Chapter 9. Introduction to Relativistic Quantum Mechanics

This chapter consists of two very different parts. Its first part is a discussion of the basic elements of the quantum theory of the electromagnetic field, usually called quantum electrodynamics (QED). We will see, in particular, that the QED may be viewed as the relativistic quantum theory of particles with zero rest mass – photons. The second part of the chapter is a brief review of the relativistic quantum theory of particles with non-zero rest mass, including the famous Dirac's theory of spin-½ particles such as electrons. These theories mark the point of entry into a more complete relativistic quantum theory – the quantum field theory – which is beyond the scope of this course.

9.1. Electromagnetic field quantization[1]

Classical physics gives us[2] the following general relativistic relation between the momentum **p** and energy E of a free particle with rest mass m, which may be simplified in two limits – non-relativistic and ultra-relativistic:

Free particle's relativistic energy

$$E = \left[(pc)^2 + (mc^2)^2\right]^{1/2} \to \begin{cases} mc^2 + p^2/2m, & \text{for } p << mc, \\ pc, & \text{for } p >> mc. \end{cases} \tag{9.1}$$

In both limits, the transfer from classical to quantum mechanics is easier than in the arbitrary case. Since all the previous contents of this course were committed to the first, non-relativistic limit, I will now jump to a brief discussion of the ultra-relativistic limit $p >> mc$, for a particular but very important system – the electromagnetic field. Since the excitations of this field, called *photons*, are currently believed to have zero rest mass m,[3] the ultra-relativistic relation $E = pc$ is exactly valid for any photon energy E, and the quantization scheme is rather straightforward.

As usual, the quantization has to be based on the classical theory of the system – in this case, the Maxwell equations. As the simplest case, let us consider the electromagnetic field inside a finite free-space volume limited by ideal walls, which reflect incident waves perfectly.[4] Inside the volume, the Maxwell equations give a simple wave equation[5] for the electric field

$$\nabla^2 \mathscr{E} - \frac{1}{c^2}\frac{\partial^2 \mathscr{E}}{\partial t^2} = 0, \tag{9.2}$$

and an absolutely similar equation for the magnetic field $\mathscr{B}$. We may look for the general solution of Eq. (2) in the variable-separating form

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[1] The described approach was pioneered by the same P. A. M. Dirac as early as 1927.

[2] See, e.g., EM Chapter 9, in particular Eq. (9.78).

[3] By now, this fact has been verified experimentally with an accuracy of at least 10^{-18} eV/c^2, i.e. ~10^{-24} m_e – see, e.g. the review by C. Amsler *et al. (Particle Data Group), Phys. Lett. B* **667**, 1 (2008).

[4] In the case of finite energy absorption in the walls, or in the wave propagation media, the system is not energy-conserving (Hamiltonian), i.e. interacts with a dissipative environment as was discussed in Chapter 7. Specific cases of such interaction will be considered in Sections 2 and 3 below.

[5] See, e.g., EM Eq. (7.3), for the particular case $\varepsilon = \varepsilon_0$, $\mu = \mu_0$, so $v^2 \equiv 1/\varepsilon\mu = 1/\varepsilon_0\mu_0 \equiv c^2$.

$$\mathscr{E}(\mathbf{r},t)=\sum_j \mathscr{E}_j(\mathbf{r},t), \quad \text{with } \mathscr{E}_j(\mathbf{r},t)=p_j(t)\mathbf{e}_j(\mathbf{r}). \tag{9.3}$$

Physically, each term of this sum is a standing wave whose spatial distribution and polarization ("*mode*") are described by the vector function $\mathbf{e}_j(\mathbf{r})$, while its temporal dynamics follows the function $p_j(t)$. Plugging an arbitrary term of this sum into Eq. (2), and separating the variables exactly as we did, for example, in the Schrödinger equation in Sec. 1.5, we get

$$\frac{\nabla^2\mathbf{e}_j}{\mathbf{e}_j}=\frac{1}{c^2}\frac{\ddot{p}_j}{p_j}=\text{const}\equiv -k_j^2, \tag{9.4}$$

so the spatial distribution of the mode satisfies the following 3D Helmholtz equation:

$$\boxed{\nabla^2\mathbf{e}_j+k_j^2\mathbf{e}_j=0.} \tag{9.5}$$

Equation for spatial distribution

The set of solutions of this equation, with appropriate boundary conditions, determines the set of the functions $\mathbf{e}_j$, and simultaneously the spectrum of the wave number magnitudes k_j. The latter values determine the mode eigenfrequencies, following from Eq. (4):

$$\ddot{p}_j+\omega_j^2 p_j=0, \quad \text{with } \omega_j\equiv k_j c. \tag{9.6}$$

There is a big philosophical difference between the quantum-mechanical approach to Eqs. (5) and (6), despite their single origin (4). The first (Helmholtz) equation may be rather difficult to solve in realistic geometries,[6] but it remains intact in the basic quantum electrodynamics, with the scalar components of the vector functions $\mathbf{e}_j(\mathbf{r})$ still treated (at each point $\mathbf{r}$) as *c*-numbers. In contrast, the classical Eq. (6) is readily solvable (giving sinusoidal oscillations with frequency ω_j), but this is exactly where we can make the transfer to quantum mechanics because we already know how to quantize a mechanical 1D harmonic oscillator, which in classics obeys the same equation.

As usual, we need to start with the appropriate Hamiltonian – the operator corresponding to the classical Hamiltonian function H of the proper set of generalized coordinates and momenta. The electromagnetic field's Hamiltonian function (which in this case coincides with the field's energy) is[7]

$$H=\int d^3r\left(\frac{\varepsilon_0\mathscr{E}^2}{2}+\frac{\mathscr{B}^2}{2\mu_0}\right). \tag{9.7}$$

Let us represent the magnetic field in a form similar to Eq. (3),[8]

$$\mathscr{B}(\mathbf{r},t)=\sum_j \mathscr{B}_j(\mathbf{r},t), \quad \text{with } \mathscr{B}_j(\mathbf{r},t)=-\omega_j q_j(t)\mathbf{b}_j(\mathbf{r}). \tag{9.8}$$

[6] See, e.g., the cases discussed in EM Sec. 7.9.

[7] See, e.g., EM Sec. 9.8, in particular, Eq. (9.225). Here I am using SI units, with $\varepsilon_0\mu_0\equiv c^{-2}$; in the Gaussian units, the coefficients ε_0 and μ_0 disappear, but there is an additional common factor $1/4\pi$ in the formula H. However, if we modify the normalization conditions (see below) accordingly, all the subsequent results, starting from Eq. (10), look similar in any system of units.

[8] Here I am using the letter q_j, instead of x_j, for the generalized coordinate of the field oscillator, in order to emphasize the difference between the former variable and one of the Cartesian coordinates, i.e. one of the arguments of the *c*-number functions $\mathbf{e}_j(\mathbf{r})$ and $\mathbf{b}_j(\mathbf{r})$.

