come from small oscillations of the particles near the equilibrium position  $r_{12} = 2D$ . In order to find the oscillation frequency, let us introduce, besides the difference angle  $\varphi$  defined by Eq. (\*), another independent linear combination of particles' coordinates:

$$\phi = \frac{\varphi_1 + \varphi_2}{2}, \quad (**)$$

characterizing their joint rotation – just as it was done in the two previous problems. Solving the system of equations (\*) and (\*\*) for  $\varphi_{1,2}$ , and plugging the result,

$$\varphi_1 = \phi + \frac{\varphi}{2}, \quad \varphi_2 = \phi - \frac{\varphi}{2},$$

into the classical expression for the kinetic energy of the system,

$$T = \frac{m(R\dot{\varphi}_1)^2}{2} + \frac{m(R\dot{\varphi}_2)^2}{2},$$

we get

$$T = T_{\text{rot}} + T_{\text{osc}}, \quad \text{with } T_{\text{rot}} = \frac{I}{2}\dot{\phi}^2, \quad \text{and } T_{\text{osc}} = \frac{I'}{2}\dot{\varphi}^2,$$

where  $I \equiv (2m)R^2$  is the total moment of inertia of the system, while  $I' \equiv m_{\text{ef}}R^2 = (m/2)R^2$  is the “reduced moment of inertia”, similar to the “reduced mass”  $m_{\text{ef}} = m/2$  in other two-body problems with equal masses of the components. Now we may Taylor-expand the potential energy near its minimum value:

$$U = \frac{q^2}{4\pi\epsilon_0 r_{12}} = \frac{q^2}{8\pi\epsilon_0 R \sin|\varphi/2|} = U_0 + \tilde{U}, \quad \text{with } \tilde{U} \approx \kappa_{\text{ef}} \frac{\tilde{\varphi}^2}{2}, \quad \text{where } \tilde{\varphi} \equiv \varphi - \pi,$$

to calculate the effective spring constant  $\kappa_{\text{ef}}$  for small oscillations  $\tilde{\varphi}$  of the angular distance  $\varphi$ . A straightforward calculation yields

$$\kappa_{\text{ef}} \equiv \left. \frac{d^2U}{d\varphi^2} \right|_{\varphi=\pi} = \frac{q^2}{32\pi\epsilon_0 R}.$$

so the total energy of the oscillations is

$$E_{\text{osc}} = T_{\text{osc}} + \tilde{U} = \frac{I'}{2}\dot{\tilde{\varphi}}^2 + \frac{\kappa_{\text{ef}}}{2}\tilde{\varphi}^2 \equiv \frac{I'}{2}\dot{\tilde{\varphi}}^2 + \frac{I'\omega_0^2}{2}\tilde{\varphi}^2, \quad \text{with } \omega_0 \equiv \left( \frac{\kappa_{\text{ef}}}{I'} \right)^{1/2} = \left( \frac{q^2}{4\pi\epsilon_0} \frac{1}{4mR^3} \right)^{1/2}.$$

As we know from classical mechanics, the  $\omega_0$  so defined is the small oscillations' frequency.

Now proceeding to quantum mechanics, Eqs. (\*) and (\*\*), and the replacement  $U \rightarrow \tilde{U}$  allow us to rewrite the initial Hamiltonian in the form of the sum of two independent components:<sup>24</sup>

$$\hat{H} = \hat{H}_{\text{rot}} + \hat{H}_{\text{osc}}, \quad \text{with } \hat{H}_{\text{rot}} = -\frac{\hbar^2}{4mR^2} \frac{\partial^2}{\partial \phi^2}, \quad \hat{H}_{\text{osc}} = -\frac{\hbar^2}{2I'} \frac{\partial^2}{\partial \tilde{\varphi}^2} + \frac{I'\omega_0^2}{2} \tilde{\varphi}^2,$$

whose stationary energies may be calculated separately, and then added. The oscillation part, which was repeatedly discussed in this course, immediately yields

$$E_{\text{osc}} = \hbar\omega_0 \left( n + \frac{1}{2} \right) \equiv \hbar \left( \frac{q^2}{4\pi\epsilon_0} \frac{1}{4mR^3} \right)^{1/2} \left( n + \frac{1}{2} \right), \quad \text{with } n = 0, 1, 2, \dots$$

The eigenfunctions of the rotational Hamiltonian, which has only a simple kinetic-energy component, have been also discussed several times, starting from Sec. 3.5:

<sup>24</sup> An alternative way to get these expressions is to use the solution of Problem 8.8, taking  $\hat{\mathbf{L}} = \mathbf{n}_z \hat{L}_z$ , where  $\mathbf{n}_z$  is the unit vector normal to the ring's plane.

$$\psi(\phi) = \frac{1}{(2\pi)^{1/2}} e^{im\phi}. \quad (***)$$

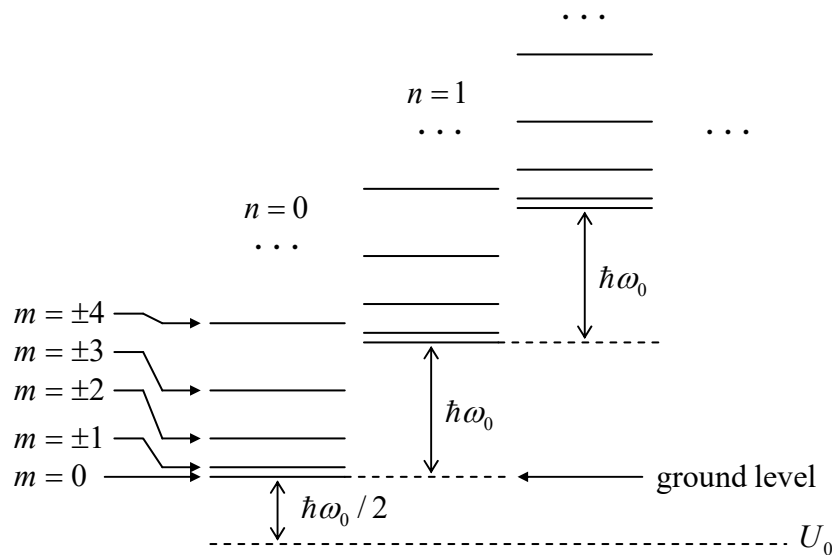
However, at this point, we need to be very careful, because now this wavefunction describes the joint rotation of a *two-particle* system, and their permutation properties are important. If the particles are distinguishable (either by their nature or by the state of some internal degrees of freedom),  $\psi(\phi)$  should be invariant with respect to the system's rotation by  $\Delta\phi = 2\pi$  (and its multiples), just as in the case of a single-particle rotor. This condition immediately gives the equality  $\exp\{im2\pi\} = 1$ , i.e. forces  $m$  to be an integer, giving the energy spectrum<sup>25</sup>

$$E_{\text{rot}} = \frac{\hbar^2}{4mR^2} m^2, \quad \text{with } m = 0, \pm 1, \pm 2, \dots \quad (***)$$

The figure below shows the scheme of the system's lowest energy levels for this case. Note the double rotational degeneracy of all levels (besides those with  $m = 0$ ), and the level hierarchy due to the strong relation between the gaps between adjacent rotational and oscillational energies,

$$\Delta E_{\text{osc}} = \hbar\omega_0 = \hbar \left( \frac{q^2}{4\pi\epsilon_0} \frac{1}{4mR^3} \right)^{1/2} \sim (U_0 \Delta E_{\text{rot}})^{1/2} \gg \Delta E_{\text{rot}},$$

which is valid in our case of very strong particle interaction ( $U_0 \gg \Delta E_{\text{rot}}$ ).



If the particles are indistinguishable, the situation is more complicated. Indeed, let the background (spin plus vibrational) state of the system be symmetric with respect to the particle permutation. (This is true, for example, if the particles are spinless bosons, and the system is in an even vibrational state with  $n = 2n'$ , with integer  $n'$ , for example, in the ground state with  $n = 0$ .) Then the system's rotation by just  $\pm\pi$  results in an identical quantum state, so we have to require that the wavefunction (\*\*\*) satisfies the condition  $\psi(\phi \pm \pi) = \psi(\phi)$ , i.e. that  $\exp\{im\pi\} = 1$ . This requirement allows only *even* values of  $m$ , thus decimating the rotational energy spectrum (\*\*\*)).

<sup>25</sup> Let me hope that the difference between the fonts used for the “magnetic” quantum number ( $m$ ) and the particle mass ( $m$ ) is sufficient to avoid any confusion.



On the other hand, in an odd vibrational state of the bosonic system, with  $n = 2n' + 1$ , the oscillator's wavefunction changes sign at the replacement  $\varphi \rightarrow -\varphi$ . According to the definition of the angles  $\varphi$  and  $\phi$  (see, e.g., the figure above), such replacement is equivalent, modulo  $2\pi$ , to the replacement  $\phi \rightarrow \phi \pm \pi$ , so the sign change of the total wavefunction may be compensated by that of  $\psi(\phi)$ , but only if  $\exp\{im\pi\} = -1$ , i.e. if  $m$  is *odd*. Hence, the rotational spectrum (\*\*\*\*) is decimated again, but now by *forbidding* the energy levels with even  $m$ , notably including the pseudo-ground state with  $m = 0$ .

This effect becomes even more involved in the case of two indistinguishable spin- $\frac{1}{2}$  fermions – e.g., electrons or protons. As was discussed in Sec. 8.2 of the lecture notes, in this case, the necessary antisymmetry of the system's wavefunction to particle permutation may be achieved either via the spin asymmetry (in the singlet spin state with  $S = 0$ ) or the orbital asymmetry, with a symmetric (triplet) spin state, with  $S = 1$ . For our system, this means, for example, that in the ground vibrational state ( $n = 0$ ), there are two sets of spin-rotational states: spin-singlet states with  $m$  even, and spin-triplet states with  $m$  odd.

Rather counter-intuitively, such symmetry effects may affect readily observable properties of real systems (for example, such important diatomic molecules as  $O_2$  and  $N_2$ ) even when they are imposed by *nuclear* spins, despite their extremely weak interaction with other degrees of freedom – see the next problem.

**Problem 8.14.** Low-energy spectra of many diatomic molecules may be well described by modeling the molecule as a system of two particles connected with a light and elastic but very stiff spring. Calculate the energy spectrum of a molecule within this model. Discuss possible effects of nuclear spins on spectra of the so-called *homonuclear* diatomic molecules formed by two similar atoms.

*Solution:* In the specified model, the system's Hamiltonian is

$$\hat{H} = \frac{\hat{p}_1^2}{2m_1} + \frac{\hat{p}_2^2}{2m_2} + \frac{\kappa(r-a)^2}{2}, \quad \text{with } \mathbf{r} \equiv \mathbf{r}_1 - \mathbf{r}_2,$$

where  $a$  is the equilibrium distance between the two atomic nuclei. By using the solution of Problem 11 to transform the kinetic-energy part of the Hamiltonian, we may rewrite it as

$$\hat{H} = \frac{\hat{P}^2}{2M} + \frac{\hat{p}^2}{2m} + \frac{\kappa(r-a)^2}{2}, \quad (*)$$

where  $M \equiv m_1 + m_2$  is the total mass of the molecule,

$$m \equiv \frac{m_1 m_2}{M} \equiv \left( \frac{1}{m_1} + \frac{1}{m_2} \right)^{-1},$$

$m$  is the reduced mass of the mutual motion of its components, and the momenta operators,

$$\hat{\mathbf{P}} \equiv \hat{\mathbf{p}}_1 + \hat{\mathbf{p}}_2, \quad \text{and} \quad \hat{\mathbf{p}} \equiv \frac{m_2}{M} \hat{\mathbf{p}}_1 - \frac{m_1}{M} \hat{\mathbf{p}}_2,$$

commute in the usual (“canonical”) way with, respectively, the radius vector  $\mathbf{R}$  of the center of mass of the molecule, and the distance radius vector  $\mathbf{r}$ .

As Eq. (\*) shows, the system's spectrum is a sum of two independent contributions: the kinetic energy of the molecule as a whole, with the mass  $M$ , free to move in space, and an "effective" single particle, with the reduced mass  $m$ , moving in the spherically symmetric potential  $U = \kappa(r - a)^2/2$ . As we know well, the former motion is simple, giving a continuous energy spectrum (1.89), while the latter is generally complex, and is simplified only if the spring is rather stiff:

$$\kappa a^2 \gg \frac{\hbar^2}{ma^2}. \quad (**)$$

In this limit, we may separate the general 3D motion of the effective particle into its rotation at the fixed distance  $r = a$ , and small radial (1D) oscillations about this point, and use Eqs. (2.262) and (3.163) to write the total energy spectrum as the sum

$$E = \frac{\hbar^2 k^2}{2M} + \frac{\hbar^2 l(l+1)}{2ma^2} + \hbar \omega_0 \left( n + \frac{1}{2} \right), \quad \text{with } \omega_0 \equiv \left( \frac{\kappa}{m} \right)^{1/2}, \quad (***)$$

where the wave vector  $\mathbf{k}$  may take arbitrary values,<sup>26</sup> while  $l$  and  $n$  are integer quantum numbers that take independent values from the similar sets: 0, 1, 2, ...

For most diatomic molecules, the rotational energy scale  $\hbar^2/ma^2$  is in the range from  $10^{-5}$  to  $10^{-2}$  eV. (In the extreme case of the hydrogen molecule  $\text{H}_2$ , with its very light nuclei,  $m_{1,2} \approx 1.7 \times 10^{-27}$  kg and a small equilibrium distance  $a \approx 0.074$  nm  $\approx 1.4 r_B$  between them,  $\hbar^2/ma^2 \approx 7.6$  meV.) As a result, at room temperatures  $T \sim 300$  K, with  $k_B T \sim 25$  meV, thermal fluctuations are sufficient to excite quite a few lower rotational levels with  $l > 0$ . On the other hand, the vibration frequencies  $\omega_0/2\pi$  are between  $10^{12}$  and  $10^{14}$  Hz, so even the lowest oscillation energies are in a much higher range from  $\sim 10^{-2}$  to  $\sim 1$  eV. (In the same ultimate case of  $\text{H}_2$ ,  $\hbar \omega_0 \approx 0.54$  eV.) As a result, at room temperatures, the vibrational levels with  $n > 0$  are virtually *not* populated. The electronic state excitations have comparable or even higher energies, in the a-few-eV ballpark, because they do not involve the motion of relatively heavy particles such as nuclei. This hierarchy justifies the model explored in this problem, and in particular the stiff-spring condition (\*\*).

This is essentially the whole story for *heteronuclear* molecules, such as CO, NO, or HCl, consisting of different and hence distinguishable atoms. On the other hand, for *homonuclear* molecules, such as  $\text{H}_2$ ,  $\text{O}_2$ , or  $\text{N}_2$ , the indistinguishability effects may be important even at room temperatures, because (as was discussed above) most molecules are in their ground electronic and vibrational states, and hence are either symmetric or antisymmetric with respect to atom permutation, depending on their total spin, including not only its electronic but also its nuclear component.

For example, the  $^{16}\text{O}$  nucleus (of the oxygen isotope most abundant at natural conditions) has its total spin equal to zero, while the total (orbital + spin) ground-state electronic wavefunction of the oxygen molecule is *antisymmetric* with respect to the nuclei permutation. As a result, just as was discussed in the solution of the previous problem, the rotational wavefunction has to be antisymmetric with respect to the replacement  $\mathbf{r} \rightarrow -\mathbf{r}$ , i.e. to the simultaneous replacement  $\theta \rightarrow \pi - \theta$ , and  $\varphi \rightarrow \varphi + \pi$  (modulo  $2\pi$ ), where  $\theta$  and  $\varphi$  are the usual polar angles of the distance radius vector  $\mathbf{r}$ . As we know from the properties of the spherical harmonics (see, e.g., Eqs. (3.168) and (3.171), or just Fig. 3.20 of the

<sup>26</sup> The quantum transitions used for most spectral measurements are unaffected by the translational motion, described by the first term in Eq. (\*\*\*), so this component will be ignored in the forthcoming discussion.

lecture notes), this condition may be only fulfilled for odd values of the quantum number  $l$ . This means, rather counter-intuitively, that the ground state of the  $O_2$  molecule corresponds to  $l = 1$ , i.e. essentially, to its rotation:

$$E_g = (E_g)_{\text{electronic}} + \frac{\hbar^2}{ma^2} + \frac{\hbar\omega_0}{2}.$$

Even more interesting (and historically, more important) are the properties of the nitrogen molecule  $N_2$ , with the nitrogen atoms of the (dominating) isotope  $^{14}\text{N}$ . This nucleus has seven protons and seven neutrons, and its ground state has the net spin  $I = 1$ . At the same time, the ground orbital electronic state of the (covalent-bound)  $N_2$  molecule is *symmetric* with respect to the nuclei permutation.<sup>27</sup> As a result, the lowest rotational energy of the molecule depends on the net spin  $I_\Sigma$  of the two nuclei. Since the operator of the total spin is a vector sum similar to those discussed in Secs. 5.7 and 8.2 of the lecture notes:

$$\hat{\mathbf{I}}_\Sigma = \hat{\mathbf{I}}_1 + \hat{\mathbf{I}}_2, \quad \text{with } I_1 = I_2 = 1,$$

and obeys relations similar to those given by Eq. (8.48), we may use the solution of Problem 9, with  $s = 1$ , to conclude that the nuclear spin system has six symmetric states (allowing only even values of  $l$ ) and three antisymmetric states (allowing only odd values of  $l$ ). Since for these molecules, at room temperature,  $k_B T \gg \hbar^2/ma^2$ , many lower-energy rotational states are thermally excited, with the number of such states with even values of  $l$  twice larger than that for odd values of  $l$ .

The selection rules discussed in Sec. 5.6 of the lecture notes (see also the solution of Problem 5.41) enable experimental determination of  $l$ 's parity by measuring which quantum (in particular, optical) transitions from such state to a fixed final state are allowed. In the late 1920s, i.e. before the experimental discovery of neutrons in 1932, the observation of this 2:1 ratio in experimental molecular spectra of  $N_2$  molecules (by L. Ornstein) helped to establish the fact that the spin  $I$  of the  $^{14}\text{N}$  nucleus is indeed equal to 1, and hence to discard the then-plausible model in which the nucleus would consist of 14 protons and 7 electrons, also giving it the observed mass  $m \approx 14m_p$  and the net electric charge  $Q = 7e$ . (In that model, the ground-state value of  $I$  would be semi-integer, leading to a different statistics of  $I_\Sigma$ , and hence of  $l$ .)<sup>28</sup>

**Problem 8.15.** Two indistinguishable spin- $1/2$  particles are attracting each other at contact:

$$U(x_1, x_2) = -w\delta(x_1 - x_2), \quad \text{with } w > 0,$$

but are otherwise free to move along the  $x$ -axis. Find the energy and the orbital wavefunction of the ground state of the system.

*Solution:* The system's Hamiltonian is

$$\hat{H} = \hat{T} + \hat{U} = \frac{\hat{p}_1^2}{2m} + \frac{\hat{p}_2^2}{2m} - w\delta(x_1 - x_2) = -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \right) - w\delta(x_1 - x_2),$$

<sup>27</sup> Let me emphasize that this *orbital symmetry* of the ground electronic state does not contradict its fundamental *asymmetry* with respect to the permutation of any two electrons, which is provided by the singlet spin factor – see, e.g., Eq. (8.12). Such radical difference between the two symmetries is possible because each electron in such an entangled state is a “common commodity” of both nuclei, and its number cannot be associated with that of a particular nucleus.

<sup>28</sup> The author is grateful to P. van Nieuwenhuizen for sharing this historic note.

so the corresponding Schrödinger equation is satisfied, at  $x_1 \neq x_2$ , by exponential orbital wavefunctions

$$\psi_{\kappa_1, \kappa_2} = \text{const} \times \exp\{\kappa_1 x_1 + \kappa_2 x_2\}, \quad (*)$$

with any (real or complex)  $c$ -numbers  $\kappa_{1,2}$ , corresponding to the following kinetic energy:

$$E_{\kappa_1, \kappa_2} = -\frac{\hbar^2}{2m}(\kappa_1^2 + \kappa_2^2).$$

Since the potential energy  $U$  depends only on the distance  $x \equiv x_1 - x_2$  between the particles, it is natural to replace the variables by introducing, besides  $x$ , another independent linear combination of coordinates  $x_{1,2}$ , namely the position  $X \equiv (x_1 + x_2)/2$  of their center of mass. Plugging the reciprocal relation between the old and new variables,<sup>29</sup>

$$x_1 = X + \frac{x}{2}, \quad x_2 = X - \frac{x}{2},$$

into Eq. (\*), we get (for  $x \neq 0$  only):

$$\psi_{\kappa_1, \kappa_2} = \text{const} \times \exp\{\kappa x + \mathcal{K}X\}, \quad \text{with } \kappa \equiv \frac{\kappa_1 - \kappa_2}{2}, \quad \text{and } \mathcal{K} \equiv \kappa_1 + \kappa_2,$$

so

$$\kappa_1 = \frac{\mathcal{K}}{2} + \kappa, \quad \kappa_2 = \frac{\mathcal{K}}{2} - \kappa, \quad \text{and } E_{\kappa_1, \kappa_2} = -\frac{\hbar^2}{2m} \left( \frac{\mathcal{K}^2}{2} + 2\kappa^2 \right).$$

The potential energy is independent of the coordinate  $X$ , so the constant  $\mathcal{K}$  cannot have any real part (otherwise the wavefunction would diverge at either  $X \rightarrow +\infty$  or  $X \rightarrow -\infty$ ), i.e. has to be purely imaginary,  $\mathcal{K} = iK$ . But that would give a positive contribution  $\hbar^2 K^2/4m$  to the energy, so the lowest-energy eigenstates correspond to  $K = 0$ , physically meaning that in its ground state, the system as the whole is at rest (at a completely uncertain location  $X$ ), so its wavefunction reduces to

$$\psi_g(x) = \begin{cases} C_+ \exp\{\kappa_+ x\}, & \text{for } x > 0, \\ C_- \exp\{\kappa_- x\}, & \text{for } x < 0, \end{cases} \quad \text{with } \frac{\hbar^2 \kappa_{\pm}^2}{m} = -E_g. \quad (**)$$

Now we need to select the constants  $C_{\pm}$  (or rather their ratio) and the signs of  $\kappa_{\pm}$  to satisfy:

- the boundary conditions  $\psi(\pm\infty) = 0$ ,
- the symmetry of  $|\psi|^2$  with respect to the particle permutation  $x_1 \leftrightarrow x_2$ , i.e. to the replacement  $x \leftrightarrow -x$ , and
- the fermionic permutation rule – see Eq. (8.14) of the lecture notes.

The first two requirements may be satisfied by assigning to  $\kappa_{\pm}$  the opposite signs and taking  $C_- = \pm C_+$ , i.e. by taking the wavefunction in one of the following two forms:

<sup>29</sup> This transformation of coordinate and momenta is, of course, just a particular case of that discussed in Problem 11, for the particular case  $m_1 = m_2 = m$ , so the reduced mass  $m_{\text{ef}}$  equals  $m/2$ . However, due to this simple relation and the 1D character of particle motion in our current system, it is easier to carry out this transformation again more explicitly rather than to use the results of the more general solution of that problem.

$$\psi = C \times \begin{cases} \exp\{-\kappa|x|\}, \\ \text{sgn}(x)\exp\{-\kappa|x|\}, \end{cases} \quad (***)$$

where  $\kappa \equiv |\kappa_{\pm}| \geq 0$ .

The first of the functions (\*\*\*) is symmetric with respect to the permutation of our spin- $\frac{1}{2}$  particles, and hence is suitable for the description of their singlet spin state (8.21). Now using the fact that at  $x \neq 0$ , for any of the functions (\*\*\*),  $\partial^2 \psi / \partial x_1^2 = \partial^2 \psi / \partial x_2^2$ , we may recast the system's Hamiltonian in the single-particle form:

$$\hat{H} = -\frac{\hbar^2}{2m_{\text{ef}}} \frac{\partial^2}{\partial x^2} - \mathcal{W} \delta(x), \quad \text{with } m_{\text{ef}} = \frac{m}{2}.$$

The (easy) problem of finding the localized eigenstates of this Hamiltonian was solved at the beginning of Sec. 2.6 of the lecture notes: there is only one such state, given by the first of Eqs. (\*\*\*), with  $\kappa$  given by Eq. (2.161). With the due replacement  $m \rightarrow m_{\text{ef}} = m/2$ , it is

$$\kappa = \frac{m}{2\hbar^2} \mathcal{W},$$

giving the ground-state energy

$$E_g = -\frac{\hbar^2 \kappa^2}{m} = -\frac{m\mathcal{W}^2}{4\hbar^2}.$$

On the other hand, for a triplet spin state, the orbital wavefunction had to be antisymmetric, i.e. have the second form listed in Eq. (\*\*\*). However, this function is discontinuous at  $x = 0$ , and hence cannot be the solution of the Schrödinger equation – at least with our Hamiltonian. So, the system does not have a localized triplet eigenstate, and all acceptable triplet states are extended, i.e. have energies  $E \geq 0$ , higher than the negative  $E_g$  found above for the singlet spin state.

**Problem 8.16.** Two indistinguishable spin- $\frac{1}{2}$  particles are confined to move around a circle of radius  $R$ , and interact only at a very short arc distance  $l = R(\varphi_1 - \varphi_2) \equiv R\varphi$  between them, so the interaction potential  $U$  may be well approximated with a delta function of  $\varphi$ . Find the ground state and its energy, for the cases of:

- (i) the orbital (spin-independent) repulsion:  $\hat{U} = \mathcal{W} \delta(\varphi)$ ,
- (ii) the spin-spin interaction:  $\hat{U} = -\mathcal{W} \hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2 \delta(\varphi)$ ,

both with  $\mathcal{W} > 0$ . Analyze the trends of your results in the limits  $\mathcal{W} \rightarrow 0$  and  $\mathcal{W} \rightarrow \infty$ .

*Solutions:*

(i) The system's Hamiltonian is

$$\hat{H} = \frac{\hat{L}_1^2}{2mR^2} + \frac{\hat{L}_2^2}{2mR^2} + \hat{U},$$

where  $\hat{L}_{1,2}$  are the single-particle operators of the angular momentum (or more exactly, of its only Cartesian component), in the coordinate representation equal to

$$\hat{L}_{1,2} = -i\hbar \frac{\partial}{\partial \varphi_{1,2}}.$$

Since at  $\varphi \neq 0$ , the potential energy  $U$  vanishes, the two-particle Schrödinger equation corresponding to this Hamiltonian is satisfied by any product of the single-particle eigenfunctions given by Eq. (3.129) of the lecture notes:

$$\psi_{\nu_1, \nu_2} = \text{const} \times \exp\{i(\nu_1 \varphi_1 + \nu_2 \varphi_2)\}, \quad (*a)$$

with any  $c$ -numbers  $\nu_1$  and  $\nu_2$  – cf. Eq. (\*) of the model solution of the previous problem. Similarly to that solution, since  $U$  depends only on the “distance angle”  $\varphi \equiv \varphi_1 - \varphi_2$ , it is natural to replace the variables by introducing, besides  $\varphi$ , the average angle  $\phi \equiv (\varphi_1 + \varphi_2)/2$  (essentially the angular position of the system’s center of mass), so the individual particle positions are

$$\varphi_1 = \phi + \frac{\varphi}{2}, \quad \varphi_2 = \phi - \frac{\varphi}{2}.$$

Plugging these relations into Eq. (\*a), we may recast it as

$$\psi_{\nu_1, \nu_2} = \text{const} \times \exp\{i(\nu \varphi + N \phi)\}, \quad \text{with } \nu \equiv \frac{\nu_1 - \nu_2}{2}, \quad N \equiv \nu_1 + \nu_2, \quad (*b)$$

where  $N$  scales the total angular momentum of the system,  $L \equiv L_1 + L_2$ , in such a state:  $L = \hbar(\nu_1 + \nu_2) = \hbar N$ .

For each spin state of the system, we need to form a correct linear superposition of such fundamental partial solutions, which would:

- satisfy the fermionic permutation rule – see the second of Eqs. (8.14) of the lecture notes,
- satisfy the proper boundary conditions at the interaction point  $\varphi = 0$ , and
- be invariant to the physically indistinguishable translations  $\varphi_{1,2} \rightarrow \varphi_{1,2} + 2\pi$ .

Since we do not know *a priori* which spin state of the system has the lowest-energy (ground) state,<sup>30</sup> we need to consider both options. In any of the *triplet* spin states described by Eqs. (8.21) of the lecture notes, the orbital wavefunction  $\psi_t(\varphi_1, \varphi_2)$  has to be antisymmetric with respect to the particle permutation:

$$\psi_t(\varphi_1, \varphi_2) = -\psi_t(\varphi_2, \varphi_1), \quad (**)$$

and since it also has to be continuous everywhere (even at the potential’s singularity point), the wavefunction has to vanish at  $\varphi_1 \rightarrow \varphi_2$ , i.e. at  $\varphi \rightarrow 0$ . As a result, according to Eq. (2.75) applied to  $\psi_t$  as a function of any of its arguments, the orbital wavefunction of the triplet state is not affected by the interaction potential at all, and the eigenstates may be constructed as a linear superposition of the states (\*) extended to all values of  $\varphi_1$  and  $\varphi_2$ , from  $-\infty$  to  $+\infty$ . Since such extended states are linearly independent, the above periodicity-invariance condition has to apply to each of them, giving  $\nu_1 = n_1$ ,  $\nu_2 = n_2$ , with integer  $n_{1,2}$ . For the lowest-energy eigenstates, we have to select the quantum numbers  $n_{1,2}$  with the smallest  $|n_{1,2}|$  (corresponding to the lowest magnitudes of the corresponding angular momenta  $L_{1,2} = \hbar n_{1,2}$  and hence of the kinetic energy), but the choice  $n_1 = n_2 = 0$  would give  $\psi(\varphi_1, \varphi_2) = \text{const}$  and

<sup>30</sup> On the basis of the helium atom’s discussion in Sec. 8.2, and the solution of several prior problems of this chapter, we may *guess* this should be a singlet state, but it is prudent to verify this guess.

hence violate Eq. (\*\*). The next-lowest quantum number sets are  $\{n_1 = 0, n_2 = \pm 1\}$  and  $\{n_1 = \pm 1, n_2 = 0\}$ , whose eigenstates may be readily combined to satisfy Eq. (\*\*):

$$\psi_{\pm} = \psi_{\pm} = \text{const} \times (\exp\{\pm i\varphi_1\} - \exp\{\pm i\varphi_2\}).$$

For each of these two states, each of the component wavefunctions corresponds to the angular orbital momentum  $L_{1,2} = \pm\hbar$  of one particle and  $L_{2,1} = 0$  of its counterpart, and hence the total kinetic energies  $T_{\pm} = (L_1^2 + L_2^2) / 2mR^2$  of these states may be found even without their formal calculation:

$$E_{\pm} = E_{\pm} = T_{\pm} = \frac{\hbar^2}{2mR^2} > 0.$$

On the contrary, in the *singlet* spin state, the orbital wavefunction  $\psi_s(\varphi_1, \varphi_2)$  has to be symmetric:

$$\psi_s(\varphi_1, \varphi_2) = \psi_s(\varphi_2, \varphi_1). \quad (***)$$

Hence, the wavefunction does not necessarily vanish at the interaction point  $\varphi_1 = \varphi_2$ , i.e. at  $\varphi = 0$ , and may be affected by the interaction potential  $U$ . Hence it is more natural to consider it a function of the combinational arguments  $\varphi$  and  $\phi$  introduced above:

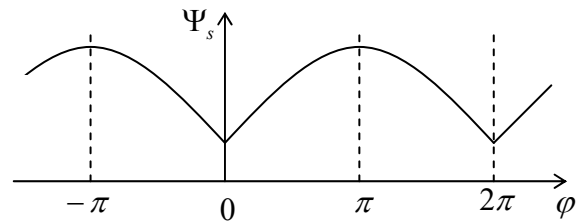
$$\Psi_s(\varphi, \phi) \equiv \psi_s(\varphi_1, \varphi_2) = \psi_s\left(\phi + \frac{\varphi}{2}, \phi - \frac{\varphi}{2}\right),$$

and try to compose the correct wavefunction from the partial functions (\*b). According to Eq. (\*\*\*),  $\Psi_s$  as a function of  $\varphi$  has to be symmetric for any  $\phi$ :

$$\Psi_s(-\varphi, \phi) = \Psi_s(\varphi, \phi)$$

– see the figure on the right. As a result, its single-side derivatives at the interaction point  $\varphi = 0$  should be equal but opposite:

$$\left. \frac{\partial \Psi_s}{\partial \varphi} \right|_{\varphi=+0} = - \left. \frac{\partial \Psi_s}{\partial \varphi} \right|_{\varphi=-0}.$$



Using this equality in Eq. (2.75) of the lecture notes, applied to  $\Psi_s$  as a function of  $\varphi$ , and with the due replacement  $m \rightarrow m_{\text{ef}} = m/2$ , we get the following boundary condition:

$$\left. \frac{\partial \Psi_s}{\partial \varphi} \right|_{\varphi=+0} = \frac{m}{\hbar^2} \omega \Psi_s \Big|_{\varphi=\pm 0}. \quad (***)$$

This relation does not affect the dependence of  $\Psi_s$  on  $\phi$ , so if we want the lowest-energy wavefunction, we should compose it of the exponential functions (\*b) with  $N = 0$ :<sup>31</sup>

$$\Psi_s = \sum_{\nu} c_{\nu} \exp\{i\nu\varphi\}.$$

<sup>31</sup> Physically, this means that we consider the system with zero total angular momentum – apparently, a natural requirement for the lowest-energy state. Note, however, that for the calculated triplet states  $\psi_{\pm}$ , the equality  $\langle L \rangle = 0$  is valid for each of the states, but *not* for each exponential component of such a state, which correspond to equal and opposite momenta  $L = \pm\hbar$ .

Due to the cusp of the function  $\Psi_s$  at  $\varphi = 0$  (see Eq. (\*\*\*) and the figure above), and its  $2\pi$ -periodicity, it is natural to limit this expansion to a  $2\pi$ -segment (say,  $[0, 2\pi]$ ) of the argument  $\varphi$ , where the function is smooth, extending it to other similar segments periodically. At this limited segment, the sum of just two terms, with  $\nu = \pm\lambda$ ,

$$\Psi_s = \text{const} \times [\exp\{+i\lambda(\varphi - \pi)\} + \exp\{-i\lambda(\varphi - \pi)\}] \propto \cos \lambda(\varphi - \pi), \quad \text{for } 0 < \varphi < 2\pi,$$

satisfies the symmetry condition (\*\*\*) for any (not necessarily integer!)  $\lambda$ . Similarly to the triplet case, it is unnecessary to calculate the eigenenergy corresponding to this linear superposition explicitly, because each of its terms has the same angular momentum magnitude  $|L_{1,2}| = \hbar\lambda$  of each particle, so

$$E_s = T_1 + T_2 = 2 \frac{L_{1,2}^2}{2mR^2} = \lambda^2 \frac{\hbar^2}{mR^2}.$$

The value of  $\lambda$ , and hence that of  $E_s$ , may be found by plugging this  $\Psi_s$  into the boundary condition (\*\*\*\*). It gives us the following characteristic equation:

$$\lambda \sin \lambda\pi = \frac{m}{\hbar^2} \omega \cos \lambda\pi,$$

which may be rewritten, more conveniently for analysis, as

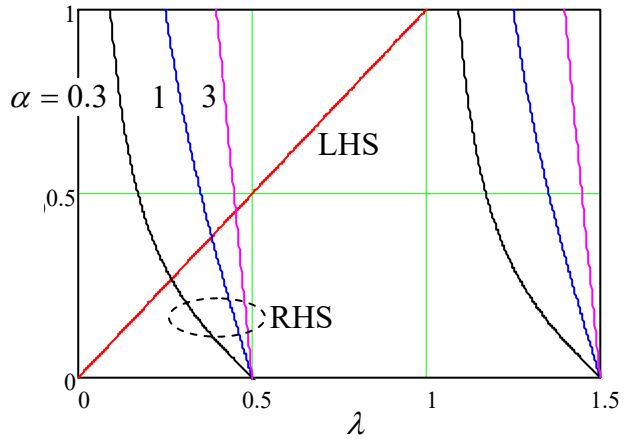
$$\lambda = \alpha \cot \lambda\pi, \quad \text{with } \alpha \equiv \frac{m}{\hbar^2} \omega.$$

Both sides of the last form of the equation are plotted, in the figure on the right, as functions of  $\lambda$ , for several values of the normalized interaction strength  $\alpha$ . Since the eigenenergy of the state scales as  $\lambda^2$ , the lowest-energy state corresponds to the smallest root of the characteristic equation, i.e. to the curve intersection point that is closest to the origin. As the figure shows, such smallest root is always confined to the segment  $0 < \lambda < 1/2$ , so for any  $\lambda$ ,

$$0 \leq E_s \leq \frac{\hbar^2}{4mR^2} \equiv \frac{1}{2} E_t.$$

Thus, as could be expected, for any dimensionless interaction parameter  $\alpha > 0$ , the spin-singlet state has its lowest energy lower than that of the spin-triplet states, i.e. it is the genuine ground state.<sup>32</sup>

If the interaction is weak,  $\alpha \rightarrow 0$ , then  $\lambda \rightarrow 0$  as well, and we may find its asymptotic value by approximating  $\sin \lambda\pi$  with  $\lambda\pi$ , and  $\cos \lambda\pi$  with 1, so  $\cot \lambda\pi \approx 1/\lambda\pi$ . With this approximation, our characteristic equation yields  $\lambda \approx (\alpha/\pi)^{1/2}$ , so<sup>33</sup>



<sup>32</sup> A thoughtful reader might ask: how do we know that all eigenstates of the system, in which the particle *do* interact, are limited to the spin singlet and triplet states, i.e. the states that may be factored according to Eq. (8.12)? An answer to this concern is that each of the 4 considered states (1 singlet and 3 triplet) are eigenstates of the problem. Since these states may be taken for the full basis in the 4-function Hilbert space of two spins- $1/2$ , this problem cannot have other independent spin eigenstates. However, this fact was *not* clear *a priori*, and may *not* be true for other problems, so the caution of this (hypothetical :- ) reader is justified.



$$E_s \approx \frac{\alpha \hbar^2}{\pi m R^2} = \frac{1}{\pi} \frac{\mathcal{W}}{R^2} \rightarrow 0.$$

On the other hand, in the limit of very strong particle repulsion ( $\alpha \rightarrow \infty$ ),  $\lambda$  tends to  $1/2$ , so the singlet state energy tends to

$$(E_s)_{\max} = \frac{\hbar^2}{4mR^2} = \frac{1}{2} E_t.$$

Since  $\cos[(\varphi - \pi)/2] = -|\sin(\varphi/2)|$ , in this limit, the singlet state's eigenfunction may be represented, for any value of  $\varphi$  ( $-\infty < \varphi < +\infty$ ), as

$$\Psi_s = \text{const} \times \left| \sin \frac{\varphi}{2} \right|,$$

approaching zero at the interaction point  $\varphi = 0$ . This fact explains why the state's energy does not increase further as the interaction factor  $\mathcal{W}$  is increased.

(ii) As was argued above, *triplet* spin states of the system are not affected by the delta-functional interaction  $U \propto \delta(\varphi)$  of the particles at all. This result does not depend on the particular form of the coefficient before the delta function, so even for the (local) spin-spin interaction, the result for  $E_t$  remains the same as above:

$$E_t = \frac{\hbar^2}{2mR^2}.$$

On the other hand, for the *singlet* state, we may use the result obtained in the solution of Problem 3,

$$\langle \mathbf{s}_1 \cdot \mathbf{s}_2 \rangle_- = -3 \left( \frac{\hbar}{2} \right)^2,$$

for the expectation value of the product  $\mathbf{s}_1 \cdot \mathbf{s}_2$  participating in the interaction  $U$ . Since, according to this solution, the singlet state is one of the eigenstates of the corresponding operator (the others being the three triplet states), its energy may be obtained from the results of part (i) of our current problem by the following simple replacement:

$$\mathcal{W} \rightarrow 3 \left( \frac{\hbar}{2} \right)^2 \mathcal{W}, \quad \text{i.e. } \alpha \rightarrow 3 \left( \frac{\hbar}{2} \right)^2 \alpha,$$

giving, in particular, the following asymptotic values:

$$E_s \rightarrow \frac{\hbar^2}{mR^2} \times \begin{cases} 3\alpha(\hbar/2)^2 / \pi \rightarrow 0, & \text{for } \alpha \rightarrow 0, \\ 1/4, & \text{for } \alpha \rightarrow \infty, \end{cases}$$

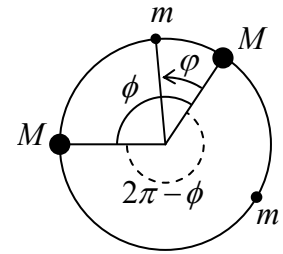
so for any  $\alpha$ ,  $E_s < E_t$ , i.e. the singlet state is the (non-degenerate) ground state of the system.