Since, according to the Maxwell equations, in our case, the magnetic field satisfies the equation similar to Eq. (2), the time-dependent amplitude q_j of each of its modes $\mathbf{b}_j(\mathbf{r})$ obeys an equation similar to Eq. (6), i.e. in the classical theory also changes in time sinusoidally, with the same frequency ω_j. Plugging Eqs. (3) and (8) into Eq. (7), we may recast it as

$$H = \sum_j \left[\frac{p_j^2}{2} \int \varepsilon_0 e_j^2(\mathbf{r}) d^3 r + \frac{\omega_j^2 q_j^2}{2} \int \frac{1}{\mu_0} b_j^2(\mathbf{r}) d^3 r \right]. \tag{9.9}$$

Now note that the distribution of constant factors between two operands in each product of Eq. (3) is so far arbitrary, so we may fix it by requiring the first integral in Eq. (9) to equal 1. Since according to the Maxwell equations, there is a specific relation between the field vector amplitudes, $\mathscr{B}_j/\mathscr{E}_j = (\varepsilon_0\mu_0)^{1/2} \equiv 1/c$,[9] this normalization makes the second integral in Eq. (9) equal 1 as well, and Eq. (9) becomes

$$H = \sum_j H_j, \qquad H_j = \frac{p_j^2}{2} + \frac{\omega_j^2 q_j^2}{2}. \tag{9.10}$$

Note that p_j is the legitimate generalized momentum corresponding to the generalized coordinate q_j, because it is equal to $\partial L / \partial \dot{q}_j$, where L is the Lagrangian function of the field – see EM Eq. (9.217):

$$L = \int d^3 r \left(\frac{\varepsilon_0 \mathscr{E}^2}{2} - \frac{\mathscr{B}^2}{2\mu_0} \right) = \sum_j L_j, \qquad L_j = \frac{p_j^2}{2} - \frac{\omega_j^2 q_j^2}{2}. \tag{9.11}$$

Hence we can carry out the standard quantization procedure, namely declare H_j, p_j, and q_j to be quantum-mechanical operators related as in Eq. (10),

Electro-magnetic mode's Hamiltonian

$$\hat{H}_j = \frac{\hat{p}_j^2}{2} + \frac{\omega_j^2 \hat{q}_j^2}{2}. \tag{9.12}$$

We see that this Hamiltonian coincides with that of a 1D harmonic oscillator with the mass m_j formally equal to 1,[10] and the frequency equal to ω_j. Moreover, since the Lagrangian function L has the same form (11) as in a set of independent harmonic oscillators with coordinates q_j and momenta p_j, the corresponding operators satisfy the following natural generalization of the commutation relations (2.14):

$$\left[\hat{q}_j, \hat{p}_{j'}\right] = i\hbar \delta_{jj'}, \tag{9.13}$$

As the reader already knows, Eqs. (12) and (13) open for us several alternative ways to proceed:

(i) Use the Schrödinger-picture wave mechanics based on wavefunctions $\Psi_j(q_j, t)$. As we know from Sec. 2.9, this way is inconvenient for most tasks, because the eigenfunctions of the harmonic oscillator are rather clumsy.

(ii) A substantially more efficient way is to write and use the Heisenberg-picture equations for the time evolution of the operators $\hat{q}_j(t)$ and $\hat{p}_j(t)$.

[9] See, e.g., EM Eqs. (7.6)-(7.7) with $\varepsilon = \varepsilon_0$, $\mu = \mu_0$, and $\mathscr{H} = \mathscr{B}/\mu_0$.

[10] Selecting a different normalization of the function $\mathbf{e}_j(\mathbf{r})$, we could readily arrange any value of m_j, so the choice corresponding to $m_j = 1$ is the best one just for the notation simplicity.

(iii) An even more convenient approach is to use equations similar to Eqs. (5.65) to decompose the Heisenberg operators $\hat{q}_j(t)$ and $\hat{p}_j(t)$ into the creation-annihilation operators $\hat{a}_j^\dagger(t)$ and $\hat{a}_j(t)$.

In this chapter, I will mostly use the last route. After the replacement of m with $m_j \equiv 1$, and ω_0 with ω_j, the last forms of Eqs. (5.65) become

$$\hat{a}_j = \left(\frac{\omega_j}{2\hbar}\right)^{1/2}\left(\hat{q}_j + i\frac{\hat{p}_j}{\omega_j}\right), \qquad \hat{a}_j^\dagger = \left(\frac{\omega_j}{2\hbar}\right)^{1/2}\left(\hat{q}_j - i\frac{\hat{p}_j}{\omega_j}\right). \tag{9.14}$$

Due to Eq. (13), these creation-annihilation operators obey the commutation similar to Eq. (5.68),

$$\left[\hat{a}_j, \hat{a}_{j'}^\dagger\right] = \hat{I}\delta_{jj'}. \tag{9.15}$$

As a result, according to Eqs. (3) and (8), the quantum-mechanical operators of the electric and magnetic fields may be represented as sums over all *field oscillators*:

$$\hat{\mathscr{E}}(\mathbf{r},t) = i\sum_j \left(\frac{\hbar\omega_j}{2}\right)^{1/2} \mathbf{e}_j(\mathbf{r})\left(\hat{a}_j^\dagger - \hat{a}_j\right), \tag{9.16a}$$

$$\hat{\mathscr{B}}(\mathbf{r},t) = \sum_j \left(\frac{\hbar\omega_j}{2}\right)^{1/2} \mathbf{b}_j(\mathbf{r})\left(\hat{a}_j^\dagger + \hat{a}_j\right), \tag{9.16b}$$

Electro-magnetic field operators

and Eq. (12) for the j^{th} mode's Hamiltonian becomes

$$\hat{H}_j = \hbar\omega_j\left(\hat{a}_j^\dagger\hat{a}_j + \frac{1}{2}\hat{I}\right) = \hbar\omega_j\left(\hat{n}_j + \frac{1}{2}\hat{I}\right), \quad \text{with } \hat{n}_j \equiv \hat{a}_j^\dagger\hat{a}_j, \tag{9.17}$$

absolutely similar to Eq. (5.72) for a mechanical oscillator.

Now comes a very important conceptual step. From Sec. 5.4, we know that the stationary (Fock) states n_j of the Hamiltonian (17) have energies

$$E_j = \hbar\omega_j\left(n_j + \frac{1}{2}\right), \quad n_j = 0,1,2,... \tag{9.18}$$

Electro-magnetic mode eigen-energies

and, according to Eq. (5.89), the operators $\hat{a}_j^\dagger$ and $\hat{a}_j$ act on the eigenkets of these partial states as

$$\hat{a}_j|n_j\rangle = (n_j)^{1/2}|n_j - 1\rangle, \qquad \hat{a}_j^\dagger|n_j\rangle = (n_j+1)^{1/2}|n_j+1\rangle, \tag{9.19}$$

regardless of the quantum states of other modes. These rules coincide with the definitions (8.64) and (8.68) of bosonic creation-annihilation operators, and hence their action may be considered as the creation/annihilation of certain bosons. Such a *quasiparticle* (actually, an *excitation*, with energy $\hbar\omega_j$, of the j^{th} field oscillator) is exactly what is, strictly speaking, called a *photon*. Note immediately that according to Eq. (16), such an excitation does not change the spatial distribution of the j^{th} mode of the field. So, such a "global" photon is an excitation created simultaneously at all points of the field confinement region.

If this picture is too contrary to the intuitive image of a particle, please recall that in Chapter 2, we discussed a similar situation with the fundamental solutions $\exp\{\pm ikx\}$ of the Schrödinger equation of a free non-relativistic particle: they represent sinusoidal de Broglie waves existing simultaneously at

all points of the particle confinement region. The (partial :-) reconciliation with the classical picture of a moving particle might be obtained by using the linear superposition principle to assemble a quasi-localized wave packet, as a group of sinusoidal waves with close wave numbers. Very similarly, we may form a similar wave packet using a linear superposition of the "global" photons with close values of $\mathbf{k}_j$ (and hence ω_j), to form a quasi-localized photon. An additional simplification here is that the dispersion relation for electromagnetic waves (at least in free space) is linear:

$$\frac{\partial \omega_j}{\partial k_j} = c = \text{const}, \qquad \text{i.e. } \frac{\partial^2 \omega_j}{\partial k_j{}^2} = 0, \tag{9.20}$$

so according to Eq. (2.39a), the electromagnetic wave packets (i.e. space-localized photons) do not spread out during their propagation. Note also that due to the fundamental classical relations $\mathbf{p} = \mathbf{n}E/c$ for the linear momentum of the traveling electromagnetic wave packet of energy E, propagating along the direction $\mathbf{n} \equiv \mathbf{k}/k$, and $\mathbf{S} = \pm\mathbf{n}E/\omega_j$ for its angular momentum,[11] such a photon may be prescribed the linear momentum $\mathbf{p} = \mathbf{n}\hbar\omega_j/c \equiv \hbar\mathbf{k}$ and the angular momentum (essentially, the spin) $\mathbf{S} = \pm\mathbf{n}\hbar$, with the sign depending on the direction of its circular polarization ("helicity").