Finally, note that both interactions considered above correspond to the effective repulsion of the particles. For the opposite sign of  $\mathcal{W}$  (particle attraction), the singlet ground states may be *bound*, i.e. localized at  $\varphi \approx 0$ , having imaginary values of  $\nu_{1,2}$ , and hence negative eigenenergies<sup>34</sup> – cf. Problem 15.

<sup>33</sup> This result may be also obtained using the perturbation theory – the additional exercise highly recommended to the reader.

<sup>34</sup> Solving this (conceptually, very similar) problem may be one more useful exercise for the reader.

**Problem 8.17.** Two particles of mass  $M$ , separated by two much lighter particles of mass  $m \ll M$ , are placed on a circle of radius  $R$  – see the figure on the right. The particles fully repulse each other at contact, but otherwise, each of them is free to move along the circle. Calculate the lower part of the system’s energy spectrum.



*Solution:* Due to the strong hierarchy of the masses, we may solve the problem in two stages: first, analyze the “fast” (high-energy) motion of the lighter particles while considering the angular positions  $\phi_1$  and  $\phi_2$  of the heavier particles fixed, and then, with the account of the kinetic energy of that motion, analyze the “slow” motion of the heavier particles.<sup>35</sup>

At the first stage, due to the strong particle repulsion at contact, we may consider the motion of one lighter particle as free but confined to a fixed angular segment of length  $\phi \equiv \phi_2 - \phi_1$ , with its wavefunction turning to zero at its ends. The Hamiltonian of this problem is the same as for the single-particle planar rotor (see Sec. 3.5 of the lecture notes):

$$\hat{H}_m = \frac{\hat{L}_z^2}{2mR^2}, \quad \text{with } \hat{L}_z = \hat{p}R = -i\hbar \frac{\partial}{\partial \varphi},$$

where  $\varphi$  is the angular position of the light particle, referred, for example, to one of the boundaries of the segment – see the figure above. The solution of the corresponding Schrödinger eigenproblem,

$$-\frac{\hbar^2}{2mR^2} \frac{d^2 \psi_n}{d\varphi^2} = E_n \psi_n, \quad \text{with } \psi_n|_{\varphi=0} = \psi_n|_{\varphi=\phi} = 0,$$

is very simple (cf. Sec. 1.7 of the lecture notes):

$$\psi_n = C \sin \frac{\pi n \varphi}{\phi}, \quad E_n = \frac{\pi^2 \hbar^2}{2mR^2 \phi^2} n^2, \quad n = 0, 1, 2, \dots$$

At  $m \rightarrow 0$ , the separation of these energy levels is very large, so for our purposes, we are interested only in the ground state of this motion, with the energy  $E_1 = \pi^2 \hbar^2 / 2mR^2 \phi^2$ . Adding, to this energy, the similar ground-state energy of motion of the second light particle on its angular segment of the length  $(2\pi - \phi)$ , we get the following total ground-state energy of the light particles:

$$E_g = U(\phi) \equiv \frac{\pi^2 \hbar^2}{2mR^2} \left[ \frac{1}{\phi^2} + \frac{1}{(2\pi - \phi)^2} \right].$$

Since this energy is a function of  $\phi$  only, it plays the role of the potential energy for the slow motion of the heavier particles. The scale of the variable  $\phi$  is of the order of  $\pi$ , so the quantization of that motion leads to additional energies of the order of  $\hbar^2 / MR^2$ , which is, at  $M \gg m$ , much lower than the scale  $\hbar^2 / mR^2$  of the function  $U(\phi)$ . This is why we are only interested in the shape of this function near

<sup>35</sup> This *Born-Oppenheimer approximation* is broadly used for the separation of electron and nuclear motion in theoretical analyses of molecular spectra and some other tasks. Due to the large ratio  $m_p/m_e \approx 1,835$ , generally, it works very well but sometimes may benefit from corrections – for example, in the description of the lightest atoms/ions such as hydrogen – see, e.g., L. Cattaneo *et al.*, *Nature Phys.* **14**, 733 (2018) and/or K. Krüget *et al.*, *Nature Chemistry* **15**, 326 (2023).

its minimum, reached at the point  $\phi_0 = \pi$ . Near this point, we may take  $\phi \equiv \pi + \tilde{\phi}$ , and Taylor-expand this function,

$$U(\phi) \equiv \frac{\pi^2 \hbar^2}{2mR^2} \left[ \frac{1}{\phi^2} + \frac{1}{(2\pi - \phi)^2} \right] \equiv \frac{\pi^2 \hbar^2}{2mR^2} \left[ \frac{1}{(\pi + \tilde{\phi})^2} + \frac{1}{(\pi - \tilde{\phi})^2} \right] \equiv \frac{\hbar^2}{mR^2} \frac{1 + (\tilde{\phi}/\pi)^2}{\left[1 - (\tilde{\phi}/\pi)^2\right]^2},$$

with respect to small  $\tilde{\phi}/\pi$ , keeping only two leading terms of the series:

$$U(\phi) \approx \frac{\hbar^2}{mR^2} \left( 1 + 3 \frac{\tilde{\phi}^2}{\pi^2} \right) \equiv U_0 + \frac{\kappa (R\tilde{\phi})^2}{2}, \quad \text{with } U_0 \equiv \frac{\hbar^2}{mR^2}, \text{ and } \kappa \equiv \frac{6\hbar^2}{\pi^2 mR^4}. \quad (*)$$

In this approximation, the Hamiltonian describing the motion of the heavier particles is

$$\hat{H}_M = \frac{\hat{P}_1^2}{2M} + \frac{\hat{P}_2^2}{2M} + U(\phi), \quad \text{with } \hat{P}_{1,2} = -i\hbar \frac{\partial}{\partial (R\phi_{1,2})}.$$

This Hamiltonian may be partitioned, exactly as this was done in several previous problems starting from Problem 11, into a sum of that of the joint rotation of both particles, with the total mass  $2M$ , around the circle, and the harmonic oscillator, with the reduced mass  $M_r = M/2$  and the effective spring constant  $\kappa$ , and hence the frequency

$$\omega_0 = \left( \frac{\kappa}{M_r} \right)^{1/2} = \frac{2\sqrt{3}\hbar}{\pi(mM)^{1/2} R^2}.$$

Adding the results of the quantization of these independent subsystems, we get the requested energy spectrum:<sup>36</sup>

$$E_{N,m} = U_0 + \frac{2\sqrt{3}\hbar^2}{\pi^2 R^2 (mM)^{1/2}} \left( N + \frac{1}{2} \right) + \frac{\hbar^2}{4MR^2} m^2, \quad \text{with } N = 0, 1, 2, \dots, \text{ and } m = 0, \pm 1, \pm 2, \dots$$

Due to the given mass relation  $m \ll M$ , the intervals between first rotational values are much narrower than those between the vibrational levels (and those, in turn, are much smaller than  $U_0$ ), so semi-quantitatively, the spectrum looks just like the one sketched in the model solution of Problem 13.

Note also that if the particles are indistinguishable, the set of quantum numbers  $m$  may be decimated, because the period of the rotational wavefunction may change from  $2\pi$  (as was assumed above) to  $\pi$  – depending on the type of the particles (bosons vs fermions) and the vibrational state's symmetry – see the solutions of Problems 13 and 14.

**Problem 8.18.** Two spin- $1/2$  particles are confined in a spherically symmetric potential well  $U_0(\mathbf{r}) = m\omega_0^2 r^2/2$ . In addition, they directly interact via a short-range potential  $U_{\text{int}} = \mathcal{W}\delta(\mathbf{r}_1 - \mathbf{r}_2)$ . In the first approximation in small  $\mathcal{W}$ , calculate the energies of

- (i) the ground state, and
- (ii) the lowest excited states of the system.

<sup>36</sup> Let me hope that the difference between the magnetic quantum number  $m$  and the lighter particle mass in this expression is absolutely clear from the context.

*Solutions:*

(i) In the absence of the direct (explicit) particle-particle interaction, the ground state of the system is the spin singlet described by Eq. (8.24) of the lecture notes,

$$\langle \mathbf{r} | \mathbf{g} \rangle = |s_-\rangle \psi_g(\mathbf{r}_1) \psi_g(\mathbf{r}_2),$$

whose spin factor is given by Eq. (8.18):

$$|s_-\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle),$$

while  $\psi_g(\mathbf{r})$  is the orbital ground-state wavefunction of a single particle in the potential  $U_0(\mathbf{r})$ . According to Eq. (3.125) with  $d = 3$ , this function may be represented in the Cartesian form<sup>37</sup>

$$\psi_g(\mathbf{r}) = \psi_{000}(\mathbf{r}) \equiv \psi_0(x) \psi_0(y) \psi_0(z),$$

where  $\psi_0$  is the ground-state wavefunction (2.275) of a 1D harmonic oscillator:

$$\psi_0(x) = \frac{1}{\pi^{1/4} x_0^{1/2}} \exp\left\{-\frac{x^2}{2x_0^2}\right\}, \quad \text{with } x_0 \equiv \left(\frac{\hbar}{m\omega_0}\right)^{1/2}.$$

The unperturbed energy of this spin-singlet state is just twice the energy of each particle, given by Eq. (3.124) with  $n_j = 0$  and  $d = 3$ :

$$E_g^{(0)} = 2\varepsilon_g = 3\hbar\omega_0.$$

The first-order correction to this value, due to the particle-particle interaction, may be found by using Eq. (6.14). Taking into account the spin independence of the perturbation potential  $U_{\text{int}}$ , we get

$$\begin{aligned} E_g^{(1)} &= \langle \mathbf{g} | \hat{U}_{\text{int}} | \mathbf{g} \rangle = \langle s_- | s_- \rangle \int d^3r_1 \int d^3r_2 \psi_{000}^*(\mathbf{r}_1) \psi_{000}^*(\mathbf{r}_2) w \delta(\mathbf{r}_1 - \mathbf{r}_2) \psi_{000}(\mathbf{r}_1) \psi_{000}(\mathbf{r}_2) = w \int \psi_{000}^4(\mathbf{r}) d^3r \\ &= w \int \psi_0^4(x) dx \int \psi_0^4(y) dy \int \psi_0^4(z) dz = w \left[ \int \psi_0^4(x) dx \right]^3 = w \left( \frac{1}{\pi x_0^2} \int_{-\infty}^{+\infty} \exp\left\{-\frac{2x^2}{x_0^2}\right\} dx \right)^3 \\ &= w \left( \frac{1}{\sqrt{2\pi} x_0} \int_{-\infty}^{+\infty} \exp\{-\xi^2\} d\xi \right)^3 = \frac{w}{(2\pi)^{3/2} x_0^3}. \end{aligned}$$

(ii) As in the helium atom discussed in Sec. 8.2 of the lecture notes, at  $\mathcal{W} = 0$ , the lowest excited states of the system are either spin singlets:

$$\langle \mathbf{r} | \mathbf{e}_-\rangle = |s_-\rangle \frac{1}{\sqrt{2}} [\psi_e(\mathbf{r}_1) \psi_g(\mathbf{r}_2) + \psi_g(\mathbf{r}_1) \psi_e(\mathbf{r}_2)]$$

or spin triplets:

$$\langle \mathbf{r} | \mathbf{e}_+\rangle = |s_+\rangle \frac{1}{\sqrt{2}} [\psi_e(\mathbf{r}_1) \psi_g(\mathbf{r}_2) - \psi_g(\mathbf{r}_1) \psi_e(\mathbf{r}_2)], \quad (*)$$

<sup>37</sup> Alternatively, as was discussed in Problem 3.27, the ground state and the lowest excited states of this isotropic 3D harmonic oscillator may be described by the spherical-harmonic wavefunction (3.200). Solving our current problem in this representation is a good additional exercise, which is highly recommended to the reader.

where  $|s_+\rangle$  is any of the kets participating in Eq. (8.21):

$$|s_+\rangle = \text{either } |\uparrow\uparrow\rangle, \text{ or } |\downarrow\downarrow\rangle, \text{ or } \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle),$$

while  $\psi_e(\mathbf{r})$  may be any of the orbital wavefunctions of the lowest excited state of a single particle:

$$\psi_e(\mathbf{r}) = \text{either } \psi_{100}(\mathbf{r}) \equiv \psi_1(x)\psi_0(y)\psi_0(z), \quad \text{or } \psi_{010}(\mathbf{r}), \quad \text{or } \psi_{001}(\mathbf{r}).$$

Here  $\psi_1$  is the wavefunction of the lowest excited state of a 1D harmonic oscillator; according to Eqs. (2.282) and (2.284),

$$\psi_1(x) = \frac{1}{\sqrt{2\pi^{1/4}x_0^{1/2}}} \exp\left\{-\frac{x^2}{2x_0^2}\right\} H_1\left(\frac{x}{x_0}\right) = \frac{\sqrt{2}}{\pi^{1/4}x_0^{1/2}} \frac{x}{x_0} \exp\left\{-\frac{x^2}{2x_0^2}\right\}. \quad (**)$$

The unperturbed energy of all these states, corresponding to a single  $\hbar\omega_0$ -excitation of just one of the component 1D oscillators, is the same:

$$E_e^{(0)} = E_g^{(0)} + \hbar\omega_0 = 4\hbar\omega_0;$$

due to the triple orbital degeneracy of all these states and the additional triple spin degeneracy of the triplet states, this energy level's total degeneracy is  $N = 3 \times (1+3) = 12$ .

As was discussed in Sec. 6.1, the main effect of a stationary perturbation  $U_{\text{int}}$  is lifting this degeneracy. The  $N$  energy shifts  $E_n^{(1)}$  describing this effect may be found as the roots of Eq. (6.27). For spelling it out for our 12 states, we, generally, would need to calculate  $N^2 = 144$  matrix elements  $H_{nn'}^{(1)}$  defined by Eq. (6.8):

$$H_{nn'}^{(1)} = \langle \mathbf{e}_n | \hat{U}_{\text{int}} | \mathbf{e}_{n'} \rangle.$$

However, due to the high symmetry of our problem, this task is not as hard as it may look at first glance.

First, due to the spin independence of  $U_{\text{int}}$ , all matrix elements relating the spin-singlet and spin-triplet states vanish because  $\langle s_{\pm} | s_{\mp} \rangle = 0$ . Hence, the  $12 \times 12$  matrix  $H_{nn'}^{(1)}$  falls apart into two independent matrices: one with  $3 \times 3 = 9$  elements, which inter-relates the spin-singlet states, and the second one with  $9 \times 9 = 81$  elements relating the spin-triplet states. Let us start with the first matrix:

$$\begin{aligned} H_{nn'}^{(1)} &= \langle (\mathbf{e}_-)_n | \hat{U}_{\text{int}} | (\mathbf{e}_-)'_{n'} \rangle = \langle s_- | s_- \rangle \int d^3r_1 \int d^3r_2 \frac{1}{\sqrt{2}} [\psi_e(\mathbf{r}_1)\psi_g(\mathbf{r}_2) + \psi_g(\mathbf{r}_1)\psi_e(\mathbf{r}_2)]_n \omega \delta(\mathbf{r}_1 - \mathbf{r}_2) \\ &\quad \times \frac{1}{\sqrt{2}} [\psi_e(\mathbf{r}_1)\psi_g(\mathbf{r}_2) + \psi_g(\mathbf{r}_1)\psi_e(\mathbf{r}_2)]_{n'}, \\ &= \frac{\omega}{2} \int [2\psi_e(\mathbf{r})\psi_g(\mathbf{r})]_n [2\psi_e(\mathbf{r})\psi_g(\mathbf{r})]_{n'} d^3r \equiv 2\omega \int [\psi_e(\mathbf{r})]_n [\psi_e(\mathbf{r})]_{n'} \psi_g^2(\mathbf{r}) d^3r. \end{aligned}$$

Here comes the second major simplification: all such integrals with  $n \neq n'$ , i.e. with different combinations of single-particle wavefunctions, vanish because the 1D functions (\*\*) are asymmetric; for example,

$$\int \psi_{100}(\mathbf{r})\psi_{010}(\mathbf{r})\psi_g^2(\mathbf{r}) d^3r = \int_{-\infty}^{+\infty} \psi_1(x)\psi_0^3(x) dx \int_{-\infty}^{+\infty} \psi_1(y)\psi_0^3(y) dy \int_{-\infty}^{+\infty} \psi_0^4(z) dz = 0,$$

and similarly for all other pairs of different indices. Only the diagonal matrix elements are different from zero; e.g., for  $\psi_e(\mathbf{r}) = \psi_1(x)\psi_0(y)\psi_0(z)$ :

$$H_{nn}^{(1)} = 2\mathcal{W} \int [\psi_e(\mathbf{r})]_n^2 \psi_g^2(\mathbf{r}) d^3r = 2\mathcal{W} \int_{-\infty}^{+\infty} \psi_1^2(x) \psi_0^2(x) dx \int_{-\infty}^{+\infty} \psi_0^4(y) dy \int_{-\infty}^{+\infty} \psi_0^4(z) dz,$$

and similarly for two other combinations. The (equal) second and third integrals were already calculated in Task (i), so what remains is to calculate the first one by using the above formulas for  $\psi_0$  and  $\psi_1$ :

$$\int_{-\infty}^{+\infty} \psi_1^2(x) \psi_0^2(x) dx = \frac{2}{\pi x_0^2} \int_{-\infty}^{+\infty} \frac{x^2}{x_0^2} \exp\left\{-\frac{2x^2}{x_0^2}\right\} dx = \frac{2}{\pi x_0} \int_{-\infty}^{+\infty} \xi^2 \exp\{-2\xi^2\} d\xi = \frac{1}{(8\pi)^{1/2} x_0},$$

and we get

$$H_{nn}^{(1)} = \frac{\mathcal{W}}{(2\pi)^{3/2} x_0^3}.$$

Hence, for the spin-singlet excited states, the determinant in Eq. (6.27) has only three equal diagonal terms, i.e. the just-calculated expression gives the energy shift of these states. (By coincidence, it is equal to the ground-state energy shift calculated in the previous task.)

Finally, the last (but not least) simplification is that *all* matrix elements  $H_{mn}^{(1)}$ , for the spin-triplet excited states vanish because of the  $\delta$ -functional character of our perturbation. Indeed, the internal integration over one of coordinates  $\mathbf{r}_{1,2}$ , leading to the replacement  $\mathbf{r}_2 \rightarrow \mathbf{r}_1 \equiv \mathbf{r}$ , turns any of the orbital factors in Eq. (\*) to zero identically. Hence, in the first order of the perturbation theory, the energy of these states does not change.

To summarize, the perturbation lifts the 12-fold degeneracy of the lowest excited energy level only partly, by separating the three spin-singlet states from the nine spin-triplet states by

$$\Delta E_e = \frac{\mathcal{W}}{(2\pi)^{3/2} x_0^3}.$$

This first-order perturbative result is quantitatively correct only if  $E^{(1)} \sim \mathcal{W}/x_0^3 \ll E^{(0)} \sim \hbar\omega_0$ .

**Problem 8.19.**  $N$  indistinguishable spin- $1/2$  particles are placed into the spherically symmetric potential well  $U(\mathbf{r}) = m\omega_0^2 r^2/2$ . Neglecting the explicit interaction of the particles, find the ground-state energy of the system.

*Solution:* As was discussed at the beginning of Sec. 8.3 of the lecture notes, solving such problems (for non-interacting particles only!), we may neglect the genuine structure of the spin states, and reduce the spin effects to the Pauli principle, with the spin degeneracy  $g = 2s + 1$  of each single-particle orbital state. Per Eq. (3.124) of the lecture notes (with  $d = 3$ ), the single-particle orbital energy spectrum in this potential is

$$\varepsilon_n = \hbar\omega_0 \left( n + \frac{3}{2} \right), \quad \text{with } n \equiv n_x + n_y + n_z, \quad \text{and } n_j = 0, 1, \dots$$

As was discussed in the model solution of Problem 3.27, the orbital degeneracy of each level may be calculated as the number of different ways to distribute  $n$  indistinguishable “balls” (the partial quantum numbers contributing to integer  $n$ ) between 3 distinct “boxes” ( $n_x$ ,  $n_y$ , and  $n_z$ ):<sup>38</sup>

$$M_n^{(3)} = \frac{(n-1+3)!}{n!(3-1)!} \equiv \frac{1}{2}(n+1)(n+2).$$

The spin- $1/2$  degeneracy  $g = 2s + 1 = 2$  doubles this orbital degeneracy. Hence, if the given number  $N$  of particles coincides with any of the following special integers,

$$N_m \equiv 2 \sum_{n=0}^{m-1} M_n^{(3)},$$

then in the ground state, exactly  $m$  single-particle levels (with  $n = 0, 1, \dots, m-1$ ) are completely filled, so the total energy is

$$E(N_m) = 2 \sum_{n=0}^{m-1} \varepsilon_n M_n^{(3)} = 2\hbar\omega_0 \sum_{n=0}^{m-1} \left(n + \frac{3}{2}\right) M_n^{(3)}.$$

Defining a new summation index as  $n' \equiv n + 1$ , so that  $n = n' - 1$ , we get

$$\begin{aligned} N_m &\equiv 2 \sum_{n=0}^{m-1} M_n^{(3)} = \sum_{n=0}^{m-1} (n+1)(n+2) \equiv \sum_{n'=1}^m n'(n'+1) \equiv \sum_{n'=1}^m n'^2 + \sum_{n'=1}^m n', \\ E(N_m) &= \hbar\omega_0 \sum_{n=0}^{m-1} \left(n + \frac{3}{2}\right) (n+1)(n+2) \equiv \hbar\omega_0 \left( \sum_{n'=1}^m n'^3 + \frac{3}{2} \sum_{n'=1}^m n'^2 + \frac{1}{2} \sum_{n'=1}^m n' \right). \end{aligned}$$

Now by using the well-known formulas for the summation of several first natural numbers, their squares, and their cubes,<sup>39</sup> we obtain

$$N_m = \frac{1}{3}m(m+1)(m+2), \quad E(N_m) = \frac{1}{4}m(m+1)(m^2 + 3m + 2)\hbar\omega_0.$$

As the easiest sanity check, for  $m = 1$  (i.e. for only the lowest, ground-state level completely filled), these formulas yield  $N_m = 2$ ,  $E(N_m) = 3\hbar\omega_0$ , i.e. the evidently correct results.

In the case when  $N = N_m + N'$ , with  $0 < N' < 2(M_{m+1}^{(3)} - M_m^{(3)}) \equiv 4(m+1)(m+2)$ , additional  $N'$  particles have to occupy the next level, with  $n = m$ , and  $\varepsilon_n = \varepsilon_m = \hbar\omega_0(m + 3/2)$ , so

$$E(N) = E(N_m) + \varepsilon_m N' = \hbar\omega_0 \left[ \frac{1}{4}m(m+1)(m^2 + 3m + 2) + N' \left(m + \frac{3}{2}\right) \right].$$

In the limit  $N \gg 1$ ,  $m$  is large as well, and these results may be approximated as

$$N \approx \frac{m^3}{3}, \quad \text{so } m \approx (3N)^{1/3}, \quad \text{and } E(N) \approx \frac{\hbar\omega_0}{4}m^4 \approx \frac{\hbar\omega_0}{4}(3N)^{4/3}.$$

<sup>38</sup> This is a particular case of a formula for  $k$  boxes:  $M_n^{(k)} = (n-1+k)!/n!(k-1)!$  – see, e.g., MA Eq. (2.4).

<sup>39</sup> See, e.g., MA Eqs. (2.5b), (2.6a), and (2.6b).

**Problem 8.20.** Use the Hund rules to evaluate the quantum numbers  $L$ ,  $S$ , and  $J$  in the ground states of carbon and nitrogen atoms. Write down the Russell-Saunders symbols for these states.

*Solution:* As the table in Fig. 3.24 of the lecture notes shows, the ground state of the carbon (C) atom has two electrons in the (completely filled) He shell, two electrons in the  $2s$  orbital state ( $n = 2$ ,  $l = 0$ ), and two electrons in the  $2p$  sub-shell ( $n = 2$ ,  $l = 1$ ). As it follows from the discussion in Sec. 8.2 of the lecture notes, each pair of the  $s$ -state electrons has to be in the same orbital state and in the spin-singlet state, with zero net orbital momentum and zero net spin, so they do not contribute to the net quantum numbers  $L$ ,  $S$ , and  $J$  of the atom, and we need to discuss only the two  $2p$  electrons, with  $l = 1$ . Due to the triple degeneracy ( $m_l = +1, 0, -1$ ) of their orbital states, and the double degeneracy ( $m_s = \pm 1/2$ ) of the spin states, the Pauli principle allows up to six electrons in this sub-shell, so we need to use the Hund rules to understand which exactly of these states our two electrons would take.

The highest Rule 1 of Hund's hierarchy says that  $S$  has to take the largest value possible. Since, according to Eq. (8.48),  $S \equiv \max |M_S| = \max |(m_s)_1 + (m_s)_2|$ , such a maximum,  $S = 1$ , is evidently achieved in a linear superposition of the triplet spin states. These states are symmetric with respect to the electron permutation; hence to satisfy the Pauli principle, the involved orbital states have to be different, i.e. their quantum numbers,  $(m_l)_1$  and  $(m_l)_2$ , have to take different values from the available set  $\{+1, 0, -1\}$ ,<sup>40</sup> so the quantum number  $L \equiv \max |(m_l)_1 + (m_l)_2|$  can only take values 0 or 1. Now by using Rule 2, we have to select the highest of these values,  $L = 1$ . Finally, the Hund Rule 3 says that since this sub-shell is filled by less than half, then  $J = |L - S| = 0$ . As a result, the Russell-Saunders symbol (defined by Eq. (8.59) of the lecture notes) of this ground state is  $^3P_0$ .

The atom of nitrogen (N) is different from that of carbon "only" by one more, third electron in the same sub-shell  $\{n = 2, l = 1\}$ , so again, non-zero contributions to the net quantum numbers  $L$ ,  $S$ , and  $J$  may be given only by the (now, three) electrons of this sub-shell, with three different orbital states. Indeed, if the electrons are in different orbital states, their magnetic spin numbers  $m_s$  may take equal values without violating the Pauli principle. Such configurations:  $(m_s)_1 = (m_s)_2 = (m_s)_3 = \pm 1/2$ , are evidently the best ones for the Hund Rule 1, providing the highest possible value  $S \equiv \max |M_S| = \max |(m_s)_1 + (m_s)_2 + (m_s)_3| = 3/2$ , so  $2S + 1 = 4$ . Any such spin state is fully symmetric with respect to the permutation of any two particles, so the orbital state of the system has to be a linear superposition fully antisymmetric with respect to such permutation, similar to the Slater determinant (8.60a), of all possible six states with different  $m_l = \{+1, 0, -1\}$ . Since in this superposition, the coefficient moduli (and hence the spin orientation probabilities) are equal, then  $M_S = (m_s)_1 + (m_s)_2 + (m_s)_3 = 0$ . Translating what we know from Sec. 8.2 about the case of two spins- $1/2$ , and from the solution of Problem 10 about two spins-1, to the orbital-momentum language, we may conclude that such an antisymmetric state has to have  $L = 0$ .<sup>41</sup> Hence  $J = S = 3/2$  (so the Hund Rules 2 and 3 are redundant here). Thus, the Russell-Saunders symbol of the ground state of nitrogen is  $^4S_{3/2}$ .

**Problem 8.21.**  $N \gg 1$  indistinguishable quantum particles, not interacting directly, are placed into a hard-wall rectangular box with sides  $a_x$ ,  $a_y$ , and  $a_z$ . Calculate the ground-state energy of the

<sup>40</sup> For this case, as well as for the nitrogen atom discussed below, the physical origin of the first Hund rule is very clear: the Coulomb repulsion of the electrons forces them into different  $p$ -orbitals, thus maximizing their average distance from each other – see, e.g., the second row of Fig. 3.20.

<sup>41</sup> An explicit proof of this result, using the same approach as in Problem 8.3, and Eq. (5.164) of the lecture notes (with  $l = 1$ ), is a good additional exercise, recommended to the reader.



system and the average forces it exerts on each face of the box. Can we characterize the forces by certain pressure  $\mathcal{P}$ ?

*Hint:* Consider separately the cases of bosons and fermions.

*Solution:* Non-interacting *bosons* may occupy the same single-particle energy level  $\varepsilon$ , so the ground-state energy  $E_g$  of  $N$  of them is just  $N\varepsilon_g$ . Using Eq. (1.86) of the lecture notes, with  $n_x = n_y = n_z = 1$ , for  $\varepsilon_g$ , we get

$$E_g = N \frac{\pi^2 \hbar^2}{2m} \left( \frac{1}{a_x^2} + \frac{1}{a_y^2} + \frac{1}{a_z^2} \right).$$

Just as was discussed in the model solution of Problem 1.11, this expression shows that the force-to-area ratios for each wall of the box are generally different. For example, for the faces normal to the  $x$ -axis, of area  $A_x = a_y a_z$ ,

$$\mathcal{P}_x \equiv \frac{\langle F_x \rangle}{A_x} = \frac{1}{a_y a_z} \left( -\frac{\partial E_g}{\partial a_x} \right) = N \frac{\pi^2 \hbar^2}{m a_x^3 a_y a_z} = \frac{\pi^2 \hbar^2}{m a_x^2} \frac{N}{V},$$

where  $V = a_x a_y a_z$  is the box volume. Hence the exerted forces generally *cannot* be characterized by a unique pressure  $\mathcal{P}$  (which by definition should be isotropic), and only for a cubic box, with  $a_x = a_y = a_z \equiv a$ , we may write

$$\mathcal{P}_x = \mathcal{P}_y = \mathcal{P}_z \equiv \mathcal{P} = N \frac{\pi^2 \hbar^2}{m a^5} = \frac{\pi^2 \hbar^2 N}{m V^{5/3}} \equiv \frac{2}{3} \frac{E_g}{V}.$$

In contrast, because of the Pauli principle, indistinguishable *fermions* cannot be in the same quantum state. Hence, to form the ground state with the lowest energy, we may place, in each single-particle orbital state, only  $g$  fermions, where  $g = 2s + 1$  is their spin degeneracy. (For electrons, as spin- $\frac{1}{2}$  particles,  $g = 2$ .) Since, according to Eq. (1.90) of the lecture notes, the density of such states in the wave vector space is constant, the set of  $N_{\text{orb}} \equiv N/g \gg 1$  orbital states with the lowest possible energies form, in the  $\mathbf{k}$ -space, a sphere<sup>42</sup> of certain radius  $k_F$ . This radius and the total ground energy of the system may be readily calculated by writing, for them, two very similar expressions and then transforming them by using Eqs. (1.90) and, in the second case, Eq. (1.89) as well:<sup>43</sup>

$$N = \int_{k < k_F} g dN_{\text{orb}} = \frac{gV}{(2\pi)^3} \int_{k < k_F} d^3k = \frac{gV}{(2\pi)^3} \int_0^{k_F} 4\pi k^2 dk = \frac{gV}{(2\pi)^3} \frac{4\pi k_F^3}{3},$$

$$E_g = \int_{k < k_F} g \varepsilon_k dN_o = \frac{gV}{(2\pi)^3} \int_{k < k_F} \frac{\hbar^2 k^2}{2m} d^3k = \frac{gV \hbar^2}{(2\pi)^3 2m} \int_0^{k_F} k^2 4\pi k^2 dk = \frac{gV \hbar^2}{(2\pi)^3 2m} \frac{4\pi k_F^5}{5},$$

where, in our current case,  $V = a_x a_y a_z$ . By expressing  $k_F$  from the first of these formulas and plugging the result into the second one, we finally get

<sup>42</sup> This is exactly what is called the *Fermi sphere* – a particular case of the *Fermi surface*, for free particles. As a reminder, at particle motion in periodic potentials, the constant-energy surfaces (and hence the Fermi surfaces) may be non-spherical – see, e.g., Sec. 3.4 of the lecture notes.

<sup>43</sup> Due to its importance, this simple calculation is virtually repeated in SM Sec. 3.3, where it serves as a background for a discussion of fermion gas properties at non-zero temperatures.

$$E_g = \frac{3}{5} \varepsilon_F N,$$

where  $\varepsilon_F$  is the so-called *Fermi energy* – the largest single-particle energy on the occupied levels:

$$\varepsilon_F \equiv \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m} \left( \frac{6\pi^2 N}{g V} \right)^{2/3}.$$

This result shows that the energy of the system depends on each linear dimension of the box only via its volume  $V$ . Hence the average forces exerted on its walls *may be* characterized by an isotropic pressure:

$$\mathcal{P} \equiv -\frac{\partial E_g}{\partial V} = \left( \frac{6\pi^2}{g} \right)^{2/3} \frac{\hbar^2 N^{2/3}}{3mV^{5/3}} \equiv \frac{2}{3} \frac{E_g}{V},$$

for any ratio  $a_x:a_y:a_z$  of the cubic box – or even for any other shape of the particle-confining volume.

**Problem 8.22.** A system of three similar spins- $1/2$  is described by the Heisenberg Hamiltonian

$$\hat{H} = -J(\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2 + \hat{\mathbf{s}}_2 \cdot \hat{\mathbf{s}}_3 + \hat{\mathbf{s}}_3 \cdot \hat{\mathbf{s}}_1),$$

where  $J$  is a spin interaction constant (cf. Problems 6 and 7). Find the stationary states and energies of this system, and give an interpretation of your results.

*Solution:* The uncoupled-representation  $z$ -basis of the system has  $2^3 = 8$  states corresponding to the  $\uparrow$  and  $\downarrow$  orientations of each spin. Let us see what is the result of the Hamiltonian operator's action upon each of these states. This is especially easy to do by using the intermediate results of the model solution of Problem 3 for two spins- $1/2$ ,<sup>44</sup>

$$\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2 |\uparrow\uparrow\rangle = \left(\frac{\hbar}{2}\right)^2 |\uparrow\uparrow\rangle, \quad \hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2 |\downarrow\downarrow\rangle = \left(\frac{\hbar}{2}\right)^2 |\downarrow\downarrow\rangle, \quad (*)$$

$$\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2 |\uparrow\downarrow\rangle = \left(\frac{\hbar}{2}\right)^2 (2|\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle), \quad \hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2 |\downarrow\uparrow\rangle = \left(\frac{\hbar}{2}\right)^2 (2|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle). \quad (**)$$

For example, since the operator  $\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2$  does not affect the state of the third spin, Eqs. (\*) yield

$$\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2 |\uparrow\uparrow\uparrow\rangle = \left(\frac{\hbar}{2}\right)^2 |\uparrow\uparrow\uparrow\rangle, \quad \hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2 |\downarrow\downarrow\downarrow\rangle = \left(\frac{\hbar}{2}\right)^2 |\downarrow\downarrow\downarrow\rangle.$$

These results evidently do not depend on the indices of the operator product components, so their summation for all three index combinations yield

$$(\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2 + \hat{\mathbf{s}}_2 \cdot \hat{\mathbf{s}}_3 + \hat{\mathbf{s}}_3 \cdot \hat{\mathbf{s}}_1) |\uparrow\uparrow\uparrow\rangle = 3 \left(\frac{\hbar}{2}\right)^2 |\uparrow\uparrow\uparrow\rangle, \quad (\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2 + \hat{\mathbf{s}}_2 \cdot \hat{\mathbf{s}}_3 + \hat{\mathbf{s}}_3 \cdot \hat{\mathbf{s}}_1) |\downarrow\downarrow\downarrow\rangle = 3 \left(\frac{\hbar}{2}\right)^2 |\downarrow\downarrow\downarrow\rangle.$$

This means that we have already found two stationary states of the system, with the same energy

<sup>44</sup> I am again using the standard shorthand notation, in which the spin's number is coded with its position inside the ket-vector.

$$E_{\uparrow\uparrow\uparrow} = E_{\downarrow\downarrow\downarrow} = E_0 \equiv -3J\left(\frac{\hbar}{2}\right)^2. \quad (***)$$

Thanks to Eqs. (\*\*), the calculations for the “mixed” (entangled) spin states are only slightly bulkier. For example, let us calculate

$$(\hat{s}_1 \cdot \hat{s}_2 + \hat{s}_2 \cdot \hat{s}_3 + \hat{s}_3 \cdot \hat{s}_1)|\downarrow\uparrow\uparrow\rangle \equiv \hat{s}_1 \cdot \hat{s}_2|\downarrow\uparrow\uparrow\rangle + \hat{s}_2 \cdot \hat{s}_3|\downarrow\uparrow\uparrow\rangle + \hat{s}_3 \cdot \hat{s}_1|\downarrow\uparrow\uparrow\rangle.$$

Applying the second of Eqs. (\*\*) to the first term on the right-hand side, its analog for indices 1 and 3, to the third term, and the analog of the first of Eqs. (\*) for indices 2 and 3, to the second term, we get

$$\begin{aligned} (\hat{s}_1 \cdot \hat{s}_2 + \hat{s}_2 \cdot \hat{s}_3 + \hat{s}_3 \cdot \hat{s}_1)|\downarrow\uparrow\uparrow\rangle &= \left(\frac{\hbar}{2}\right)^2 \left[ (2|\uparrow\downarrow\uparrow\rangle - |\downarrow\uparrow\uparrow\rangle) + |\downarrow\uparrow\uparrow\rangle + (2|\uparrow\uparrow\downarrow\rangle - |\downarrow\uparrow\uparrow\rangle) \right] \\ &\equiv \left(\frac{\hbar}{2}\right)^2 (2|\uparrow\downarrow\uparrow\rangle + 2|\uparrow\uparrow\downarrow\rangle - |\downarrow\uparrow\uparrow\rangle). \end{aligned}$$

It is useful to formulate this result verbally: the action of the sum of all two-spin operator products on a ket with just one spin down yields, besides the multiplication by  $(\hbar/2)^2$ , the ket of the same state with the minus sign, plus two other possible kets with one spin down, each multiplied by a factor of 2. This rule, which may be readily verified to be valid for any state with one spin down, means that the three states of this group are only coupled to each other, so their interaction, in units of  $-J(\hbar/2)^2$ , may be described by the following  $3 \times 3$  matrix:

$$\begin{pmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{pmatrix}. \quad (****)$$

(Due to the symmetry of the matrix, it is not even important what exactly states correspond to its rows/columns.) The eigenvalues of this matrix may be found from the corresponding characteristic equation

$$\begin{vmatrix} -1-\lambda & 2 & 2 \\ 2 & -1-\lambda & 2 \\ 2 & 2 & -1-\lambda \end{vmatrix} = 0, \quad \text{giving } f(\mu) \equiv \mu^3 - 12\mu - 16 = 0, \quad \text{where } \mu \equiv \lambda + 1.$$

One root:  $\mu_+ = -2$ , i.e.  $\lambda_+ \equiv \mu_+ - 1 = -3$ , of this simple cubic equation may be readily guessed;<sup>45</sup> after that, dividing the polynomial  $f(\mu)$  by  $(\mu - \mu_+) \equiv (\mu + 2)$ , we get the quadratic polynomial  $g(\mu) = \mu^2 - 2\mu - 8$ , whose roots are easy to calculate:  $\mu = \mu_+ = -2$ ,  $\mu_0 = +4$ , so  $\lambda_+ = \lambda_- = -3$ ,  $\lambda_0 = +3$ . As a result, the eigenenergies corresponding to the one-spin-down states are  $E_+ = E_- = -E_0$  and  $+E_0$ , where  $E_0$  is given by Eq. (\*\*).

Due to the spin up-down symmetry of the Hamiltonian, it is obvious (and may be checked by the absolutely similar calculation) that the three states with one spin up also are coupled to each other, and

<sup>45</sup> If you do not like guessing, it is useful to have a look at the numerical plot of function  $f(\mu)$ , which touches the horizontal axis (i.e. has a double root) at the point  $\mu = -2$ . Another (much harder) option is to use the cumbersome (“quasi-analytical”) Tartaglia-Cardano formulas for the roots of an arbitrary cubic equation.

have similar eigenenergies: two eigenstates with energy  $-E_0$ , and one state with energy  $+E_0$ . To summarize: our system has just two energy levels, each of them four-degenerate: one level with energy  $+E_0$ , corresponding to the two states with all spins aligned (in any direction), plus two linear superpositions of three states with one spin misaligned, while the level with energy  $-E_0$  corresponds to four other linear superpositions of the states with one spin misaligned, each superposition consisting of the same number of spins-up and spins-down.