This electromagnetic field quantization scheme should look very straightforward, but it raises an important conceptual issue of ground state energy. Indeed, Eq. (18) implies that the total ground-state (i.e., the lowest) energy of the field is

Ground-state energy of EM field

$$E_g = \sum_j (E_g)_j = \sum_j \frac{\hbar\omega_j}{2}. \tag{9.21}$$

Since for any realistic model of the field-confining volume, either infinite or not, the density of electromagnetic field modes only grows with frequency,[12] this sum diverges on its upper limit, leading to infinite ground-state energy per unit volume. This infinite-energy paradox cannot be dismissed by declaring the ground-state energy of field oscillators unobservable, because this would contradict numerous experimental observations – starting perhaps from the famous *Casimir effect*.[13]

The simplest implementation of this effect involves two parallel, perfectly conducting plates of area A, separated by a vacuum gap of thickness $t << A^{1/2}$ (Fig. 1).

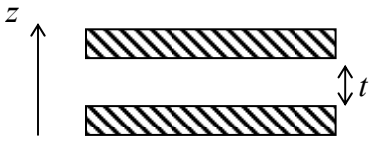

Fig. 9.1. The simplest geometry of the Casimir effect manifestation.

[11] See, e.g., EM Sections 7.7 and 9.8 (where the angular momentum of the field is denoted **L**).

[12] See, e.g., Eq. (1.1), which is similar to Eq. (1.90) for the de Broglie waves, derived in Sec. 1.7.

[13] This effect was predicted in 1948 by Hendrik Casimir and Dirk Polder, and confirmed semi-quantitatively in experiments by M. Sparnaay, *Nature* **180**, 334 (1957). After that and several other experiments, a decisive error bar reduction (to about ~5%), providing a quantitative confirmation of the Casimir formula (23), was achieved by S. Lamoreaux, *Phys. Rev. Lett.* **78**, 5 (1997) and by U. Mohideen and A. Roy, *Phys. Rev. Lett.* **81**, 004549 (1998). Note also that there are other experimental confirmations of the reality of the ground-state electromagnetic field, including, for example, the experiments by R. Koch *et al*. already discussed in Sec. 7.5, and the recent spectacular direct observations by C. Riek *et al*., *Science* **350**, 420 (2015).

Rather counterintuitively, the plates attract each other with a force F proportional to the area A and rapidly increasing with the decrease of t, even in the absence of any explicit electromagnetic field sources. The effect's explanation is that the energy of each electromagnetic field mode, including its ground-state energy, exerts average pressure,

$$\left\langle \mathcal{P}_j \right\rangle = -\frac{\partial E_j}{\partial V}, \tag{9.22}$$

on the walls constraining it to volume V. While the field's pressure on the external surfaces on the plates is due to the contributions (22) of all free-space modes, with arbitrary values of k_z (the z-component of the wave vector $\mathbf{k}_j$), in the gap between the plates, the spectrum of k_z is limited to the multiples of π/t, so the pressure on the internal surfaces is lower. This is why the net force exerted on the plates may be calculated as the sum of the contributions (22) from all "missing" low-frequency modes in the gap, with the minus sign. In the simplest model when the plates are made of an ideal conductor, which provides simple boundary conditions $\mathscr{E}_\tau = \mathscr{B}_n = 0$ on their surfaces,[14] such calculation is quite straightforward (and is hence left for the reader's exercise), and its result is

$$F = -\frac{\pi^2 A\hbar c}{240 t^4}. \tag{9.23}$$

Casimir effect

Note that for such calculation, the high-frequency divergence of Eq. (21) is not important, because it participates in the forces exerted on all surfaces of each plate, and cancels out from the net pressure. In this way, the Casimir effect not only confirms Eq. (21), but also teaches us an important lesson on how to deal with the divergences of such sums at $\omega_j \to \infty$. The lesson is: just get accustomed to the idea that the divergence exists, and ignore this fact while you can, i.e. if the final result you are interested in is finite. However, for some more complex problems of quantum electrodynamics (and the quantum theory of any other fields), this simplest approach becomes impossible, and then more complex, *renormalization* techniques become necessary. For their study, I have to refer the reader to a quantum field theory course – see the references at the end of this chapter.

9.2. Photon absorption and counting

As a matter of principle, the Casimir effect may be used to observe not only the electromagnetic field's ground state but also the field arriving from active sources – lasers, etc. However, usually, such studies may be done by simpler detectors, in which the absorption of a photon by a single atom leads to its ionization. This ionization, i.e. the emission of a free electron, triggers an avalanche-like chain reaction (e.g., an electric discharge in a Geiger-type counter), which may be readily registered using

[14] For realistic conductors, the reduction of t below ~1 μm causes significant deviations from this simple model, and hence from Eq. (23). The reason is that for gaps so narrow, the depth of field penetration into the conductors (see, e.g., EM Sec. 6.2), at the important frequencies $\omega \sim c/t$, becomes comparable with t, and an adequate theory of the Casimir effect has to involve a certain model of the penetration. (It is curious that in-depth analyses of this problem, pioneered in 1956 by E. Lifshitz, have revealed a deep relation between the Casimir effect and the London dispersion force which was the subject of Problems 3.16, 5.15, and 6.18 – for a review see, e.g., either I. Dzhyaloshinskii *et al.*, *Sov. Phys. Uspekhi* **4**, 153 (1961), or K. Milton, *The Casimir Effect*, World Scientific, 2001. Recent experiments in the 100 nm – 2 μm range of t, with an accuracy better than 1%, have enabled not only a clear observation of field penetration effects on the Casimir force but even a selection between some approximate models of the penetration – see D. Garcia-Sanchez *et al.*, *Phys. Rev. Lett.* **109**, 027202 (2012).

appropriate electronic circuitry. In good photon counters, the first step, the "trigger" atom ionization, is the bottleneck of the whole process (the *photon count*), so to analyze their statistics, it is sufficient to consider the field's interaction with just this atom.

Its ionization is a quantum transition from a discrete initial state of the atom to its final, ionized state with a continuous energy spectrum, induced by an external electromagnetic field. This is exactly the situation shown in Fig. 6.12, so we may apply to it the Golden Rule of quantum mechanics in the form (6.149), with system *a* associated with the electromagnetic field, and system *b* with the trigger atom. The atom's size is typically much smaller than the radiation wavelength, so the field-atom interaction may be adequately described in the electric-dipole approximation (6.146)

$$\hat{H}_{\rm int} = -\hat{\mathscr{E}} \cdot \hat{\mathbf{d}}, \tag{9.24}$$

where $\hat{\mathbf{d}}$ is the dipole moment's operator. Hence we may associate this operator with the operand $\hat{B}$ in Eqs. (6.145)-(6.149), while the electric field operator $\hat{\mathscr{E}}$ is associated with the operand $\hat{A}$ in those relations. First, let us assume that our field consists of only one mode of frequency ω. Then we can keep only one term in the sum (16a), and drop the index j, so Eq. (6.149) may be rewritten as