The misaligned-spin superpositions may be readily found by plugging the calculated values of  $\lambda$  into the linear system of equations with the matrix (\*\*\*\*), and then the normalization – just as was repeatedly done in the examples and exercises of Chapter 4. The results for the one-spin-down states may be represented in the form

$$|0\rangle = \frac{1}{\sqrt{3}}(|\downarrow\uparrow\uparrow\rangle + |\uparrow\downarrow\uparrow\rangle + |\uparrow\uparrow\downarrow\rangle), \quad |\pm\rangle = \frac{1}{\sqrt{3}}\left(|\downarrow\uparrow\uparrow\rangle + \frac{-1 \pm i\sqrt{3}}{2}|\uparrow\downarrow\uparrow\rangle + \frac{-1 \mp i\sqrt{3}}{2}|\uparrow\uparrow\downarrow\rangle\right);$$

the one-spin-up eigenstates are similar. The physical meaning of these three eigenstates becomes more transparent by rewriting them all in a similar wave form:

$$|\alpha\rangle = \frac{1}{\sqrt{3}}\left(\exp\left\{i\alpha\frac{0\cdot 2\pi}{3}\right\}|\downarrow\uparrow\uparrow\rangle + \exp\left\{+i\alpha\frac{2\pi}{3}\right\}|\uparrow\downarrow\uparrow\rangle + \exp\left\{-i\alpha\frac{2\pi}{3}\right\}|\uparrow\uparrow\downarrow\rangle\right), \quad \text{with } \alpha = 0, \pm 1.$$

If we interpret the system's Hamiltonian as a model of interaction of the spins located at three equidistant positions on a circle, for example at angles  $\varphi = 0$ , and  $\pm\Delta\varphi = \pm 2\pi/3$ , then each state is just a traveling wave of propagation of the spin-down “excitation”, with the equal phase shifts  $\alpha\Delta\varphi$  at each excitation's jump to the adjacent site, absolutely similar to that of single-particle 1D Bloch waves – see Sec. 2.7.<sup>46</sup> In this picture, the above eigenvalues of the normalized wave number  $\alpha$  (to whom any multiple of 3 may be added without changing the solution) result from the natural cycling-boundary condition  $\exp\{i\alpha 2\pi\} = 1$ . Such Bloch waves of spin orientations are called either *spin waves* or *magnon waves*.<sup>47</sup>

The spin-wave interpretation explains why the state with  $\alpha = 0$  has the energy  $(+E_0)$ ,<sup>48</sup> different from that  $(-E_0)$  of the two states with  $\alpha = \pm 1$ : in usual wave systems, with positive kinetic energy, the wave energy grows with the square of the wave number (modulo its period, in our current case  $\Delta\alpha = 3$ ). Note, however, that in the Heisenberg model (and at real spin interactions in crystals) the sign of  $J$  may be both positive and negative. Only the case  $J > 0$ , with the ground-state energy  $E_0 < 0$ , corresponds to classical wave systems. (It also describes the effect of spontaneous spin alignment, the *ferromagnetism*.)

<sup>46</sup> Such constant phase shift between the adjacent sites is the main feature of any traveling waves in periodic structures, including classical systems – see, e.g., CM Sec. 6.3.

<sup>47</sup>The fact that such waves, possibly with numerous flipped spins, are described by the Heisenberg model is the essence of the so-called *Bethe Ansatz* – named after H. Bethe who first suggested this idea in 1931. This fact enables exact analyses of some models for systems of  $N \gg 1$  spins, for which the direct approach used above is not practicable. For an introduction to the Bethe Ansatz, I can recommend, for example, a popular article by M. Batchelor, *Phys. Today* **60**, 36 (2007), or a more detailed three-part review by M. Karbach *et al.*, available online at <http://www.phys.uri.edu/gerhard/introbethe.html>.

<sup>48</sup> If the fact that this energy is equal to that of the all-spin-aligned states looks surprising to you, please revisit the discussion of the <sup>4</sup>He atom in Sec. 8.2 of the lecture notes and/or the solution of Problem 3. There, in the absence of the external field, all triplet states (either factorable or entangled) of the two-spin system also had the same energy.

For the case  $J < 0$ ,<sup>49</sup> the lowest energy of the system is  $-E_0 < 0$ , corresponding to the alternating-spin ground states. This is the Heisenberg-model description of the effect of *antiferromagnetism*;

One more (parenthetic) remark: since the two one-spin-down stationary states with  $\alpha = \pm 1$

$$|\pm\rangle = \frac{1}{\sqrt{3}} \left( |\downarrow\uparrow\uparrow\rangle + e^{\pm i2\pi/3} |\uparrow\downarrow\uparrow\rangle + e^{\mp i2\pi/3} |\uparrow\uparrow\downarrow\rangle \right),$$

correspond to the same energy  $-E_0$ , any of their linear superpositions is also a legitimate stationary state. Of such superpositions, the most notable are the combinations that exclude one of three elementary (factorable) states, for example,

$$|1\rangle \equiv \frac{-i}{\sqrt{2}} (|+\rangle - |-\rangle) = \frac{-i}{\sqrt{6}} \left( 2i \sin \frac{2\pi}{3} |\uparrow\downarrow\uparrow\rangle - 2i \sin \frac{2\pi}{3} |\uparrow\uparrow\downarrow\rangle \right) \equiv \frac{1}{\sqrt{2}} (|\uparrow\downarrow\uparrow\rangle - |\uparrow\uparrow\downarrow\rangle).$$

While the initial states ( $\pm$ ) may be interpreted as *traveling* spin waves, the state 1 represents a *standing* spin wave. On the other hand, we may write

$$|1\rangle = |\uparrow\rangle \otimes \frac{1}{\sqrt{2}} (|\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle),$$

so this state is based on the singlet of the last two spins. Evidently, there are three such states, with the same energy, which differ only by the number of the particle in the non-entangled spin state, but since they all are linear superpositions of the traveling-wave states  $\pm$ , only two of them are linearly independent. (Of course, the same is true for the one-spin-down states with  $\alpha = \pm 1$ .)

**Problem 8.23.** For a system of three spins- $\frac{1}{2}$ , find the common eigenstates and eigenvalues of the operators  $\hat{S}_z$  and  $\hat{S}^2$ , where  $\hat{\mathbf{S}} \equiv \hat{\mathbf{s}}_1 + \hat{\mathbf{s}}_2 + \hat{\mathbf{s}}_3$  is the vector operator of the total spin of the system. Do the corresponding quantum numbers  $S$  and  $M_S$  obey Eqs. (8.48) of the lecture notes?

*Solution:* Since the partial operators  $\hat{\mathbf{s}}_{1,2,3}$  are defined in different Hilbert spaces and hence commute, we may transform the operator  $\hat{S}^2$  just as in the model solution of Problem 3:

$$\hat{S}^2 \equiv (\hat{\mathbf{s}}_1 + \hat{\mathbf{s}}_2 + \hat{\mathbf{s}}_3)^2 \equiv (\hat{s}_1^2 + \hat{s}_2^2 + \hat{s}_3^2) + 2(\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2 + \hat{\mathbf{s}}_2 \cdot \hat{\mathbf{s}}_3 + \hat{\mathbf{s}}_3 \cdot \hat{\mathbf{s}}_1). \quad (*)$$

The eigenstates and the corresponding eigenvalues of the operator in the second parentheses of the last expression have been found in the solution of the previous problem. They all (as well as an arbitrary spin state of this system) may be represented as linear superpositions of  $2^3 = 8$  simple (factorable) states, with the ket-vectors (in the  $z$ -basis for each spin),

$$|\uparrow\uparrow\uparrow\rangle, |\downarrow\uparrow\uparrow\rangle, |\uparrow\downarrow\uparrow\rangle, \text{ etc.}, \quad (**)$$

which form a full uncoupled-representation basis of the system. The corresponding eigenvalues of  $\hat{S}^2$  also follow from the previous problem's results – naturally, stripped of the factor  $(-J)$ :

$$\langle \hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2 + \hat{\mathbf{s}}_2 \cdot \hat{\mathbf{s}}_3 + \hat{\mathbf{s}}_3 \cdot \hat{\mathbf{s}}_1 \rangle = \pm 3 \left( \frac{\hbar}{2} \right)^2.$$

<sup>49</sup> A negative  $J$  may result from the exchange interaction of electrons of adjacent atoms.

Next, since each of the operators in the first parentheses of the last form of Eq. (\*), namely  $\hat{S}_{1,2,3}^2$ , acts only on the corresponding component of these elementary kets, they all obey the same equality as in the case of a single spin- $1/2$  (see Chapter 4):

$$\hat{S}_{1,2,3}^2 = (\hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2)_{1,2,3} = 3 \left( \frac{\hbar}{2} \right)^2 \hat{I}.$$

This means that all the eigenstates found in the solution of the previous problem are also eigenstates of the operator in the first parentheses of Eq. (\*), with the same eigenvalue,  $9(\hbar/2)^2$ .

So, all these states are eigenstates of the total operator  $\hat{S}^2$  as well, with the following eigenvalues:

$$\langle S^2 \rangle = \left( \frac{\hbar}{2} \right)^2 \times \begin{cases} (9 + 2 \cdot 3) \equiv 15, & \text{for two spin - aligned states, and two misaligned states with } \alpha = 0, \\ (9 - 2 \cdot 3) \equiv 3, & \text{for four spin - misaligned states, with } \alpha = \pm 2\pi/3. \end{cases}$$

Now proceeding to the operator

$$\hat{S}_z \equiv \hat{S}_{1z} + \hat{S}_{2z} + \hat{S}_{3z},$$

we may note that each of the component operators on the right-hand side of this equality acts only on the corresponding spin. As a result, according to Eq. (4.128) of the lecture notes, acting on any of the factorable basis ket (\*\*), the net operator results in the same ket multiplied by the factor  $\hbar M_S$ , where<sup>50</sup>

$$M_S \equiv m_1 + m_2 + m_3.$$

For example, for the state with  $m_1 = +1/2$ ,  $m_2 = -1/2$ , and  $m_3 = +1/2$  (and hence  $M_S = +1/2$ ):

$$\hat{S}_z |\uparrow\downarrow\uparrow\rangle \equiv \hat{S}_{1z} |\uparrow\downarrow\uparrow\rangle + \hat{S}_{2z} |\uparrow\downarrow\uparrow\rangle + \hat{S}_{3z} |\uparrow\downarrow\uparrow\rangle = \frac{\hbar}{2} |\uparrow\downarrow\uparrow\rangle - \frac{\hbar}{2} |\uparrow\downarrow\uparrow\rangle + \frac{\hbar}{2} |\uparrow\downarrow\uparrow\rangle \equiv \frac{\hbar}{2} |\uparrow\downarrow\uparrow\rangle.$$

Since each of the discussed eigenstates of the operator  $\hat{S}^2$  is a linear superposition of such elementary states with the same value of  $M_S$  (the same number of up- and down-spins), they are also the eigenstates of the operator  $\hat{S}_z$ , with the following eigenvalues:

$$S_z = \hbar M_S, \quad \text{with } M_S = \begin{cases} +3/2, & \text{for the aligned state with all spins up,} \\ +1/2, & \text{for all misaligned states with two spins up,} \\ -1/2, & \text{for all misaligned states with two spins down,} \\ -3/2, & \text{for the aligned state with all spins down.} \end{cases}$$

Comparing these results with the general Eqs. (8.48) of the lecture notes, we see that they all fit, in particular satisfying the relations

$$\langle S^2 \rangle = \hbar^2 S(S+1) \quad \text{and} \quad -S \leq M_S \leq +S,$$

provided that we prescribe to the eigenstates (besides the values of  $M_S$  specified above) the following values of the quantum number  $S$ :

<sup>50</sup> Here, as in the solution of Problem 4, the index  $s$  in the magnetic quantum numbers  $m_s$  of the component spins has been dropped.

$$S = \begin{cases} 3/2, & \text{for two spin - aligned states, and two misaligned states with } \alpha = 0, \\ 1/2, & \text{for four spin - misaligned states, with } \alpha = \pm 2\pi/3. \end{cases}$$

I believe that these results, together with those for the two-spin system (discussed in Sec. 8.2 of the lecture notes and the solution of Problem 3) illuminate the physical sense of the net quantum numbers  $S$  and  $M_S$ , and in particular clarify why these numbers may take not only integer but also half-integer values.

**Problem 8.24.** Explore basic properties of the Heisenberg model (whose few-spin versions were the subjects of Problems 6, 7, and 22), for a 1D chain of  $N$  spins- $1/2$ :

$$\hat{H} = -J \sum_{\{j,j'\}} \hat{\mathbf{s}}_j \cdot \hat{\mathbf{s}}_{j'} - \gamma \mathcal{B} \cdot \sum_j \hat{\mathbf{s}}_j, \quad \text{with } J > 0,$$

where the summation is over all  $N$  spins, with the symbol  $\{j, j'\}$  meaning that the first sum is only over the adjacent spin pairs. In particular, find the ground state of the system and its lowest excited states in the absence of external magnetic field  $\mathcal{B}$ , and also the dependence of their energies on the field.

*Hint:* For the sake of simplicity, you may assume that the first sum includes the term  $\hat{\mathbf{s}}_N \cdot \hat{\mathbf{s}}_1$  as well. (Physically, this means that the chain is bent into a closed loop.<sup>51</sup>)

*Solution:* This problem is a natural generalization of Problems 6, 7, and 22, so it may be solved quickly by using some intermediate results of their model solutions. First of all, it is evident from those solutions that at least at  $\mathcal{B} = 0$ , the ground state of the system with  $J > 0$  (i.e. the Heisenberg model of *ferromagnetism*<sup>52</sup>) is one of two simple (factorable) products of  $N$  aligned spin states:

$$|g_+\rangle = |\uparrow\uparrow \dots \uparrow\uparrow\rangle, \quad |g_-\rangle = |\downarrow\downarrow \dots \downarrow\downarrow\rangle. \quad (*)$$

Indeed, acting on any of these ket-vectors by the first term of our Hamiltonian,

$$\hat{H}|_{\mathcal{B}=0} = -J \sum_{\{j,j'\}} \hat{\mathbf{s}}_j \cdot \hat{\mathbf{s}}_{j'} \equiv -J(\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2 + \hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2 + \dots + \hat{\mathbf{s}}_{N-1} \cdot \hat{\mathbf{s}}_N + \hat{\mathbf{s}}_N \cdot \hat{\mathbf{s}}_1),$$

and applying Eq. (\*) of the model solution of Problem 22 to each of  $N$  pairs of spins, we get the same ket multiplied by the following factor (which is, by definition, the state's energy):

$$E_+ = E_- = E_g \equiv -JN \left( \frac{\hbar}{2} \right)^2.$$

Moreover, as it is physically clear from the expressions for the kets  $|0\rangle$  and  $|\pm\rangle$  in the same solution, the lowest excitations of the system should be Bloch-wave-like linear superpositions,

$$|\alpha\rangle_{\pm} = C \sum_j e^{i\alpha j} |k+j\rangle_{\pm}, \quad (**)$$

<sup>51</sup> Note that for dissipative spin systems, differences between low-energy excitations of open-end and closed-end 1D chains may be substantial even in the limit  $N \rightarrow \infty$  – see, e.g., SM Sec. 4.5. However, for our Hamiltonian (and hence dissipation-free) system, the differences are relatively small.

<sup>52</sup> Solutions of the similar Heisenberg model of *antiferromagnetism*, with  $J < 0$  and  $\mathcal{B} \neq 0$ , are more involved.

of the kets  $|k\rangle_{\pm}$  corresponding to one reversed spin, in the  $k^{\text{th}}$  position:

$$|k\rangle_{+} \equiv \left| \underbrace{\uparrow\uparrow \dots \uparrow}_{k-1} \downarrow \underbrace{\uparrow\uparrow \dots \uparrow}_{N-k} \right\rangle, \quad |k\rangle_{-} \equiv \left| \underbrace{\downarrow\downarrow \dots \downarrow}_{k-1} \uparrow \underbrace{\downarrow\downarrow \dots \downarrow}_{N-k} \right\rangle,$$

where the real parameter  $\alpha$  (physically, the normalized wave number<sup>53</sup> of the spin wave) satisfies the cyclic boundary condition  $|k+N\rangle_{\pm} = |k\rangle_{\pm}$  if

$$e^{iN\alpha} = 1. \quad (***)$$

(The summation in Eq. (\*\*)) is over all  $N$  spins of the ring, with sequential numbering starting from any position – counting the positions modulo  $N$ , i.e. identifying the number  $j = j_0 + N$  with  $j_0$ .) Indeed, by applying Eqs. (\*) and (\*\*) of the model solution of Problem 22 to each pair of adjacent spins, we get similar results for any of these single-misaligned-spin states:

$$\hat{H}|_{\mathcal{B}=0}|k\rangle_{\pm} = -J\left(\frac{\hbar}{2}\right)^2 \left[ (N-4)|k\rangle_{\pm} + 2|k-1\rangle_{\pm} + 2|k+1\rangle_{\pm} \right].$$

As a result, acting by the same Hamiltonian upon any of the aggregate kets (\*\*), and then changing the summation indices in the last two partial sums from  $j$  to  $j' = j \pm 1$ , we get

$$\begin{aligned} \hat{H}|_{\mathcal{B}=0}|\alpha\rangle_{\pm} &= -J\left(\frac{\hbar}{2}\right)^2 C \left[ (N-4)\sum_j e^{i\alpha j} |k+j\rangle_{\pm} + 2\sum_j e^{i\alpha j} |k-1+j\rangle_{\pm} + 2\sum_j e^{i\alpha j} |k+1+j\rangle_{\pm} \right] \\ &\equiv -J\left(\frac{\hbar}{2}\right)^2 C \left[ (N-4)\sum_{j'} e^{i\alpha j'} |k+j'\rangle_{\pm} + 2e^{i\alpha} \sum_{j'} e^{i\alpha j'} |k+j'\rangle_{\pm} + 2e^{-i\alpha} \sum_{j'} e^{i\alpha j'} |k+j'\rangle_{\pm} \right] \\ &= -J\left(\frac{\hbar}{2}\right)^2 \left[ (N-4) + 2e^{-i\alpha} + 2e^{+i\alpha} \right] |\alpha\rangle_{\pm}. \end{aligned}$$

Hence the kets (\*\*) indeed describe the stationary states of our system, with their energies independent (at  $\mathcal{B} = 0$  only!) of the misaligned spin's orientation:

$$E_{\pm}(\alpha) = -J\left(\frac{\hbar}{2}\right)^2 \left[ (N-4) + 2e^{+i\alpha} + 2e^{-i\alpha} \right] \equiv E_g + 4J\left(\frac{\hbar}{2}\right)^2 (1 - \cos \alpha). \quad (****)$$

As a sanity check, for the particular case  $N = 3$ , when Eq. (\*\*\*\*) gives, modulo  $2\pi$ ,  $\alpha = 0, \pm 2\pi/3$ , i.e.  $\cos \alpha = +1, -1/2$ , we recover the results of Problem 22:  $E_{\pm}(0) = -3J(\hbar/2)^2 + 4J(\hbar/2)^2 \cdot 0 \equiv -3J(\hbar/2)^2$ ,  $E_{\pm}(\pm 2\pi/3) = -3J(\hbar/2)^2 + 4J(\hbar/2)^2 \cdot (1 + 1/2) \equiv +3J(\hbar/2)^2$ .

The last term of Eq. (\*\*\*\*) evidently describes the spin-wave excitation energy. For our (ferromagnetic) case  $J > 0$ , this energy is positive for any  $\alpha$ .<sup>54</sup> The excitation energy tends to zero at  $\alpha \rightarrow 0$ , so the triplet-like solution with  $\alpha = 0$  has the same energy as the ground state with all spins aligned. (If this fact looks counter-intuitive, please revisit the discussion of the two-spin triplet in Sec.

<sup>53</sup> See, e.g., Eq. (2.193) and/or CM Eq. (6.26), and the accompanying discussions.

<sup>54</sup> For the antiferromagnetic chain ( $J < 0$ ), the term is negative, showing that the spin-aligned states (\*) are unstable with respect to a single spin reversal, and hence they are *not* the ground states of the system.



8.2 of the lecture notes, and in the solution of Problem 3.) So, the first actual excitation (with  $E(\alpha) > E_g$ ) corresponds to the two lowest non-zero values of  $\alpha$  (modulo  $2\pi$ ) of the allowed set (\*\*\*):

$$E_{\pm}\left(\alpha = \frac{2\pi}{N}\right) - E_g = E_{\pm}\left(\alpha = -\frac{2\pi}{N}\right) - E_g = 4J\left(\frac{\hbar}{2}\right)^2 \left(1 - \cos\frac{2\pi}{N}\right).$$

Note that if  $N \gg 1$ , the energy of these low-energy excitations is proportional to the square of  $\alpha$ , i.e. of the normalized wave number  $k = \alpha/d$  (where  $d$  is the spatial period of the natural geometric model of the chain):

$$\hbar\omega \equiv E(\alpha) - E_g \approx 2J\left(\frac{\hbar}{2}\right)^2 \alpha^2 \equiv 2J\left(\frac{\hbar}{2}\right)^2 d^2 k^2,$$

meaning that the low-energy spin waves<sup>55</sup> have a quadratic dispersion law  $\omega(k)$ , similar to that of free non-relativistic particles (see Eq. (1.30) of the lecture notes), but very much different from that of the acoustic waves<sup>56</sup> and the electromagnetic waves in free space.<sup>57</sup>

Proceeding to the effects of a non-zero magnetic field  $\mathcal{B}$ , as we already know from the solutions of Problems 6 and 24, the states described by Eqs. (\*) and (\*\*) are also eigenstates of the sum  $\sum_j \hat{s}_{jz}$  (where the  $z$ -axis is directed along the field), with the eigenvalues  $\pm N(\hbar/2)$  and  $\pm(N-2)(\hbar/2)$ , respectively. As a result, we may immediately write their energies in the field:<sup>58</sup>

$$E_{\pm} = -JN\left(\frac{\hbar}{2}\right)^2 \mp N\frac{\hbar}{2}\gamma\mathcal{B}, \quad E_{\pm}(\alpha) = -JN\left(\frac{\hbar}{2}\right)^2 + 4J\left(\frac{\hbar}{2}\right)^2 (1 - \cos\alpha) \mp (N-2)\frac{\hbar}{2}\gamma\mathcal{B}.$$

Note, however, that at arbitrary  $\mathcal{B}$ , these (exact!) results do not allow us to say what is the ground state of the system, and what is its lowest excitation energy – because at  $\mathcal{B} \neq 0$ , more complex spin waves (with more than one spin inverted) may have comparable, and in particular lower, energies.

**Problem 8.25.** Calculate commutators of the following operators:

$$\hat{\sigma}_+ \equiv \hat{a}_1^\dagger \hat{a}_2, \quad \hat{\sigma}_- \equiv \hat{a}_2^\dagger \hat{a}_1, \quad \hat{\sigma}_z \equiv \frac{1}{2}(\hat{a}_1^\dagger \hat{a}_1 - \hat{a}_2^\dagger \hat{a}_2),$$

where  $\hat{a}_{1,2}^\dagger$  and  $\hat{a}_{1,2}$  are the operators of the creation and annihilation of bosons in two different states.

*Solution:* Let us start with calculating the following commutator:

$$[\hat{\sigma}_+, \hat{\sigma}_-] \equiv [\hat{a}_1^\dagger \hat{a}_2, \hat{a}_2^\dagger \hat{a}_1] \equiv \hat{a}_1^\dagger \hat{a}_2 \hat{a}_2^\dagger \hat{a}_1 - \hat{a}_2^\dagger \hat{a}_1 \hat{a}_1^\dagger \hat{a}_2.$$

Per Eq. (8.75) of the lecture notes, bosonic operators with different particle indices may be swapped at will, so we may continue by grouping the operators belonging to each particle, together:

<sup>55</sup> This means that the particle-like narrow- $k$  wave packets of the spin waves in systems with  $N \gg 1$ , called *magnons*, may be assigned a finite mass inversely proportional to  $J$ .

<sup>56</sup> See, e.g., CM Secs. 6.3 and 6.4, in particular, Eq. (6.31).

<sup>57</sup> See, e.g., EM Sec. 7.1, in particular, Eq. (7.13).

<sup>58</sup> Note that at  $\mathcal{B} \neq 0$ ,  $E_{\pm}(0) \neq E_{\pm}$ .

$$[\hat{\sigma}_+, \hat{\sigma}_-] = \left( \hat{a}_1^\dagger \hat{a}_1 \right) \left( \hat{a}_2 \hat{a}_2^\dagger \right) - \left( \hat{a}_1 \hat{a}_1^\dagger \right) \left( \hat{a}_2^\dagger \hat{a}_2 \right).$$

As we know from solving Chapter 5, to simplify operator expressions, it is often useful to place the basic operators, in each term, in the same order – for example, with the annihilation operators first. For bosonic operators, this may be done using the commutation relation (8.74). Applying it to the second and third parentheses of the last expression, we get

$$[\hat{\sigma}_+, \hat{\sigma}_-] = \left( \hat{a}_1^\dagger \hat{a}_1 \right) \left( \hat{a}_2^\dagger \hat{a}_2 + \hat{I} \right) - \left( \hat{a}_1^\dagger \hat{a}_1 + \hat{I} \right) \left( \hat{a}_2^\dagger \hat{a}_2 \right) \equiv \hat{a}_1^\dagger \hat{a}_1 - \hat{a}_2^\dagger \hat{a}_2 \equiv 2\hat{\sigma}_z.$$

Now we can use the same step sequence for the calculation of a different commutator:

$$\begin{aligned} 2[\hat{\sigma}_z, \hat{\sigma}_+] &\equiv \left[ \hat{a}_1^\dagger \hat{a}_1 - \hat{a}_2^\dagger \hat{a}_2, \hat{a}_1^\dagger \hat{a}_2 \right] \equiv \hat{a}_1^\dagger \hat{a}_1 \hat{a}_1^\dagger \hat{a}_2 - \hat{a}_2^\dagger \hat{a}_2 \hat{a}_1^\dagger \hat{a}_2 - \hat{a}_1^\dagger \hat{a}_2 \hat{a}_1^\dagger \hat{a}_1 + \hat{a}_1^\dagger \hat{a}_2 \hat{a}_2^\dagger \hat{a}_2 \\ &= \hat{a}_1^\dagger \hat{a}_1 \hat{a}_1^\dagger \hat{a}_2 - \hat{a}_1^\dagger \hat{a}_2^\dagger \hat{a}_2 \hat{a}_2 - \hat{a}_1^\dagger \hat{a}_1^\dagger \hat{a}_1 \hat{a}_2 + \hat{a}_1^\dagger \hat{a}_2 \hat{a}_2^\dagger \hat{a}_2 \\ &= \hat{a}_1^\dagger \left( \hat{a}_1^\dagger \hat{a}_1 + \hat{I} \right) \hat{a}_2 - \hat{a}_1^\dagger \hat{a}_2^\dagger \hat{a}_2 \hat{a}_2 - \hat{a}_1^\dagger \hat{a}_1^\dagger \hat{a}_1 \hat{a}_2 + \hat{a}_1^\dagger \left( \hat{a}_2^\dagger \hat{a}_2 + \hat{I} \right) \hat{a}_2 \equiv 2\hat{a}_1^\dagger \hat{a}_2 \equiv 2\hat{\sigma}_+. \end{aligned}$$

An absolutely similar calculation yields

$$2[\hat{\sigma}_z, \hat{\sigma}_-] = -2\hat{\sigma}_-.$$

All our results may be summarized in the following form:

$$[\hat{\sigma}_+, \hat{\sigma}_-] = 2\hat{\sigma}_z, \quad [\hat{\sigma}_z, \hat{\sigma}_\pm] = \pm\hat{\sigma}_\pm,$$

which is strikingly similar to the commutation relations (5.154) of the ladder operators  $\hat{L}_\pm$  of the orbital angular momentum – and also to those valid for similarly formed ladder operators of the spin and the total angular momentum. This similarity is used, in particular, in quantum field theory.

**Problem 8.26.** Compose the simplest model Hamiltonians, in terms of the second quantization formalism, for systems of indistinguishable particles placed in the following external potentials:

- (i) two weakly coupled potential wells, with on-site particle interactions giving additional energy  $J$  per each pair of particles in the same potential well, and
- (ii) a periodic 1D potential, with the same particle interactions, in the tight-binding limit.

*Solutions:*

(i) Let us use Eq. (8.99) of the lecture notes as the baseline, and add a term describing on-site interactions. For *bosons*, this may be done, for example, by keeping the diagonal elements in Eq. (8.114) with all  $u_{jjjj}$  equal to  $J$ . As a result, the simplest model that satisfies the assignment requirements is

$$\hat{H} = \varepsilon_1 \hat{a}_1^\dagger \hat{a}_1 + \frac{J}{2} \hat{a}_1^\dagger \hat{a}_1^\dagger \hat{a}_1 \hat{a}_1 + \varepsilon_2 \hat{a}_2^\dagger \hat{a}_2 + \frac{J}{2} \hat{a}_2^\dagger \hat{a}_2^\dagger \hat{a}_2 \hat{a}_2 + t \left( \hat{a}_1^\dagger \hat{a}_2 + \text{h.c.} \right).$$

with  $\varepsilon_{1,2} = \pm c_z$ ,  $t \equiv |c_-| = |c_+|$ . Applying the bosonic operator commutation rule to the middle pair of operators in the 4-products, just as it was done in Eq. (8.120), we may rewrite the result as

$$\hat{H} = \varepsilon_1 \hat{N}_1 + \frac{J}{2} \hat{N}_1 (\hat{N}_1 - \hat{I}) + \varepsilon_2 \hat{N}_2 + \frac{J}{2} \hat{N}_2 (\hat{N}_2 - \hat{I}) + t \left( \hat{a}_1^\dagger \hat{a}_2 + \text{h.c.} \right), \quad \text{with } \hat{N}_j \equiv \hat{a}_j^\dagger \hat{a}_j.$$

For *fermions*, such a model would not make much sense because the eigenvalues  $N_j$  may only take values 0 or 1, so the term proportional to  $J$  would equal zero for any state. This is why the simplest model for fermions may be based on the assumption of two quantum states for each site (say, with different spin orientations), so *each* of their occupancies  $N_\uparrow$  and  $N_\downarrow$  may be equal to either 0 or 1. Then, in analogy with the above expression for bosons, we may write

$$\hat{H} = \varepsilon_1 (\hat{N}_{1\uparrow} + \hat{N}_{1\downarrow}) + J \hat{N}_{1\uparrow} \hat{N}_{1\downarrow} + \varepsilon_2 (\hat{N}_{2\uparrow} + \hat{N}_{2\downarrow}) + J \hat{N}_{2\uparrow} \hat{N}_{2\downarrow} + t \left( \hat{a}_{1\uparrow}^\dagger \hat{a}_{2\uparrow} + \hat{a}_{1\downarrow}^\dagger \hat{a}_{2\downarrow} + \text{h.c.} \right).$$

This expression takes into account the fact that the orbital motion, whether this is a localized state or interwell tunneling, is typically independent of the particle's spin, so the terms proportional to  $t$  include only creation-annihilation operator products with the same spin orientation, and coefficients  $\varepsilon_j$  and  $t$  are spin-independent.

(ii) A straightforward generalization of the formula for *bosons* to an infinite 1D chain of similar localized sites (see also Eq. (8.112) of the notes) is

$$\hat{H} = \sum_{j=-\infty}^{+\infty} \left[ \frac{J}{2} \hat{N}_j (\hat{N}_j - \hat{I}) + t \left( \hat{a}_j^\dagger \hat{a}_{j+1} + \text{h.c.} \right) \right].$$

Here I have used the fact that if the potential is indeed periodic, the core energies  $\varepsilon_j$  are equal to each other, so if the total number  $N$  of particles in the system is fixed, their sum  $\varepsilon N$  is also a constant, and may be taken for the energy reference. This Hamiltonian is known as the *Bose-Hubbard model*.

A close term, the *Hubbard model*, is typically reserved for *fermions* (typically, electrons in condensed matter systems), and may be also obtained by the generalization of the above two-site model. Just as for bosons, the difference between the parameters  $\varepsilon_j$  and  $t_j$  at different sites is typically neglected, giving

$$\hat{H} = \sum_{j=-\infty}^{+\infty} \left[ J \hat{N}_{j\uparrow} \hat{N}_{j\downarrow} + t \left( \hat{a}_{j,\uparrow}^\dagger \hat{a}_{j+1,\uparrow} + \hat{a}_{j,\downarrow}^\dagger \hat{a}_{j+1,\downarrow} + \text{h.c.} \right) \right].$$

**Problem 8.27.** For each of the Hamiltonians composed in the previous problem, derive the Heisenberg equations of motion for particle creation/annihilation operators.

*Solution:* Evidently, the bosonic and fermionic models have to be considered separately.

**Bosons.** The Heisenberg equation contributions due to the terms quadratic in the creation/annihilation operators have been calculated in Sec. 8.3 (see Eqs. (8.101)-(8.106) of the lecture notes), so the only new terms we should handle for our Bose models are those proportional to  $\hat{a}_j^\dagger \hat{a}_j^\dagger \hat{a}_j \hat{a}_j$ , all with the same site index  $j$ . Dropping the index for the sake of notation simplicity, we may write a typical commutator we would need as

$$\left[ \hat{a}, \hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a} \right] \equiv \hat{a} \hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a} - \hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a} \hat{a}. \quad (*)$$

Applying the commutation rule (8.74) to the first term twice, to move the first annihilation operator to the back (rightmost) position, we get

$$\hat{a}\hat{a}^\dagger\hat{a}^\dagger\hat{a}\hat{a} = \left(\hat{I} + \hat{a}^\dagger\hat{a}\right)\hat{a}^\dagger\hat{a}\hat{a} = \hat{a}^\dagger\hat{a}\hat{a} + \hat{a}^\dagger\hat{a}\hat{a}^\dagger\hat{a}\hat{a} = \hat{a}^\dagger\hat{a}\hat{a} + \hat{a}^\dagger\left(\hat{I} + \hat{a}^\dagger\hat{a}\right)\hat{a}\hat{a} = 2\hat{a}^\dagger\hat{a}\hat{a} + \hat{a}^\dagger\hat{a}^\dagger\hat{a}\hat{a},$$

The last term in this expression cancels with that in Eq. (\*), so we get

$$\left[\hat{a}, \hat{a}^\dagger\hat{a}^\dagger\hat{a}\hat{a}\right] = 2\hat{a}^\dagger\hat{a}\hat{a}.$$

As a result, the Heisenberg equations of motion for the annihilation operators take the following forms:

– for two coupled wells:

$$i\hbar\dot{\hat{a}}_1 = \varepsilon_1\hat{a}_1 + J\hat{a}_1^\dagger\hat{a}_1\hat{a}_1 + t\hat{a}_2, \quad i\hbar\dot{\hat{a}}_2 = \varepsilon_2\hat{a}_2 + J\hat{a}_2^\dagger\hat{a}_2\hat{a}_2 + t\hat{a}_1,$$

– for the Bose-Hubbard model of a 1D chain of similar sites:

$$i\hbar\dot{\hat{a}}_j = J\hat{a}_j^\dagger\hat{a}_j\hat{a}_j + t(\hat{a}_{j-1} + \hat{a}_{j+1}).$$

(The equations for the creation operators may be obtained absolutely similarly.)

Despite the innocent look of these equations, they are nonlinear and hence do not allow exact analytical solutions.

**Fermions.** It may look that for the fermions, the situation would be easier because only the first power of each population operator participates in the Hamiltonians. However, the celebration would be premature because the creation-annihilation operators belonging to different states are not independent now. Indeed, let us crank open a typical commutator we would need (with the well's index dropped, as above):

$$\left[\hat{a}_\uparrow, \hat{N}_\uparrow\hat{N}_\downarrow\right] = \left[\hat{a}_\uparrow, \hat{a}_\uparrow^\dagger\hat{a}_\uparrow\hat{a}_\downarrow^\dagger\hat{a}_\downarrow\right] = \hat{a}_\uparrow\hat{a}_\uparrow^\dagger\hat{a}_\uparrow\hat{a}_\downarrow^\dagger\hat{a}_\downarrow - \hat{a}_\uparrow^\dagger\hat{a}_\uparrow\hat{a}_\downarrow^\dagger\hat{a}_\downarrow\hat{a}_\uparrow,$$

and start swapping operators in the first term by using the fermionic commutation rules (8.95)-(8.96):

$$\hat{a}_\uparrow\hat{a}_\uparrow^\dagger\hat{a}_\uparrow\hat{a}_\downarrow^\dagger\hat{a}_\downarrow = \left(\hat{I} - \hat{a}_\uparrow^\dagger\hat{a}_\uparrow\right)\hat{a}_\uparrow\hat{a}_\downarrow^\dagger\hat{a}_\downarrow = \hat{a}_\uparrow\hat{a}_\downarrow^\dagger\hat{a}_\downarrow - \hat{a}_\uparrow^\dagger\hat{a}_\uparrow\hat{a}_\uparrow\hat{a}_\downarrow^\dagger\hat{a}_\downarrow.$$

At this stage, we should notice that the second term in the last expression gives zero at its action upon any fermion state (because two annihilation operators follow each other), and thus may be ignored. Similarly, twice commuting the operators in the second term of the commutator, we get

$$\hat{a}_\uparrow^\dagger\hat{a}_\uparrow\hat{a}_\downarrow^\dagger\hat{a}_\downarrow\hat{a}_\uparrow = -\hat{a}_\uparrow^\dagger\hat{a}_\downarrow^\dagger\hat{a}_\uparrow\hat{a}_\downarrow\hat{a}_\uparrow = \hat{a}_\uparrow^\dagger\hat{a}_\downarrow^\dagger\hat{a}_\downarrow\hat{a}_\uparrow\hat{a}_\uparrow,$$

so it always gives zero as well. Thus, finally,

$$\left[\hat{a}_\uparrow, \hat{N}_\uparrow\hat{N}_\downarrow\right] = \hat{a}_\uparrow\hat{a}_\downarrow^\dagger\hat{a}_\downarrow.$$

This is not more complex than for the bosonic operators, but not simpler either. We may also notice that all commutators like

$$[\hat{a}_j, \hat{N}_{j'}]$$

vanish if  $j$  and  $j'$  are different (orbital and/or spin) states. As a result, the Heisenberg equations of motion are:

– for two coupled wells:

$$i\hbar\dot{\hat{a}}_{1\uparrow} = \varepsilon_1\hat{a}_{1\uparrow} + J\hat{a}_{1\uparrow}\hat{a}_{1\downarrow}^\dagger\hat{a}_{1\downarrow} + t\hat{a}_{2\uparrow}, \quad i\hbar\dot{\hat{a}}_{2\uparrow} = \varepsilon_2\hat{a}_{2\uparrow} + J\hat{a}_{2\uparrow}\hat{a}_{2\downarrow}^\dagger\hat{a}_{2\downarrow} + t\hat{a}_{1\uparrow},$$

– for the Hubbard model:

$$i\hbar\dot{\hat{a}}_{j\uparrow} = J\hat{a}_{j\uparrow}\hat{a}_{j\downarrow}^\dagger\hat{a}_{j\downarrow} + t(\hat{a}_{j-1,\uparrow} + \hat{a}_{j+1,\uparrow}),$$

and similarly for the opposite-spin states. We see that equations for the states with opposite spins are coupled via the on-site interaction term, not making their solution any easier.

**Problem 8.28.** Express the ket-vectors of all possible Dirac states of three indistinguishable

- (i) bosons, and
- (ii) fermions,

via those of the single-particle states  $\beta$ ,  $\beta'$ , and  $\beta''$  they occupy.

*Solutions:*

(i) *Bosons:* If all three single-particle states occupied in the considered Dirac states are different, we may use Eq. (8.80) of the lecture notes with  $N_1 = N_2 = N_3 = 1$ ,  $N_4 = N_5 = \dots = 0$ , so the left-hand side of this relation may be truncated just to three positions, while its right-hand side is a sum of  $N! = 3! = 6$  different kets formed by particle permutations:<sup>59</sup>

$$|1,1,1\rangle = \frac{1}{\sqrt{6}}(|\beta\beta'\beta''\rangle + |\beta\beta''\beta'\rangle + |\beta'\beta\beta''\rangle + |\beta'\beta''\beta\rangle + |\beta''\beta\beta'\rangle + |\beta''\beta'\beta\rangle), \quad (*)$$

where the possible zeros in the left-hand ket (expressing unoccupied states) are suppressed.

If two of the single-particle states (say,  $\beta'$  and  $\beta''$ ) are identical, i.e. there are just two different single-particle states,  $\beta$  and  $\beta'$ , then the Dirac ket may be truncated even more, to show just two first positions, say with  $N_1 = 1$  and  $N_2 = 2$ , and the right-hand side of Eq. (8.80) has only three permutations:

$$|1,2\rangle = \left(\frac{2!}{3!}\right)^{1/2} (|\beta\beta'\beta'\rangle + |\beta'\beta\beta'\rangle + |\beta'\beta'\beta\rangle) \equiv \frac{1}{\sqrt{3}}(|\beta\beta'\beta'\rangle + |\beta'\beta\beta'\rangle + |\beta'\beta'\beta\rangle).$$

Absolutely similarly,

$$|2,1\rangle = \frac{1}{\sqrt{3}}(|\beta\beta\beta'\rangle + |\beta'\beta\beta\rangle + |\beta\beta'\beta\rangle).$$

<sup>59</sup> Note again that the symbol positions within the kets on two sides of this relation have very different meanings: in the second quantization language (the left-hand side) they code the single-particle *state* numbers, while those in the “usual” notation (the right-hand side), the *particle* numbers. To emphasize the difference, I always separate the *state* numbers by commas.

Finally, if all three particles are in the same single-particle state (say,  $\beta$ ), then we may take  $N_1 = 3, N_2 = N_3 = \dots = 0$ , and Eq. (8.80) yields simply

$$|3\rangle = \left(\frac{3!}{3!}\right)^{1/2} |\beta\beta\beta\rangle \equiv |\beta\beta\beta\rangle.$$

Note that the general state of a three-particle system may be a linear superposition of the Dirac states of these three types, with various  $\beta, \beta'$ , and  $\beta''$ , i.e. it is not necessarily one of the Dirac states.

(ii) *Fermions*: Per the Pauli principle, all occupied states  $\beta, \beta'$ , and  $\beta''$  have to be different, so suppressing all zeros in the Dirac ket-vector again, we may spell out the Slater determinant (8.60) as

$$\begin{aligned} |1,1,1\rangle &= \frac{1}{\sqrt{3!}} \begin{vmatrix} |\beta\rangle & |\beta'\rangle & |\beta''\rangle \\ |\beta\rangle & |\beta'\rangle & |\beta''\rangle \\ |\beta\rangle & |\beta'\rangle & |\beta''\rangle \end{vmatrix} \\ &\equiv \frac{1}{\sqrt{6}} (|\beta\beta'\beta''\rangle - |\beta\beta''\beta'\rangle - |\beta'\beta\beta''\rangle + |\beta'\beta''\beta\rangle + |\beta''\beta\beta'\rangle - |\beta''\beta'\beta\rangle), \end{aligned}$$

where the last expression uses the same shorthand notation (with the symbol position coding of the particle numbers) as used in Task (i) of this solution. Evidently, it differs from Eq. (\*) only by sign alternation, which ensures the state asymmetry (rather than symmetry) with respect to the permutation of any two particles.

**Problem 8.29.** Explain why the general perturbative result (8.126), when applied to the  $^4\text{He}$  atom, gives the correct<sup>60</sup> expression (8.29) for the ground singlet state, and correct Eqs. (8.39)-(8.42) (with the minus sign in the first of these relations) for the excited triplet states, but cannot describe these results, with the plus sign in Eq. (8.39), for the excited singlet state.

*Solution:* In the numbered-particle language, the unperturbed ground (singlet) state used for the calculation of Eq. (8.29) is represented by Eq. (8.24) and may be described by the ket-vector

$$|\text{gg}\rangle \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \equiv \frac{1}{\sqrt{2}} (|g_\uparrow\rangle \otimes |g_\downarrow\rangle - |g_\downarrow\rangle \otimes |g_\uparrow\rangle), \quad (*)$$

where “g” denotes the orbital factor of the single-particle ground state:  $\langle \mathbf{r} | g \rangle \equiv \psi_{100}(\mathbf{r})$ , and each ket on the right-hand side of this expression is a spin-orbital – see Eq. (8.125). On the other hand, with the states  $g_\uparrow$  and  $g_\downarrow$  taken for the single-particle basis ( $\beta$  and  $\beta'$ ) for the Dirac representation, the two-electron Dirac state ket,  $|N_1, N_2\rangle = |1, 1\rangle$ , i.e. the Slater determinant (8.60a), is represented by the ket

$$\frac{1}{\sqrt{2}} (|\beta\beta'\rangle - |\beta'\beta\rangle) \equiv \frac{1}{\sqrt{2}} (|\beta\rangle \otimes |\beta'\rangle - |\beta'\rangle \otimes |\beta\rangle) \equiv \frac{1}{\sqrt{2}} (|g_\uparrow\rangle \otimes |g_\downarrow\rangle - |g_\downarrow\rangle \otimes |g_\uparrow\rangle),$$

i.e. exactly the same state as Eq. (\*).

<sup>60</sup> Correct in the sense of the first order of the perturbation theory.

However, for the analysis of the  $^4\text{He}$  atom in Sec. 8.2 of the lecture notes, we have described the excited singlet state by its orbital wavefunction (8.35), with the plus sign, i.e. by the following total (orbital + spin) ket-vector:

$$\frac{1}{\sqrt{2}}(|ge\rangle + |eg\rangle) \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \equiv \frac{1}{2}(|g\rangle \otimes |e\rangle + |e\rangle \otimes |g\rangle)(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle),$$

where “e” means the orbital part of a single-particle excited state:  $\langle \mathbf{r} | e \rangle \equiv \psi_{nlm}(\mathbf{r})$  with  $n > 1$ . Multiplying the parentheses, we may represent this expression as a sum of four terms:

$$\frac{1}{2}(|g_{\uparrow}\rangle \otimes |e_{\downarrow}\rangle - |g_{\downarrow}\rangle \otimes |e_{\uparrow}\rangle + |e_{\uparrow}\rangle \otimes |g_{\downarrow}\rangle - |e_{\downarrow}\rangle \otimes |g_{\uparrow}\rangle),$$

which may be regrouped as

$$\frac{1}{\sqrt{2}} \left[ \frac{1}{\sqrt{2}}(|g_{\uparrow}\rangle \otimes |e_{\downarrow}\rangle - |e_{\downarrow}\rangle \otimes |g_{\uparrow}\rangle) + \frac{1}{\sqrt{2}}(|e_{\uparrow}\rangle \otimes |g_{\downarrow}\rangle - |g_{\downarrow}\rangle \otimes |e_{\uparrow}\rangle) \right].$$

Each of the two components of this linear superposition is a  $2 \times 2$  Slater determinant in the particle-number representation, i.e. a single Dirac ket  $|N_1, N_2\rangle = |1, 1\rangle$ . However, since these two kets have different spin-orbital state bases ( $g_{\uparrow}$  and  $e_{\downarrow}$  vs.  $e_{\uparrow}$  and  $g_{\downarrow}$ ), their coherent sum is *not* a single Dirac ket, such as those used at the derivation of Eq. (8.126).

The same is also true for the entangled excited triplet state,

$$\frac{1}{\sqrt{2}}(|ge\rangle - |eg\rangle) \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \equiv \frac{1}{2}(|g\rangle \otimes |e\rangle - |e\rangle \otimes |g\rangle)(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle),$$

which is just another, linearly-independent superposition of the two same Dirac kets:

$$\frac{1}{\sqrt{2}} \left[ \frac{1}{\sqrt{2}}(|g_{\uparrow}\rangle \otimes |e_{\downarrow}\rangle - |e_{\downarrow}\rangle \otimes |g_{\uparrow}\rangle) - \frac{1}{\sqrt{2}}(|e_{\uparrow}\rangle \otimes |g_{\downarrow}\rangle - |g_{\downarrow}\rangle \otimes |e_{\uparrow}\rangle) \right].$$

On the other hand, the two “simple” (factorable) triplet states, for example

$$\frac{1}{\sqrt{2}}(|ge\rangle - |eg\rangle)|\uparrow\uparrow\rangle \equiv \frac{1}{\sqrt{2}}(|g_{\uparrow}\rangle \otimes |e_{\uparrow}\rangle - |e_{\uparrow}\rangle \otimes |g_{\uparrow}\rangle),$$

are single Slater determinants, i.e. single Dirac kets.

Hence, the fact that Eq. (8.126), with  $N = 2$ , does describe a negative contribution from the exchange interaction is only due to the existence of the corresponding factorable triplet states.

**Problem 8.30.\*** Explore the *Thomas-Fermi model*<sup>61</sup> of a heavy atom, with the nuclear charge  $Q = Ze \gg e$ , in which the interaction between electrons is limited to their contributions to the common electrostatic potential  $\phi(\mathbf{r})$ . In particular, derive the ordinary differential equation obeyed by the radial distribution of the potential, and use it to estimate the effective radius of the atom.

<sup>61</sup> It was suggested in 1927 independently by L. Thomas and E. Fermi.

*Solution:* In the case  $Z \gg 1$ , due to the Pauli principle, we may expect the characteristic radius  $r_{\text{TF}}(Z)$  of the atom (i.e. of the electron cloud surrounding the point-like nucleus) to be much larger than the characteristic radius  $r_0$  of the single-electron ground-state wavefunctions in the Coulomb field of a bare nucleus with charge  $Q = Ze$ :

$$r_0 = \frac{r_{\text{B}}}{Z},$$

where  $r_{\text{B}}$  is the Bohr radius given by Eqs. (1.10) and (3.192) of the lecture notes. (This assumption,  $r_{\text{TF}} \gg r_0$ , will be confirmed by our solution.) Due to this relation, which means that the electron's electrostatic potential energy  $U(\mathbf{r}) = -e\phi(\mathbf{r})$  changes in space slowly on the  $r_0$ -scale, we may calculate the electron density  $n(\mathbf{r}) \equiv dN/dV$  in a small local volume  $dV$ , with  $r_0 \ll (dV)^{1/3} \ll r_{\text{TF}}$ , by neglecting the gradient of  $U(\mathbf{r})$ , i.e. considering each electron as a *locally free* particle with the full energy

$$\varepsilon = \frac{p^2}{2m_e} - e\phi(\mathbf{r}), \quad (*)$$

where the second term is treated, at each location  $\mathbf{r}$ , as a local constant. As a result, we may apply to this small local volume of this gas, at a negligible temperature,<sup>62</sup> the analysis carried out for fermions in the model solution of Problem 21, with the spin degeneracy  $g = 2s + 1 = 2$ , to calculate the *local Fermi energy*, i.e. the highest kinetic energy level filled by the electrons at point  $\mathbf{r}$ :

$$\varepsilon_{\text{F}}(\mathbf{r}) = \frac{\hbar^2}{2m_e} [3\pi^2 n(\mathbf{r})]^{2/3}. \quad (**)$$

Now comes the most non-trivial point of this solution. If we accept the free electron energy at distance  $r \rightarrow \infty$  from the nucleus for the reference, i.e. take  $\phi(\infty) = 0$ , then the largest value of the full energy (\*), for any  $\mathbf{r}$ , should equal zero because an electrically-neutral atom should be in dynamic equilibrium with free electrons in the environment.<sup>63</sup> Hence the maximum value (\*\*) of the local kinetic energy has to be equal to  $-q\phi(\mathbf{r}) \equiv e\phi(\mathbf{r})$ . This equality yields

$$n(\mathbf{r}) = \frac{1}{3\pi^2} \left[ \frac{2m_e e\phi(\mathbf{r})}{\hbar^2} \right]^{3/2}. \quad (***)$$

The second relation between the functions  $n(\mathbf{r})$  and  $\phi(\mathbf{r})$  is given by the Poisson equation of electrostatics,<sup>64</sup>

<sup>62</sup> The apparent scale of temperatures at which this assumption certainly becomes invalid is given by the Hartree energy  $E_{\text{H}} \approx 27.2$  eV (see Eq. (1.13) and its discussion), corresponding to  $T_{\text{K}} = E_{\text{H}}/k_{\text{B}} \sim 3 \times 10^5$  K – about a thousand times higher than the standard room temperature of 300 K. Actually, the solution of the next problem will show that the validity limit for temperature is even  $\sim Z^{4/3} \gg 1$  times higher.

<sup>63</sup> Note that in statistical physics, this situation is called *chemical equilibrium*, and the corresponding value of energy (in our case, accepted for zero), is called the *chemical potential*, commonly denoted as  $\mu$ . A more general introduction of this notion in statistical physics enables one to streamline this reasoning, and also generalize the calculations to arbitrary temperatures. This is why I gave this problem and the next one again, and provided their more formal solutions, in the SM part of this series.

<sup>64</sup> See, e.g., EM Eq. (1.41). Let me hope that the difference between the single-particle energy  $\varepsilon$  and the electric constant  $\varepsilon_0$  (see, e.g., *Appendix UCA*) is absolutely clear from the context.



$$\nabla^2 \phi(\mathbf{r}) = -\frac{\rho(\mathbf{r})}{\epsilon_0} \equiv -\frac{e[Z\delta(\mathbf{r}) - n(\mathbf{r})]}{\epsilon_0},$$

because the electric charge density  $\rho(\mathbf{r})$  consists of the point-like positive charge  $Q = Ze$  of the nucleus at the origin and the space-distributed negative charge of the electron cloud, with the density  $-en(\mathbf{r})$ . Plugging in the  $n(\mathbf{r})$  from Eq. (\*\*), and spelling out the Laplace operator for our spherically-symmetric problem,<sup>65</sup> we get the following *Thomas-Fermi equation* for the radial distribution of the electrostatic potential  $\phi$ :

$$\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d\phi}{dr} \right) = \frac{e}{3\pi^2 \epsilon_0} \left( \frac{2m_e e \phi}{\hbar^2} \right)^{3/2}, \quad \text{for } r > 0.$$

This ordinary differential equation has to be solved with the following boundary conditions. Close to the atomic nucleus, the potential has to approach its field alone:

$$\phi(r) \rightarrow \frac{Q}{4\pi\epsilon_0 r} \equiv \frac{Ze}{4\pi\epsilon_0 r}, \quad \text{at } r \rightarrow 0.$$

On the other hand, at large distances, due to the atom's electroneutrality, its electrostatic potential should not only tend to zero but also do it faster than that of any non-zero net charge:<sup>66</sup>

$$r\phi(r) \rightarrow 0, \quad \text{at } r \rightarrow \infty.$$

It is convenient to recast this boundary problem by introducing the dimensionless distance  $\xi$  from the origin, defined as

$$\xi \equiv \frac{r}{r_{\text{TF}}(Z)}, \quad \text{with } r_{\text{TF}}(Z) \equiv b \frac{r_{\text{B}}}{Z^{1/3}} = br_0 Z^{2/3} \gg r_0, \quad \text{and } b \equiv \frac{1}{2} \left( \frac{3\pi}{4} \right)^{2/3} \approx 0.8853, \quad (\text{****})$$

and also a dimensionless function  $\chi(\xi)$  defined by the following equality:

$$\phi(r) \equiv \frac{Ze}{4\pi\epsilon_0 r} \chi(\xi).$$

With these definitions, our boundary problem becomes “universal” (i.e. free of parameters, in particular, independent of the atomic number  $Z$ ):

$$\frac{d^2 \chi}{d^2 \xi} = \frac{\chi^{3/2}}{\xi^{1/2}}, \quad \text{with } \chi(\xi) \rightarrow \begin{cases} 1, & \text{at } \xi \rightarrow 0, \\ 0, & \text{at } \xi \rightarrow \infty. \end{cases}$$

Unfortunately, this nonlinear differential equation may be solved only numerically, but this is not a big loss: the solution shows that as its argument  $\xi$  is increased, the function  $\chi(\xi)$  goes down from

<sup>65</sup> See, e.g., MA Eq. (10.9) with  $\partial/\partial\theta = \partial/\partial\phi = 0$ .

<sup>66</sup> A useful sanity check of the Thomas-Fermi model's self-consistency may be performed by using the above relations to prove that the total number of electrons, calculated as

$$N = \int n(\mathbf{r}) d^3 r \equiv 4\pi \int_0^\infty n(r) r^2 dr,$$

equals exactly  $Z$  – a simple exercise, highly recommended to the reader.

unity at  $\xi = 0$  to zero at  $\xi \rightarrow \infty$  monotonically (and very uneventfully), at distances  $\xi \sim 1$ . (For example,  $\chi(1) \approx 0.4$ .) This is why, even without the exact solution on hand, we may conclude that the constant  $r_{\text{TF}}(Z)$  defined by Eq. (\*\*\*\*) gives a fair scale of the atom's size. That formula shows that this size decreases with the atomic number  $Z$  very slowly, as  $r_{\text{B}}/Z^{1/3}$ , and hence, at  $Z \gg 1$ , is much smaller than  $r_0 = r_{\text{B}}/Z$  – confirming, in particular, our initial assumption. This result is in good agreement (for  $Z \gg 1$ ) with those given by more accurate models describing quantized energy spectra of heavy atoms.

**Problem 8.31.**\* Use the Thomas-Fermi model explored in the previous problem to calculate the total binding energy of a heavy atom. Compare the result with that of the simpler model, in that the Coulomb electron-electron interaction is completely ignored.

*Solution:* The binding energy of an atom may be calculated, for example, as

$$E_{\text{b}} = \sum_{Z'=Z}^0 \mathcal{W}(Z'), \quad (*)$$

where  $\mathcal{W}(Z')$  is the work necessary to *decrease* the atomic number from  $Z'$  to  $(Z' - 1)$ . In order to find  $\mathcal{W}(Z')$ , let us note that the process of decreasing the atomic number by one may be decomposed into two moves: taking one electron out of the electron cloud, and then one proton, of charge  $+e$ , out of the nucleus. By removing this electron from the Fermi surface, i.e. at its total energy equal to zero, the first step of the process requires no work, while the second step requires work  $\mathcal{W}(Z') = -e\phi_{\text{e}}(0)$ , where  $\phi_{\text{e}}(r)$  is the part of the potential  $\phi(r)$  that is due to electrons only.<sup>67</sup> Using the relations derived in the previous problem, with the notation replacement  $Z \rightarrow Z'$ , we get

$$\phi_{\text{e}}(r) = \phi(r) - \frac{Z'e}{4\pi\epsilon_0 r} \equiv \frac{Z'e}{4\pi\epsilon_0 r} \chi(\xi) - \frac{Z'e}{4\pi\epsilon_0 r} \equiv \frac{Z'e}{4\pi\epsilon_0} \frac{\chi(\xi) - 1}{r}.$$

Since  $\chi(0) - 1 = 0$  by construction, at  $r \rightarrow 0$ , the last fraction tends to  $(d\chi/dr)_{r=0}$  and we get

$$\mathcal{W}(Z') = -e\phi_{\text{e}}(0) = -\frac{Z'e^2}{4\pi\epsilon_0} \left( \frac{d\chi}{dr} \right)_{r=0} \equiv \frac{Z'e^2}{4\pi\epsilon_0 r_{\text{TF}}(Z')} \left( -\frac{d\chi}{d\xi} \right)_{\xi=0}.$$

Due to the properties of the universal function  $\chi(\xi)$ , discussed at the end of the previous problem's solution, we may expect the derivative  $d\chi/d\xi$  to be negative, with a modulus of the order of 1 at  $\xi = 0$ . Indeed, a numerical solution of the boundary problem for the function  $\chi(\xi)$  yields

$$a \equiv \left( -\frac{d\chi}{d\xi} \right)_{\xi=0} \approx 1.5881,$$

so  $\mathcal{W}(Z') > 0$  for any  $Z'$ . As a result, the total binding energy  $E_{\text{b}}$  given by Eq. (\*) is positive as well. (This means that the atom's components, after they have been brought far apart, have higher energy than

<sup>67</sup> Of course, the removed proton also interacts (and very strongly) with the initial  $Z'$  protons in the nucleus. However, our goal is to calculate the *binding* energy, i.e. difference between the sum of energies of the "assembled" nucleus and individual electrons, all far apart from each other, and that of the fully "assembled" atom. At the calculation of such difference, the change of the intrinsic energy of the nucleus cancels.

the initial atom, ensuring that the latter is stable.) Due to the condition  $Z \gg 1$ , the sum (\*) may be calculated as the integral

$$E_b = \int_0^Z \mathcal{W}(Z') dZ' = a \int_0^Z \frac{Z'e^2}{4\pi\epsilon_0 r_{\text{TF}}(Z')} dZ' \equiv \frac{a}{b} \frac{e^2}{4\pi\epsilon_0 r_B} \int_0^Z Z'^{4/3} dZ' = \frac{3a}{7b} Z^{7/3} \frac{e^2}{4\pi\epsilon_0 r_B}.$$

But the last fraction is just the Hartree energy  $E_H$ , so we finally get

$$E_b = \frac{3a}{7b} Z^{7/3} E_H \approx 0.7688 Z^{7/3} E_H \gg E_H, \quad \text{for } Z \gg 1.$$

Note the very nontrivial scaling of the binding energy with the atomic number  $Z$ .

Now let us consider a simpler model,<sup>68</sup> in which the electron-electron interaction is completely ignored. Using the same arguments as in the previous problem's solution, we still may use its Eq. (\*\*),

$$\varepsilon_F(\mathbf{r}) = \frac{\hbar^2}{2m_e} [3\pi^2 n(\mathbf{r})]^{2/3}, \quad (**)$$

for the local Fermi energy  $\varepsilon_F(\mathbf{r})$ , i.e. the largest kinetic energy of electrons at the location  $\mathbf{r}$ , and find its dependence on  $r$  from the requirement that the largest total energy of the electron,

$$\mu \equiv \varepsilon_F(\mathbf{r}) + q\phi(\mathbf{r}) = \varepsilon_F(\mathbf{r}) - e\phi(\mathbf{r}),$$

is spatially independent. However, in this simple model, the electrostatic potential  $\phi(\mathbf{r})$  is given by the bare Coulomb field of the nuclear point charge  $Ze$ , so this condition becomes

$$\mu = \varepsilon_F(\mathbf{r}) - \frac{Ze^2}{4\pi\epsilon_0 r} = \text{const}, \quad (***)$$

with  $\mu$  not known in advance. In order to have the electrons localized near the nucleus,  $\mu$  cannot be positive (i.e. larger than the potential energy value at  $r \rightarrow \infty$ ), so  $\varepsilon_F$  (and hence the electron density  $n$ ) has to turn to zero at some finite radius  $r_{\text{ef}}$ , which, in this model, plays the role of the atom's radius.<sup>69</sup> Per Eq. (\*\*\*), this radius is related to  $\mu$  as

$$\frac{Ze^2}{4\pi\epsilon_0 r_{\text{ef}}} \equiv -\mu \geq 0,$$

so Eqs. (\*\*) and (\*\*\*) yield

$$n(\mathbf{r}) = \frac{1}{3\pi^2} \left[ \frac{m_e e^2 Z}{2\pi\epsilon_0 \hbar^2} \left( \frac{1}{r} - \frac{1}{r_{\text{ef}}} \right) \right]^{3/2}.$$

Now we may calculate the constant  $r_{\text{ef}}$  (and hence  $\mu$ ) by requiring the atom as the whole to be neutral, i.e. the number of electrons to be equal to  $Z$ :

<sup>68</sup> Very unfortunately, this model is sometimes called “statistical” – why??

<sup>69</sup> Note that in contrast to the Thomas-Fermi approximation, this simple model is not self-consistent because it implies that  $\phi(r_{\text{ef}}) = -\mu \neq 0$ , while the electrostatic potential of a neutral and spherically symmetrical atom should vanish at its effective surface.

$$\int_{r \leq R} n(\mathbf{r}) d^3 r = Z.$$

Carrying out the integration, we get

$$\begin{aligned} \int_{r \leq R} n(\mathbf{r}) d^3 r &= 4\pi \int_0^R n(\mathbf{r}) r^2 dr = 4\pi \frac{1}{3\pi^2} \left( \frac{m_e e^2 Z}{2\pi\epsilon_0 \hbar^2} \right)^{3/2} \int_0^R \left( \frac{1}{r} - \frac{1}{r_{\text{ef}}} \right)^{3/2} r^2 dr \\ &\equiv \frac{4}{3\pi} \left( \frac{m_e e^2 Z r_{\text{ef}}}{2\pi\epsilon_0 \hbar^2} \right)^{3/2} \int_0^1 (1-\xi)^{3/2} \xi^{1/2} d\xi. \end{aligned}$$

By using the substitution  $\xi \equiv \sin^2 \alpha$ , the last integral may be recast into a sum of elementary integrals, which may be readily worked out using MA Eqs. (3.3d) and (3.4). The final result is  $\pi/16$ , so the electron counting yields the following equation:

$$\frac{4}{3\pi} \left( \frac{m_e e^2 Z r_{\text{ef}}}{2\pi\epsilon_0 \hbar^2} \right)^{3/2} \frac{\pi}{16} = Z, \quad (****)$$

giving

$$r_{\text{ef}} = (18)^{1/3} \frac{4\pi\epsilon_0 \hbar^2}{e^2 m_e} \frac{1}{Z^{1/3}} \equiv (18)^{1/3} \frac{r_B}{Z^{1/3}} \approx 2.621 \frac{r_B}{Z^{1/3}}.$$

So, for the effective radius of the atom, this simple model gives the same functional dependence on  $Z$  as  $r_{\text{TF}}$  in the Thomas-Fermi model. The fact that  $r_{\text{ef}} \sim r_{\text{TF}} \gg r_0 = r_B/Z$  shows that, at least in this system, the implicit interaction of electrons via the Pauli principle, taken into account in this model, is more important than their explicit Coulomb interaction – completely ignored in it.

Now let us calculate the binding energy (\*) within this model. In order to avoid the calculation of the electron potential  $\phi_e(0)$  felt by the nuclear charges, the partial work  $\mathcal{W}(Z')$  may be calculated differently than for the Thomas-Fermi model. Namely, let us calculate the radius  $r_{\text{ef}}(Z')$  and  $\mu(Z')$  of an ion, with  $Z'$  electrons, but the nuclear charge  $Q$  is still equal to  $Ze$ . Reviewing the above calculations, we see that this may be done by replacing  $Z$  on the right-hand side of Eq. (\*\*\*\*) with  $Z'$ :

$$\frac{4}{3\pi} \left[ \frac{m_e e^2 Z' r_{\text{ef}}(Z')}{2\pi\epsilon_0 \hbar^2} \right]^{3/2} \frac{\pi}{16} = Z', \quad \text{giving } r_{\text{ef}}(Z') = (18)^{1/3} \frac{Z'^{2/3}}{Z} r_B,$$

and then calculating  $\mu$  as

$$-\mu(Z') = \frac{Ze^2}{4\pi\epsilon_0 r_{\text{ef}}(Z')} = \frac{1}{(18)^{1/3}} \frac{Ze^2}{4\pi\epsilon_0 r_B} \frac{Z}{Z'^{2/3}} \equiv \frac{E_H}{(18)^{1/3}} \frac{Z^2}{Z'^{2/3}}.$$

The work  $\mathcal{W}(Z')$  necessary for the removal of an additional electron from the ion to infinity is  $-\mu(Z')$ , so, replacing the sum (\*) with the corresponding integral, we get

$$E_b = -\int_0^Z \mu(Z') dZ' = \frac{E_H}{(18)^{1/3}} Z^2 \int_0^Z \frac{dZ'}{Z'^{2/3}} = \frac{3}{(18)^{1/3}} Z^{7/3} E_H \approx 1.145 Z^{7/3} E_H.$$

Very naturally, this value is higher than that calculated in the solution of the previous problem for the Thomas-Fermi model because, in the current simple model, each electron is attracted to the

nucleus by its Coulomb field unscreened by other electrons, making their interaction stronger. Note, however, that the difference is not too large – just about 50%.

**Problem 8.32.** Suggest and explore a simple model of dephasing in a system consisting of  $N$  similar, distinct, non-interacting components. In particular, how does the dephasing time scale with  $N$ ?

*Solution:* To piggyback on our discussion of dephasing in two-level (spin- $1/2$ -like) systems in Sec. 7.3 of the lecture notes, let us explore a system of  $N$  similar, distinct two-level components whose quantum-mechanical phases  $\varphi$ , defined by Eqs. (5.1) and (5.11) with  $\gamma = -\varphi/2$ ,

$$|\alpha\rangle \equiv \alpha_{\uparrow}|\uparrow\rangle + \alpha_{\downarrow}|\downarrow\rangle = \cos\frac{\theta}{2}e^{-i\varphi/2}|\uparrow\rangle + \sin\frac{\theta}{2}e^{+i\varphi/2}|\downarrow\rangle \quad (*)$$

(where the Bloch-sphere angles  $\theta$  and  $\varphi$  are real), obey the diffusion law (7.85):

$$\langle(\Delta\varphi)^2\rangle \equiv \langle[\varphi(t) - \varphi(0)]^2\rangle = 2D_{\varphi}t, \quad (**)$$

while  $\theta$  stays constant.<sup>70</sup> Let us further assume that the phase difference we are interested in (say, the one defining quantum interference in the system) is the sum

$$\varphi_{\Sigma}(t) \equiv C \sum_{k=1}^N \varphi_k(t), \quad (***)$$

over all two-level components, with a constant coefficient  $C$ .

In this case, we may write

$$\Delta\varphi_{\Sigma} \equiv C \sum_{k=1}^N \Delta\varphi_k, \quad \text{so} \quad \langle(\Delta\varphi_{\Sigma})^2\rangle = C^2 \sum_{k,k'=1}^N \langle\Delta\varphi_k \Delta\varphi_{k'}\rangle.$$

Under the natural assumption that the fluctuation sources  $f_k(t)$  participating in each of Eqs. (7.70) and resulting in the phase diffusion (\*\*\*) are independent of each other,<sup>71</sup> all terms with  $k \neq k'$  vanish, and we get

$$\langle[\Delta\varphi_{\Sigma}]^2\rangle = C^2 \sum_{k=1}^N \langle(\Delta\varphi_k)^2\rangle = NC^2 \langle(\Delta\varphi)^2\rangle \equiv 2D_{\Sigma}t, \quad \text{with} \quad D_{\Sigma} = NC^2D_{\varphi}.$$

Since according to Eq. (7.89), the dephasing time  $T_2$  is inversely proportional to the phase diffusion coefficient, we get

$$(T_2)_{\Sigma} = \frac{T_2}{NC^2}.$$

This result shows that at least in this simple model, for any reasonable and  $N$ -independent value of  $C$ , the dephasing time in a typical macroscopic system (with, say,  $N \sim N_A \sim 10^{23}$ ) is extremely small.

<sup>70</sup> As a reminder, these results follow from the simple model described by Eqs. (7.69), (7.70), and (7.82), and, per Eq. (7.142), agree with the more general Eq. (7.210). Note, however, that this model, in which there is no diffusion of the phase  $\theta$ , is only valid for the interaction Hamiltonian (7.70) diagonal in the  $z$ -basis.

<sup>71</sup> If this assumption is violated, the final result may be an even stronger function of  $N$ .

**Problem 8.33.** The notion of the reduced density operator  $\hat{w}$  defined by Eq. (7.160) is sometimes used for the characterization of entanglement in multi-qubit systems. Calculate  $\hat{w}$  for one qubit of a two-qubit system that is in an arbitrary pure state, and analyze the result.

*Solution:* Let  $\hat{w}_\Sigma$  be the density operator of the two-bit system. As was discussed in Sec. 7.1 of the lecture notes, if a system is in a pure state, we may always select a basis in which the operator has the simple form following from Eqs. (7.15)-(7.16):

$$\hat{w}_\Sigma = |w_j\rangle\langle w_j|, \quad (*)$$

where the index  $j$  lists the states of the full system. In our current case of a two-qubit system, we may represent any pure state as a linear superposition of the 4 basis states of the composite  $2 \times 2$ -dimensional Hilbert space:

$$|w_j\rangle = a_{00}|0\rangle \otimes |0\rangle + a_{01}|0\rangle \otimes |1\rangle + a_{10}|1\rangle \otimes |0\rangle + a_{11}|1\rangle \otimes |1\rangle, \quad (**)$$

where the qubit number is coded, as usual, by the position of its ket-vector,<sup>72</sup> while  $|0\rangle$  and  $|1\rangle$  are the basis states of each qubit – in the same basis that is used in Eq. (\*).

Now let us form the reduced density operator  $\hat{w}_1$  of the first qubit as prescribed by Eq. (7.160), i.e. by taking the partial trace of the full density operator over the states of its “environment” – in this case, of the second qubit:

$$\hat{w}_1 \equiv \text{Tr}_2 \hat{w}_\Sigma = \langle 0|\hat{w}_\Sigma|0\rangle + \langle 1|\hat{w}_\Sigma|1\rangle = \langle 0|w_j\rangle\langle w_j|0\rangle + \langle 1|w_j\rangle\langle w_j|1\rangle,$$

where the single kets are those of the second qubit. For the state (\*\*), the short brackets participating in the last form may be readily calculated; for example,

$$\begin{aligned} \langle 0|w_j\rangle &= \langle 0|(a_{00}|0\rangle \otimes |0\rangle + a_{01}|0\rangle \otimes |1\rangle + a_{10}|1\rangle \otimes |0\rangle + a_{11}|1\rangle \otimes |1\rangle) \\ &= a_{00}\langle 0|0\rangle \otimes \langle 0|0\rangle + a_{01}\langle 0|0\rangle \otimes \langle 0|1\rangle + a_{10}\langle 0|1\rangle \otimes \langle 0|0\rangle + a_{11}\langle 0|1\rangle \otimes \langle 0|1\rangle = a_{00}|0\rangle + a_{10}|1\rangle; \end{aligned}$$

in the last form, the single kets are those of the first qubit. Acting absolutely similarly, we get

$$\langle 1|w_j\rangle = a_{01}|0\rangle + a_{11}|1\rangle,$$

so, finally:

$$\begin{aligned} \hat{w}_1 &= (a_{00}|0\rangle + a_{10}|1\rangle)(a_{00}^*\langle 0| + a_{10}^*\langle 1|) + (a_{01}|0\rangle + a_{11}|1\rangle)(a_{01}^*\langle 0| + a_{11}^*\langle 1|) \\ &\equiv (a_{00}a_{00}^* + a_{10}a_{10}^*)|0\rangle\langle 0| + (a_{00}a_{10}^* + a_{01}a_{11}^*)|0\rangle\langle 1| + (a_{10}a_{00}^* + a_{11}a_{01}^*)|1\rangle\langle 0| + (a_{10}a_{10}^* + a_{11}a_{11}^*)|1\rangle\langle 1|. \end{aligned} \quad (***)$$

Let us analyze this result, taking into account that the coefficients in Eq. (\*\*\*) have to satisfy the normalization requirement

$$\langle w_j|w_j\rangle \equiv |a_{00}|^2 + |a_{01}|^2 + |a_{10}|^2 + |a_{11}|^2 = 1.$$

<sup>72</sup> As a reminder, the qubits are “always” (or at least in this course) considered distinguishable – say, by their spatial positions.

We may immediately notice that for any factorable (i.e. unentangled) state of the two-qubit system, the reduced density operator has only one ket-bra combination, i.e. formally coincides with the genuine density operator of the first qubit, describing its pure state. For example, if  $|w_j\rangle = |0\rangle\otimes|0\rangle$ , i.e. if  $a_{00} = 1$  while all other coefficients in Eq. (\*\*\*) equal zero, then

$$\hat{w}_1 = |0\rangle\langle 0|. \quad (****)$$

Also, the state  $|w_j\rangle = |0\rangle\otimes|1\rangle$  (described by Eq. (\*\*\*) if  $a_{01} = 1$  while all other coefficients vanish) gives the same result. On the other hand, such states as the singlet or the entangled triplet:  $|w_j\rangle = (1/\sqrt{2})(|0\rangle\otimes|1\rangle \pm |1\rangle\otimes|0\rangle)$  give the reduced operator

$$\hat{w}_1 = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|),$$

corresponding to a 50/50 classical mixture.

Let us prove that *all* entangled states of the two-bit system give a mixed state of  $\hat{w}_1$ . For example, let us find out what values the coefficients  $a_{kk'}$  may have to give Eq. (\*\*\*\*). From the last form of Eq. (\*\*\*) , this requires, in particular, the coefficient before the operator  $|1\rangle\langle 1|$  to vanish:

$$a_{11}a_{11}^* + a_{10}a_{10}^* \equiv |a_{11}|^2 + |a_{10}|^2 = 0.$$

But this may be only if  $a_{11} = a_{10} = 0$ . Plugging the first of these results into the requirement for the coefficient before  $|0\rangle\langle 1|$  to vanish as well,

$$a_{00}a_{10}^* + a_{01}a_{11}^* = 0,$$

we get  $a_{00}a_{10}^* = 0$ , so at least one of these coefficients has to equal 0. Per Eq. (\*\*), this means that the direct product states listed above,

$$|w_j\rangle = |0\rangle\otimes|0\rangle \quad \text{and} \quad |w_j\rangle = |0\rangle\otimes|1\rangle$$

are the only ones that yield Eq. (\*\*\*\*). An absolutely similar analysis of the opposite case,

$$\hat{w}_1 = |1\rangle\langle 1|,$$

shows that it also results only from any of the direct products

$$|w_j\rangle = |1\rangle\otimes|1\rangle \quad \text{and} \quad |w_j\rangle = |1\rangle\otimes|0\rangle,$$

but not from any entangled state.

Hence, the so-reduced density operator may indeed be used for entanglement characterization.

**Problem 8.34.** For a system of two distinct qubits (i.e. two-level systems), introduce a reasonable uncoupled-representation  $z$ -basis and write, in this basis, the  $4\times 4$  matrix of the operator that swaps their states.

*Solution:* The requested basis should obviously include all four possible uncoupled-representation states:

$$\uparrow\uparrow, \quad \uparrow\downarrow, \quad \downarrow\uparrow, \quad \downarrow\downarrow, \quad (*)$$

but in order to prescribe definite 4-component vectors to the states, and hence definite 4×4 matrices to the linear operators acting in this joint Hilbert space, a certain order of the basis states should be selected. (For one spin-1/2, the traditional order, used in particular in this course, is natural: ↑ first, then ↓.) Generally, the order may be selected at will, but it makes sense to establish it in a way that makes possible generalization to more than two spins natural. In this sense, the order given by Eq. (\*), in which the rightmost spins are altered first, is very reasonable. This may be confirmed by rewiring it in the notation accepted in qubit applications (with ↑ denoted as 0, and ↓ as 1 – see the beginning of Sec. 8.5 of the lecture notes):

$$00, 01, 10, 11.$$

Indeed, if these zeros and ones are understood in the sense of classical bits, this line corresponds to the naturally ordered sequence of binary numbers, in the decimal system equal to 0, 1, 2, and 3.

With this order accepted, the ket-vector of an arbitrary pure state of this composite system,

$$|\alpha\rangle = a|\uparrow\uparrow\rangle + b|\uparrow\downarrow\rangle + c|\downarrow\uparrow\rangle + d|\downarrow\downarrow\rangle,$$

is represented by the column

$$\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix},$$

and the operator  $\hat{X}$  swapping the spin states,

$$\hat{X}|\alpha\rangle \equiv \hat{X}(a|\uparrow\uparrow\rangle + b|\uparrow\downarrow\rangle + c|\downarrow\uparrow\rangle + d|\downarrow\downarrow\rangle) = a|\uparrow\uparrow\rangle + b|\downarrow\uparrow\rangle + c|\uparrow\downarrow\rangle + d|\downarrow\downarrow\rangle,$$

should just swap the coefficients  $b$  and  $c$ , so its matrix  $X$ , in the accepted basis, should act as

$$X \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \begin{pmatrix} a \\ c \\ b \\ d \end{pmatrix}.$$

Evidently, this operation is achieved by the following 4×4 matrix:

$$X = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

**Problem 8.35.** Find a time-independent Hamiltonian that causes the qubit evolution described by Eqs. (8.155) of the lecture notes. Discuss the relation between your result and the time-dependent Hamiltonian (6.86).



*Solution:* In the lecture notes, Eqs. (8.155) were obtained as solutions of Eqs. (6.94), for the particular case of exact frequency tuning,  $\Delta = 0$ . In the notation of Sec. 8.5, they are

$$i\hbar\dot{a}_0 = Aa_1, \quad i\hbar\dot{a}_1 = A^*a_0. \quad (*)$$

They may be evidently interpreted as the set of two Schrödinger equations,

$$i\hbar\dot{a}_0 = H_{00}a_0 + H_{01}a_1, \quad i\hbar\dot{a}_1 = H_{10}a_0 + H_{11}a_1,$$

with the following matrix coefficients of an effective time-independent Hamiltonian (in the basis of the states 0 and 1):

$$H_{00} = H_{11} = 0, \\ H_{01} = A \equiv |A|e^{i\varphi} \equiv |A|(\cos\varphi + i\sin\varphi), \quad H_{10} = A^* \equiv |A|e^{-i\varphi} = |A|(\cos\varphi - i\sin\varphi).$$

Recalling the definition (4.105) of the Pauli matrices, we may represent this matrix as

$$\mathbf{H} \equiv \begin{pmatrix} H_{00} & H_{01} \\ H_{10} & H_{11} \end{pmatrix} = |A|\cos\varphi \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - |A|\sin\varphi \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \equiv |A|(\cos\varphi\sigma_x - \sin\varphi\sigma_y).$$

Hence, for the requested Hamiltonian operator itself, we may write the following expression (valid in any basis):

$$\hat{H} = |A|(\cos\varphi\hat{\sigma}_x - \sin\varphi\hat{\sigma}_y) \equiv \hat{\sigma}_x \operatorname{Re} A - \hat{\sigma}_y \operatorname{Im} A. \quad (**)$$

This expression may be interpreted as the result of time averaging of the product of the time-dependent Hamiltonian (6.86), whose perturbative treatment in Sec. 6.5 has led us to Eqs. (\*), by the factor  $\exp\{i\omega_0 t\}$  which compensates the re-definition (6.82) of the probability amplitudes. Let me hope that the reader remembers that such an averaging, as an alternative method of performing the rotating wave approximation (RWA) was repeatedly used in Chapter 7.