$$\begin{aligned} \Gamma &= \frac{2\pi}{\hbar}\left|\left\langle \text{ fin}\left|\hat{\mathscr{E}}(\mathbf{r},t)\right|\text{ ini}\right\rangle\right|^2 \left|\left\langle \text{ fin}\left|\hat{\mathbf{d}}(t)\cdot\mathbf{n}_e\right|\text{ ini}\right\rangle\right|^2 \rho_{\rm a} \\ &= \frac{2\pi}{\hbar}\frac{\hbar\omega}{2}\left|\left\langle \text{ fin}\left|\left[\hat{a}^\dagger(t)-\hat{a}(t)\right]e(\mathbf{r})\right|\text{ ini}\right\rangle\right|^2 \left|\left\langle \text{ fin}\left|\hat{\mathbf{d}}(t)\cdot\mathbf{n}_e\right|\text{ ini}\right\rangle\right|^2 \rho_{\rm a}, \end{aligned} \tag{9.25}$$

where $\mathbf{n}_e \equiv \mathbf{e}(\mathbf{r})/e(\mathbf{r})$ is the local direction of the vector $\mathbf{e}(\mathbf{r})$, symbols "ini" and "fin" denote the initial and final states of the corresponding subsystem (the electromagnetic field in the first long bracket, and the atom in the second bracket), and the density $\rho_{\rm a}$ of the atomic state continuum should be calculated at the final energy $E_{\rm fin} = E_{\rm ini} + \hbar\omega$.

As a reminder, in the Heisenberg picture of quantum dynamics, the initial and final states are time-independent, while the creation-annihilation operators are functions of time. In the Golden Rule formula (25), as in any perturbative result, this time dependence has to be calculated ignoring the perturbation – in this case, the field-atom interaction. For the field's creation-annihilation operators, this dependence coincides with that of the usual 1D oscillator – see Eq. (5.141), in which ω_0 should be, in our current notation, replaced with ω:

$$\hat{a}(t) = \hat{a}(0)e^{-i\omega t}, \quad \hat{a}^\dagger(t) = \hat{a}^\dagger(0)e^{+i\omega t}. \tag{9.26}$$

Hence Eq. (25) becomes

$$\Gamma = \pi\omega\left|\left\langle \text{ fin}\left|\left[\hat{a}^\dagger(0)e^{i\omega t} - \hat{a}(0)e^{-i\omega t}\right]e(\mathbf{r})\right|\text{ ini}\right\rangle\right|^2 \left|\left\langle \text{ fin}\left|\hat{\mathbf{d}}(t)\cdot\mathbf{n}_e\right|\text{ ini}\right\rangle\right|^2 \rho_{\rm a}. \tag{9.27a}$$

Now let us multiply the first long bracket by $\exp\{i\omega t\}$, and the second one by $\exp\{-i\omega t\}$:

$$\Gamma = \pi\omega\left|\left\langle \text{ fin}\left|\left[\hat{a}^\dagger(0)e^{2i\omega t} - \hat{a}(0)\right]e(\mathbf{r})\right|\text{ ini}\right\rangle\right|^2 \left|\left\langle \text{ fin}\left|\hat{\mathbf{d}}(t)\cdot\mathbf{n}_e e^{-i\omega t}\right|\text{ ini}\right\rangle\right|^2 \rho_{\rm a}. \tag{9.27b}$$

This, mathematically equivalent form of the previous relation shows more clearly that at resonant photon absorption, only the *annihilation* operator gives a significant time-averaged contribution to the

first bracket matrix element. (As a reminder, the quantum-mechanical Golden Rule for time-dependent perturbations is a result of averaging over a time interval much larger than $1/\omega$ – see Sec. 6.6.) Similarly, according to Eq. (4.199), the Heisenberg operator of the dipole moment corresponding to the *increase* of the atom's energy by $\hbar\omega$, has the Fourier components that differ in frequency from ω only by $\sim\Gamma << \omega$, so its time dependence virtually compensates the additional factor in the second bracket of Eq. (27b), and this bracket also may have a substantial time average. Hence, in the first bracket, we may neglect the fast-oscillating term, whose average over time interval $\sim 1/\Gamma$ is very close to zero.[15]

Now let us assume, first, that we use the same detector, characterized by the same matrix element of the quantum transition, i.e. the same second bracket in Eq. (27), and the same final state density ρ_a, for measurement of various electromagnetic fields – or just of the same field at different points **r**. Then we are only interested in the behavior of the first, field-related bracket, and may write

$$\Gamma \propto \left|\left\langle \text{fin}\left|\hat{a}e(\mathbf{r})\right|\text{ini}\right\rangle\right|^2 \equiv \left\langle \text{fin}\left|\hat{a}e(\mathbf{r})\right|\text{ini}\right\rangle\left\langle \text{fin}\left|\hat{a}e(\mathbf{r})\right|\text{ini}\right\rangle^* \equiv \left\langle \text{ini}\left|\hat{a}^\dagger e^*(\mathbf{r})\right|\text{fin}\right\rangle\left\langle \text{fin}\left|\hat{a}e(\mathbf{r})\right|\text{ini}\right\rangle, \quad (9.28)$$

where the creation-annihilation operators are implied to be taken at $t = 0$, i.e. in the Schrödinger picture, and the initial and final states are those of the field alone. Second, let us now calculate the *total* rate of transitions to *all* available final states of the given mode **e**(**r**). If such states formed a full and orthonormal set, we could use the closure relation (4.44) applied to the final states to write

$$\Gamma \propto \sum_{\text{fin}} \left\langle \text{ini}\left|\hat{a}^\dagger e^*(\mathbf{r})\right|\text{fin}\right\rangle\left\langle \text{fin}\left|\hat{a}e(\mathbf{r})\right|\text{ini}\right\rangle = \left\langle \text{ini}\left|\hat{a}^\dagger\hat{a}\right|\text{ini}\right\rangle e^*(\mathbf{r})e(\mathbf{r}) = \langle n\rangle_{\text{ini}}\left|e(\mathbf{r})\right|^2, \quad (9.29)$$

Photon counting rate

where, for a given field mode, $\langle n\rangle_{\text{ini}}$ is the expectation value of the operator $\hat{n} \equiv \hat{a}^\dagger\hat{a}$ for the initial state of the electromagnetic field. In the more realistic case of fields in relatively large volumes, $V >> \lambda^3$, with their virtually continuous spectrum of the final states, the middle equality in this relation is not strictly valid, but it is correct to a constant multiplier,[16] which we are currently not interested in. Note, however, that Eq. (29) may be substantially wrong for high-Q electromagnetic resonators ("cavities"), which may make just one (or a few) modes available for transitions. (Quantum electrodynamics of such cavities will be briefly discussed in Sec. 4 below.)

Let us apply Eq. (29) to several possible quantum states of the mode.

(i) First, as a sanity check, the ground initial state, $n = 0$, gives no photon absorption at all. The interpretation is easy: the ground state field, cannot emit a photon that would ionize an atom in the counter. Again, this does not mean that the ground-state "motion" is not observable (if you still think so, please review the Casimir effect discussion in Sec. 1), just that it cannot ionize the trigger atom – because it does not have any *spare* energy for doing that.

(ii) All other coherent states (Fock, Glauber, squeezed, etc.) of the field oscillator give the same counting rate, provided that their $\langle n\rangle_{\text{ini}}$ is the same. This result may be less evident if we apply Eq. (29) to the interference of two light beams from the same source – say, in the double-slit or the Bragg-scattering configurations. In this case, we may represent the spatial distribution of the field as a sum

[15] This is essentially the same rotating wave approximation (RWA) that was already used in Sec. 6.5 and beyond – see, e.g., the transition from Eq. (6.90) to the first of Eqs. (6.94).

[16] As the Golden Rule shows, this multiplier is proportional to the density ρ_f of the final states of the field.

$$e(\mathbf{r}) = e_1(\mathbf{r}) + e_2(\mathbf{r}) . \tag{9.30}$$

Here each term describes one possible wave path, so the operator product in Eq. (29) may be a rapidly changing function of the detector position. For this configuration, our result (29) means that the interference pattern (and its contrast) are independent of the particular state of the electromagnetic field's mode.