Note also that according to Eq. (4.163a), for a spin- $\frac{1}{2}$  particle with a non-zero gyromagnetic ratio  $\gamma$ , the Hamiltonian (\*\*) may be created by applying a time-independent magnetic field with its vector  $\mathcal{B}$  within the  $[x, y]$  plane, with the angle  $(-\varphi)$  between it and the  $x$ -axis.

## Chapter 9. Elements of Relativistic Quantum Mechanics

**Problem 9.1.** Prove the Casimir formula (see Eq. (9.23) of the lecture notes) by calculating the net force  $F = \mathcal{P}A$  exerted by the electromagnetic field, in its ground state, on two perfectly conducting parallel plates of area  $A$ , separated with a free-space gap of width  $t \ll A^{1/2}$ .

*Hint:* Calculate the field's energy in the gap's volume with and without the account of the plate effect, and then apply the Euler-Maclaurin formula<sup>73</sup> to the difference between these two results.

*Solution:* Let us calculate the electromagnetic energy in the volume  $At$  of the gap as a sum over all possible sinusoidal standing waves<sup>74</sup> with wave vectors  $\mathbf{k} = \{\mathbf{k}_\rho, k_z\}$ , where the  $z$ -axis is normal to the plates, and  $\rho \equiv \{x, y\}$  is the 2D radius vector in the plane of their surfaces:

$$E = 2 \sum_{\omega} \frac{\hbar\omega}{2} \equiv \hbar c \sum_{\mathbf{k}} |\mathbf{k}| = \hbar c \sum_{\mathbf{k}_\rho, k_z} (k_\rho^2 + k_z^2)^{1/2} \quad (*)$$

(where the front factor 2 is due to two different electromagnetic field modes, with orthogonal polarizations, for each wave vector  $\mathbf{k}$ ), with and without the effect of the plates. To avoid the high- $k$  divergence, we may cut both sums at the same, sufficiently large ( $k_{\max} \gg 1/t \gg 1/A^{1/2}$ ) value of  $k \equiv |\mathbf{k}|$  because the higher modes are not affected by the plates.

Thanks to the strong condition  $A^{1/2} \gg t$ , the in-plane wave vector quantization may be replaced with an integral, by using the electromagnetic-wave analog of Eq. (1.92) of the lecture notes:

$$\sum_{\mathbf{k}_\rho} (...) = \int_{n_x \geq 0} dn_x \int_{n_y \geq 0} dn_y (...) = \frac{a_x}{\pi} \int_{k_x \geq 0} dk_x \frac{a_y}{\pi} \int_{k_y \geq 0} dk_y (...) \equiv \frac{A}{\pi^2} \int_{k_x \geq 0} dk_x \int_{k_y \geq 0} dk_y (...). \quad (**)$$

On the other hand, the values of  $k_z$  are significantly limited to a discrete set,

$$k_z = \frac{\pi n}{t}, \quad \text{with } n = 0, 1, 2, \dots,$$

by the boundary conditions on the plate surfaces.<sup>75</sup> As a result, Eq. (\*) becomes

$$E = \frac{A\hbar c}{\pi^2} \sum'_{n \geq 0} \int_{k_x \geq 0} dk_x \int_{k_y \geq 0} dk_y \left[ k_\rho^2 + \left( \frac{\pi n}{t} \right)^2 \right]^{1/2},$$

where the symbol  $\sum'$  means that the term with  $n = 0$  is taken with the additional factor  $1/2$ , because for this special value of  $n$ , the boundary conditions allow only one wave polarization, with the electric field normal to the plate surfaces.

<sup>73</sup> See, e.g., MA Eq. (2.12).

<sup>74</sup> As implied by the discussion in Sec. 9.1 (but perhaps was not sufficiently emphasized there), the analogy between an electromagnetic field mode and that of the simple ("lumped") 1D harmonic oscillator is direct only for a standing (rather than traveling) wave.

<sup>75</sup> See, e.g., EM Eq. (7.196).

Now it is convenient to use the fact that the function under the integral is symmetric with respect to all Cartesian components of the wave vector, and extend the summation and integration to all (positive and negative) values of  $n$ ,  $k_x$ , and  $k_y$ , compensating this extension by an extra multiplier  $1/2^3 \equiv 1/8$ , and then make, in the double integral, the transfer from the Cartesian to the polar coordinates:

$$E = \frac{A\hbar c}{\pi^2} \frac{1}{8} \sum_n \int_{\mathbf{k}_\rho} \left[ k_\rho^2 + \left( \frac{\pi n}{t} \right)^2 \right]^{1/2} d^2 k_\rho = \frac{A\hbar c}{8\pi^2} \sum_n \int_{k_\rho \geq 0} \left[ k_\rho^2 + \left( \frac{\pi n}{t} \right)^2 \right]^{1/2} 2\pi k_\rho dk_\rho.$$

(Note that the exception for  $n = 0$  in the sum  $\sum$  is automatically absorbed into  $\sum$ , making it regular.) Since  $2k_\rho dk_\rho \equiv d(k_\rho^2) \equiv d[k_\rho^2 + (\pi n/t)^2]$ , the integration is elementary, giving

$$E = \frac{A\hbar c}{12\pi} \sum_n \left[ k_\rho^2 + \left( \frac{\pi n}{t} \right)^2 \right]^{3/2} \Big|_{k_\rho=0}^{k=k_{\max}} \equiv \frac{A\hbar c}{12\pi} \sum_{n=-n_{\max}}^{+n_{\max}} \left[ k_{\max}^3 - \left| \frac{\pi n}{t} \right|^3 \right],$$

where  $n_{\max} \equiv k_{\max} t / \pi \gg 1$ .

Now let us repeat the calculation for the same volume but disregarding the effect of the plates, so the summation over  $k_z$  may be replaced with the integration similar to that over  $k_x$  and  $k_y$ :

$$\sum_{k_z > 0} (\dots) = \frac{t}{\pi} \int_{k_z \geq 0} (\dots) dk_z = \frac{t}{2\pi} \int_{k_z} (\dots) dk_z,$$

where the last integration is in symmetric limits. The result is

$$E_0 = \hbar c \frac{A}{4\pi^2} \frac{t}{2\pi} \int_{k_z} dk_z (k_\rho^2 + k_z^2)^{3/2} \Big|_{k_\rho=0}^{k=k_{\max}} = \frac{A\hbar c}{12\pi} \frac{t}{\pi} \int_{-k_{\max}}^{+k_{\max}} (k_{\max}^3 - |k_z|^3) dk_z.$$

The difference between these two energy values, describing the effect of the conducting plates,

$$\Delta E \equiv E - E_0 = \frac{A\hbar c}{12\pi} \left[ \sum_{n=-n_{\max}}^{+n_{\max}} \left( k_{\max}^3 - \left| \frac{\pi n}{t} \right|^3 \right) - \frac{t}{\pi} \int_{-k_{\max}}^{+k_{\max}} (k_{\max}^3 - |k_z|^3) dk_z \right],$$

may be recast into a simpler form by introducing a continuous dimensionless variable  $\xi \equiv k_z t / \pi$ .

$$\Delta E \equiv E - E_0 = \frac{A\hbar c}{12\pi} \left[ \sum_{n=-n_{\max}}^{+n_{\max}} f(n) - \int_{-n_{\max}}^{+n_{\max}} f(\xi) d\xi \right], \quad \text{where } f(\xi) \equiv k_{\max}^3 - \left| \frac{\pi \xi}{t} \right|^3.$$

The expression in the square brackets may be evaluated using the Euler-Maclaurin formula. However, since the function  $f(\xi)$  is not infinitely differentiable (it has a “soft cusp” at  $\xi = 0$ ), we may apply that formula only separately to each of the two similar “wings” of the symmetric function  $f(\xi)$ , with  $-n_{\max} \leq \xi < 0$  and  $0 < \xi \leq n_{\max}$ . (At this separation, the term  $f(0)$  may be either delegated to one of the partial sums or, more logically, accounted for separately.) Summing up these three contributions, we get

$$\sum_{n=-n_{\max}}^{+n_{\max}} f(n) - \int_{-n_{\max}}^{+n_{\max}} f(\xi) d\xi = f(0) + 2 \cdot \left[ \sum_{n=1}^{n_{\max}} f(n) - \int_0^{n_{\max}} f(\xi) d\xi \right]$$

$$= f(0) + 2 \left\{ \frac{1}{2} [f(n_{\max}) - f(+0)] + \frac{1}{6} \cdot \frac{1}{2!} \left[ \frac{df}{d\xi}(n_{\max}) - \frac{df}{d\xi}(+0) \right] - \frac{1}{30} \cdot \frac{1}{4!} \left[ \frac{d^3 f}{d\xi^3}(n_{\max}) - \frac{d^3 f}{d\xi^3}(+0) \right] + \dots \right\}.$$

At  $\xi = n_{\max}$ , our function  $f(\xi)$  vanishes due to the definition of the parameter  $n_{\max}$ , while its derivatives at this point may be ignored because the mode summation cutoff at  $k_{\max}$  may be made smoothly spread over an interval  $\pi/t \ll \Delta k \ll k_{\max}$ , without a substantial effect on the calculation. As a result, using the derivatives,

$$\frac{df}{d\xi} = -3 \left( \frac{\pi}{t} \right)^3 \xi^2 \operatorname{sgn}(\xi), \quad \frac{d^3 f}{d\xi^3} = -6 \left( \frac{\pi}{t} \right)^3 \operatorname{sgn}(\xi), \quad \frac{d^n f}{d\xi^n} = 0 \quad \text{for } n > 3 \text{ and } \xi \neq 0,$$

we obtain the final result (which, as could be expected, is independent of the artificial cutoff  $k_{\max}$ ):

$$\sum_{n=-n_{\max}}^{+n_{\max}} f(n) - \int_{-n_{\max}}^{+n_{\max}} f(\xi) d\xi = -2 \cdot \frac{1}{30} \cdot \frac{1}{4!} \cdot 6 \left( \frac{\pi}{t} \right)^3, \quad \text{giving } \Delta E = -\frac{\pi^2 A \hbar c}{720 t^3}. \quad (***)$$

The result shows that the energy difference is negative, and its magnitude grows as  $t$  is decreased, i.e. the plates attract each other. The differentiation over  $t$ ,  $F = -\partial(\Delta E)/\partial t$ , immediately yields the Casimir formula (9.23):

$$F = -\frac{\pi^2 A \hbar c}{240 t^4}.$$

Note also that the numerical coefficient apart, Eq. (\*\*\*) is a great case for its derivation from dimensionality arguments, without solving the problem exactly. Indeed, since we are dealing with quantum mechanics of the electromagnetic field in free space, the final expression for the ratio  $\Delta E/A$  may only include the Planck constant  $\hbar$ , the free-space speed of light  $c$ , and the only significant geometric parameter of the problem,  $t$ . Now by writing the dimensionalities of these constants (correct in any system of units):

$$[\hbar] = \text{energy} \times \text{time}, \quad [c] = \frac{\text{length}}{\text{time}}, \quad [t] = \text{length},$$

we see that the only way they may be combined to give the correct dimensionality of the result,

$$\left[ \frac{\Delta E}{A} \right] = \frac{\text{energy}}{(\text{length})^2},$$

is in the fraction  $\hbar c/t^3$ . However, the reader should not think that all their hard work on the problem was “only” the calculation of the numerical factor before this fraction. A more important reward is that the solution yields a very clear physical picture of the Casimir effect, while the dimensionality-based “derivation” cannot bring this clarity.

**Problem 9.2.** Electromagnetic radiation of some single-mode quantum sources may have such a high degree of coherence that it is possible to observe the interference of waves from two independent sources with virtually the same frequency, incident on one detector.

- (i) Generalize Eq. (9.29) of the lecture notes to this case.

(ii) Use this generalized expression to show that incident waves in different Fock states do not create an interference pattern.

*Solutions:*

(i) Let us rewrite the second form of Eq. (9.29),

$$\Gamma \propto \langle \text{ini} | \hat{a}^\dagger \hat{a} | \text{ini} \rangle e^*(\mathbf{r})e(\mathbf{r}),$$

as follows:

$$\Gamma \propto \langle \text{ini}(\mathbf{r}) | \hat{a}^\dagger \hat{a} | \text{ini}(\mathbf{r}) \rangle, \quad \text{with } | \text{ini}(\mathbf{r}) \rangle \equiv | \mathbf{e}(\mathbf{r}) | \text{ini} \rangle, \quad \text{and } \langle \text{ini}(\mathbf{r}) | \equiv \langle \text{ini} | \mathbf{e}^*(\mathbf{r}). \quad (*)$$

A sum of two waves of the same frequency may be described by the ket-vector

$$| \text{ini}(\mathbf{r}) \rangle = | \text{ini}_1(\mathbf{r}) \rangle + | \text{ini}_2(\mathbf{r}) \rangle = \mathbf{e}_1(\mathbf{r}) | \text{ini}_1 \rangle + \mathbf{e}_2(\mathbf{r}) | \text{ini}_2 \rangle,$$

where each component wave is proportional to its own spatial distribution factor  $\mathbf{e}_j(\mathbf{r})$  and may be in its own quantum state. Plugging this expression, and the corresponding expression for the bra-vector, into the first of Eqs. (\*), and opening the parentheses, we may represent  $\Gamma$  as a sum of four terms including the following two terms describing the waves' interference:

$$\Gamma_{\text{int}} \propto \langle \text{ini}_1 | \hat{a}^\dagger \hat{a} | \text{ini}_2 \rangle \mathbf{e}_1^*(\mathbf{r}) \cdot \mathbf{e}_2(\mathbf{r}) + \text{c.c.} \quad (**)$$

For plane waves,  $\mathbf{e}_1(\mathbf{r}) \propto \exp\{i(\mathbf{k}_1 \cdot \mathbf{r} + \text{const}_1)\}$ ,  $\mathbf{e}_2(\mathbf{r}) \propto \exp\{i(\mathbf{k}_2 \cdot \mathbf{r} + \text{const}_2)\}$ , so the product  $\mathbf{e}_1^*(\mathbf{r}) \cdot \mathbf{e}_2(\mathbf{r})$  is proportional to  $\exp\{i\varphi_{12}\}$ , with  $\varphi_{12} = (\mathbf{k}_1 - \mathbf{k}_2) \cdot \mathbf{r} + \text{const}$ ; the same is approximately true for quasi-plane-wave situations – see Sec. 3.1. If the wave frequencies  $\omega$  are slightly different, the phase shift  $\varphi_{12}$  slowly drifts in time due to the difference between the two values of  $k = \omega/c$ , so the interference still can be measured if this is done relatively fast in order not to be averaged out.

(ii) Let the component waves be in some Fock states:

$$| \text{ini}_{1,2} \rangle = | n_{1,2} \rangle;$$

then the interference terms in Eq. (\*\*) are proportional to the following long bracket:

$$\langle n_1 | \hat{a}^\dagger \hat{a} | n_2 \rangle = \langle n_1 | \hat{N} | n_2 \rangle.$$

But the number operator  $\hat{N} \equiv \hat{a}^\dagger \hat{a}$  is diagonal in the stationary (Fock) state basis – see, e.g., Eq. (5.74) of the lecture notes. As a result, if the component waves are in different Fock states, with  $n_1 \neq n_2$ , then  $\Gamma_{\text{int}} = 0$ , i.e. the interference pattern disappears.

**Problem 9.3.** Calculate the zero-delay value  $g^{(2)}(0)$  of the second-order correlation function of a single-mode electromagnetic field in the so-called *cat state* (see Problem 7.4): a coherent superposition of two Glauber states with equal but sign-opposite parameters  $\alpha$  and a certain phase shift between them.

*Solution:* The initial state of this field may be represented by the following ket-vector:

$$| \text{cat} \rangle = C \left( | +\alpha \rangle + | -\alpha \rangle e^{i\varphi} \right),$$

where each ket  $|\alpha\rangle$  represents the Glauber state with the complex “shift parameter”  $\alpha$  that participates in the basic Eqs. (5.102) and (5.124) of the lecture notes. The normalization constant  $C$  may be found by requiring the superposition state to be normalized,  $\langle \text{cat} | \text{cat} \rangle = 1$  (just as the component states  $\pm\alpha$  are), giving the following equation:

$$|C|^2 \left( \langle +\alpha | + e^{-i\varphi} \langle -\alpha | \right) \left( |+\alpha\rangle + |-\alpha\rangle e^{i\varphi} \right) = 1.$$

Opening the parentheses, we get

$$|C|^2 = \frac{1}{1 + 1 + \langle +\alpha | -\alpha \rangle e^{i\varphi} + \langle -\alpha | +\alpha \rangle e^{-i\varphi}}.$$

The inner products participating in this expression may be calculated, for example, by using the Fock-state expansions (5.134) of the Glauber states:<sup>76</sup>

$$|+\alpha\rangle = \exp\left\{-\frac{|\alpha|^2}{2}\right\} \sum_{n=0}^{\infty} \frac{(+\alpha)^n}{(n!)^{1/2}} |n\rangle, \quad |-\alpha\rangle = \exp\left\{-\frac{|-\alpha|^2}{2}\right\} \sum_{n=0}^{\infty} \frac{(-\alpha)^n}{(n!)^{1/2}} |n\rangle,$$

giving

$$\langle +\alpha | -\alpha \rangle = \langle -\alpha | +\alpha \rangle = \exp\{-|\alpha|^2\} \sum_{n=0}^{\infty} \frac{(-\alpha\alpha^*)^n}{n!} = \exp\{-2|\alpha|^2\}, \quad (*)$$

so

$$|C|^2 = \frac{1}{2 + 2 \exp\{-2|\alpha|^2\} \cos\varphi}. \quad (**)$$

(For the particular case  $\varphi = 0$ , this result was already obtained in the solution of Problem 7.4.)

Now we can use the basic Eq. (5.124) and its bra-vector counterpart,

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle, \quad \langle\alpha|\hat{a}^\dagger = \alpha^*\langle\alpha|,$$

to calculate the numerator of the ratio (9.35), at the final steps of the calculation using Eqs. (\*) and (\*\*) again:

$$\begin{aligned} \langle \hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a} \rangle_{\text{cat}} &\equiv \langle \text{cat} | \hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a} | \text{cat} \rangle = |C|^2 \left( \langle +\alpha | + \langle -\alpha | e^{-i\varphi} \right) \hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a} \left( |+\alpha\rangle + |-\alpha\rangle e^{i\varphi} \right) \\ &\equiv |C|^2 \times \left( \begin{aligned} &\langle +\alpha | \hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a} | +\alpha \rangle + \langle -\alpha | \hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a} | -\alpha \rangle \\ &+ \langle +\alpha | \hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a} | -\alpha \rangle e^{i\varphi} + \langle -\alpha | \hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a} | +\alpha \rangle e^{-i\varphi} \end{aligned} \right) \\ &= |C|^2 \left( \begin{aligned} &\alpha^* \alpha^* \alpha \alpha + (-\alpha)^* (-\alpha)^* (-\alpha)(-\alpha) \\ &+ \alpha^* \alpha^* (-\alpha)(-\alpha) e^{i\varphi} + (-\alpha)^* (-\alpha)^* \alpha \alpha e^{-i\varphi} \langle -\alpha | +\alpha \rangle \end{aligned} \right) \\ &= |C|^2 |\alpha|^4 \left( 2 + 2 \exp\{-2|\alpha|^2\} \cos\varphi \right) = |\alpha|^4. \end{aligned}$$

The inner product in its denominator may be calculated similarly:

<sup>76</sup> Another way to get the same final result for  $C$  is to use the coordinate representation (5.107) of the Glauber state.

$$\begin{aligned}
\langle \hat{a}^\dagger \hat{a} \rangle_{\text{cat}} &= \langle \text{cat} | \hat{a}^\dagger \hat{a} | \text{cat} \rangle = |C|^2 \left( \langle +\alpha | + e^{-i\varphi} \langle -\alpha | \right) \hat{a}^\dagger \hat{a} \left( |+\alpha\rangle + |-\alpha\rangle e^{i\varphi} \right) \\
&\equiv |C|^2 \left( \langle +\alpha | \hat{a}^\dagger \hat{a} | +\alpha \rangle + \langle -\alpha | \hat{a}^\dagger \hat{a} | -\alpha \rangle + \right. \\
&\quad \left. \langle +\alpha | \hat{a}^\dagger \hat{a} | -\alpha \rangle e^{i\varphi} + \langle -\alpha | \hat{a}^\dagger \hat{a} | +\alpha \rangle e^{-i\varphi} \langle +\alpha | -\alpha \rangle \right) \\
&= |C|^2 \left( \alpha^* \alpha + (-\alpha)^* (-\alpha) + \alpha^* (-\alpha) e^{i\varphi} \langle +\alpha | -\alpha \rangle \right. \\
&\quad \left. + (-\alpha)^* \alpha e^{-i\varphi} \langle -\alpha | +\alpha \rangle \right) \\
&= |C|^2 |\alpha|^2 \left( 2 - 2 \exp\{-2|\alpha|^2\} \cos \varphi \right) = |\alpha|^2 \frac{1 - \exp\{-2|\alpha|^2\} \cos \varphi}{1 + \exp\{-2|\alpha|^2\} \cos \varphi},
\end{aligned}$$

so, finally,

$$g^{(2)}(0) = \frac{\langle \hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a} \rangle}{\langle \hat{a}^\dagger \hat{a} \rangle^2} = \left( \frac{1 + \exp\{-2|\alpha|^2\} \cos \varphi}{1 - \exp\{-2|\alpha|^2\} \cos \varphi} \right)^2.$$

The result shows that the second-order correlation function is the largest at  $\varphi = 0$ ,

$$\max_{\varphi} g^{(2)}(0) = \left( \frac{1 + \exp\{-2|\alpha|^2\}}{1 - \exp\{-2|\alpha|^2\}} \right)^2 \equiv \coth^2(|\alpha|^2), \quad (***)$$

is always larger than 1, and may be much larger than 2.<sup>77</sup> Such *super-bunching*, with  $g^{(2)}(0) > 2$ , may be obtained with other field states as well – see the next problem.

**Problem 9.4.** Calculate the zero-delay value  $g^{(2)}(0)$  of the second-order correlation function of a single-mode electromagnetic field in the squeezed ground state  $\zeta$  defined by Eq. (5.142) of the lecture notes.

*Solution:* Let us reuse the important intermediate result,

$$\hat{b} \hat{b}^\dagger = \hat{b}^\dagger \hat{b} + \hat{I}, \quad (*)$$

obtained in the model solution of Problem 5.22 for the squeezing operators  $\hat{b}^\dagger$  and  $\hat{b}$ . These operators are defined by Eq. (5.144), which may be rewritten as

$$\hat{a} = \mu \hat{b} - \nu \hat{b}^\dagger, \quad \hat{a}^\dagger = \mu \hat{b}^\dagger - \nu^* \hat{b},$$

where  $\mu$  and  $\nu$  are the  $c$ -number squeezing parameters:

$$\mu \equiv \cosh r, \quad \nu \equiv e^{i\theta} \sinh r.$$

As was discussed in the same solution, the squeezed ground state is an eigenstate of the operator  $\hat{b}$ , with zero eigenvalue:

<sup>77</sup> The result (\*\*\*) even tends to infinity at  $\alpha \rightarrow 0$ , but we should remember that if  $\alpha = 0$  exactly, the field is in its ground state, and according to Eq. (9.29) with  $n = 0$ , there are no photon counts at all to speak about.

$$\hat{b}|\zeta\rangle = 0, \quad \langle\zeta|\hat{b}^\dagger = 0, \quad (**)$$

and is normalized:

$$\langle\zeta|\zeta\rangle = 1.$$

The average participating in the denominator of (9.35) for the requested value

$$g^{(2)}(0) = \frac{\langle\hat{a}^\dagger\hat{a}^\dagger\hat{a}\hat{a}\rangle}{\langle\hat{a}^\dagger\hat{a}\rangle^2},$$

was already calculated in the model solution of Problem 5.23:

$$\langle\hat{a}^\dagger\hat{a}\rangle \equiv \langle\zeta|\hat{a}^\dagger\hat{a}|\zeta\rangle = \nu\nu^* \equiv \sinh^2 r,$$

so we only need to calculate the expectation value in the numerator of that fraction:

$$\begin{aligned} \langle\hat{a}^\dagger\hat{a}^\dagger\hat{a}\hat{a}\rangle &\equiv \langle\zeta|\hat{a}^\dagger\hat{a}^\dagger\hat{a}\hat{a}|\zeta\rangle = \langle\zeta|\left(\mu\hat{b}^\dagger - \nu^*\hat{b}\right)^2\left(\mu\hat{b} - \nu\hat{b}^\dagger\right)^2|\zeta\rangle \\ &= \langle\zeta|\left[\mu^2\hat{b}^\dagger\hat{b}^\dagger + (\nu^*)^2\hat{b}\hat{b} - \mu\nu^*(\hat{b}^\dagger\hat{b} + \hat{b}\hat{b}^\dagger)\right]\left[\mu^2\hat{b}\hat{b} + \nu^2\hat{b}^\dagger\hat{b}^\dagger - \mu\nu(\hat{b}^\dagger\hat{b} + \hat{b}\hat{b}^\dagger)\right]|\zeta\rangle. \end{aligned}$$

The multiplication of the square brackets gives 16 operator-product terms but due to Eqs. (\*\*), we may immediately discard those with the operator products either starting with  $\hat{b}^\dagger$ , or ending with  $\hat{b}$ , or both – because, acting on the state  $\zeta$ , they would give null states. The remaining four terms give

$$\begin{aligned} \langle\hat{a}^\dagger\hat{a}^\dagger\hat{a}\hat{a}\rangle &= \mu^2\nu\nu^*\langle\zeta|\hat{b}\hat{b}^\dagger\hat{b}\hat{b}^\dagger|\zeta\rangle + \nu^2(\nu^*)^2\langle\zeta|\hat{b}\hat{b}\hat{b}^\dagger\hat{b}^\dagger|\zeta\rangle \\ &\quad - \mu\nu^2\nu^*\langle\zeta|\hat{b}\hat{b}^\dagger\hat{b}^\dagger\hat{b}|\zeta\rangle - \mu\nu(\nu^*)^2\langle\zeta|\hat{b}\hat{b}\hat{b}^\dagger|\zeta\rangle. \end{aligned}$$

Let us calculate each of the averages by applying the commutation relation (\*). It makes sense to start with calculating an auxiliary two-operator product:<sup>78</sup>

$$\langle\zeta|\hat{b}\hat{b}^\dagger|\zeta\rangle = \langle\zeta|\left(\hat{b}^\dagger\hat{b} + \hat{I}\right)|\zeta\rangle \equiv \langle\zeta|\hat{b}^\dagger\hat{b}|\zeta\rangle + \langle\zeta|\hat{I}|\zeta\rangle = 0 + 1 \equiv 1,$$

and then use this result, together with Eqs. (\*\*), to calculate the four-operator averages one by one:

$$\begin{aligned} \langle\zeta|\hat{b}\hat{b}^\dagger\hat{b}\hat{b}^\dagger|\zeta\rangle &\equiv \langle\zeta|\hat{b}\hat{b}^\dagger\left(\hat{b}\hat{b}^\dagger\right)|\zeta\rangle = \langle\zeta|\hat{b}\hat{b}^\dagger\left(\hat{b}^\dagger\hat{b} + \hat{I}\right)|\zeta\rangle \\ &\equiv \langle\zeta|\hat{b}\hat{b}^\dagger\hat{b}^\dagger\hat{b}|\zeta\rangle + \langle\zeta|\hat{b}\hat{b}^\dagger|\zeta\rangle = 0 + 1 \equiv 1, \\ \langle\zeta|\hat{b}\hat{b}\hat{b}^\dagger\hat{b}^\dagger|\zeta\rangle &\equiv \langle\zeta|\hat{b}\left(\hat{b}\hat{b}^\dagger\right)\hat{b}^\dagger|\zeta\rangle = \langle\zeta|\hat{b}\left(\hat{b}^\dagger\hat{b} + \hat{I}\right)\hat{b}^\dagger|\zeta\rangle \\ &\equiv \langle\zeta|\hat{b}\hat{b}^\dagger\hat{b}\hat{b}^\dagger|\zeta\rangle + \langle\zeta|\hat{b}\hat{b}^\dagger|\zeta\rangle = 1 + 1 \equiv 2, \end{aligned}$$

<sup>78</sup> Actually, it was also calculated in the model solution of Problem 5.23.



$$\begin{aligned}
\langle \zeta | \hat{b} \hat{b}^\dagger \hat{b}^\dagger \hat{b}^\dagger | \zeta \rangle &\equiv \langle \zeta | \left( \hat{b} \hat{b}^\dagger \right) \hat{b}^\dagger \hat{b}^\dagger | \zeta \rangle = \langle \zeta | \left( \hat{b}^\dagger \hat{b} + \hat{I} \right) \hat{b}^\dagger \hat{b}^\dagger | \zeta \rangle \\
&\equiv \langle \zeta | \hat{b}^\dagger \hat{b} \hat{b}^\dagger \hat{b}^\dagger | \zeta \rangle + \langle \zeta | \hat{b}^\dagger \hat{b}^\dagger | \zeta \rangle = 0 + 0 \equiv 0, \\
\langle \zeta | \hat{b} \hat{b} \hat{b} \hat{b}^\dagger | \zeta \rangle &\equiv \langle \zeta | \hat{b} \hat{b} \left( \hat{b} \hat{b}^\dagger \right) | \zeta \rangle = \langle \zeta | \hat{b} \hat{b} \left( \hat{b}^\dagger \hat{b} + \hat{I} \right) | \zeta \rangle \\
&\equiv \langle \zeta | \hat{b} \hat{b} \hat{b}^\dagger \hat{b} | \zeta \rangle + \langle \zeta | \hat{b} \hat{b} | \zeta \rangle = 0 + 0 \equiv 0.
\end{aligned}$$

Thus, we finally have

$$\langle \hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a} \rangle = \mu^2 \nu \nu^* + 2\nu^2 (\nu^*)^2 \equiv \cosh^2 r \sinh^2 r + 2 \sinh^4 r,$$

so

$$g^{(2)}(0) = \frac{\langle \hat{a}^\dagger \hat{a}^\dagger \hat{a} \hat{a} \rangle}{\langle \hat{a}^\dagger \hat{a} \rangle^2} = \frac{\cosh^2 r \sinh^2 r + 2 \sinh^4 r}{(\sinh^2 r)^2} \equiv \coth^2 r + 2. \quad (***)$$

Since  $\coth^2 r$  of the real argument  $r \equiv |\zeta|$  is always larger than 1, our result shows that  $g^{(2)}(0) \geq 3$ , indicating the super-bunching effect mentioned at the end of Sec. 9.2 of the lecture notes and in the previous problem.<sup>79</sup> Note that, paradoxically, at  $r \rightarrow 0$ , the result (\*\*\*) does not tend to Eq. (9.37),  $g^{(2)}(0) = 1$ , for the Glauber state, i.e. in the absence of squeezing. However, there is no actual contradiction here, because at  $r = 0$  and  $\alpha = 0$ , both results yield an uncertainty due to the vanishing denominator, physically corresponding to the absence of photon counts from the field in the usual ground state.

**Problem 9.5.** Calculate the rate of spontaneous photon emission (into unrestricted free space) by a hydrogen atom, initially in the  $2p$  state ( $n = 2, l = 1$ ) with  $m = 0$ . Would the result be different for  $m = \pm 1$ ? for the  $2s$  state ( $n = 2, l = 0, m = 0$ )? Discuss the relation between these quantum-mechanical results and those given by the classical theory of radiation for the simplest classical model of the atom.

*Solution:* For this single-particle system, we may use the general formula (9.53) of the lecture notes, for the electric-dipole radiation into free space, with  $\mathbf{d} = -e\mathbf{r}$ :

$$\Gamma_s = \frac{1}{4\pi\epsilon_0} \frac{4\omega^3}{3\hbar c^3} \langle \text{fin} | \hat{\mathbf{d}} | \text{ini} \rangle \cdot \langle \text{ini} | \hat{\mathbf{d}} | \text{fin} \rangle^* = \frac{e^2}{4\pi\epsilon_0} \frac{4\omega^3}{3\hbar c^3} \langle \text{fin} | \hat{\mathbf{r}} | \text{ini} \rangle \cdot \langle \text{ini} | \hat{\mathbf{r}} | \text{fin} \rangle^*,$$

in the first case, with  $\langle \text{fin} | \equiv \langle n, l, m |_{\text{fin}} = \langle 1, 0, 0 |$  and  $| \text{ini} \rangle \equiv | n, l, m \rangle_{\text{ini}} = | 2, 1, 0 \rangle$ . Due to the axial symmetry of these two states, the only non-zero contribution to the matrix element of the radius vector's operator is provided by its  $z$ -component:

$$\begin{aligned}
\langle 2, 1, 0 | \hat{z} | 1, 0, 0 \rangle &= \langle 2, 1, 0 | r \cos \theta | 1, 0, 0 \rangle = \\
&= \int_0^{2\pi} d\varphi \int_0^\pi \sin \theta d\theta \int_0^\infty r^2 dr \times \mathcal{R}_{1,0}(r) Y_0^0(\theta, \varphi) \times r \cos \theta \times \mathcal{R}_{2,1}(r) Y_1^0(\theta, \varphi).
\end{aligned}$$

This matrix element was already calculated in the solution of Problem 6.20:

<sup>79</sup> For recent experimental observations of super-bunching see, e.g., Y. Bromberg *et al.*, *Nature Photonics* **4**, 721 (2010), and references therein.

$$\langle 2,1,0 | r \cos \theta | 1,0,0 \rangle = \frac{2^{15/2}}{3^5} r_B,$$

so, finally,

$$\Gamma_s = \frac{e^2}{4\pi\epsilon_0} \frac{2^{15}}{3^{10}} \frac{4\omega^3 r_B^2}{3\hbar c^3}. \quad (*)$$

Now we may plug into this result the expressions for the Bohr radius  $r_B$  (see Eq. (1.10) of the lecture notes), and the radiation frequency, following from Eqs. (1.12)-(1.13):

$$\omega = \frac{E_{\text{ini}} - E_{\text{fin}}}{\hbar} = \frac{E_H}{2\hbar} \left( -\frac{1}{2^2} + \frac{1}{1^2} \right) \equiv \frac{3E_H}{8\hbar} = \frac{3}{8} \frac{m_e}{\hbar^3} \left( \frac{e^2}{4\pi\epsilon_0} \right)^2,$$

and get Eq. (\*) in a form more convenient for evaluation:

$$\frac{\Gamma_s}{\omega} = \frac{2^{11}}{3^9} \alpha^3 \approx 0.104 \alpha^3,$$

thus confirming the estimate (9.54). Numerically,  $\omega \approx 1.6 \times 10^{16} \text{ s}^{-1}$ ,  $\Gamma_s \approx 6.3 \times 10^8 \text{ s}^{-1}$ , so the relative half-width of the spectral line  $\Gamma_s/\omega \approx 4 \times 10^{-8} \ll 1$ .

Superficially, it may look like for other  $2p$  initial states, with  $m = \pm 1$ , the rate vanishes because the initial function under the matrix element integral is now proportional to  $\exp\{\pm im\varphi\}$ , and the integral over the azimuthal angle equals zero. However, this is only true for the  $z$ -component of the dipole moment operator; for two other components, the solid-angle integral becomes

$$\begin{aligned} & \int_0^{2\pi} d\varphi \int_0^\pi \sin \theta d\theta Y_0^0(\theta, \varphi) (\mathbf{n}_x \cos \varphi + \mathbf{n}_y \sin \varphi) Y_1^{\pm 1}(\theta, \varphi) \\ &= \mp \left( \frac{3}{2} \right)^{1/2} \frac{1}{4\pi} \int_0^{2\pi} (\mathbf{n}_x \cos \varphi + \mathbf{n}_y \sin \varphi) e^{\pm i\varphi} d\varphi \int_0^\pi \sin \theta d\theta = \mp \left( \frac{3}{2} \right)^{1/2} \frac{1}{2} (\mathbf{n}_x \pm i\mathbf{n}_y), \end{aligned}$$

so

$$|\langle 2,1,\pm 1 | \mathbf{r} | 1,0,0 \rangle|^2 = |\langle 2,1,\pm 1 | (\mathbf{n}_x x + \mathbf{n}_y y) | 1,0,0 \rangle|^2 = \left( \frac{2^{15/2}}{3^5} r_B \right)^2 \frac{1}{2} |\mathbf{n}_x \pm i\mathbf{n}_y|^2 = \left( \frac{2^{15/2}}{3^5} r_B \right)^2,$$

i.e. exactly the same result as for  $m = 0$ . In hindsight, this is very natural, because the wavefunctions of all three  $2p$  states with different  $m$  are similar, besides their spatial orientation – see, e.g., the second row of Fig. 3.20 of the lecture notes.

On the other hand, for the initial  $2s$  state, the initial and final wavefunctions are both independent of  $\theta$  and  $\varphi$ ; hence all Cartesian components of the solid-angle integral of the product  $\psi_f^* \mathbf{r} \psi_i$  are equal to zero, so the electric dipole transition rate vanishes. This zero result is a particular manifestation of the orbital selection rules (mentioned in Sec. 5.6 of the lecture notes, and proved in the model solution of Problem 5.41): in the absence of spin effects, the electric dipole transitions are possible only if  $\Delta l \equiv l_{\text{ini}} - l_{\text{fin}} = \pm 1$ .

In order to compare Eq. (\*) with the classical theory of radiation, let us take into account that due to the general exponential decay law (see, e.g., Eqs. (2.151) or (6.114) of the lecture notes), the ensemble-averaged radiation power of an atom, immediately after its definite placement into the initial state, is

$$\langle \mathcal{P}_Q \rangle = \hbar \omega \Gamma_s.$$

Using Eq. (\*), this power at the  $2p \rightarrow 1s$  transition may be represented as

$$\langle \mathcal{P}_Q \rangle = \frac{2^{14}}{3^9} \frac{e^2}{4\pi\epsilon_0} \frac{\omega^4 r_B^2}{3c^3} \approx 0.83 \frac{e^2}{4\pi\epsilon_0} \frac{\omega^4 r_B^2}{3c^3}.$$

This quantum-mechanical result may be compared with the following classical result for the power radiated by a charge  $q = -e$  moving, with the angular velocity  $\omega$ , around a circle of radius  $R$ :<sup>80</sup>

$$\mathcal{P}_C = 2 \frac{e^2}{4\pi\epsilon_0} \frac{\omega^4 R^2}{3c^3}.$$

The comparison of the two formulas shows that the quantum and classical expressions are close if we parallel  $R$  and  $r_B$ .<sup>81</sup> However, not only the numerical coefficients but (more importantly) the very spirit of these results are very much different. The classical theory depends only on the initial, but not on the final state (and hence there are no selection rules), does not have a good analog of the most important  $s$ -states (with  $l = 0$ ), and even more importantly, does not have the fundamental notion of the ground state with a non-zero spatial extension – which produces no spontaneous radiation at all. Still, it may be shown that the quantum-mechanical results approach the classical ones for transitions between the so-called *Rydberg states*, with  $n \gg 1$  and hence with  $\langle r \rangle \gg r_B$ .

**Problem 9.6.** An electron has been placed on the lowest excited level of a spherically symmetric, quadratic potential well  $U(\mathbf{r}) = m_e \omega^2 r^2 / 2$ . Calculate the rate of its relaxation to the ground state, with the emission of a photon (into unrestricted free space). Compare the rate with that for a similar transition of the hydrogen atom, for the case when the radiation frequencies of these two systems are equal.