(iii) The last statement is also valid for a classical mixture of the different eigenstates of the same field mode, for example for its thermal-equilibrium state. Indeed, in this case, we need to average Eq. (29) over the corresponding classical ensemble, but it would only result in a different meaning of averaging n in that equation; the field part describing the interference pattern is not affected.

The last result may look a bit counter-intuitive because common sense tells us that the stochasticity associated with thermal equilibrium has to suppress the interference pattern contrast. These expectations are (partly :-) justified because a typical thermal source of radiation produces many field modes j, rather than one mode we have analyzed. These modes may have different wave numbers k_j and hence different field distribution functions $\mathbf{e}_j(\mathbf{r})$, resulting in shifted interference patterns. Their summation would indeed smear the interference, suppressing its contrast.

So the use of one photon detector is not the best way to distinguish different quantum states of an electromagnetic field mode. This task, however, may be achieved using the photon counting correlation technique shown in Fig. 2.[17]

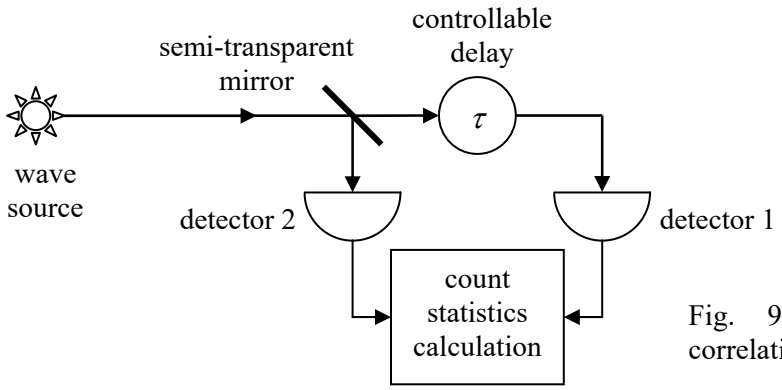

Fig. 9.2. Photon count correlation measurement.

In this experiment, the counting statistics may be characterized by the so-called *second-order correlation function* of the detector count rates,

Second-order correlation function

$$g^{(2)}(\tau) \equiv \frac{\langle \Gamma_1(t)\Gamma_2(t) \rangle}{\langle \Gamma_1(t) \rangle \langle \Gamma_2(t) \rangle}, \tag{9.31}$$

where the averaging may be carried out either over many similar experiments, or over a relatively long time interval $t >> \tau$, with usual field sources – due to their ergodicity.[18] Using the normalized correlation

[17] It was pioneered as early as the mid-1950s (i.e. before the advent of lasers), by Robert Hanbury Brown and Richard Twiss. Their second experiment was also remarkable for the rather unusual light source – the star Sirius! (Their work was an effort to improve astrophysics interferometry techniques.)

[18] This is why the argument t in Eq. (31) is just symbolic, and for the rates $\Gamma_{1,2}$, we can use Eq. (29), even though its derivation involved averaging over times much longer than $1/\omega$.

function (31) is very convenient because the characteristics of both detectors and the beam splitter (e.g., a semi-transparent mirror, see Fig. 2) drop out from this fraction.

Very unexpectedly for the mid-1950s, Hanbury Brown and Twiss discovered that the correlation function depends on the time delay τ in the way shown (schematically) with the solid line in Fig. 3. It is evident from Eq. (31) that if the counting events are completely independent, $g^{(2)}(\tau)$ should be equal to 1 – which is always the case in the limit $\tau \to \infty$. (As will be shown in the next section, the characteristic time of this approach is usually between 10^{-11}s and 10^{-8}s, so for its measurement, the delay time control may be provided just by moving one of the detectors by a human-scale distance between a few millimeters to a few meters.) Hence, the observed behavior at $\tau \to 0$ corresponds to a *positive* correlation of detector counts at small time delays, i.e. to a *higher* probability of the nearly simultaneous arrival of photons to both counters. This rather counterintuitive effect is called *photon bunching*.

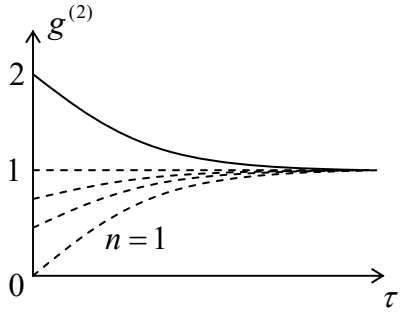

Fig. 9.3. Photon bunching (solid line) and antibunching for various n (dashed lines). The lines approach the level $g^{(2)} = 1$ at $\tau \to \infty$ (on the time scale depending on the light source).

Let us use our simple single-mode model to analyze this experiment, assuming that the time delay τ includes the difference between the times of the wave propagation from the source to detectors 1 and 2. Then the elementary quantum process characterized by the numerator of Eq. (31) is the correlated ionization of two trigger atoms, at two spatial-temporal points $\{\mathbf{r}_1, t\}$ and $\{\mathbf{r}_2, t - \tau\}$, by the same field mode, so we need to make the following replacement in the first of Eqs. (25):

$$\hat{\mathscr{E}}(\mathbf{r},t) \to \text{const} \times \hat{\mathscr{E}}(\mathbf{r}_1,t)\hat{\mathscr{E}}(\mathbf{r}_2,t-\tau)\,. \tag{9.32}$$

Then repeating all the manipulations performed above for the single-counter case, we get

$$\langle \Gamma_1(t)\Gamma_2(t)\rangle \propto \langle \text{ini}|\hat{a}(t)^\dagger \hat{a}(t-\tau)^\dagger \hat{a}(t-\tau)\hat{a}(t)|\text{ini}\rangle\, e^*(\mathbf{r}_1)e^*(\mathbf{r}_2)e(\mathbf{r}_1)e(\mathbf{r}_2). \tag{9.33}$$

Plugging this formula, as well as Eq. (29) for single-counter rates, into Eq. (31), we see that the field distribution factors (as well as the detector-specific brackets and the density of states ρ_a) cancel, giving a very simple final expression:

$$g^{(2)}(\tau) = \frac{\left\langle \hat{a}^\dagger(t)\hat{a}^\dagger(t-\tau)\hat{a}(t-\tau)\hat{a}(t)\right\rangle}{\left\langle \hat{a}^\dagger(t)\hat{a}(t)\right\rangle^2}, \tag{9.34}$$

where the averaging should be carried out, as before, over the initial state of the field.

Still, the calculation of this expression for arbitrary τ may be quite involved because in most practical cases, the relaxation of the correlation function to the asymptotic value $g^{(2)}(\infty)$ is due to the interaction of the light source with its environment, and hence requires the open-system techniques that

were discussed in Chapter 7. However, the zero-delay value $g^{(2)}(0)$ may be calculated straightforwardly, because the time arguments of all operators are equal, so we may write

Zero-delay correlation

$$g^{(2)}(0) = \frac{\left\langle \hat{a}^\dagger \hat{a}^\dagger \hat{a}\hat{a} \right\rangle}{\left\langle \hat{a}^\dagger \hat{a} \right\rangle^2}. \tag{9.35}$$

Let us evaluate this ratio for the simplest states of the field.