*Solution:* Just like in the previous problem, the spontaneous photon emission rate of this single-particle system, due to its electric dipole moment  $\mathbf{d} = q\mathbf{r}$ , may be calculated as

$$\Gamma_s = \frac{e^2}{4\pi\epsilon_0} \frac{4\omega^3}{3\hbar c^3} \langle \text{fin} | \hat{\mathbf{r}} | \text{ini} \rangle \cdot \langle \text{ini} | \hat{\mathbf{r}} | \text{fin} \rangle^*, \quad (*)$$

so the problem is reduced to the calculation of the proper matrix element for the isotropic 3D harmonic oscillator. As was discussed in Sec. 3.5 of the lecture notes, and in the model solution of Problem 3.27, its eigenfunctions may be represented either in the spherical-coordinate form or the Cartesian form. In the latter representation (which is a bit easier for calculations) the final, ground-state wavefunction is a product of similar 1D functions:

$$\psi_{\text{fin}}(\mathbf{r}) = \psi_0(x)\psi_0(y)\psi_0(z),$$

<sup>80</sup> This expression follows from the well-known Larmor formula for radiation at 1D motion (see, e.g., EM Eq. (8.29) for the free space, in which  $Z = Z_0 = 1/\epsilon_0 c$  and  $v = c$ ), with the extra factor of 2, due to the radiation by two non-zero oscillating Cartesian components of the rotating electric dipole moment – see the model solution of EM Problem 8.1.

<sup>81</sup> In the view of the original Bohr's theory, and the exact relations (3.210)-(3.211), this is a reasonable (though an approximate) estimate.

while the excited energy level is triple-degenerate, with wavefunctions of the type

$$\psi_{\text{ini}}(\mathbf{r}) = \psi_1(x)\psi_0(y)\psi_0(z),$$

with two other eigenfunctions different only by the argument swaps – and hence giving the same radiation rate. (Here  $\psi_0$  and  $\psi_1$  describe, respectively, the ground state and the first excited state of the 1D oscillator.) Hence the matrix element participating in Eq. (\*) may be calculated as

$$\begin{aligned} \langle \text{ini} | \hat{\mathbf{r}} | \text{fin} \rangle &\equiv \langle \text{ini} | \mathbf{n}_x \hat{x} + \mathbf{n}_y \hat{y} + \mathbf{n}_z \hat{z} | \text{fin} \rangle \\ &= \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \int_{-\infty}^{+\infty} dz \psi_1^*(x)\psi_0^*(y)\psi_0^*(z) (\mathbf{n}_x x + \mathbf{n}_y y + \mathbf{n}_z z) \psi_0(x)\psi_0(y)\psi_0(z). \end{aligned} \quad (**)$$

Since  $\psi_0$  is an even function, while  $\psi_1$  is an odd function of their arguments (see, e.g., Eq. (2.284) and/or Fig. 2.35 of the lecture notes), only the first one of the resulting three 1D integrals does not vanish, giving

$$\langle \text{ini} | \hat{\mathbf{r}} | \text{fin} \rangle = \mathbf{n}_x \int_{-\infty}^{+\infty} \psi_1^*(x)x\psi_0(x)dx \int_{-\infty}^{+\infty} \psi_0^*(y)\psi_0(y)dy \int_{-\infty}^{+\infty} \psi_0^*(z)\psi_0(z)dz.$$

Since Eq. (\*) assumes that all participating wavefunctions are normalized, each of the two last integrals equals 1, while the first one, by definition, is the matrix element  $x_{10}$ . According to Eq. (5.92), with  $n' = 1$  and  $n = 0$ , for our system (with  $\omega_0 = \omega$  and  $m = m_e$ ) it is equal to  $(\hbar/2m_e\omega)^{1/2}$ . As a result, we get

$$\Gamma_s = \frac{e^2}{4\pi\epsilon_0} \frac{4\omega^3}{3\hbar c^3} \times \frac{\hbar}{2m_e\omega}.$$

According to Eq. (5.95), the last fraction is just the ground-state expectation value of  $x^2$ , so comparing this result with the solution of the previous problem, we get a physically transparent result:

$$\frac{(\Gamma_s)_{\text{oscillator}}}{(\Gamma_s)_{\text{H atom}}} = \frac{3^{10} \langle x^2 \rangle_g}{2^{15} r_B^2}.$$

Since the difference between the adjacent energy levels of a harmonic oscillator is  $\hbar\omega$ , its radiation frequency is just  $\omega$ , so for the matching of its value with that of the hydrogen atom's radiation (at the  $n = 2$  to  $n = 1$  transition),

$$\omega = \frac{E_H}{\hbar} \left[ \left( -\frac{1}{2 \cdot 2^2} \right) - \left( -\frac{1}{2} \right) \right] = \frac{3}{8} \frac{E_H}{\hbar} \equiv \frac{3}{8} \frac{\hbar}{m_e r_B^2},$$

we get

$$\langle x^2 \rangle_g = \frac{\hbar}{2m_e\omega} = \frac{\hbar}{2m_e} \bigg/ \frac{3}{8} \frac{\hbar}{m_e r_B^2} = \frac{4}{3} r_B^2, \quad \text{so} \quad \frac{(\Gamma_s)_{\text{oscillator}}}{(\Gamma_s)_{\text{H atom}}} = \frac{3^{10}}{2^{15}} \frac{4}{3} \equiv \frac{3^9}{2^{13}} \approx 2.403 > 1.$$

This result is natural because, in the hydrogen atom, the wavefunctions are more pressed to the center by the rapidly diverging Coulomb potential  $U(r) \propto -1/r$ , and hence provide a smaller dipole moment  $d$ , for the same frequency.

**Problem 9.7.** Derive an analog of Eq. (9.53) for the spontaneous photon emission (into free space) due to a change of the *magnetic* dipole moment  $\mathbf{m}$  of a small-size system.

*Solution:* The derivation is straightforward due to the similarity between the Hamiltonians describing the interaction of the electric and magnetic dipole moments of a small system with the corresponding electromagnetic field components:

$$\hat{H}_{\text{electric}} = -\hat{\mathcal{E}} \cdot \hat{\mathbf{d}}, \quad \hat{H}_{\text{magnetic}} = -\hat{\mathcal{B}} \cdot \hat{\mathbf{m}},$$

and of the expressions of the field operators via the photon creation/annihilation operators – see Eqs. (9.16) of the lecture notes:

$$\hat{\mathcal{E}}(\mathbf{r}, t) = i \sum_j \left( \frac{\hbar \omega_j}{2} \right)^{1/2} \mathbf{e}_j(\mathbf{r}) \left( \hat{a}_j^\dagger - \hat{a}_j \right), \quad \hat{\mathcal{B}}(\mathbf{r}, t) = \sum_j \left( \frac{\hbar \omega_j}{2} \right)^{1/2} \mathbf{b}_j(\mathbf{r}) \left( \hat{a}_j^\dagger + \hat{a}_j \right).$$

(As a reminder, the *c*-number vector functions  $\mathbf{e}_j(\mathbf{r})$  and  $\mathbf{b}_j(\mathbf{r})$ , describing the spatial distribution of the electric and magnetic fields in the  $j^{\text{th}}$  mode, are similarly normalized,

$$\int e_j^2(\mathbf{r}) d^3r = \frac{1}{\epsilon_0}, \quad \int b_j^2(\mathbf{r}) d^3r = \mu_0,$$

so they similarly drop out at the averaging over free-space modes,<sup>82</sup> besides the replacement of  $1/\epsilon_0$  in the electric field case with  $\mu_0$  in the magnetic field case.) As a result, reproducing the calculations carried out in Secs. 9.2-9.3 for the electric dipole case, we get

$$\Gamma_{\text{magnetic}} = \frac{\mu_0}{4\pi} \frac{4\omega^3}{3\hbar c^3} \left| \langle \text{fin} | \hat{\mathbf{m}} | \text{ini} \rangle \right|^2.$$

Due to the identity  $\mu_0 \equiv 1/\epsilon_0 c^2$ , this relation may be rewritten as

$$\Gamma_{\text{magnetic}} = \frac{1}{4\pi\epsilon_0} \frac{4\omega^3}{3\hbar c^3} \frac{1}{c^2} \left| \langle \text{fin} | \hat{\mathbf{m}} | \text{ini} \rangle \right|^2. \quad (*)$$

Its comparison with Eq. (9.53) of the lecture notes,

$$\Gamma_{\text{electric}} = \frac{1}{4\pi\epsilon_0} \frac{4\omega^3}{3\hbar c^3} \left| \langle \text{fin} | \hat{\mathbf{d}} | \text{ini} \rangle \right|^2, \quad (**)$$

shows that their relation parallels that between the classical expressions for the intensity of the electric-dipole and magnetic-dipole radiation, with an extra factor  $c^2$  in the denominator in the latter case.<sup>83</sup> Due to this factor, for an orbital motion of a charged particle with velocity  $v \ll c$ , its magnetic-dipole radiation power is of the order of  $\sim (v/c)^2$  of the electric-dipole one. This weakness is the justification for the focus on the latter radiation in Sec. 9.3 of the lecture notes; however, if a system does not change its electric dipole moment at a quantum transition, its magnetic-dipole radiation may be important – see, e.g., the next problem.

<sup>82</sup> This is not true for electromagnetic cavities, where the exact position of the emitting particle in the standing wave field may play an important role, in particular affecting the coupling constant  $\kappa$  – see Sec. 9.4 of the lecture notes and also Problem 11 below.

<sup>83</sup> See, e.g., EM Eqs. (8.26) and (8.139).

**Problem 9.8.** A spin- $1/2$  particle with a gyromagnetic ratio  $\gamma$  is in its orbital ground state in a static magnetic field  $\mathcal{B}_0$ . Calculate the rate of its spontaneous transition from the higher to the lower spin energy level, with the emission of a photon into unrestricted free space. Evaluate this rate for an electron in a field of 10 T, and discuss the implications of this result for laboratory experiments with electron spins.

*Solution:* Since the particle remains in the same (ground) orbital state, its electromagnetic radiation at such quantum transition may be only due to the flip of its magnetic dipole moment  $\mathbf{m} = \gamma\mathbf{S}$ , with the emission of a photon with the frequency<sup>84</sup>

$$\omega = \frac{|E_{\uparrow} - E_{\downarrow}|}{\hbar} = \frac{2|\mathbf{m} \cdot \mathcal{B}_0|}{\hbar} = \frac{2|\gamma\mathbf{S} \cdot \mathcal{B}_0|}{\hbar} = |\gamma\boldsymbol{\sigma} \cdot \mathcal{B}_0| = |\gamma| \mathcal{B}_0.$$

Hence we may use the result of the previous problem for the rate of such spontaneous transition:

$$\Gamma_{\text{magnetic}} = \frac{1}{4\pi\epsilon_0} \frac{4\omega^3}{3\hbar c^3} \frac{1}{c^2} \left| \langle \text{fin} | \hat{\mathbf{m}} | \text{ini} \rangle \right|^2.$$

In order to evaluate the matrix element participating in this formula, we may use the standard spin  $z$ -basis, with the axis  $z$  directed along the magnetic field. In this case, for  $\gamma > 0$ , the initial spin state (with the higher energy) is  $\downarrow$ , and the final one is  $\uparrow$ , i.e.

$$\begin{aligned} \langle \text{fin} | \hat{\mathbf{m}} | \text{ini} \rangle &= \langle \uparrow | \hat{\mathbf{m}} | \downarrow \rangle = \gamma (\mathbf{n}_x \langle \uparrow | \hat{S}_x | \downarrow \rangle + \mathbf{n}_y \langle \uparrow | \hat{S}_y | \downarrow \rangle + \mathbf{n}_z \langle \uparrow | \hat{S}_z | \downarrow \rangle) \\ &= \gamma \frac{\hbar}{2} (\mathbf{n}_x \langle \uparrow | \hat{\sigma}_x | \downarrow \rangle + \mathbf{n}_y \langle \uparrow | \hat{\sigma}_y | \downarrow \rangle + \mathbf{n}_z \langle \uparrow | \hat{\sigma}_z | \downarrow \rangle). \end{aligned}$$

By now, the reader hopefully knows the matrix elements on the right-hand side by heart,<sup>85</sup> and we get

$$\langle \text{fin} | \hat{\mathbf{m}} | \text{ini} \rangle = \gamma \frac{\hbar}{2} (\mathbf{n}_x - i\mathbf{n}_y), \quad \text{so} \quad \left| \langle \text{fin} | \hat{\mathbf{m}} | \text{ini} \rangle \right|^2 = \left( \gamma \frac{\hbar}{2} \right)^2 |\mathbf{n}_x - i\mathbf{n}_y|^2 = 2 \left( \gamma \frac{\hbar}{2} \right)^2.$$

As a result, we get

$$\Gamma_{\text{magnetic}} = \frac{1}{4\pi\epsilon_0} \frac{4\omega^3}{3\hbar c^3} \frac{\gamma^2 \hbar^2}{2c^2}.$$

For an electron with  $\gamma = \gamma_e = -e/m_e$ , this expression may be rewritten as

$$\Gamma_{\text{magnetic}} = \frac{e^2}{4\pi\epsilon_0} \frac{4\omega^3}{3\hbar c^3} \frac{1}{2} \left( \frac{\hbar}{m_e c} \right)^2 \equiv \frac{e^2}{4\pi\epsilon_0} \frac{4\omega^3}{3\hbar c^3} \frac{\alpha^2}{2} r_B^2,$$

where  $\alpha \equiv e^2/4\pi\epsilon_0\hbar c \approx 1/137$  is the fine structure constant. Comparing this expression with the solution of Problem 5 for the electric-dipole emission by a hydrogen atom,

$$\Gamma_{\text{electric}} \sim \frac{e^2}{4\pi\epsilon_0} \frac{4\omega^3}{3\hbar c^3} r_B^2,$$

<sup>84</sup> The conservation of the net angular momentum of this system is achieved by the emission of a circularly polarized photon, carrying away a momentum of magnitude  $\hbar$ .

<sup>85</sup> If not, see, e.g. Eq. (4.128) of the lecture notes.

we see that the decay rate due to the spin flip in atoms is much (by a factor  $\sim \alpha^2$ ) smaller than that due to the electric-dipole radiation, even if the radiation frequency  $\omega$  is the same.

The same is even more true for experiments with electrons in realistic magnetic fields, where the spin-flip radiation frequency  $\omega = |\gamma|\mathcal{B}_0 = e\mathcal{B}_0/m_e$  is much lower than those ( $\omega \sim 10^{16} \text{ s}^{-1}$ ) of the optical transitions in atoms. For example, even for  $\mathcal{B}_0 = 10 \text{ T}$  (which is a pretty high field for a laboratory),  $\omega \approx 1.76 \times 10^{12} \text{ s}^{-1}$ . As a result, the rate of the spontaneous spin flips is extremely low: for the above case,  $\Gamma_{\text{magnetic}} \approx 4.4 \times 10^{-8} \text{ s}$ . This means that the lifetime  $\tau = 1/\Gamma$  of the excited spin states is limited by such flips to  $\sim 2.3 \times 10^7 \text{ s} \approx 265 \text{ days}$  – the time more than sufficient to carry out virtually any imaginable experiment (say, of the Stern-Gerlach type) with electron spins.

**Problem 9.9.** Calculate the rate of spontaneous transitions between the two sublevels of the ground state of a hydrogen atom, formed as a result of its hyperfine splitting. Discuss the implications of the result for the width of the 21-cm spectral line of hydrogen.

*Solution:* As was discussed in the model solution of Problem 8.5, the hyperfine splitting of the ground state energy of the hydrogen atom, due to the interaction between the spins of its electron and nucleus (proton), separates the three spin-triplet states with the ( $z$ -basis) ket-vectors

$$|s_+\rangle = \frac{1}{\sqrt{2}} \left( |\uparrow\rangle_e |\downarrow\rangle_p + |\downarrow\rangle_e |\uparrow\rangle_p \right), \quad |s_{\uparrow\uparrow}\rangle = |\uparrow\rangle_e |\uparrow\rangle_p, \quad \text{and} \quad |s_{\downarrow\downarrow}\rangle = |\downarrow\rangle_e |\downarrow\rangle_p, \quad (*)$$

from the singlet spin state with the ket-vector

$$|s_-\rangle = \frac{1}{\sqrt{2}} \left( |\uparrow\rangle_e |\downarrow\rangle_p - |\downarrow\rangle_e |\uparrow\rangle_p \right), \quad (**)$$

giving the states (\*) a slightly higher energy. Since the magnitude of the proton's gyromagnetic ratio  $\gamma_p = g_p e/2m_p$ , is much smaller than that of the electron,  $\gamma_e = -g_e e/2m_e \approx -e/m_e$  (due to the proton's larger mass,  $m_p \gg m_e$ ), its interaction with the electromagnetic field is proportionally smaller, and may be neglected. As a result, the radiation is dominantly due to the flip of the electron's spin, and its rate may be calculated using the formula derived in the solution of Problem 7:

$$\Gamma_s = \frac{1}{4\pi\epsilon_0} \frac{4\omega^3}{3\hbar c^3} \frac{1}{c^2} \left| \langle \text{fin} | \hat{\mathbf{m}} | \text{ini} \rangle \right|^2,$$

with the magnetic dipole moment operator  $\hat{\mathbf{m}} = \gamma_e \hat{\mathbf{S}}_e$  – just as in the previous problem. However, now this rate has to be calculated for each of the three initial states (\*), at the same final state (\*\*).

Let us start from the first, entangled-triplet initial state  $s_+$ :

$$\langle \text{fin} | \hat{\mathbf{m}} | \text{ini} \rangle = \langle s_- | \hat{\mathbf{m}} | s_+ \rangle = \gamma_e \langle s_- | \hat{\mathbf{S}}_e | s_+ \rangle = \gamma_e \left( \mathbf{n}_x \langle s_- | \hat{S}_{ex} | s_+ \rangle + \mathbf{n}_y \langle s_- | \hat{S}_{ey} | s_+ \rangle + \mathbf{n}_z \langle s_- | \hat{S}_{ez} | s_+ \rangle \right).$$

These three matrix elements may be calculated, for example, using Eqs. (4.128) of the lecture notes; for example:

$$\langle s_- | \hat{S}_{ex} | s_+ \rangle = \frac{1}{\sqrt{2}} \left( \langle \uparrow | \langle \downarrow | - \langle \downarrow | \langle \uparrow | \right) \frac{\hbar}{2} \left( |\uparrow\rangle_e \langle \downarrow|_e + |\downarrow\rangle_e \langle \uparrow|_e \right) \frac{1}{\sqrt{2}} \left( |\uparrow\rangle_e |\downarrow\rangle_p + |\downarrow\rangle_e |\uparrow\rangle_p \right).$$

Due to the orthonormality of the proton spin states, this expression reduces to

$$\langle s_- | \hat{S}_{ex} | s_+ \rangle = \frac{\hbar}{4} \langle \uparrow |_e (|\uparrow\rangle_e \langle \downarrow |_e + |\downarrow\rangle_e \langle \uparrow |_e) | \uparrow \rangle_e - \frac{\hbar}{4} \langle \downarrow |_e (|\uparrow\rangle_e \langle \downarrow |_e + |\downarrow\rangle_e \langle \uparrow |_e) | \downarrow \rangle_e = 0 - 0 \equiv 0.$$

The result for the  $y$ -component of the spin operator is similar, but the  $z$ -component bracket is different from zero:

$$\begin{aligned} \langle s_- | \hat{S}_{ez} | s_+ \rangle &= \frac{1}{\sqrt{2}} \left( \langle \uparrow |_e \langle \downarrow |_p - \langle \downarrow |_e \langle \uparrow |_p \right) \frac{\hbar}{2} \left( |\uparrow\rangle_e \langle \uparrow |_e - |\downarrow\rangle_e \langle \downarrow |_e \right) \frac{1}{\sqrt{2}} \left( |\uparrow\rangle_e |\downarrow\rangle_p + |\downarrow\rangle_e |\uparrow\rangle_p \right) \\ &= \frac{\hbar}{4} \langle \uparrow |_e (|\uparrow\rangle_e \langle \uparrow |_e - |\downarrow\rangle_e \langle \downarrow |_e) | \uparrow \rangle_e - \frac{\hbar}{4} \langle \downarrow |_e (|\uparrow\rangle_e \langle \uparrow |_e - |\downarrow\rangle_e \langle \downarrow |_e) | \downarrow \rangle_e = \frac{\hbar}{4} + \frac{\hbar}{4} \equiv \frac{\hbar}{2}. \end{aligned}$$

As a result, we get

$$\langle \text{fin} | \hat{\mathbf{m}} | \text{ini} \rangle = \gamma_e \frac{\hbar}{2} \mathbf{n}_z, \quad \langle \text{fin} | \hat{\mathbf{m}} | \text{ini} \rangle^2 = \left( \gamma_e \frac{\hbar}{2} \right)^2 \mathbf{n}_z^2 \equiv \left( \gamma_e \frac{\hbar}{2} \right)^2 \equiv \left( \frac{e\hbar}{2m_e} \right)^2. \quad (***)$$

(Note that the last value is twice smaller than that in the previous problem, due to a different, entangled two-spin character of the initial and final states in our current case.)

Now let us perform a similar calculation for the first simple (factorable) triplet state,  $s_{\uparrow\uparrow}$ . For this state, the  $z$ -component's matrix element vanishes:

$$\begin{aligned} \langle s_- | \hat{S}_{ez} | s_{\uparrow\uparrow} \rangle &= \frac{1}{\sqrt{2}} \left( \langle \uparrow |_e \langle \downarrow |_p - \langle \downarrow |_e \langle \uparrow |_p \right) \frac{\hbar}{2} \left( |\uparrow\rangle_e \langle \uparrow |_e - |\downarrow\rangle_e \langle \downarrow |_e \right) \left( |\uparrow\rangle_e |\uparrow\rangle_p \right) \\ &= -\frac{\hbar}{2\sqrt{2}} \langle \downarrow |_e (|\uparrow\rangle_e \langle \uparrow |_e - |\downarrow\rangle_e \langle \downarrow |_e) | \uparrow \rangle_e = 0 - 0 \equiv 0, \end{aligned}$$

but the  $x$ - and  $y$ -components do not. Due to the similar structure of their operators (see Eq. (4.128) again), it is convenient to calculate them in one shot:

$$\begin{aligned} &\langle s_- | \mathbf{n}_x \hat{S}_{ex} + \mathbf{n}_y \hat{S}_{ey} | s_{\uparrow\uparrow} \rangle \\ &= \frac{1}{\sqrt{2}} \left( \langle \uparrow |_e \langle \downarrow |_p - \langle \downarrow |_e \langle \uparrow |_p \right) \frac{\hbar}{2} \left[ (\mathbf{n}_x - i\mathbf{n}_y) |\uparrow\rangle_e \langle \downarrow |_e + (\mathbf{n}_x + i\mathbf{n}_y) |\downarrow\rangle_e \langle \uparrow |_e \right] \left( |\uparrow\rangle_e |\uparrow\rangle_p \right) \\ &= -\frac{\hbar}{2\sqrt{2}} \langle \downarrow |_e \left[ (\mathbf{n}_x - i\mathbf{n}_y) |\uparrow\rangle_e \langle \downarrow |_e + (\mathbf{n}_x + i\mathbf{n}_y) |\downarrow\rangle_e \langle \uparrow |_e \right] | \uparrow \rangle_e = -\frac{\hbar}{2\sqrt{2}} (\mathbf{n}_x + i\mathbf{n}_y), \end{aligned}$$

so

$$\langle \text{fin} | \hat{\mathbf{m}} | \text{ini} \rangle^2 = \gamma_e^2 \left( \frac{\hbar}{2\sqrt{2}} \right)^2 |\mathbf{n}_x + i\mathbf{n}_y|^2 = \gamma_e^2 \left( \frac{\hbar}{2\sqrt{2}} \right)^2 \cdot 2 \equiv \left( \gamma_e \frac{\hbar}{2} \right)^2 \equiv \left( \frac{e\hbar}{2m_e} \right)^2,$$

i.e. the same result as in Eq. (\*\*\*). An absolutely similar calculation for the second factorable initial state,  $s_{\downarrow\downarrow}$ , gives the same final result. So, the spontaneous photon emission rate,

$$\Gamma_s = \frac{e^2}{4\pi\epsilon_0} \frac{4\omega_{ss}^3}{3\hbar c^3} \left( \frac{\hbar}{2m_e c} \right)^2, \quad \text{giving} \quad \frac{\Gamma_s}{\omega_{ss}} = \frac{4\alpha}{3} \left( \frac{\hbar\omega_{ss}}{m_e c^2} \right)^2,$$

where  $\alpha$  is the fine structure constant, does not depend on which exactly of the states (\*), or what their linear superposition, the system initially was in.



Plugging in the fundamental constants, and the radiation frequency  $\omega = \omega_{ss} \approx 0.892 \times 10^{10} \text{ s}^{-1}$  (the famous 21-cm line – see the model solution of Problem 8.5), we get  $\Gamma_s \approx 2.86 \times 10^{-15} \text{ s}^{-1}$ .<sup>86</sup> Thus, the “natural” (fundamental) broadening of the 21-cm line, due to the spontaneous radiation, is extremely small:

$$\frac{\Gamma_s}{\omega_{ss}} \approx 3.2 \times 10^{-25}.$$

The much larger width ( $\Delta\omega \sim 10^{-3} \omega_{ss}$ ) of the 21-cm radiation line observed from various space regions is mostly due to the Doppler effect caused by the random thermal velocities of the emitting hydrogen atoms.

**Problem 9.10.** Find the eigenstates and eigenvalues of the Jaynes-Cummings Hamiltonian (9.78), and discuss their behavior near the resonance point  $\omega = \Omega$ .

*Solution:* The functional form of both eigenstates with energies close to  $E_n$  (9.80) is given by Eq. (9.82) of the lecture notes:

$$|\alpha\rangle = c_+ |+\rangle + c_- |-\rangle, \quad (*)$$

where

$$|+\rangle \equiv |\uparrow\rangle \otimes |n-1\rangle, \quad |-\rangle \equiv |\downarrow\rangle \otimes |n\rangle.$$

Plugging this solution into the stationary Schrödinger equation corresponding to the Jaynes-Cummings Hamiltonian (9.78),

$$\left( \frac{\hbar\Omega}{2} \hat{\sigma}_z + \hbar\omega \hat{a}^\dagger \hat{a} + \frac{\hbar\kappa}{2} \hat{\sigma}_+ \hat{a} + \frac{\hbar\kappa}{2} \hat{\sigma}_- \hat{a}^\dagger \right) |\alpha\rangle = E |\alpha\rangle,$$

and taking into account the following results of operator actions on the component states  $|\pm\rangle$  (which readily follow from what the reader already knows about two-level systems and harmonic oscillators),

$$\begin{aligned} \hat{\sigma}_z |\pm\rangle &= \pm |\pm\rangle, & \hat{a}^\dagger \hat{a} |+\rangle &\equiv (n-1) |+\rangle, & \hat{a}^\dagger \hat{a} |-\rangle &\equiv n |-\rangle, \\ \hat{\sigma}_+ \hat{a} |+\rangle &= 0, & \hat{\sigma}_+ \hat{a} |-\rangle &= 2n^{1/2} |+\rangle, & \hat{\sigma}_- \hat{a}^\dagger |+\rangle &= 2n^{1/2} |-\rangle, & \hat{\sigma}_- \hat{a}^\dagger |-\rangle &= 0, \end{aligned}$$

we get the following system of two linear algebraic equations for the coefficients  $c_\pm$ :

$$\begin{aligned} \frac{\hbar\Omega}{2} c_+ + \hbar\omega(n-1)c_+ + \hbar\kappa n^{1/2} c_- &= E c_+, \\ -\frac{\hbar\Omega}{2} c_- + \hbar\omega n c_- + \hbar\kappa n^{1/2} c_+ &= E c_-. \end{aligned}$$

With the definitions (9.70) and (9.80) of parameters  $\xi$  and  $E_n$ , and a natural notation for eigenenergy’s deviation from the central value  $E_n$ :

<sup>86</sup> Reformulated into the decay time  $\tau_s \equiv 1/\Gamma_s \sim 3 \times 10^{14} \text{ s} \sim 10^7$  years, this result means that such *spontaneous* radiation events are extremely rare. Indeed, most of the observed 21-line radiation by the hydrogen atoms in space is due to their transitions (both up and down across the hyperfine energy gap) that are *induced* by electromagnetic radiation from other sources, including the cosmic microwave background.

$$\tilde{E} \equiv E - E_n,$$

the system takes a very symmetric form,

$$\begin{aligned} \left(\frac{\hbar\xi}{2} - \tilde{E}\right)c_+ + \hbar\kappa n^{1/2}c_- &= 0, \\ \hbar\kappa n^{1/2}c_+ + \left(-\frac{\hbar\xi}{2} - \tilde{E}\right)c_- &= 0, \end{aligned} \quad (**)$$

so the condition of its consistency,

$$\begin{vmatrix} \frac{\hbar\xi}{2} - \tilde{E} & \hbar\kappa n^{1/2} \\ \hbar\kappa n^{1/2} & -\frac{\hbar\xi}{2} - \tilde{E} \end{vmatrix} = 0, \quad \text{i.e. } \tilde{E}^2 - \left(\frac{\hbar\xi}{2}\right)^2 = (\hbar\kappa)^2 n,$$

gives the following simple result for the Jaynes-Cummings eigenenergies:

$$\tilde{E}_{\pm} \equiv E - E_n = \pm \left[ \left(\frac{\hbar\xi}{2}\right)^2 + (\hbar\kappa)^2 n \right]^{1/2}. \quad (***)$$

At  $\kappa \rightarrow 0$ , this result is reduced to Eq. (9.79) of the lecture notes, while at  $\kappa \neq 0$ , it describes an anticrossing diagram similar to those encountered in the course so many times (see, e.g., Fig. 5.1), with the minimum sublevel splitting (at the exact resonance,  $\Omega = \omega$ )

$$\Delta E_n \equiv \tilde{E}_+ - \tilde{E}_- = 2\hbar\kappa n^{1/2}, \quad \text{for } \xi = 0.$$

Now we need to find the eigenstate vectors  $|\alpha\rangle_{\pm}$  corresponding to the calculated eigenenergies. Since we already know their functional form (\*), it is sufficient to calculate the pair of the coefficients  $c_{\pm}$  for each eigenstate.<sup>87</sup> For that, we need to plug each of the two solutions (\*\*\*) back into any of Eqs. (\*\*), use it to calculate the corresponding coefficient ratios. For example, the first equation yields

$$\left(\frac{c_+}{c_-}\right)_{\pm} = \frac{\hbar\kappa n^{1/2}}{\tilde{E}_{\pm} - \hbar\xi/2}.$$

By using the normalization condition  $|c_+|^2 + |c_-|^2 = 1$ , this result may be represented in the following convenient form:

$$(c_+)_{+} = (c_-)_{-} = \cos\theta, \quad (c_-)_{+} = \sin\theta, \quad (c_+)_{-} = -\sin\theta, \quad \text{where } \theta \equiv \frac{1}{2} \arctan \frac{\kappa n^{1/2}}{\xi},$$

which makes it easy to analyze the basic properties of the distribution coefficients. In particular:

(i) If the detuning's magnitude  $|\xi|$  is much larger than the coupling factor  $\kappa n^{1/2}$ , the angle  $\theta$  is close to 0, and the magnitude of one of the coefficients is much larger than that of the other one, i.e. the

<sup>87</sup> Note that they are frequently called *distribution coefficients*, because they specify how exactly each eigenstate is distributed between the simple "partial" states of the system, in our particular case, between  $|\pm\rangle$ . Such coefficients are also an important notion of the classical theory of oscillations and waves – see, e.g., CM Secs. 5.5-5.6 and 6.1-6.3.

system essentially resides in one of the component states  $|\pm\rangle$ , meaning that the interaction of the two-level and oscillator subsystems has virtually no effect on the system's properties.

(ii) In the opposite, most interesting limit  $|\xi| \ll \kappa n^{1/2}$ , we have  $\theta = \pm\pi/4$ , i.e. the distribution coefficients are equal by magnitude,  $|c_{\pm}| = 1/\sqrt{2}$ , with opposite signs of the ratio  $c_+/c_-$  at the upper and lower sublevels, so (apart from an inconsequential common phase multiplier), we may write

$$|\alpha\rangle = \frac{1}{\sqrt{2}} \times \begin{cases} \left( |\uparrow\rangle \otimes |n-1\rangle + |\downarrow\rangle \otimes |n\rangle \right), & \text{with } E = E_n + \hbar\kappa n^{1/2}, \\ \left( |\uparrow\rangle \otimes |n-1\rangle - |\downarrow\rangle \otimes |n\rangle \right), & \text{with } E = E_n - \hbar\kappa n^{1/2}, \end{cases}$$

in exact analogy with Eqs. (2.169) and (2.175), and also Eqs. (4.114). This means that near the exact resonance, the partial states  $|\pm\rangle$  interact most strongly. As was discussed in Sec. 9.4 of the lecture notes, the physics of this fact is that at  $\omega \approx \Omega$ , the partial energies of the two components of the coherent superposition (\*) are very close, enabling their strong coherent mixing (“hybridization”).

**Problem 9.11.** Analyze the Purcell effect, mentioned in Secs. 9.3 and 9.4 of the lecture notes, quantitatively. In particular, calculate the so-called *Purcell factor*  $F_P$  defined as the ratio of the rate  $\Gamma_s$  of an atom's spontaneous emission into a resonant cavity tuned exactly to the quantum transition frequency, to that into free space.

*Solution:* If the cavity's coupling to its environment is sufficiently large to suppress the phase coherence of the components of the states (9.82),<sup>88</sup> the photon emission by the atom is an incoherent effect, which may be described by the Golden Rule – just as it was done for the emission into free space at the beginning of Sec. 9.3. The main necessary modification is that of the density of states because Eq. (9.50) is valid only in the free space.

As we know from classical electrodynamics, in the absence of dissipation, i.e. of coupling to the environment, the frequency spectrum of a resonant cavity is discrete, so its density of states, participating in Eq. (9.49) as  $\rho_f$ , is a sum of delta functions  $\delta(E - \hbar\omega_j)$  at energies corresponding to the resonance frequencies  $\omega_j$ . Each of these delta functions is essentially an infinitely narrow resonance curve, well known from the classical theory of oscillations.<sup>89</sup> A small but non-zero dissipation gives the resonance a small but non-zero width<sup>90</sup>

$$\rho_f(E) = \delta(E - \hbar\omega_j) \rightarrow \frac{\delta}{\pi\hbar} \frac{1}{\delta^2 + \xi^2}, \quad \text{with } \xi \equiv \frac{E}{\hbar} - \omega_j, \quad (*)$$

where  $\delta$  is the damping constant related as  $\delta = \omega_j/2Q$  to the  $Q$ -factor of the resonance,<sup>91</sup> and the constant factor before the fraction is selected to satisfy the normalization condition

<sup>88</sup> The corresponding condition is  $\delta \gg \kappa, |\xi|$ , where the constants  $\kappa$  and  $\xi$  are defined in Sec. 9.4 of the lecture notes, and  $\delta$  is the damping constant – see below.

<sup>89</sup> See, e.g., CM Sec. 5.1.

<sup>90</sup> See, e.g., Eq. (7.150) – which duplicates CM Eq. (5.22).

<sup>91</sup> Generally, the factors  $\delta$  (and hence  $Q$ ) depend on the resonance number  $j$ ; I do not use the corresponding indices only to avoid formula cluttering. Note also that Eq. (\*) is strictly valid only if both  $\delta$  and  $|\xi|$  are much smaller than  $\omega_j$ , meaning in particular that  $Q \gg 1$ .

$$\int_{E \approx \hbar \omega_j} \rho_f(E) dE = 1.$$

In particular, at the exact tuning ( $E = \hbar \omega_j$ ), Eq. (\*) yields

$$\rho_f(\hbar \omega_j) = \frac{1}{\pi \hbar \delta} = \frac{2Q}{\pi \hbar \omega_j},$$

which should be used instead of Eq. (9.50).

Also, the  $e_d$  defined by Eq. (9.52) has to be replaced with some  $e_d \leq e_{\max}$ , where

$$e_{\max}^2 = \frac{1}{\epsilon_0 V_{\text{cavity}}},$$

reflecting the facts that, first, the atom may not be necessarily placed into the point where the electric field of the cavity mode is the largest, and, second, that only one mode is involved. With these replacements, the Purcell factor is

$$F_p \equiv \frac{(\Gamma_s)_{\text{cavity}}}{(\Gamma_s)_{\text{free space}}} = \frac{(\rho_f e_d^2)_{\text{cavity}}}{(\rho_f e_d^2)_{\text{free space}}} = 6\pi \frac{Q}{V_{\text{cavity}}} \left(\frac{c}{\omega}\right)^3 \left(\frac{e_d}{e_{\max}}\right)^2.$$

At the “best” location of the atom (in the electric field’s maximum), the last factor equals 1, and we get

$$F_p = 6\pi \frac{Q}{V_{\text{cavity}}} \left(\frac{c}{\omega}\right)^3 = \frac{3}{4\pi^2} Q \frac{\lambda^3}{V_{\text{cavity}}}.$$

In the lowest-frequency modes of a typical resonant cavity, the last ratio is of the order of 1 (see, e.g., EM Sec. 7.9), so the Purcell factor of a cavity scales as its  $Q$ -factor. For transitions between the adjacent Rydberg states, with very high values of the principal quantum number  $n$ , the electric dipole transition frequencies may be lowered to the microwave band ( $\omega \sim 10^{11} \text{ s}^{-1}$ ), in which superconducting cavities may have very high values of  $Q$  (up to  $\sim 10^{12}$ ), so the Purcell factor may be made extremely large.

As was mentioned in Sec. 9.3 of the lecture notes, this resonant increase of the radiation rate at frequencies  $\omega \approx \omega_j$  is compensated by its suppression between the resonances.

**Problem 9.12.** Use Eqs. (9.84) of the lecture notes to prove the continuity relation (1.52), with the probability density  $w$  and the current density  $\mathbf{j}$  given by Eqs. (9.89).

*Solution:* Multiplying all terms of the Klein-Gordon equation (9.84) by  $\Psi^*$  and of its complex-conjugate, by  $\Psi$ , and then subtracting the results, we get

$$\frac{1}{c^2} \left( \Psi^* \frac{\partial^2 \Psi}{\partial t^2} - \Psi \frac{\partial^2 \Psi^*}{\partial t^2} \right) - \left( \Psi^* \nabla^2 \Psi - \Psi \nabla^2 \Psi^* \right) = 0. \quad (*)$$

Now by using the same mathematical identity (1.45) as was employed at a similar calculation for the non-relativistic case,

$$\Psi^* \nabla^2 \Psi - \Psi \nabla^2 \Psi^* = \nabla \cdot (\Psi^* \nabla \Psi - \Psi \nabla \Psi^*),$$

and a similar identity for the time derivatives

$$\Psi^* \frac{\partial^2 \Psi}{\partial t^2} - \Psi \frac{\partial^2 \Psi^*}{\partial t^2} = \frac{\partial}{\partial t} \left( \Psi^* \frac{\partial \Psi}{\partial t} - \Psi \frac{\partial \Psi^*}{\partial t} \right),$$

and multiplying all terms of Eq. (\*) by  $i\hbar/2m$ , we may rewrite it as

$$\frac{\partial}{\partial t} \left[ \frac{i\hbar}{2mc^2} \left( \Psi^* \frac{\partial \Psi}{\partial t} - \text{c.c.} \right) \right] + \nabla \cdot \left[ \frac{i\hbar}{2m} \left( \Psi^* \nabla \Psi - \text{c.c.} \right) \right] = 0.$$

But this is exactly the continuity equation (1.52),

$$\frac{\partial w}{\partial t} + \nabla \cdot \mathbf{j} = 0,$$

with the probability and the probability current density given by Eqs. (9.89):

$$w = \frac{i\hbar}{2mc^2} \left( \Psi^* \frac{\partial \Psi}{\partial t} - \text{c.c.} \right), \quad \mathbf{j} = \frac{i\hbar}{2m} \left( \Psi^* \nabla \Psi - \text{c.c.} \right).$$

**Problem 9.13.** Prove that the Klein-Gordon equation (9.84) may be rewritten in a form similar to the non-relativistic Schrödinger equation (1.25) but for a two-component wavefunction, with the Hamiltonian represented (in the usual  $z$ -basis) by the following  $2 \times 2$ -matrix:

$$H = -(\sigma_z + i\sigma_y) \frac{\hbar^2}{2m} \nabla^2 + mc^2 \sigma_z.$$

Use your solution to discuss the physical meaning of the wavefunction's components.

*Solution:* Plugging the general form of the two-component wavefunction,<sup>92</sup>

$$\psi = \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix},$$

where (in contrast with the apparently similar Eq. (9.123) of the lecture notes)  $\psi_{\pm}$  are some spin-independent scalar wavefunctions, into the Schrödinger equation to be proved,

$$i\hbar \frac{\partial \psi}{\partial t} = -(\sigma_z + i\sigma_y) \frac{\hbar^2}{2m} \nabla^2 \psi + mc^2 \sigma_z \psi,$$

and spelling out the Pauli matrices, we get

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} = - \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} \frac{\hbar^2}{2m} \nabla^2 \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} + mc^2 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix}.$$

<sup>92</sup> Here  $\psi_{\pm}$  are functions of both  $\mathbf{r}$  and  $t$ , and the lower-case letter is used just to distinguish this two-component function from the scalar (single-component) function  $\Psi(\mathbf{r}, t)$  obeying the same Klein-Gordon equation in the scalar form (9.84).