(i) The n^{th} Fock state. In this case, it is convenient to act with the annihilation operators upon the ket-vectors, and by the creation operators, upon the bra-vectors, using Eqs. (19):

Photon anti-bunching

$$g^{(2)}(0) = \frac{\left\langle n \middle| \hat{a}^\dagger \hat{a}^\dagger \hat{a}\hat{a} \middle| n \right\rangle}{\left\langle n \middle| \hat{a}^\dagger \hat{a} \middle| n \right\rangle^2} = \frac{\left\langle n-2 \middle| \left[n(n-1)\right]^{1/2} \left[n(n-1)\right]^{1/2} \middle| n-2 \right\rangle}{\left\langle n-1 \middle| n^{1/2} n^{1/2} \middle| n-1 \right\rangle^2} = \frac{n(n-1)}{n^2} \equiv 1 - \frac{1}{n}. \tag{9.36}$$

We see that the correlation function at small delays is below 1, i.e. below the value for fully independent counts – see the dashed lines in Fig. 3. This *photon antibunching* effect has a very simple handwaving explanation: a single photon emitted by the wave source may be absorbed by just one of the detectors. For the initial state $n = 1$, this is the only option, and it is very natural that Eq. (36) predicts no simultaneous counts at $\tau = 0$. Despite this theoretical simplicity, reliable observations of the antibunching have not been carried out until 1977,[19] due to the experimental difficulty of driving electromagnetic field oscillators into their Fock states – see Sec. 4 below.

(ii) The Glauber state α. A similar procedure, but now using Eq. (5.124) and its Hermitian conjugate, $\left\langle \alpha \middle| \hat{a}^\dagger = \left\langle \alpha \middle| \alpha^* \right.\right.$, yields

Glauber field statistics

$$g^{(2)}(0) = \frac{\left\langle \alpha \middle| \hat{a}^\dagger \hat{a}^\dagger \hat{a}\hat{a} \middle| \alpha \right\rangle}{\left\langle \alpha \middle| \hat{a}^\dagger \hat{a} \middle| \alpha \right\rangle^2} = \frac{\alpha^* \alpha^* \alpha\alpha}{(\alpha^* \alpha)^2} \equiv 1, \tag{9.37}$$

for any parameter α. We see that the result is different from that for the Fock states, unless in the latter case $n \to \infty$. (We know that the Fock and Glauber properties should also coincide for the ground state, but at that state, the correlation function's value is uncertain because there are no photon counts at all.)

(iii) Classical mixture. From Chapter 7, we know that such statistical ensembles cannot be described by single-state vectors, and require the density matrix w for their description. Here, we may combine Eqs. (35) and (7.5) to write

$$g^{(2)}(0) = \frac{\mathrm{Tr}\left(\hat{w}\hat{a}^\dagger \hat{a}^\dagger \hat{a}\hat{a}\right)}{\left[\mathrm{Tr}\left(\hat{w}\hat{a}^\dagger \hat{a}\right)\right]^2}. \tag{9.38}$$

Spelling out this expression is easy for the field in thermal equilibrium at some temperature T, because its density matrix is diagonal in the basis of the Fock states n – see Eqs. (7.24):

[19] By H. J. Kimble *et al.*, *Phys. Rev. Lett.* **39**, 691 (1977). For a detailed review of photon antibunching, see, e.g., H. Paul, *Rev. Mod. Phys*. **54**, 1061 (1982).

$$w_{nn'} = W_n \delta_{nn'}, \quad W_n = \exp\left\{-\frac{E_n}{k_B T}\right\} \Big/ Z \equiv \lambda^n \Big/ \sum_{n=0}^{\infty} \lambda^n, \quad \text{where } \lambda \equiv \exp\left\{-\frac{\hbar\omega}{k_B T}\right\}. \tag{9.39}$$

So, for the operators in the numerator and denominator of Eq. (38) we also need just the diagonal terms of the operator products, which have already been calculated – see Eq. (36). As a result, we get

$$g^{(2)}(0) = \frac{\sum_{n=0}^{\infty} W_n n(n-1)}{\left(\sum_{n=0}^{\infty} W_n n\right)^2} = \frac{\sum_{n=0}^{\infty} \lambda^n n(n-1) \times \sum_{n=0}^{\infty} \lambda^n}{\left(\sum_{n=0}^{\infty} \lambda^n n\right)^2}. \tag{9.40}$$

One of the three series in the last expression is just the usual geometric progression,

$$\sum_{n=0}^{\infty} \lambda^n = \frac{1}{1-\lambda}, \tag{9.41}$$

and the remaining two series may be readily calculated by its differentiation over the parameter λ:

$$\begin{aligned} &\sum_{n=0}^{\infty} \lambda^n n \equiv \lambda \sum_{n=0}^{\infty} \lambda^{n-1} n = \lambda \frac{d}{d\lambda} \sum_{n=0}^{\infty} \lambda^n = \lambda \frac{d}{d\lambda} \frac{1}{1-\lambda} = \frac{\lambda}{(1-\lambda)^2}, \\ &\sum_{n=0}^{\infty} \lambda^n n(n-1) \equiv \lambda^2 \sum_{n=0}^{\infty} \lambda^{n-2} n(n-1) = \lambda^2 \frac{d^2}{d^2\lambda} \left(\sum_{n=0}^{\infty} \lambda^n\right) = \lambda^2 \frac{d^2}{d\lambda^2} \frac{1}{1-\lambda} = \frac{2\lambda^2}{(1-\lambda)^3}, \end{aligned} \tag{9.42}$$

and for the correlation function, we get an extremely simple result independent of the parameter λ and hence of temperature:

$$g^{(2)}(0) = \frac{\left[2\lambda^2/(1-\lambda)^3\right]\left[1/(1-\lambda)\right]}{\left[\lambda/(1-\lambda)^2\right]^2} \equiv 2. \tag{9.43}$$

Photon bunching

This is exactly the photon bunching effect first observed by Hanbury Brown and Twiss – see Fig. 3. We see that in contrast to antibunching, this is an essentially classical (statistical) effect. Indeed, Eq. (43) allows for a purely classical derivation. In the classical theory, the counting rate (of a single counter) is proportional to the wave intensity I, so Eq. (31) with $\tau = 0$ is reduced to

$$g^{(2)}(0) = \frac{\langle I^2 \rangle}{\langle I \rangle^2}, \quad \text{with } I \propto \overline{E^2(t)} \propto E_\omega E_\omega^*. \tag{9.44}$$

For a sinusoidal field, the intensity is constant, and $g^{(2)}(0) = 1$. (This is also evident from Eq. (37), because the classical state may be considered a Glauber state with $\alpha \to \infty$.) On the other hand, if the intensity fluctuates (either in time or from one experiment to another), the averages in Eq. (44) should be calculated as

$$\langle I^k \rangle = \int_0^{\infty} w(I) I^k dI, \quad \text{with } \int_0^{\infty} w(I) dI = 1, \quad \text{and } k = 1, 2, \tag{9.45}$$

where $w(I)$ is the probability density. Per Eq. (39), for classical statistics, the probability is an exponential function of the electromagnetic field energy, and hence its intensity:

$$w(I) = Ce^{-\beta I}, \quad \text{where } \beta \propto 1/k_B T, \tag{9.46}$$

so Eqs. (45) yield:[20]

$$\int_0^\infty C\exp\{-\beta I\}dI \equiv C/\beta = 1, \quad \text{and hence } C = \beta,$$

$$\left\langle I^k \right\rangle = \int_0^\infty w(I) I^k dI = C\int_0^\infty \exp\{-\beta I\} I^k dI = \frac{1}{\beta^k}\int_0^\infty \exp\{-\xi\}\xi^k d\xi = \begin{cases} 1/\beta, & \text{for } k = 1, \\ 2/\beta^2, & \text{for } k = 2. \end{cases} \tag{9.47}$$

Plugging these results into Eq. (44), we get $g^{(2)}(0) = 2$, in complete agreement with Eq. (43).

For some field states, including the squeezed ground states ζ discussed at the end of Sec. 5.5, the values of $g^{(2)}(0)$ may be even higher than 2 – the so-called *super-bunching*. Analyses of two cases of such super-bunching are offered for the reader's exercise – see the problem list at the chapter's end.

9.3. Photon emission: spontaneous and stimulated

In the last section, we considered how the counter's trigger atom *absorbs* a photon. Now let us have a look at the opposite process of *spontaneous emission* of a photon by an atom at its transition from an excited quasi-stationary (metastable) state to a state with an energy lower by $\Delta E = \hbar\omega$.[21] By using the same electric-dipole approximation (24) for the atom-to-field interaction, we may still use the Golden Rule for the model depicted in Fig. 6.12, but now the roles of its two component systems change: we have to associate the operator $\hat{A}$ with the electric dipole moment of the atom, while the operator $\hat{B}$, with the electric field, so the continuous spectrum of the system b represents the plurality of the electromagnetic field states into which the spontaneous radiation may happen. Since now the transition *increases* the energy of the electromagnetic field, and *decreases* that of the atom, after the multiplication of the field bracket in Eq. (27a) by $\exp\{-i\omega t\}$, and the second, by $\exp\{+i\omega t\}$, we may keep only the photon *creation* operator whose time evolution (26) compensates this additional fast "rotation". As a result, the Golden Rule takes the following form:

Spontaneous photon emission rate

$$\Gamma_s = \pi\omega \left| \langle \text{fin} | \hat{a}^\dagger | 0 \rangle \right|^2 \left| \langle \text{fin} | \hat{\mathbf{d}} \cdot \mathbf{e}(\mathbf{r}) | \text{ini} \rangle \right|^2 \rho_f, \tag{9.48}$$

where all operators and states are time-independent, and ρ_f is the density of final states of the electromagnetic field – which in this problem plays the role of the atom's environment.[22] Here the electromagnetic field oscillator has been assumed to be initially in the ground state – the assumption that will be changed later in this section.

This relation, together with Eq. (19), shows that for the field's matrix element to be different from zero, the final field has to be its first excited Fock state, $n = 1$. (By the way, *this* is exactly the most practicable way of generating an excited Fock state of a field oscillator.) With that, Eq. (48) yields

[20] See, e.g., MA Eq. (6.7c) with $n = 0$ and $n = 1$.

[21] A straightforward Fourier transform of Eq. (6.114) (which is the inseparable counterpart of the Golden Rule we are going to use) shows that the emitted radiation has the Lorentzian line centered to the frequency ω, with the half-width equal to the transition rate Γ_s that we will calculate.

[22] Here the summation over all electromagnetic field modes j may be smuggled back. Since in the quasistatic approximation $k_j a << 1$, which is necessary for the validity of Eq. (24), the matrix elements in Eq. (48) are independent of the field vector direction, and their magnitudes are fixed by ω, this summation is reduced to the calculation of the total ρ_f for all modes, and the spatial averaging of $e^2(\mathbf{r})$ – see below.

$$\Gamma_s = \pi\omega \left| \langle \text{fin} | \hat{\mathbf{d}} \cdot \mathbf{e}(\mathbf{r}) | \text{ini} \rangle \right|^2 \rho_f \equiv \pi\omega \left| \langle \text{fin} | \hat{d} e_d(\mathbf{r}) | \text{ini} \rangle \right|^2 \rho_f , \tag{9.49}$$

where e_d is the Cartesian component of the vector $\mathbf{e}(\mathbf{r})$ along the electric dipole's direction, and ρ_f is now the density of *electromagnetic modes* at the frequency ω. The expression for it follows from our first formula in this course – see Eq. (1.1):

$$\rho_f \equiv \frac{dN}{dE} = V \frac{\omega^2}{\pi^2 \hbar c^3}, \tag{9.50}$$

where the volume V should be large enough to ensure the spectrum's virtual continuity:[23] $V >> \lambda^3 = (2\pi c/\omega)^3$. Because of that, in the normalization condition used to simplify Eq. (9), we may consider $e^2(\mathbf{r})$ constant. Let us represent this square as a sum of squares of the three Cartesian components of the vector $\mathbf{e}(\mathbf{r})$, with one of those (e_d) aligned with the dipole's direction; due to the space isotropy we may write

$$e^2 \equiv e_d^2 + e_{\perp 1}^2 + e_{\perp 2}^2 = 3e_d^2. \tag{9.51}$$

As a result, the normalization condition yields

$$e_d^2 = \frac{1}{3\varepsilon_0 V}. \tag{9.52}$$

and Eq. (49) gives the famous (and very important) formula[24]

$$\Gamma_s = \frac{1}{4\pi\varepsilon_0} \frac{4\omega^3}{3\hbar c^3} \left| \langle \text{fin} | \hat{\mathbf{d}} | \text{ini} \rangle \right|^2 \equiv \frac{1}{4\pi\varepsilon_0} \frac{4\omega^3}{3\hbar c^3} \langle \text{fin} | \hat{\mathbf{d}} | \text{ini} \rangle \cdot \langle \text{ini} | \hat{\mathbf{d}} | \text{fin} \rangle^* . \tag{9.53}$$

Free-space spontaneous emission rate

Leaving a comparison of this formula with the classical theory of radiation,[25] and the exact evaluation of Γ_s for a particular transition in the hydrogen atom, for the reader's exercises, let me just estimate its order of magnitude. Assuming that $d \sim e r_B \equiv e\hbar^2/m_e(e^2/4\pi\varepsilon_0)$ and $\hbar\omega \sim E_H \equiv m_e(e^2/4\pi\varepsilon_0)^2/\hbar^2$, and taking into account the definition (6.62) of the fine-structure constant $\alpha \approx 1/137$, we get

$$\frac{\Gamma_s}{\omega} \sim \left(\frac{e^2}{4\pi\varepsilon_0 \hbar c} \right)^3 \equiv \alpha^3 \sim 3\times 10^{-7}. \tag{9.54}$$

This estimate shows that the emission lines at atomic transitions are typically very sharp. With the present-day availability of high-speed electronics, it also makes sense to evaluate the time scale $\tau = 1/\Gamma$ of a typical quantum transition: for a typical optical frequency $\omega \sim 3\times 10^{15}$ s^{-1}, it is close to 1 ns. This is exactly the time constant that determines the time-delay dependence of the photon counting statistics of the spontaneously emitted radiation – see Fig. 3. Very colloquially, this is the temporal scale of the

[23] In the opposite case when the same atom is placed into a high-Q resonant cavity with a discrete spectrum (see, e.g., EM 7.9), the rate of its photon emission is strongly suppressed at frequencies between the cavity resonances (where $\rho_f \to 0$) – see, e.g., the review by S. Haroche and D. Klepner, *Phys. Today* **42**, 24 (Jan. 1989). On the other hand, the emission is strongly (by a factor ~ $(\lambda^3/V)Q$, where V is the cavity's volume) enhanced at resonance frequencies – the so-called *Purcell effect*, discovered by E. Purcell in the 1940s. For a brief discussion of this and other quantum electrodynamic effects in cavities, see the next section.

[24] This was the breakthrough result obtained by P. Dirac in 1927, which jumpstarted the whole field of quantum electrodynamics. An equivalent expression was obtained from more formal arguments in 1930 by V. Weisskopf and E. Wigner, so sometimes Eq. (53) is (very unfairly) called the "Weisskopf-Wigner formula".

[25] See, e.g., EM Sec. 8.2, in particular Eq. (8.29).

photon emitted by an atom. Note that the scale $c\tau$ of the spatial extension of the corresponding wave packet is surprisingly macroscopic – of the order of 30 cm. Such a "human" size of spontaneously emitted photons makes the usual optical table, with its 1-cm-scale components, the key equipment for many optical experiments – see, e.g., Fig. 2.