Performing the matrix-by-vector multiplications, and requiring both elements of the resulting columns on the left-hand and right-hand sides to be equal, we get the following two scalar equations:

$$\begin{aligned} i\hbar \frac{\partial \psi_+}{\partial t} &= -\frac{\hbar^2}{2m} \nabla^2 (\psi_+ + \psi_-) + mc^2 \psi_+, \\ i\hbar \frac{\partial \psi_-}{\partial t} &= +\frac{\hbar^2}{2m} \nabla^2 (\psi_+ + \psi_-) - mc^2 \psi_-. \end{aligned} \quad (*)$$

Comparing these equations with Eq. (9.84), rewritten in the form

$$\frac{1}{c^2} \frac{\partial^2 \Psi}{\partial t^2} = \nabla^2 \Psi - \frac{m^2 c^2}{\hbar^2} \Psi, \quad (**)$$

we see that their major difference is the absence of the second derivative over time in Eqs. (\*). This is why it is natural to look for the relation between the functions  $\psi_{\pm}$  and  $\Psi$  in the following form:

$$\psi_{\pm} = C_{\pm} \Psi + D_{\pm} \frac{\partial \Psi}{\partial t}, \quad (***)$$

where  $C_{\pm}$  and  $D_{\pm}$  are some  $c$ -number constants, so the left-hand sides of Eqs. (\*) would have terms proportional to  $\partial^2 \Psi / \partial t^2$ . However, the comparison of Eqs. (\*) and (\*\*) shows that the sum ( $\psi_+ + \psi_-$ ) should not contain the derivative  $\partial \Psi / \partial t$ ; this is only possible if the coefficients  $D_{\pm}$  in Eq. (\*\*\*) are equal and opposite. Also, for two Eqs. (\*) to give the same single Eq. (\*\*), the coefficients  $C_{\pm}$  have to be equal. With these observations, Eq. (\*\*\*) is reduced to

$$\psi_{\pm} = C \Psi \pm D \frac{\partial \Psi}{\partial t} \equiv C \left( \Psi \pm \lambda \frac{\partial \Psi}{\partial t} \right), \quad \text{with } \lambda \equiv \frac{D}{C}.$$

Plugging this relation into Eqs. (\*), we see that they, after the cancellation of the normalization constant  $C$ , give two equivalent equations:

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \left( \Psi + \lambda \frac{\partial \Psi}{\partial t} \right) &= -\frac{\hbar^2}{2m} \nabla^2 (2\Psi) + mc^2 \left( \Psi + \lambda \frac{\partial \Psi}{\partial t} \right), \\ i\hbar \frac{\partial}{\partial t} \left( \Psi - \lambda \frac{\partial \Psi}{\partial t} \right) &= +\frac{\hbar^2}{2m} \nabla^2 (2\Psi) - mc^2 \left( \Psi - \lambda \frac{\partial \Psi}{\partial t} \right), \end{aligned}$$

which differ from Eq. (\*\*) only by the presence of the terms proportional to  $\partial \Psi / \partial t$ . However, these terms cancel if the constant  $\lambda$  is selected as

$$\lambda = \frac{i\hbar}{mc^2}, \quad \text{so that } \psi_{\pm} \equiv C \left( \Psi \pm \frac{i\hbar}{mc^2} \frac{\partial \Psi}{\partial t} \right),$$

giving two equivalent equations,

$$\mp \frac{\hbar^2}{mc^2} \frac{\partial^2 \Psi}{\partial t^2} = \mp \frac{\hbar^2}{m} \nabla^2 \Psi \pm mc^2 \Psi,$$

which, after the division of all terms by  $\mp \hbar^2 / m$ , coincide with the Klein-Gordon equation (\*\*).

In order to interpret the two-component function  $\psi$ , note a substantial (though incomplete) similarity between Eqs. (\*) for the stationary states, i.e. with  $\partial / \partial t \rightarrow E / i\hbar$ :

$$\begin{aligned}(E - mc^2)\psi_+ &= -\frac{\hbar^2}{2m}\nabla^2(\psi_+ + \psi_-), \\ (E + mc^2)\psi_- &= \frac{\hbar^2}{2m}\nabla^2(\psi_+ + \psi_-),\end{aligned}$$

and Eqs. (9.126) of the lecture notes, with  $U(\mathbf{r}) = 0$ , for a free spin- $1/2$  particle:

$$\begin{aligned}(E - mc^2)\psi_+ &= c\hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{p}}\psi_-, \\ (E + mc^2)\psi_- &= c\hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{p}}\psi_+.\end{aligned}$$

From this analogy, and the discussion of the Dirac equation in Secs. 9.6 and 9.7 of the lecture notes, we may conclude that in both cases,  $\psi_{\pm}$  describe, respectively, the particle and antiparticle components of the composite wavefunction. Not surprisingly, for spinless particles, which obey the Klein-Gordon equation, these components are just scalar functions of  $\mathbf{r}$  and  $t$ , while for spin- $1/2$  particles described by the Dirac equation, each of the  $\psi_{\pm}$  is itself a two-component column (spinor), with each component describing the states with  $S_z = \pm\hbar/2$ .

**Problem 9.14.** Calculate and discuss the energy spectrum of a relativistic, spinless, charged particle placed into an external uniform, time-independent magnetic field  $\mathcal{B}$ . Use the result to formulate the condition of validity of the non-relativistic theory for this case.

*Solution:* In the absence of spin and particle creation/annihilation effects, we may use the relativistic Schrödinger equation that may be obtained by making the general replacements (9.90), with the momentum and Hamiltonian operators given by Eqs. (9.83), in the Klein-Gordon equation – see, e.g., the bottom-right cell of Table 9.1. The replacement yields

$$\left(i\hbar\frac{\partial}{\partial t} - q\phi\right)^2\Psi = c^2(-i\hbar\nabla - q\mathbf{A})^2\Psi + (mc^2)^2\Psi. \quad (*)$$

In a time-independent magnetic field, with  $\mathbf{A} = \mathbf{A}(\mathbf{r})$  and  $\phi = 0$ , this equation has a set of stationary solutions similar in general structure to those in the non-relativistic case:

$$\Psi(\mathbf{r}, t) = \psi(\mathbf{r})\exp\left\{-i\frac{E}{\hbar}t\right\}.$$

Plugging such a solution into Eq. (\*), we get the following stationary relativistic Schrödinger equation

$$E^2\psi = c^2(-i\hbar\nabla - q\mathbf{A})^2\psi + (mc^2)^2\psi, \quad \text{i.e.} \quad \frac{1}{2m}(-i\hbar\nabla - q\mathbf{A})^2\psi = \frac{E^2 - (mc^2)^2}{2mc^2}\psi.$$

Let us compare the last equation with the non-relativistic Schrödinger equation for the same problem (see, e.g., Eq. (3.27) with  $\phi = 0$ ), with some effective energy referred (as usual in the non-relativistic theory) to the rest energy  $mc^2$  of the particle:

$$\frac{1}{2m}(-i\hbar\nabla - q\mathbf{A})^2\psi = E_{\text{ef}}\psi,$$

We see that these two equations are identical, provided that

$$E_{\text{cf}} = \frac{E^2 - (mc^2)^2}{2mc^2}, \quad \text{i.e. } E = \pm \left[ (mc^2)^2 + 2mc^2 E_{\text{cf}} \right]^{1/2},$$

where the two signs before the square root describe, respectively, the particle and the antiparticle.<sup>93</sup>

Hence we may use the solution of the non-relativistic problem (see, e.g., Sec. 3.2 of the lecture notes and the solution of Problem 3.6 with  $\ell = 0$ ), in particular, its energy spectrum,

$$\varepsilon_n(p_z) = \hbar\omega_c \left( n + \frac{1}{2} \right) + \frac{p_z^2}{2m}, \quad \text{with } \omega_c \equiv \frac{|q\mathcal{B}|}{m}, \quad n = 0, 1, 2, \dots, \quad \text{and } -\infty < p_z < +\infty,$$

where the  $z$ -axis is directed along the magnetic field, to get the (exact!) energy spectrum of the relativistic problem:

$$E_n(p_z) = \pm \left[ (mc^2)^2 + 2mc^2 \varepsilon_n \right]^{1/2} \equiv \pm \left[ (mc^2)^2 + c^2 \hbar q \mathcal{B} (2n+1) + c^2 p_z^2 \right]^{1/2}.$$

This means that as in the non-relativistic case, due to the free motion of the particle along the magnetic field, the spectrum consists of parabolic continuous bands (each corresponding to a specific quantum number  $n$ ) with the following bottom values corresponding to the purely transverse motion with  $p_z = 0$ :

$$\min_{p_z} |E_n| = \left[ (mc^2)^2 + c^2 \hbar q \mathcal{B} (2n+1) \right]^{1/2} \equiv mc^2 \left[ 1 + \frac{\hbar\omega_c}{mc^2} (2n+1) \right]^{1/2}.$$

From here we may return to the non-relativistic result for the Landau levels by expanding the right-hand side in the small dimensionless parameter  $\hbar\omega_c/mc^2 \ll 1$  and keeping only two leading terms. Hence, the non-relativistic theory is valid only if, first,  $cp_z \ll mc^2$  (i.e.  $v_z \ll c$ ), and second, if

$$\hbar\omega_c \ll mc^2, \quad \text{i.e. } |\mathcal{B}| \ll \frac{m^2 c^2}{\hbar |q|}.$$

Even for a particle as light as the electron, the right-hand side of the last relation is close to  $4 \times 10^9$  T – the value much higher than the strongest static fields ( $\sim 10^2$  T) created in laboratory. However, it is comparable to the fields conjectured to exist in the so-called *magnetars* – a specific variety of neutron stars.<sup>94</sup> (In a “usual” neutron star,  $\mathcal{B} \sim 10^6$  T.)

**Problem 9.15.** Prove Eq. (9.91) of the lecture notes for the energy spectrum of a hydrogen-like atom/ion, starting from the relativistic Schrödinger equation.

*Hint:* A mathematical analysis of Eq. (3.193) shows that its eigenvalues are still given by Eq. (3.201),  $\varepsilon_n = -1/2n^2$  with  $n = l + 1 + n_r$ , where  $n_r = 0, 1, 2, \dots$ , even if the parameter  $l$  is not an integer.

*Solution:* For the Coulomb field of the nucleus with charge  $Q = +Ze$ ,

$$\phi = \frac{Ze}{4\pi\varepsilon_0 r}, \quad \mathbf{A} = 0,$$

<sup>93</sup> Comparing the last expression with Eq. (9.1) of the lecture notes, we can see that  $E_{\text{cf}}$  is just  $p^2/2m$ , where  $\mathbf{p} = \mathbf{P} - q\mathbf{A}$  is the relativistic kinetic (“ $Mv$ –”) momentum of the particle.

<sup>94</sup> For a recent review, see e.g., R. Turolla *et al.*, *Rep. Prog. Phys.* **78**, 116901 (2015).



the relativistic Schrödinger equation (see, e.g., Eq. (\*) of the model solution of the previous problem), for an electron with the electric charge  $q = -e$  and the rest mass  $m = m_e$ , takes the form

$$\left( i\hbar \frac{\partial}{\partial t} + \frac{Ze^2}{4\pi\epsilon_0 r} \right)^2 \Psi = -\hbar^2 c^2 \nabla^2 \Psi + (m_e c^2)^2 \Psi,$$

so the stationary Schrödinger equation is

$$\left( E + \frac{Ze^2}{4\pi\epsilon_0 r} \right)^2 \psi = -\hbar^2 c^2 \nabla^2 \psi + (m_e c^2)^2 \psi.$$

Looking for its solution in the same form (3.200) that was used in the non-relativistic case,

$$\psi(\mathbf{r}) = \mathcal{R}_l(r) Y_l^m(\theta, \varphi),$$

we get the following equation for the radial function  $\mathcal{R}_l$ :

$$\left( E + \frac{Ze^2}{4\pi\epsilon_0 r} \right)^2 \mathcal{R}_l = -\hbar^2 c^2 \left[ \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d}{dr} \right) - \frac{l(l+1)}{r^2} \right] \mathcal{R}_l + (m_e c^2)^2 \mathcal{R}_l.$$

By squaring the parentheses, grouping the terms with the same power of  $1/r$ , and dividing all terms by  $2m_e c^2$ , this equation may be rewritten in the form

$$-\frac{\hbar^2}{2m_e r^2} \left\{ \frac{d}{dr} \left( r^2 \frac{d}{dr} \right) - \left[ l(l+1) - \frac{1}{\hbar^2 c^2} \left( \frac{Ze^2}{4\pi\epsilon_0} \right)^2 \right] \right\} \mathcal{R}_l - \frac{E}{m_e c^2} \frac{Ze^2}{4\pi\epsilon_0 r} \mathcal{R}_l = \frac{E^2 - (m_e c^2)^2}{2m_e c^2} \mathcal{R}_l,$$

which is similar to the non-relativistic equation (see Eq. (3.181) of the lecture notes, with  $U(r)$  given by Eq. (3.190) with  $C = Ze^2/4\pi\epsilon_0$  and  $m = m_e$ ),

$$-\frac{\hbar^2}{2m_e r^2} \left[ \frac{d}{dr} \left( r^2 \frac{d}{dr} \right) - l_{\text{ef}}(l_{\text{ef}} + 1) \right] \mathcal{R}_l - \frac{Z_{\text{ef}} e^2}{4\pi\epsilon_0 r} \mathcal{R}_l = E_{\text{ef}} \mathcal{R}_l,$$

with the following effective parameters:

$$l_{\text{ef}}(l_{\text{ef}} + 1) \equiv l(l+1) - Z^2 \alpha^2, \quad Z_{\text{ef}} \equiv \frac{E}{m_e c^2} Z, \quad E_{\text{ef}} \equiv \frac{E^2 - (m_e c^2)^2}{2m_e c^2}, \quad (*)$$

where  $\alpha$  is the fine structure constant. Hence, we may use the energy spectrum of the non-relativistic problem, given by Eq. (3.201) with  $C = Ze^2/4\pi\epsilon_0$ , and the fact provided in the *Hint*, to write

$$E_{\text{ef}} = -\frac{E_{\text{H}}}{2n_{\text{ef}}^2} Z_{\text{ef}}^2 \equiv -\frac{\alpha^2 m_e c^2}{2[(n_r + 1/2) + (l_{\text{ef}} + 1/2)]^2} Z_{\text{ef}}^2 \equiv -\frac{\alpha^2 m_e c^2}{2\{(n_r + 1/2) + [l_{\text{ef}}(l_{\text{ef}} + 1) + 1/4]^{1/2}\}^2} Z_{\text{ef}}^2. \quad (**)$$

Now using the identity  $l(l+1) + 1/4 \equiv (l + 1/2)^2$ , we get from Eqs. (\*) and (\*\*) the following simple equation for  $E$ :

$$\frac{E^2 - (m_e c^2)^2}{2m_e c^2} = -\frac{\alpha^2 m_e c^2}{2\{(n_r + 1/2) + [(l + 1/2)^2 - Z^2 \alpha^2]^{1/2}\}^2} \left( \frac{E}{m_e c^2} Z \right)^2.$$

Solving it, we get

$$E = m_e c^2 \left( 1 + \frac{Z^2 \alpha^2}{\left\{ (n_r + 1/2) + \left[ (l + 1/2)^2 - Z^2 \alpha^2 \right]^{1/2} \right\}^2} \right)^{-1/2}.$$

With the notation

$$\lambda \equiv (n_r + 1/2) + \left[ (l + 1/2)^2 - Z^2 \alpha^2 \right]^{1/2} \equiv n + \left[ (l + 1/2)^2 - Z^2 \alpha^2 \right]^{1/2} - (l + 1/2),$$

this is just Eq. (9.91) of the lecture notes.

**Problem 9.16.** Derive a general expression for the differential cross-section of elastic scattering of a spinless relativistic particle by a static potential  $U(\mathbf{r})$ , in the Born approximation, and formulate the conditions of its validity. Use these results to calculate the differential cross-section of scattering of a particle with the electric charge  $-e$  by the Coulomb electrostatic potential  $\phi(\mathbf{r}) = Ze/4\pi\epsilon_0 r$ .

*Solution:* In the absence of spin and of particle creation/annihilation, we may use the relativistic Schrödinger equation which may be obtained by using the replacements (9.90), and the momentum and Hamiltonian operators given by Eqs. (9.83), in the Klein-Gordon equation – see, e.g., the bottom-right cell of Table 9.1 of the lecture notes.<sup>95</sup> In our case,  $q\phi = U(\mathbf{r})$  and  $\mathbf{A} = 0$ , so the replacement yields

$$\left[ i\hbar \frac{\partial}{\partial t} - U(\mathbf{r}) \right]^2 \Psi = -\hbar^2 c^2 \nabla^2 \Psi + (mc^2)^2 \Psi. \quad (*)$$

As was discussed in Sec. 3.3 of the lecture notes, the elastic scattering may be analyzed using definite-energy wavefunctions – wave packets of a formally infinite spatial extension, so we may look for the particular solution of Eq. (\*) in the usual form

$$\Psi(\mathbf{r}, t) = \psi(\mathbf{r}) \exp\left\{ -i \frac{E}{\hbar} t \right\}.$$

The equation is obviously satisfied provided that the spatial factor  $\psi(\mathbf{r})$  obeys the following stationary equation:

$$[E - U(\mathbf{r})]^2 \psi = -\hbar^2 c^2 \nabla^2 \psi + (mc^2)^2 \psi.$$

Dividing both sides of this equation by  $2mc^2$ , we may rewrite it as

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + U_{\text{ef}}(\mathbf{r}) \psi = E_{\text{ef}} \psi,$$

with

$$U_{\text{ef}}(\mathbf{r}) \equiv \frac{U(\mathbf{r})[2E - U(\mathbf{r})]}{2mc^2} \quad \text{and} \quad E_{\text{ef}} \equiv \frac{E^2 - (mc^2)^2}{2mc^2}.$$

But this equation exactly coincides with the non-relativistic Schrödinger equation (with the effective potential energy profile  $U_{\text{ef}}(\mathbf{r})$  and effective particle energy  $E_{\text{ef}}$ ) that was used, in particular, in

<sup>95</sup> See also the model solutions of the two previous problems..

Sec. 3.3 of the lecture notes to derive Eq. (3.88) for the differential cross-section of scattering in the Born approximation. Hence we may use that result, in the form

$$\frac{d\sigma}{d\Omega} = \left( \frac{m}{2\pi\hbar^2} \right)^2 \left| \int U_{\text{ef}}(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}} d^3r \right|^2, \quad \text{with } \mathbf{q} \equiv \mathbf{k} - \mathbf{k}_0, \quad (**)$$

keeping in mind that the  $\mathbf{k}$  and  $\mathbf{k}_0$  are now effective rather than the actual wave vectors whose magnitude is related, by the very familiar Eq. (1.89), to not the actual but the effective energy of the particle:

$$k = k_0 = \left( \frac{2mE_{\text{ef}}}{\hbar^2} \right)^{1/2} = \frac{1}{\hbar c} \left[ E^2 - (mc^2)^2 \right]^{1/2}.$$

Note that the last expression has a simple physical sense:  $\hbar k = \hbar k_0 = p$ , where the free-particle momentum  $p$  is given by the basic Eq. (9.1):

$$E^2 = (pc)^2 + (mc^2)^2.$$

The condition of validity of Eq. (\*\*) may be obtained by the corresponding replacements in the non-relativistic condition (3.77):

$$(U_{\text{ef}})_0 \ll \frac{\hbar^2}{ma^2} \max[1, ka], \quad (***)$$

where  $(U_{\text{ef}})_0$  is a proper scale of the effective potential's magnitude, and  $a$  denotes its characteristic spatial extension. Let us specify these conditions for our particular case of the Coulomb potential:

$$U(\mathbf{r}) = -\frac{Ze^2}{4\pi\epsilon_0 r}, \quad \text{so } U_{\text{ef}}(\mathbf{r}) = -\frac{Ze^2}{4\pi\epsilon_0 r} \frac{E}{mc^2} + \left( \frac{Ze^2}{4\pi\epsilon_0 r} \right)^2 \frac{1}{2mc^2}.$$

As was discussed in the model solution of Problem 3.11, the effective radius  $a$  of an exponentially screened Coulomb potential tends to infinity as the screening is gradually removed ( $\lambda \rightarrow 0$ ); as a result, the expression on the right-hand side of Eq. (\*\*\*) is reduced to  $(\hbar^2/ma^2)(ka) \equiv \hbar^2 k/ma$ . Repeating the arguments given at the end of that solution, with the additional factor  $E/mc^2 = M/m$  (where  $M \equiv m/(1 - v^2/c^2)^{1/2}$  is the relativistic mass and  $v$  is the particle's velocity), and replacing the non-relativistic relation  $p = mv$  used there with the relativistic one,  $p = Mv$ ,<sup>96</sup> the relation takes exactly the same form as in the non-relativistic case:

$$Z\alpha \ll \frac{v}{c} \leq 1,$$

where  $\alpha \approx 1/137$  is the fine structure constant.

Now let us notice that if this condition is satisfied, the second term in the last expression for  $U_{\text{ef}}(\mathbf{r})$  is much smaller than the first one, at all distances of interest:  $r > 1/k$ . Indeed,

<sup>96</sup> See, e.g., EM Sec. 9.3 – in particular, Eqs. (9.70), (9.71), and (9.73). Note again that since the relativistic Schrödinger equation for a free particle is the quantum-mechanical generalization of the classical relations of special relativity, they are *exactly* valid for the plane-wave solutions  $\psi \propto \exp\{i(\mathbf{p}\cdot\mathbf{r} - Et)/\hbar\}$  with definite  $c$ -number values of  $\mathbf{p}$  and  $E$ .

$$\left| \frac{2^{\text{nd}} \text{ term}}{1^{\text{st}} \text{ term}} \right| = \frac{Ze^2}{4\pi\epsilon_0 r} \frac{1}{2E} < \frac{Ze^2 k}{4\pi\epsilon_0} \frac{1}{2E} \equiv \frac{Ze^2}{4\pi\epsilon_0 c\hbar} \frac{cp}{2E} \equiv Z\alpha \frac{cp}{2E} \leq \frac{Z\alpha}{2} \ll 1.$$

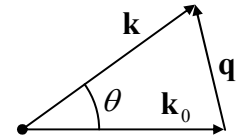
Hence we have the right to not only ignore the effect of this term on the Born approximation's validity condition (\*\*\*) but also, in this approximation, drop it at the calculation of the differential cross-section (\*\*). Since the remaining (1<sup>st</sup>) term of  $U_{\text{ef}}(\mathbf{r})$  differs from  $U(\mathbf{r})$  only by the additional factor  $E/mc^2$ , we may reuse the solution of the same Problem 3.11, getting

$$\frac{d\sigma}{d\Omega} = \left( \frac{Ze^2}{4\pi\epsilon_0} \frac{E}{mc^2} \frac{2m}{\hbar^2 q^2} \right)^2 \equiv \left( \frac{Ze^2}{4\pi\epsilon_0} \frac{2E}{\hbar^2 q^2 c^2} \right)^2.$$

Since the relativistic replacements keep intact the usual geometric relation between the magnitude  $k$  of the vectors  $\mathbf{k}$  and  $\mathbf{k}_0$ , and that of the vector  $\mathbf{q}$ ,

$$q = 2k \sin \frac{\theta}{2},$$

where  $\theta$  is the scattering angle (see the figure on the right), we may rewrite our result for the differential cross-section as



$$\frac{d\sigma}{d\Omega} = \left( \frac{Ze^2}{4\pi\epsilon_0} \frac{E}{2\hbar^2 k^2 c^2} \right)^2 \frac{1}{\sin^4(\theta/2)} \equiv \left( \frac{Ze^2}{4\pi\epsilon_0} \frac{E}{2p^2 c^2} \right)^2 \frac{1}{\sin^4(\theta/2)}.$$

Hence the angular dependence of  $d\sigma/d\Omega$  remains the same as in the non-relativistic quantum mechanics (and as in the classical mechanics), with a strong (non-integrable) divergence at  $\theta \rightarrow 0$  and hence a formally infinite total cross-section.

**Problem 9.17.** Starting from Eqs. (9.95)-(9.98) of the lecture notes, prove that the probability density  $w$  given by Eq. (9.101) and the probability current density  $\mathbf{j}$  defined by Eq. (9.102) do indeed satisfy the continuity equation (1.52):  $\partial w/\partial t + \nabla \cdot \mathbf{j} = 0$ .

*Solution:* Very similarly to what was done in Sec. 1.4 of the lecture notes for the non-relativistic Schrödinger equation, let us write Eq. (9.95), with the Dirac Hamiltonian (9.97), in the coordinate representation:

$$i\hbar \frac{\partial \Psi}{\partial t} = c\hat{\alpha} \cdot \hat{\mathbf{p}} \Psi + mc^2 \hat{\beta} \Psi, \quad \text{i.e. } i\hbar \frac{\partial \Psi}{\partial t} = -i\hbar (c\hat{\alpha} \cdot \nabla \Psi) + mc^2 (\hat{\beta} \Psi), \quad (*)$$

and left-multiply all its terms by the Hermitian-conjugate wavefunction  $\Psi^\dagger$ :

$$i\hbar \Psi^\dagger \frac{\partial \Psi}{\partial t} = -i\hbar c \Psi^\dagger \hat{\alpha} \cdot \nabla \Psi + mc^2 \Psi^\dagger \hat{\beta} \Psi. \quad (**)$$

(Since according to Eq. (9.96), both  $\Psi$  and  $\Psi^\dagger$  are matrix rows/columns, while according to Eqs. (9.98),  $\hat{\alpha}$  and  $\hat{\beta}$  are square matrices, all multiplications here and below should be understood in the matrix sense.)

Let us also write the Hermitian conjugate of Eq. (\*):<sup>97</sup>

$$-i\hbar \frac{\partial \Psi^\dagger}{\partial t} = i\hbar c (\nabla \Psi^\dagger \cdot \hat{\alpha}) + mc^2 (\Psi^\dagger \hat{\beta}),$$

right-multiply all its terms by  $\Psi$ :

$$-i\hbar \frac{\partial \Psi^\dagger}{\partial t} \Psi = i\hbar c \nabla \Psi^\dagger \cdot \hat{\alpha} \Psi + mc^2 \Psi^\dagger \hat{\beta} \Psi,$$

and then subtract this relation from Eq. (\*\*). After the cancellation of the last terms and of the common factor  $i\hbar$  in the remaining terms, the result takes the form

$$\left( \Psi^\dagger \frac{\partial \Psi}{\partial t} + \frac{\partial \Psi^\dagger}{\partial t} \Psi \right) + c (\Psi^\dagger \hat{\alpha} \cdot \nabla \Psi + \nabla \Psi^\dagger \cdot \hat{\alpha} \Psi) = 0. \quad (***)$$

Now taking into account the identities<sup>98</sup>

$$\frac{\partial}{\partial t} (\Psi^\dagger \Psi) = \Psi^\dagger \frac{\partial \Psi}{\partial t} + \frac{\partial \Psi^\dagger}{\partial t} \Psi, \quad \text{and} \quad \nabla \cdot (\Psi^\dagger \hat{\alpha} \Psi) = \Psi^\dagger \hat{\alpha} \cdot \nabla \Psi + \nabla \Psi^\dagger \cdot \hat{\alpha} \Psi,$$

Eq. (\*\*\*) may be spelled out as

$$\frac{\partial}{\partial t} (\Psi^\dagger \Psi) + \nabla \cdot (\Psi^\dagger c \hat{\alpha} \Psi) = 0,$$

i.e. as the continuity equation for the probability density (9.101) and the probability current (9.102).

**Problem 9.18.** Calculate the commutator of the operator  $\hat{L}^2$  and the Dirac Hamiltonian of a free particle. Compare the result with that for the non-relativistic Hamiltonian, and interpret the difference.

*Solution:* As was discussed in Sec. 9.6 of the lecture notes, since the vector operator  $\hat{\mathbf{L}} \equiv \hat{\mathbf{r}} \times \hat{\mathbf{p}}$  is defined in the Hilbert space of orbital states of the particle, it commutes with the spin operators (9.98), and hence with the second term of the Dirac Hamiltonian (9.97). So it is sufficient to calculate the commutator of its  $j^{\text{th}}$  Cartesian component  $L_j$  with the first term of that Hamiltonian:<sup>99</sup>

$$[\hat{L}_j, \hat{H}] = [\hat{L}_j, c \hat{\alpha} \cdot \hat{\mathbf{p}}] = c \sum_{j'=1}^3 [\hat{L}_j, \hat{\alpha}_{j'} \hat{p}_{j'}] = c \sum_{j'=1}^3 \hat{\alpha}_{j'} [\hat{L}_j, \hat{p}_{j'}].$$

According to the second of Eqs. (5.149), the last commutator equals the sum of  $i\hbar p_j \epsilon_{jj'}$ , where  $\epsilon_{jj'}$  is the Levi-Civita symbol, over all  $j'$ , so

<sup>97</sup> Note the change of operators' order in their products; it follows from the basic rule of the Hermitian conjugation of operator products:  $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger \hat{A}^\dagger$  – see, e.g., Problem 4.1(iii).

<sup>98</sup> See, e.g., MA Eqs. (4.1) and (11.4a). (It is straightforward to verify that these relations remain valid for multi-component functions like  $\Psi$  and vector matrices like  $\alpha$ .)

<sup>99</sup> Actually, this is just a straightforward generalization of the calculation made for  $L_x$  in the lecture notes – see Eq. (9.106).

$$[\hat{L}_j, \hat{H}] = i\hbar c \sum_{j', j''=1}^3 \hat{\alpha}_{j'} \hat{p}_{j''} \varepsilon_{jjj''} . \quad (*)$$

Rewriting this commutation relation as

$$\hat{L}_j \hat{H} = \hat{H} \hat{L}_j + i\hbar c \sum_{j', j''=1}^3 \hat{\alpha}_{j'} \hat{p}_{j''} \varepsilon_{jjj''} ,$$

we may use it to calculate

$$\begin{aligned} [\hat{L}_j^2, \hat{H}] &\equiv \hat{L}_j \hat{L}_j \hat{H} - \hat{H} \hat{L}_j \hat{L}_j \equiv \hat{L}_j (\hat{L}_j \hat{H}) - \hat{H} \hat{L}_j \hat{L}_j = \hat{L}_j \left( \hat{H} \hat{L}_j + i\hbar c \sum_{j', j''=1}^3 \hat{\alpha}_{j'} \hat{p}_{j''} \varepsilon_{jjj''} \right) - \hat{H} \hat{L}_j \hat{L}_j \\ &\equiv (\hat{L}_j \hat{H}) \hat{L}_j - \hat{H} \hat{L}_j \hat{L}_j + i\hbar c \sum_{j', j''=1}^3 \hat{\alpha}_{j'} \hat{L}_j \hat{p}_{j''} \varepsilon_{jjj''} \\ &= \left( \hat{H} \hat{L}_j + i\hbar c \sum_{j', j''=1}^3 \hat{\alpha}_{j'} \hat{p}_{j''} \varepsilon_{jjj''} \right) \hat{L}_j - \hat{H} \hat{L}_j \hat{L}_j + i\hbar c \sum_{j', j''=1}^3 \hat{\alpha}_{j'} \hat{L}_j \hat{p}_{j''} \varepsilon_{jjj''} = i\hbar c \sum_{j', j''=1}^3 \hat{\alpha}_{j'} \{ \hat{L}_j, \hat{p}_{j''} \} \varepsilon_{jjj''} , \end{aligned}$$

where the curly brackets denote the anticommutator – see Eq. (4.34).

Now the sum of these relations over all  $j = 1, 2, 3$  yields the required commutator:

$$[\hat{L}^2, \hat{H}] \equiv \left[ \sum_{j=1}^3 \hat{L}_j^2, \hat{H} \right] \equiv \sum_{j=1}^3 [\hat{L}_j^2, \hat{H}] = i\hbar c \sum_{j, j', j''=1}^3 \hat{\alpha}_{j'} \{ \hat{L}_j, \hat{p}_{j''} \} \varepsilon_{jjj''} . \quad (**)$$

Since this commutator is not equal to zero, the expectation value of  $L^2$  of a free spin- $1/2$  particle is *not* conserved at its free motion – and neither are its Cartesian components  $L_j$ . This result differs from the situation in non-relativistic quantum mechanics, where the free-particle Hamiltonian,

$$\hat{H} = \frac{\hat{p}^2}{2m} ,$$

commutes with the operators of  $L^2$  and all  $L_j$ , so the orbital angular momentum is conserved – see, for example, the solution of Problem 5.25. This difference shows that in the Dirac theory (and in the physical reality :- ) the orbital and spin degrees of the particle are generally related, and only in the non-relativistic limit, this relation weakens, manifesting itself only in small artifacts such as the spin-orbit coupling (9.122) and its results including, most notably, the fine structure of atomic levels – see Sec. 6.3 of the lecture notes.

**Problem 9.19.** Calculate commutators of the operators  $\hat{S}^2$  and  $\hat{J}^2$  with the Dirac Hamiltonian (9.97) and give an interpretation of the results.

*Solution:* Let us first generalize Eqs. (9.109) of the lecture notes to arbitrary Cartesian components of the vector operators  $\hat{\mathbf{S}}$ ,  $\hat{\boldsymbol{\alpha}}$ , and  $\hat{\boldsymbol{\beta}}$ . This may be readily done not only in the explicit  $4 \times 4$  matrix form, by using Eqs. (9.98b) and (9.107b), but even in the shorthand  $2 \times 2$  matrix form, by using Eqs. (9.98a) and (9.107a):<sup>100</sup>

<sup>100</sup> While doing that, we have to remember that the “elements” of these  $2 \times 2$  matrices are still the Pauli matrices, so their product components, generally, cannot be swapped.

$$\begin{aligned} \mathbf{S}_j \boldsymbol{\alpha}_{j'} &= \frac{\hbar}{2} \begin{pmatrix} \sigma_j & 0 \\ 0 & \sigma_j \end{pmatrix} \begin{pmatrix} 0 & \sigma_{j'} \\ \sigma_{j'} & 0 \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 0 & \sigma_j \sigma_{j'} \\ \sigma_j \sigma_{j'} & 0 \end{pmatrix}, \\ \boldsymbol{\alpha}_{j'} \mathbf{S}_j &= \frac{\hbar}{2} \begin{pmatrix} 0 & \sigma_{j'} \\ \sigma_{j'} & 0 \end{pmatrix} \begin{pmatrix} \sigma_j & 0 \\ 0 & \sigma_j \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 0 & \sigma_{j'} \sigma_j \\ \sigma_{j'} \sigma_j & 0 \end{pmatrix}. \end{aligned} \quad (*)$$

From here, the commutator of these matrices is

$$[\mathbf{S}_j, \boldsymbol{\alpha}_{j'}] \equiv \mathbf{S}_j \boldsymbol{\alpha}_{j'} - \boldsymbol{\alpha}_{j'} \mathbf{S}_j = \frac{\hbar}{2} \begin{pmatrix} 0 & [\sigma_j, \sigma_{j'}] \\ [\sigma_j, \sigma_{j'}] & 0 \end{pmatrix}.$$

With the Pauli matrix commutation rule (whose calculation was one of the tasks of Problem 4.3), this relation becomes

$$[\mathbf{S}_j, \boldsymbol{\alpha}_{j'}] = \frac{\hbar}{2} \sum_{j''=1}^3 \begin{pmatrix} 0 & 2i\sigma_{j''} \varepsilon_{jj''} \\ 2i\sigma_{j''} \varepsilon_{jj''} & 0 \end{pmatrix} \equiv i\hbar \sum_{j''=1}^3 \begin{pmatrix} 0 & \sigma_{j''} \\ \sigma_{j''} & 0 \end{pmatrix} \varepsilon_{jj''}.$$

Now by using the definition (9.98a) of the vector matrix  $\boldsymbol{\alpha}$  again, we may rewrite this result just as<sup>101</sup>

$$[\mathbf{S}_j, \boldsymbol{\alpha}_{j'}] = i\hbar \sum_{j''=1}^3 \boldsymbol{\alpha}_{j''} \varepsilon_{jj''}, \quad \text{i.e.} \quad [\hat{S}_j, \hat{\boldsymbol{\alpha}}_{j'}] = i\hbar \sum_{j''=1}^3 \hat{\boldsymbol{\alpha}}_{j''} \varepsilon_{jj''}.$$

An absolutely similar calculation for  $\hat{\boldsymbol{\beta}}$  yields quite a different result:

$$\begin{aligned} [\mathbf{S}_j, \boldsymbol{\beta}_{j'}] &\equiv \mathbf{S}_j \boldsymbol{\beta}_{j'} - \boldsymbol{\beta}_{j'} \mathbf{S}_j = \frac{\hbar}{2} \left[ \begin{pmatrix} \sigma_j & 0 \\ 0 & \sigma_j \end{pmatrix} \begin{pmatrix} \mathbf{I} & 0 \\ 0 & -\mathbf{I} \end{pmatrix} - \begin{pmatrix} \mathbf{I} & 0 \\ 0 & -\mathbf{I} \end{pmatrix} \begin{pmatrix} \sigma_j & 0 \\ 0 & \sigma_j \end{pmatrix} \right] \\ &= \frac{\hbar}{2} \left[ \begin{pmatrix} \sigma_j & 0 \\ 0 & -\sigma_j \end{pmatrix} - \begin{pmatrix} \sigma_j & 0 \\ 0 & -\sigma_j \end{pmatrix} \right] = 0, \quad \text{i.e.} \quad [\hat{S}_j, \hat{\boldsymbol{\beta}}_{j'}] = \hat{0}. \end{aligned}$$

Now using Eq. (9.97), we get

$$[\hat{S}_j, \hat{H}] = \left[ \hat{S}_j, c \sum_{j'=1}^3 \hat{\boldsymbol{\alpha}}_{j'} \hat{p}_{j'} + mc^2 \hat{\boldsymbol{\beta}} \right] = c \sum_{j'=1}^3 [\hat{S}_j, \hat{\boldsymbol{\alpha}}_{j'}] \hat{p}_{j'} = i\hbar c \sum_{j', j''=1}^3 \hat{\boldsymbol{\alpha}}_{j''} \hat{p}_{j'} \varepsilon_{jj''}.$$

For the purposes of comparison with the commutator  $[\hat{L}_j, \hat{H}]$ , which was calculated as a by-product in the model solution of the previous problem, let us swap the indices  $j'$  and  $j''$ , and then use the property  $\varepsilon_{jj''j'} = -\varepsilon_{jj'j''}$  of the Levi-Civita symbol to write

$$[\hat{S}_j, \hat{H}] = i\hbar c \sum_{j', j''=1}^3 \hat{\boldsymbol{\alpha}}_{j'} \hat{p}_{j''} \varepsilon_{jj''j'} \equiv -i\hbar c \sum_{j', j''=1}^3 \hat{\boldsymbol{\alpha}}_{j'} \hat{p}_{j''} \varepsilon_{jj'j''}. \quad (**)$$

So, the commutator  $[\hat{S}_j, \hat{H}]$  differs from the commutator  $[\hat{L}_j, \hat{H}]$  (see the solution of the previous problem) only by the sign.

<sup>101</sup> Note that in the “Dirac basis” used in this course (and most textbooks), the notions of an operator and the corresponding  $2 \times 2$  matrix are identical, so we may switch between the operator and matrix notations at will.

One might expect the commutators  $[\hat{S}^2, \hat{H}]$  and  $[\hat{L}^2, \hat{H}]$  to be similar as well. However, this is not so. Indeed, rewriting Eq. (\*\*) as

$$\hat{S}_j \hat{H} = \hat{H} \hat{S}_j - i\hbar c \sum_{j', j''=1}^3 \hat{\alpha}_{j'} \hat{p}_{j''} \varepsilon_{jj'j''},$$

we may use this relation twice to calculate

$$\begin{aligned} [\hat{S}_j^2, \hat{H}] &\equiv \hat{S}_j \hat{S}_j \hat{H} - \hat{H} \hat{S}_j \hat{S}_j \equiv \hat{S}_j (\hat{S}_j \hat{H}) - \hat{H} \hat{S}_j \hat{S}_j = \hat{S}_j \left( \hat{H} \hat{S}_j - i\hbar c \sum_{j', j''=1}^3 \hat{\alpha}_{j'} \hat{p}_{j''} \varepsilon_{jj'j''} \right) - \hat{H} \hat{S}_j \hat{S}_j \\ &\equiv (\hat{S}_j \hat{H}) \hat{S}_j - \hat{H} \hat{S}_j \hat{S}_j - i\hbar c \sum_{j', j''=1}^3 \hat{\alpha}_{j'} \hat{S}_j \hat{p}_{j''} \varepsilon_{jj'j''} \\ &= \left( \hat{H} \hat{S}_j - i\hbar c \sum_{j', j''=1}^3 \hat{\alpha}_{j'} \hat{p}_{j''} \varepsilon_{jj'j''} \right) \hat{S}_j - \hat{H} \hat{S}_j \hat{S}_j - i\hbar c \sum_{j', j''=1}^3 \hat{\alpha}_{j'} \hat{S}_j \hat{p}_{j''} \varepsilon_{jj'j''} \equiv -i\hbar c \sum_{j', j''=1}^3 \{ \hat{S}_j, \hat{\alpha}_{j'} \} \hat{p}_{j''} \varepsilon_{jj'j''}. \end{aligned}$$

The last anticommutator may be readily calculated using Eq. (\*) and the well-known property  $\{ \sigma_j, \sigma_{j'} \} = 2i\delta_{jj'}$  of the Pauli matrices:<sup>102</sup>

$$\begin{aligned} \{ \mathbf{S}_j, \boldsymbol{\alpha}_{j'} \} &\equiv \mathbf{S}_j \boldsymbol{\alpha}_{j'} + \boldsymbol{\alpha}_{j'} \mathbf{S}_j = \frac{\hbar}{2} \begin{pmatrix} 0 & \sigma_j \sigma_{j'} \\ \sigma_j \sigma_{j'} & 0 \end{pmatrix} + \frac{\hbar}{2} \begin{pmatrix} 0 & \sigma_{j'} \sigma_j \\ \sigma_{j'} \sigma_j & 0 \end{pmatrix} \\ &\equiv \frac{\hbar}{2} \begin{pmatrix} 0 & \{ \sigma_j, \sigma_{j'} \} \\ \{ \sigma_j, \sigma_{j'} \} & 0 \end{pmatrix} = \hbar \begin{pmatrix} 0 & \mathbf{I} \\ \mathbf{I} & 0 \end{pmatrix} \delta_{jj'}. \end{aligned}$$

However, by the very definition of the Kronecker and Levi-Civita symbols, the product  $\delta_{jj'} \varepsilon_{jj'j''}$  equals zero for any combination of indices, so

$$[\hat{S}_j^2, \hat{H}] = \hat{0}, \quad \text{and hence } [\hat{S}^2, \hat{H}] \equiv \left[ \sum_{j=1}^3 \hat{S}_j^2, \hat{H} \right] \equiv \sum_{j=1}^3 [\hat{S}_j^2, \hat{H}] = \hat{0}, \quad (***)$$

i.e. the observable  $S^2$  is conserved (at least) at the free motion of the particle. This result might be expected because, in the non-relativistic theory, this observable is firmly fixed by the particle's spin  $s$ ,  $S^2 = \hbar^2 s(s+1)$ , so for a spin- $1/2$  particle,  $S^2 = (3/4)\hbar^2$  in any of its quantum states. As an easy direct calculation using Eq. (9.107) shows,<sup>103</sup> the last result is also valid in the relativistic Dirac theory (which covers only spin- $1/2$  particles).

Now the second task of the problem's assignment becomes very easy. With the definition (9.111) of the total angular momentum, which may be represented in its Cartesian components as

$$\hat{\mathbf{J}}_j = \hat{\mathbf{L}}_j + \hat{\mathbf{S}}_j,$$

we may use the relation (\*\*) derived above, together with Eq. (\*\*) of the model solution of the previous problem, to get<sup>104</sup>

<sup>102</sup> See, e.g., the model solution of the same Problem 4.3.

<sup>103</sup> This additional exercise is highly recommended to the reader.

<sup>104</sup> This result confirms the fact already stated in Sec. 9.6 of the lecture notes: at the free motion of a particle, any component of its full angular momentum  $\mathbf{J} \equiv \mathbf{L} + \mathbf{S}$  is conserved.



$$[\hat{J}_j, \hat{H}] \equiv [\hat{L}_j + \hat{S}_j, \hat{H}] = [\hat{L}_j, \hat{H}] + [\hat{S}_j, \hat{H}] = i\hbar c \sum_{j', j''=1}^3 \hat{\alpha}_{j'} \hat{p}_{j''} \varepsilon_{jjj''} - i\hbar c \sum_{j', j''=1}^3 \hat{\alpha}_{j'} \hat{p}_{j''} \varepsilon_{jjj''} = \hat{0}.$$

Since all operators of  $J_j$  commute with the Hamiltonian, so do the operators of  $J_j^2$  and of  $J^2 = J_1^2 + J_2^2 + J_3^2$ . So, in contrast with the orbital momentum  $\mathbf{L}$ , the expectation values of all Cartesian components and of the square of the *total* angular momentum  $\mathbf{J} = \mathbf{L} + \mathbf{S}$  of a free particle are conserved in the Dirac theory.

**Problem 9.20.** In the Heisenberg picture of quantum dynamics, derive an equation describing the time evolution of a free electron's velocity in the Dirac theory. Solve the equation for the simplest state with definite energy and momentum, and interpret the oscillations (so-called *Zitterbewegung* or "trembling motion") appearing in the solution.

*Solution:* Let us start with finding what operator corresponds to the particle's velocity in the Dirac theory. With the Dirac Hamiltonian (9.97),

$$\hat{H} = c\hat{\boldsymbol{\alpha}} \cdot \hat{\mathbf{p}} + \hat{\beta} mc^2, \quad (*)$$

the Heisenberg equation (4.199) for the  $j^{\text{th}}$  Cartesian component of the electron's radius vector becomes

$$i\hbar \frac{d\hat{r}_j}{dt} = [\hat{r}_j, \hat{H}] \equiv [\hat{r}_j, c\hat{\boldsymbol{\alpha}} \cdot \hat{\mathbf{p}}] + [\hat{r}_j, \hat{\beta}] mc^2.$$

Operators  $\hat{\boldsymbol{\alpha}}$  and  $\hat{\beta}$ , which are defined in the Hilbert space of spin states, commute with the Cartesian coordinate operators, which are defined in the Hilbert space of orbital states, while the momentum operator in the Dirac theory is defined just in the non-relativistic quantum mechanics, and hence its Cartesian components obey the usual commutation relations (2.14). As a result, the second commutator in the last expression vanishes, while the first one is

$$[\hat{r}_j, c\hat{\boldsymbol{\alpha}} \cdot \hat{\mathbf{p}}] = \left[ \hat{r}_j, \sum_{j'=1}^3 c\hat{\alpha}_{j'} \hat{p}_{j'} \right] \equiv \sum_{j'=1}^3 c\hat{\alpha}_{j'} [\hat{r}_j, \hat{p}_{j'}] = \sum_{j'=1}^3 c\hat{\alpha}_{j'} i\hbar \delta_{jj'} = c\hat{\alpha}_j i\hbar.$$

So, for the particle's velocity, we get a very simple result:

$$\hat{v}_j \equiv \frac{d\hat{r}_j}{dt} = c\hat{\alpha}_j, \quad \text{i.e. } \hat{\mathbf{v}} \equiv \frac{d\hat{\mathbf{r}}}{dt} = c\hat{\boldsymbol{\alpha}}.$$

This is a formal confirmation of the conclusion, made in the lecture notes on the basis of a comparison of Eqs. (9.101) and (9.102), that the operator  $c\hat{\boldsymbol{\alpha}}$  corresponds to the particle's velocity.<sup>105</sup>

Now let us use the same Eqs. (4.199) and (9.97) to find the equation of motion of this operator – or rather its  $j^{\text{th}}$  Cartesian component:

<sup>105</sup> Still, please remember that in the spin Hilbert space, each Cartesian component of this operator is represented by a  $4 \times 4$  matrix (see Eqs. (9.98) of the lecture notes), and acts upon the 4-component bispinor (9.96), rather than on a scalar wavefunction as in the wave mechanics.

$$\begin{aligned}
i\hbar \frac{d\hat{v}_j}{dt} &= [\hat{v}_j, \hat{H}] = [c\hat{\alpha}_j, c\hat{\boldsymbol{\alpha}} \cdot \hat{\mathbf{p}}] + [c\hat{\alpha}_j, \hat{\beta}] mc^2 \equiv c^2 \sum_{j'=1}^3 [\hat{\alpha}_j, \hat{\alpha}_{j'}] \hat{p}_{j'} + c [\hat{\alpha}_j, \hat{\beta}] mc^2 \\
&\equiv c^2 \sum_{\substack{j'=1 \\ j' \neq j}}^3 (\hat{\alpha}_j \hat{\alpha}_{j'} - \hat{\alpha}_{j'} \hat{\alpha}_j) \hat{p}_{j'} + c (\hat{\alpha}_j \hat{\beta} - \hat{\beta} \hat{\alpha}_j) mc^2.
\end{aligned}$$

Using the anticommutation relations (9.99)-(9.100), we get

$$i\hbar \frac{d\hat{v}_j}{dt} = c^2 \sum_{\substack{j'=1 \\ j' \neq j}}^3 (2\hat{\alpha}_j \hat{\alpha}_{j'}) \hat{p}_{j'} + c (2\hat{\alpha}_j \hat{\beta}) mc^2 \equiv 2\hat{v}_j \left( \sum_{\substack{j'=1 \\ j' \neq j}}^3 c\hat{\alpha}_{j'} \hat{p}_{j'} + \hat{\beta} mc^2 \right). \quad (**)$$

Now by noticing that for an arbitrary choice of the index  $j$ , Eq. (\*) may be rewritten as

$$\hat{H} = \left( \sum_{\substack{j'=1 \\ j' \neq j}}^3 c\hat{\alpha}_{j'} \hat{p}_{j'} + \hat{\beta} mc^2 \right) + c\hat{\alpha}_j \hat{p}_j,$$

we may simplify Eq. (\*\*) as

$$i\hbar \frac{d\hat{v}_j}{dt} = 2\hat{v}_j (\hat{H} - c\hat{\alpha}_j \hat{p}_j) = 2\hat{v}_j \hat{H} - 2c^2 \hat{\alpha}_j \hat{\alpha}_j \hat{p}_j = 2\hat{v}_j \hat{H} - 2c^2 \hat{p}_j,$$

where for the last step, Eq. (9.99) was used again. Thus, we have obtained a simple equation for each of the three Cartesian components of the velocity; their set may be rewritten in the vector form:

$$i\hbar \frac{d\hat{\mathbf{v}}}{dt} = 2\hat{\mathbf{v}}\hat{H} - 2c^2 \hat{\mathbf{p}}. \quad (***)$$

For a free particle, the Hamiltonian and momentum operators do not depend on time. (The first fact follows from the Heisenberg equation of motion for *any* system with time-independent Hamiltonian, while the second one is obvious from Eq. (\*) because the momentum operator commutes with itself and both spin operators.) Hence a free Dirac particle may be placed into a simple state with definite and time-independent values of energy  $E$  and momentum  $\mathbf{p}$ . For such a state, Eq. (\*\*\*) becomes

$$i\hbar \frac{d\hat{\mathbf{v}}}{dt} = 2\hat{\mathbf{v}}E - 2c^2 \mathbf{p} \hat{I},$$

where the identity operator is in the Hilbert space of the particle's spin. This linear differential equation may be readily integrated, giving

$$\hat{\mathbf{v}}(t) = \frac{\mathbf{p}}{M} \hat{I} + \left( \hat{\mathbf{v}}(0) - \frac{\mathbf{p}}{M} \hat{I} \right) e^{-i\omega t}, \quad \text{with } M \equiv \frac{E}{c^2} \quad \text{and } \omega \equiv \frac{2E}{\hbar}. \quad (***)$$

So, on top of the constant velocity  $\mathbf{p}/M$  (where  $M$  is the relativistic, i.e. velocity-dependent mass), which might be expected for a free particle, the velocity operator performs sinusoidal oscillations. As Eq. (4.191) shows, this conclusion is valid for the expectation value  $\langle \mathbf{v} \rangle(t)$  of the particle's velocity (and as a result, of its spatial position) as well, unless the initial state is set up so that  $\langle \mathbf{v} \rangle(0)$  is exactly equal to  $\mathbf{p}/M$ .<sup>106</sup>

<sup>106</sup> An additional task for the reader: spell out how exactly such calculation of  $\langle \mathbf{v} \rangle(t)$  should be performed. Note a useful sanity check: since the velocity is an observable, the procedure should give a purely real function of time.

This curious effect of *Zitterbewegung* (German for “trembling motion”)<sup>107</sup> is essentially the “usual” quantum oscillations, with the frequency  $\omega = (E_1 - E_2)/\hbar$ , between two partial states of the particle, which were repeatedly discussed in this course starting from Sec. 2.6. In this particular case, one of the energies is that of the particle,  $E_1 = E$ , while another one is that of its antiparticle,  $E_2 = -E$  (see Fig. 9.6 in the lecture notes), so  $E_1 - E_2 = 2E$ . So, the oscillations may be interpreted as a result of the periodic conversion of the electron from the particle to its antiparticle (positron) and back.

Unfortunately, a direct experimental observation of this effect would require using either a very specific measurement tool or an intermediate agent (a photon or another particle/field) with its energy quantum  $\hbar\omega$  at least as high as  $2E$ , i.e. larger than  $2m_e c^2 \approx 1$  MeV. But such an agent, interacting with the original electron, may create multiple other electrons (the situation beyond the Dirac theory), which may mask the *Zitterbewegung*. As a result, to the best of my knowledge, this effect has not been directly observed yet – though a few of its close analogs have been.<sup>108</sup>

However, the *Zitterbewegung* effect finds its indirect confirmation in the existence of the so-called *Darwin term* (mentioned in Sec. 6.3 of the lecture notes)

$$\hat{H}_D = \frac{\hbar^2}{8m^2 c^2} \nabla^2 U$$

in the interaction of a relativistic particle with an external potential  $U(\mathbf{r})$ . In an atom, this term (non-vanishing only inside the nucleus) contributes to the fine-structure correction of the energies of  $s$ -states (with  $l = 0$  and hence with non-zero wavefunction values at  $r \rightarrow 0$ ), which is necessary for Eq. (6.60) to be valid for these states.

**Problem 9.21.** Calculate the energy spectrum of a relativistic spin- $\frac{1}{2}$  particle with an electric charge  $q$ , placed into a time-independent uniform external magnetic field  $\mathcal{B}$ . Compare the calculated spectrum with that following from the non-relativistic theory and the relativistic Schrödinger equation.

*Solution:* Let us look for the solution of the Dirac equation (9.112) for a particle in a time-independent magnetic field (i.e. for  $\phi = 0$ , but  $\mathbf{A} \neq 0$ ),

$$\left[ \hat{\boldsymbol{\alpha}} \cdot c(-i\hbar\nabla - q\mathbf{A}) + \hat{\beta}mc^2 - \hat{H} \right] \Psi = 0,$$

in the same form (9.125) as in Sec. 9.7 of the lecture notes:

$$\Psi(\mathbf{r}, t) = \begin{pmatrix} \psi_+(\mathbf{r}) \\ \psi_-(\mathbf{r}) \end{pmatrix} \exp\left(-i\frac{E}{\hbar}t\right).$$

where each of the elements  $\psi_{\pm}$  is a two-component column (spinor) of the type (9.123), representing two spin states of the particle (index  $+$ ) and the antiparticle (index  $-$ ). Plugging this solution into the Dirac equation, instead of Eqs. (9.126) of the lecture notes (which are valid in the opposite case when  $\phi \neq 0$  but  $\mathbf{A} = 0$ ), we get the following set of two equations:

<sup>107</sup> This feature of the Dirac theory was first revealed in 1930 by E. Schrödinger.

<sup>108</sup> See, e.g., R. Gerritsma *et al.*, *Nature* **463**, 68 (2010).

$$\begin{aligned}(E - mc^2)\psi_+ - c\hat{\boldsymbol{\sigma}} \cdot (-i\hbar\nabla - q\mathbf{A})\psi_- &= 0, \\ (E + mc^2)\psi_- - c\hat{\boldsymbol{\sigma}} \cdot (-i\hbar\nabla - q\mathbf{A})\psi_+ &= 0.\end{aligned}$$

Eliminating  $\psi_-$  from this system, we get the following equation for the particle's spinor:

$$\left\{ \left[ E^2 - (mc^2)^2 \right] - c^2 [\hat{\boldsymbol{\sigma}} \cdot (-i\hbar\nabla - q\mathbf{A})]^2 \right\} \psi_+ = 0. \quad (*)$$

Let us spell out the second term by using the fact that the Pauli operators (9.98) defined in the spin Hilbert space, and the momentum operator defined in the orbital Hilbert space, commute:

$$[\hat{\boldsymbol{\sigma}} \cdot (-i\hbar\nabla - q\mathbf{A})]^2 = \left[ \sum_{j=1}^3 \hat{\sigma}_j (-i\hbar\nabla_j - qA_j) \right]^2 = \sum_{j,j'=1}^3 \hat{\sigma}_j \hat{\sigma}_{j'} (-i\hbar\nabla_j - qA_j) (-i\hbar\nabla_{j'} - qA_{j'}),$$

where  $\nabla_j \equiv \partial/\partial r_j$ . Now by using the identity<sup>109</sup>

$$\hat{\sigma}_j \hat{\sigma}_{j'} = \hat{I} \delta_{jj'} + i \sum_{j''=1}^3 \hat{\sigma}_{j''} \varepsilon_{jjj''},$$

where  $\varepsilon_{jjj''}$  is the Levi-Civita symbol, we get

$$\begin{aligned}[\hat{\boldsymbol{\sigma}} \cdot (-i\hbar\nabla - q\mathbf{A})]^2 &= \sum_{j,j'=1}^3 \left( \hat{I} \delta_{jj'} + i \sum_{j''=1}^3 \hat{\sigma}_{j''} \varepsilon_{jjj''} \right) (-i\hbar\nabla_j - qA_j) (-i\hbar\nabla_{j'} - qA_{j'}) \\ &\equiv \sum_{j=1}^3 (-i\hbar\nabla_j - qA_j)^2 + i \sum_{j,j',j''=1}^3 \hat{\sigma}_{j''} (i\hbar\nabla_j + qA_j) (i\hbar\nabla_{j'} + qA_{j'}) \varepsilon_{jjj''} \\ &= (-i\hbar\nabla - q\mathbf{A})^2 - \hbar q \sum_{j''=1}^3 \hat{\sigma}_{j''} \sum_{j,j'=1}^3 (\nabla_j A_{j'}) \varepsilon_{jjj''}.\end{aligned}$$

However, according to Eq. (5.18), the last sum is just the  $(j'')$ <sup>th</sup> component of the vector  $\nabla \times \mathbf{A} \equiv \mathcal{B}$ , so

$$\begin{aligned}[\hat{\boldsymbol{\sigma}} \cdot (-i\hbar\nabla - q\mathbf{A})]^2 &= (-i\hbar\nabla - q\mathbf{A})^2 - \hbar q \sum_{j''=1}^3 \hat{\sigma}_{j''} \mathcal{B}_{j''} \\ &\equiv (-i\hbar\nabla - q\mathbf{A})^2 - \hbar q \hat{\boldsymbol{\sigma}} \cdot \mathcal{B} = (-i\hbar\nabla - q\mathbf{A})^2 - 2q \hat{\mathbf{S}} \cdot \mathcal{B},\end{aligned}$$

where the last step used the basic Eq. (4.116) for the spin- $1/2$  operator. Plugging this expression into Eq. (\*), and dividing all its terms by  $2mc^2$ , we may rewrite that equation as

$$-\frac{\hbar^2}{2m} \left( \nabla - i \frac{q}{\hbar} \mathbf{A} \right)^2 \psi_+ - \frac{q}{m} \hat{\mathbf{S}} \cdot \mathcal{B} \psi_+ = E_{\text{ef}} \psi_+, \quad (**)$$

where  $E_{\text{ef}} = p^2/2m$  is the same effective energy that appears in solutions of the relativistic Schrödinger equation:<sup>110</sup>

$$E_{\text{ef}} \equiv \frac{E^2 - (mc^2)^2}{2mc^2}. \quad (***)$$

<sup>109</sup> See, e.g., the solution of Problem 4.3.

<sup>110</sup> See the model solutions of Problems 14-16.

However, besides the replacement  $E \rightarrow E_{\text{ef}}$ , Eq. (\*\*) is the non-relativistic Schrödinger equation of a particle with the gyromagnetic ratio  $\gamma \equiv gq/2m = q/m$  (i.e., with the  $g$ -factor equal to exactly 2) in the magnetic field. As we know from the discussion in Chapters 3 and 5,<sup>111</sup> its energy spectrum consists of continuous bands, each corresponding to various values of the momentum  $p_z$  (where the  $z$ -axis is directed along the magnetic field), with discrete interband offsets due to the Landau-level quantization within the  $[x, y]$  plane, plus the spin orientation energy with the same energy spacing:<sup>112</sup>

$$E_{\text{ef}} = \frac{p_z^2}{2m} + \hbar\omega_c \left( n + \frac{1}{2} - m_s \operatorname{sgn} q \right),$$

with

$$-\infty < p_z < +\infty, \quad \omega_c \equiv \frac{|q\mathcal{B}|}{m}, \quad n = 0, 1, 2, \dots, \quad \text{and } m_s = \pm 1/2.$$

So, to get the spectrum of the genuine relativistic energy  $E$ , we need just to plug this result into the relation that follows from Eq. (\*\*\*):

$$E = \pm mc^2 \left( 1 + \frac{2E_{\text{ef}}}{mc^2} \right)^{1/2}.$$

In the non-relativistic limit, this recalculation becomes trivial:

$$E \approx \pm (mc^2 + E_{\text{ef}}), \quad \text{at } E_{\text{ef}} \ll mc^2.$$

On the other hand, as has been shown in the solution of Problem 14, the analysis of the same situation using the relativistic Schrödinger equation gives for  $E_{\text{ef}}$  (and hence for  $E$ ) a similar spectrum but without the  $m_s$ -term describing the spin.

**Problem 9.22.\*** Following the discussion at the end of Section 9.7 of the lecture notes, introduce quantum field operators  $\hat{\psi}$  that would be related to the usual wavefunctions  $\psi$  just as the electromagnetic field operators (9.16) are related to the classical EM fields, and explore the basic properties of these operators. (For this preliminary study, consider the fixed-time situation.)

*Solution:* In an analogy with Eqs. (9.16) of the lecture notes but taking into account the scalar nature of the “matter field” (wavefunction)  $\psi$ , we may define the field operator and its Hermitian conjugate as

$$\hat{\psi}(\mathbf{r}) \equiv \sum_j \psi_j(\mathbf{r}) \hat{a}_j, \quad \hat{\psi}^\dagger(\mathbf{r}) \equiv \sum_j \psi_j^*(\mathbf{r}) \hat{a}_j^\dagger.$$

Here  $\psi_j(\mathbf{r})$  are members of some full, orthonormal set of single-particle wavefunctions of a multiparticle system (where the index  $j$  numbers both the orbital and spin degrees of freedom),<sup>113</sup> while  $\hat{a}_j^\dagger$  and  $\hat{a}_j$  are the particle creation and annihilation operators discussed in Secs. 8.3-8.4 of the lecture notes.

<sup>111</sup> See, in particular, the model solutions of Problem 5.50.

<sup>112</sup> As Eq. (\*\*) shows, the eigenstates of the relativistic problem are also similar to those of the corresponding non-relativistic problem.

<sup>113</sup> When dealing with free (or nearly free) particles, the natural and hence a very popular choice of the base functions  $\psi_j(\mathbf{r})$  is the plane waves  $\psi_{\mathbf{k}}(\mathbf{r}) \propto \exp\{i\mathbf{k}\cdot\mathbf{r}\}$ . (Since their spectrum is continuous, the summation over  $j$  in

Let us explore the properties of the state (called, say,  $\alpha$ ) that is created by the action of the operator  $\hat{\psi}^\dagger(\mathbf{r})$  upon the vacuum Dirac state:

$$|\alpha\rangle = \hat{\psi}^\dagger(\mathbf{r})|0,0,\dots,0\rangle \equiv \sum_j \psi_j^*(\mathbf{r}) \hat{a}_j^\dagger |0,0,\dots,0\rangle = \sum_j \psi_j^*(\mathbf{r}) |0,0,\dots,1_j,\dots,0\rangle.$$

The last ket describes a single particle in the state number  $j$ , so we may represent it just as  $|j\rangle$ , and rewrite the above relation as

$$|\alpha\rangle = \sum_j \psi_j^*(\mathbf{r}) |j\rangle. \quad (*)$$

Let us calculate the wavefunction  $\psi_\alpha(\mathbf{r}')$  of this single-particle state at some arbitrary point  $\mathbf{r}'$ , for now not necessarily equal to the argument  $\mathbf{r}$  of the field operator. The obvious 3D generalization of the definition (4.233) of the wavefunction, in the single-particle representation, is<sup>114</sup>

$$\psi_\alpha(\mathbf{r}') = \langle \mathbf{r}' | \alpha \rangle, \quad \text{while } \psi_j^*(\mathbf{r}) = \langle \mathbf{r} | j \rangle^* = \langle j | \mathbf{r} \rangle. \quad (**)$$

Now combining Eqs. (\*) and (\*\*), we get

$$\psi_\alpha(\mathbf{r}') = \langle \mathbf{r}' | \sum_j \langle j | \mathbf{r} \rangle | j \rangle \equiv \langle \mathbf{r}' | \sum_j | j \rangle \langle j | \mathbf{r} \rangle.$$

Using the closure relation (4.44), and the evident 3D generalization of Eq. (4.231), we get

$$\psi_\alpha(\mathbf{r}') = \langle \mathbf{r}' | \hat{I} | \mathbf{r} \rangle \equiv \langle \mathbf{r}' | \mathbf{r} \rangle = \delta(\mathbf{r} - \mathbf{r}').$$

This means that the operator  $\hat{\psi}^\dagger(\mathbf{r})$ , acting upon the free space, creates a particle localized definitely at point  $\mathbf{r}$ . An absolutely similar calculation shows that its Hermitian conjugate, the operator  $\hat{\psi}(\mathbf{r})$ , annihilates a particle at this location. This is very natural because the field operators are just the sums of the creation/annihilation operators weighed by the wavefunctions of the corresponding states.

In contrast to these general properties, the commutation relations of the field operators depend on whether we are dealing with bosons or fermions. In the former case, we may use Eqs. (8.75)-(8.76) of the lecture notes to get, for example,

$$\left[ \hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}') \right] = \sum_{jj'} \psi_j(\mathbf{r}) \psi_{j'}^*(\mathbf{r}') \left[ \hat{a}_j, \hat{a}_{j'}^\dagger \right] = \sum_{jj'} \psi_j(\mathbf{r}) \psi_{j'}^*(\mathbf{r}') \hat{I} \delta_{jj'} = \sum_j \psi_j(\mathbf{r}) \psi_j^*(\mathbf{r}') \hat{I}.$$

Now using Eqs. (\*\*), with the argument replacements  $\mathbf{r} \leftrightarrow \mathbf{r}'$ , we may complete this calculation as

$$\left[ \hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}') \right] = \sum_j \langle \mathbf{r} | j \rangle \langle j | \mathbf{r}' \rangle \hat{I} = \hat{I} \delta(\mathbf{r} - \mathbf{r}').$$

Acting absolutely similarly, for the bosonic operators we may also get

the above formulas is then replaced with the integration over the 3D space of the wave vectors  $\mathbf{k}$ , plus the summation over the involved spin states.)

<sup>114</sup> Since all calculations in this solution are for a fixed moment of time, the wavefunction may be denoted as  $\psi$ , rather than  $\Psi$  in Eq. (4.233).

$$[\hat{\psi}(\mathbf{r}), \hat{\psi}(\mathbf{r}')] = [\hat{\psi}^\dagger(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')] = \hat{0},$$

while for the fermionic operators, Eqs. (8.95)-(8.96) of the lecture notes yield similar relations for the anticommutators:

$$\{\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')\} = \hat{I}\delta(\mathbf{r} - \mathbf{r}'), \quad \{\hat{\psi}(\mathbf{r}), \hat{\psi}(\mathbf{r}')\} = \{\hat{\psi}^\dagger(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')\} = \hat{0}.$$

Next, let us consider the following operator integral,

$$\hat{F} \equiv \int \hat{\psi}^\dagger(\mathbf{r}) \hat{f}(\mathbf{r}) \hat{\psi}(\mathbf{r}) d^3r, \quad (***)$$

where  $\hat{f}(\mathbf{r})$  is a single-particle operator. Plugging into this expression the field operator definitions, we obtain

$$\hat{F} = \sum_{j,j'} \hat{a}_j^\dagger \hat{a}_{j'} \int \psi_{j'}^*(\mathbf{r}) \hat{f}(\mathbf{r}) \psi_j(\mathbf{r}) d^3r \equiv \sum_{j,j'} f_{jj'} \hat{a}_j^\dagger \hat{a}_{j'}.$$

where  $f_{jj'}$  are the usual matrix elements of the operator  $\hat{f}$ . But the last expression exactly coincides with the right-hand side of Eq. (8.87) of the lecture notes; hence the integral (\*\*\*) is an equivalent representation of the similar single-particle components:

$$\hat{F} = \sum_{k=1}^N \hat{f}(\mathbf{r}_k).$$

The most important particular cases of such operators are those of the full momentum and the full kinetic energy of the system, which are equal to, respectively,

$$\hat{P} \equiv \sum_{k=1}^N \hat{p}_k = -i\hbar \sum_{k=1}^N \nabla_k, \quad \text{and} \quad \hat{T} \equiv -\frac{\hbar^2}{2m} \sum_{k=1}^N \nabla_k^2$$

in the “usual” (particle-number) representation, where  $m$  is the mass of a *single* particle.<sup>115</sup> According to Eq. (\*\*\*), in the second-quantization language, these operators may be represented as

$$\hat{P} = -i\hbar \int \hat{\psi}^\dagger(\mathbf{r}) \nabla \hat{\psi}(\mathbf{r}) d^3r \quad \text{and} \quad \hat{T} = -\frac{\hbar^2}{2m} \int \hat{\psi}^\dagger(\mathbf{r}) \nabla^2 \hat{\psi}(\mathbf{r}) d^3r.$$

Very similarly, the pair-interaction operators of the type (8.113),

$$\hat{U}_{\text{int}} = \frac{1}{2} \sum_{\substack{k,k'=1 \\ k \neq k'}}^N \hat{u}_{\text{int}}(\mathbf{r}_k, \mathbf{r}_{k'}),$$

may be expressed via the field operators as

$$\hat{U}_{\text{int}} = \frac{1}{2} \int d^3r \int d^3r' \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') \hat{u}_{\text{int}}(\mathbf{r}, \mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}). \quad (***)$$

Using the relations (\*\*\*) and (\*\*\*), one may express the Hamiltonians of many important models of interacting particle systems via the field operators. After that, the equations of motion of these

<sup>115</sup> A useful (and simple :-)) optional exercise for the reader: explore how these operators commute with the field operators, separately for bosons and fermions.

operators (for example, in the Heisenberg picture) may be obtained and analyzed, forming the fabric of the quantum field theory. Evidently, the most important new feature of such theory, in comparison with the plain-vanilla quantum mechanics discussed in this course, is its ability to describe, in a natural way, the creation and annihilation of particles – just as the creation and annihilation of photons were studied in Secs. 9.2-9.4. These phenomena are most significant at particle energies higher than  $2mc^2$  but also show up as small corrections to the results of the “usual” (particle-number-conserving) quantum mechanics at lower energies.



## Chapter 10. Making Sense of Quantum Mechanics

10.1.\* The original (circa 1964) J. Bell's inequality was derived for the results of SG measurements performed on two non-interacting particles with zero net spin, by using the following local-reality-based assumption: the result of each single-particle measurement is uniquely determined (besides the experimental setup) by some  $c$ -number hidden parameter  $\lambda$  that may be random, i.e. change from experiment to experiment. Derive such inequality for the experiment shown in Fig. 10.4 of the lecture notes and compare it with the corresponding quantum-mechanical result for the singlet state (10.24).

*Solution:* Let us calculate the statistical average  $\langle s_1(\mathbf{a})s_2(\mathbf{b}) \rangle$ , where  $s_1(\mathbf{a})$  is the component of the spin of the first particle along some direction  $\mathbf{a}$ , and  $s_2(\mathbf{b})$  is the similar projection of the second particle's spin on another direction,  $\mathbf{b}$ . If we accept the hidden-variable assumption described in the assignment, then we may write

$$\langle s_1(\mathbf{a})s_2(\mathbf{b}) \rangle = \int s_1(\mathbf{a}, \lambda)s_2(\mathbf{b}, \lambda)\rho(\lambda)d\lambda, \quad (*)$$

where  $\rho(\lambda) \geq 0$  is the normalized probability density of the random hidden parameter  $\lambda$ , with

$$\int \rho(\lambda)d\lambda = 1, \quad (**)$$

and the integration is over the whole range of possible values of this parameter. Since the total spin of the pair is definitely zero,  $s_2(\mathbf{b}, \lambda)$  has to be equal to  $-s_1(\mathbf{b}, \lambda)$ , so that we may rewrite Eq. (\*) as

$$\langle s_1(\mathbf{a})s_2(\mathbf{b}) \rangle = -\int s_1(\mathbf{a}, \lambda)s_1(\mathbf{b}, \lambda)\rho(\lambda)d\lambda.$$

Now let us write a similar expression for  $\langle s_1(\mathbf{a})s_2(\mathbf{c}) \rangle$ , where  $\mathbf{c}$  is one more direction, and subtract them:

$$\langle s_1(\mathbf{a})s_2(\mathbf{b}) \rangle - \langle s_1(\mathbf{a})s_2(\mathbf{c}) \rangle = -\int s_1(\mathbf{a}, \lambda)[s_1(\mathbf{b}, \lambda) - s_1(\mathbf{c}, \lambda)]\rho(\lambda)d\lambda.$$

Next, let each measured value of  $s_1$  have only two equal and opposite possible values – just as it is the case for any spin- $\frac{1}{2}$ . If (just for the notation simplicity) we measure these values in the units of  $\hbar/2$ , then  $s_1 = \pm 1$ , i.e.  $(s_1)^2 = 1$ . So we can multiply the second term in the square brackets in the last displayed expression by  $s_1(\mathbf{b}, \lambda)s_1(\mathbf{b}, \lambda) = 1$ , and rewrite it as

$$\langle s_1(\mathbf{a})s_2(\mathbf{b}) \rangle - \langle s_1(\mathbf{a})s_2(\mathbf{c}) \rangle = -\int s_1(\mathbf{a}, \lambda)s_1(\mathbf{b}, \lambda)[1 - s_1(\mathbf{b}, \lambda)s_1(\mathbf{c}, \lambda)]\rho(\lambda)d\lambda.$$

But since  $-1 \leq s_1(\mathbf{a}, \lambda)s_1(\mathbf{b}, \lambda) \leq +1$ , and  $-1 \leq s_1(\mathbf{b}, \lambda)s_1(\mathbf{c}, \lambda) \leq +1$  as well, i.e.  $[1 - s_1(\mathbf{b}, \lambda)s_1(\mathbf{c}, \lambda)] \geq 0$ , while  $\rho(\lambda) \geq 0$  by definition, we may write

$$|\langle s_1(\mathbf{a})s_2(\mathbf{b}) \rangle - \langle s_1(\mathbf{a})s_2(\mathbf{c}) \rangle| \leq \int [1 - s_1(\mathbf{b}, \lambda)s_1(\mathbf{c}, \lambda)]\rho(\lambda)d\lambda \equiv \int \rho(\lambda)d\lambda - \int s_1(\mathbf{c}, \lambda)s_1(\mathbf{b}, \lambda)\rho(\lambda)d\lambda.$$

Now by using Eq. (\*\*), the equality  $s_1(\mathbf{c}, \lambda) = -s_2(\mathbf{c}, \lambda)$ , and then the definition of  $\langle s_1(\mathbf{b}, \lambda)s_2(\mathbf{c}, \lambda) \rangle$  similar to the one given by Eq. (\*), we get the original Bell's inequality:

$$\left| \langle s_1(\mathbf{a})s_2(\mathbf{b}) \rangle - \langle s_1(\mathbf{a})s_2(\mathbf{c}) \rangle \right| \leq 1 + \langle s_1(\mathbf{b})s_2(\mathbf{c}) \rangle. \quad (***)$$

While its derivation (in contrast to E. Wigner's version described in Sec. 10.3 of the lecture notes) requires explicit use of the parameter  $\lambda$ , whose randomness is intended to explain the intrinsic uncertainty of measurement results in quantum mechanics, the made assumptions are still so natural that it is hard to imagine a more general hidden-parameter theory.

Now let us see whether the predictions of quantum mechanics satisfy Eq. (\*\*\*) for the simple geometry shown in Fig. 10.4. For a pure entangled state such as the singlet (10.24), the average of  $s_1(\mathbf{a})s_2(\mathbf{b})$ , i.e. its expectation value, may be calculated as

$$\langle s_1(\mathbf{a})s_2(\mathbf{b}) \rangle = \langle s_{12} | \hat{P}_1(\mathbf{a})\hat{P}_2(\mathbf{b}) | s_{12} \rangle = \frac{1}{2} \left( \langle \uparrow\downarrow | - \langle \downarrow\uparrow | \right) \hat{P}_1(\mathbf{a})\hat{P}_2(\mathbf{b}) \left( | \uparrow\downarrow \rangle - | \downarrow\uparrow \rangle \right), \quad (***)$$

where each  $\hat{P}(\mathbf{n})$  is the single-particle projection operator

$$\hat{P}(\mathbf{n}) = \hat{\boldsymbol{\sigma}} \cdot \mathbf{n} = n_x \hat{\sigma}_x + n_y \hat{\sigma}_y + n_z \hat{\sigma}_z,$$

and  $\mathbf{n}$  is a unit vector that may point in any of the three directions  $\mathbf{a}$ ,  $\mathbf{b}$ , and  $\mathbf{c}$ . In our case (Fig. 10.4) when all the directions are in the same plane, we may take their azimuthal angles for zero, so that  $n_x = \sin\theta$ ,  $n_y = 0$ ,  $n_z = \cos\theta$ , and in the usual  $z$ -basis, the operator's matrix elements are

$$\langle \uparrow | \hat{P}(\mathbf{n}) | \uparrow \rangle = \cos\theta, \quad \langle \uparrow | \hat{P}(\mathbf{n}) | \downarrow \rangle = \langle \downarrow | \hat{P}(\mathbf{n}) | \uparrow \rangle = \sin\theta, \quad \langle \downarrow | \hat{P}(\mathbf{n}) | \downarrow \rangle = -\cos\theta.$$

Using these expressions, we may readily calculate any of the four averages arising at opening the parentheses in Eq. (\*\*\*), for example

$$\langle \uparrow\downarrow | \hat{P}_1(\mathbf{a})\hat{P}_2(\mathbf{b}) | \uparrow\downarrow \rangle = \langle \uparrow | \hat{P}_1(\mathbf{a}) | \uparrow \rangle \langle \downarrow | \hat{P}_2(\mathbf{b}) | \downarrow \rangle = -\cos\theta_a \cos\theta_b, \quad \text{etc.}$$

The final result is

$$\langle s_1(\mathbf{a})s_2(\mathbf{b}) \rangle = \frac{1}{2} (-2\cos\theta_a \cos\theta_b - 2\sin\theta_a \sin\theta_b) \equiv -\cos(\theta_a - \theta_b)$$

(very naturally depending only on the angle between the directions  $\mathbf{a}$  and  $\mathbf{b}$ , but not on their orientation relative to the  $z$ -axis), with similar expressions for  $\langle s_1(\mathbf{b})s_2(\mathbf{c}) \rangle$  and  $\langle s_1(\mathbf{a})s_2(\mathbf{c}) \rangle$ , so that in the simple case shown in Fig. 10.4,

$$\langle s_1(\mathbf{a})s_2(\mathbf{b}) \rangle = -\cos 2\varphi, \quad \langle s_1(\mathbf{b})s_2(\mathbf{c}) \rangle = \langle s_1(\mathbf{a})s_2(\mathbf{c}) \rangle = -\cos\varphi.$$

These results show that the hidden-variable-based Bell's inequality (\*\*\*) is *not* satisfied at  $\varphi \leq \pi/2$ ; for example, at  $\varphi \ll 1$ , its left-hand side,

$$\left| \langle s_1(\mathbf{a})s_2(\mathbf{b}) \rangle - \langle s_1(\mathbf{a})s_2(\mathbf{c}) \rangle \right| = | -\cos 2\varphi + \cos\varphi | \approx \frac{3}{2}\varphi^2,$$

is larger rather than smaller than its right-hand side

$$1 + \langle s_1(\mathbf{b})s_2(\mathbf{c}) \rangle = 1 - \cos\varphi \approx \frac{1}{2}\varphi^2,$$

leading to the same conclusions as the version discussed in the lecture notes.