Note, however, that the above estimate of τ is only valid for a transition with a non-zero electric-dipole matrix element. If it equals zero, i.e. the transition does not satisfy the *selection rules*,[26] – say, due to the initial and final state symmetry – it is "forbidden". The "forbidden" transition may still take place due to a different, smaller interaction (say, via a magnetic dipole field of the atom, or its quadrupole electric field[27]), but takes much longer. In some cases the increase of τ is rather dramatic – sometimes to hours! Such long-lasting radiation is called *fluorescence*. (If the initial excitation is followed first by a series of non-radiative transitions down the energy level ladder, which delay the final radiative transition, the resulting radiation is called either *phosphorescence* or *luminescence*.)

Now let us consider a more general case when the electromagnetic field mode of frequency ω is initially in an arbitrary Fock state n, and from it may either get energy $\hbar\omega$ from the atomic system (*photon emission*) or, vice versa, give such energy back to the atom (*photon absorption*). For the photon emission rate, an evident generalization of Eq. (48) gives

$$\frac{\Gamma_e}{\Gamma_s} \equiv \frac{\Gamma_{n\to \text{fin}}}{\Gamma_{0\to 1}} = \frac{\left|\left\langle \text{fin}\left|\hat{a}^\dagger\right|n\right\rangle\right|^2}{\left|\left\langle 1\left|\hat{a}^\dagger\right|0\right\rangle\right|^2}, \tag{9.55}$$

where both brackets should be calculated in the Schrödinger picture, and Γ_s is the spontaneous emission rate (48) of the same atomic system. According to the second of Eqs. (19), at the photon emission, the final field state has to be the Fock state with $n' = n + 1$, and Eq. (55) yields

Stimulated photon emission rate

$$\Gamma_e = (n+1)\Gamma_s . \tag{9.56}$$

Thus the initial field increases the photon emission rate; this effect is called the *stimulated emission of radiation*. Note that the spontaneous emission may be considered a particular case of the stimulated emission for $n = 0$, and hence interpreted as the emission stimulated by the ground state of the electromagnetic field – one more manifestation of the non-trivial nature of this "vacuum" state.

On the other hand, following the arguments of Sec. 2,[28] for the description of radiation *absorption*, the photon creation operator has to be replaced with the annihilation operator, giving the rate ratio

[26] As was already discussed in Sec. 5.6, for a single spin-less particle moving in a spherically symmetric potential (e.g., a hydrogen-like atom), the orbital selection rules are simple: the only allowed electric-dipole transitions are those with $\Delta l \equiv l_{\text{fin}} - l_{\text{ini}} = \pm 1$ and $\Delta m \equiv m_{\text{fin}} - m_{\text{ini}} = 0$ or ± 1. The simplest example of the transition that does *not* satisfy this rule, i.e. is "forbidden", is that between the s-states ($l = 0$) with $n = 2$ and $n = 1$; because of that, the lifetime of the lowest excited s-state of a hydrogen atom is as long as ~0.15 s.

[27] See, e.g., EM Sec. 8.9.

[28] Mind, however, a major difference between the rate Γ discussed in Sec. 2, and Γ_a in Eq. (57). In our current case, the atomic transition is still between two *discrete* energy levels (see Fig. 4 below), so the rate Γ_a is proportional to ρ_f, the density of final states of the electromagnetic *field*, i.e. the same density as in Eq. (48) and

$$\frac{\Gamma_a}{\Gamma_s} = \frac{\left|\langle \text{fin}|\, \hat{a}\, |\, n\rangle\right|^2}{\left|\langle 1\,|\hat{a}^\dagger|\,0\rangle\right|^2}. \tag{9.57}$$

According to this relation and the first of Eqs. (19), the final state of the field at the photon absorption has to be the Fock state with $n' = n - 1$, and Eq. (57) yields

$$\boxed{\Gamma_a = n\Gamma_s}. \tag{9.58}$$

Photon absorption rate

The results (56) and (58) are sometimes formulated in terms of relations between the *Einstein coefficients* A and B defined in the way shown in Fig. 4, where the two energy levels are those of the atom, Γ_a is the rate of photon absorption from the electromagnetic field, Γ_e is that of photon emission into the field, and u is the electromagnetic field density in thermal equilibrium – see Eq. (1.3). Since per Eq. (7.26b), the ratio $u/\langle n\rangle$ is a constant independent of $\langle n\rangle$ (and temperature), the statistical averaging of Eqs. (56) and (58) yields[29]

$$A_{21} = B_{21}\frac{u}{\langle n\rangle} = B_{12}\frac{u}{\langle n\rangle}, \tag{9.59}$$

Einstein coefficients' relation

because each of these expressions equals the spontaneous emission rate Γ_s.

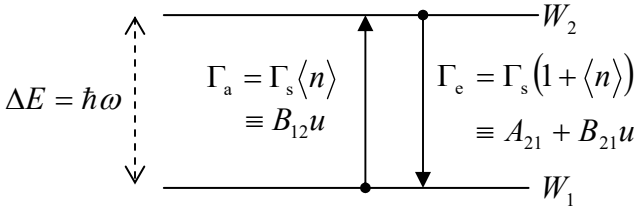

Fig. 9.4. The Einstein coefficients on the atomic quantum transition diagram – cf. Fig. 7.6.

I cannot resist the temptation to use this point for a small detour – an alternative derivation of the Bose-Einstein statistics for photons. Indeed, in the thermodynamic equilibrium we have just discussed, the average probability flows between levels 1 and 2 (see Fig. 4 again) should be equal:[30]

$$W_2\Gamma_e = W_1\Gamma_a, \tag{9.60}$$

where W_1 and W_2 are the probabilities for the atomic system to occupy the corresponding levels, so Eqs. (56) and (58) yield

$$W_2\Gamma_s\big(\langle n\rangle + 1\big) = W_1\Gamma_s\langle n\rangle, \qquad \text{i.e. } \frac{W_2}{W_1} = \frac{\langle n\rangle}{\langle n\rangle + 1}. \tag{9.61}$$

But, on the other hand, for an atomic subsystem only weakly coupled to its electromagnetic environment, we ought to have the Gibbs distribution of these probabilities:

$$\frac{W_2}{W_1} = \frac{\exp\{-E_2/k_BT\}}{\exp\{-E_1/k_BT\}} = \exp\left\{-\frac{\Delta E}{k_BT}\right\} = \exp\left\{-\frac{\hbar\omega}{k_BT}\right\}. \tag{9.62}$$

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beyond, while the rate (27) is proportional to ρ_a, the density of final (ionized) states of the photon counter's "trigger" *atom* – more exactly, of it's the electron released at its ionization.

[29] These relations were conjectured, from general statistical arguments, by Albert Einstein as early as 1916.

[30] This is just a particular embodiment of the detailed balance equation (7.198).

By requiring Eqs. (61) and (62) to give the same result for the probability ratio, we readily get the Bose-Einstein distribution for the electromagnetic field in thermal equilibrium:

$$\langle n \rangle = \frac{1}{\exp\{\hbar\omega / k_B T\} - 1}, \tag{9.63}$$

i.e. the same result (7.26b) as that obtained in Sec. 7.1 by other means.

Now returning to the discussion of Eqs. (56) and (58), their very important implication is the possibility to achieve the stimulated emission of coherent radiation using the level *occupancy inversion*. Indeed, if the ratio W_2/ W_1 is larger than that given by Eq. (62), the net power flow from the atomic system into the electromagnetic field,

$$\text{power } = \hbar\omega \times \Gamma_s \left[W_2 \left(\langle n \rangle + 1 \right) - W_1 \langle n \rangle \right], \tag{9.64}$$

may be positive. The necessary inversion may be produced using several ways, notably by intensive quantum transitions to level 2 from an even higher energy level (which, in turn, is populated, e.g., by absorption of external radiation, usually called *pumping*, at a higher frequency.)

A less obvious but crucial feature of the stimulated emission is spelled out by Eq. (55): as was mentioned above, it shows that the final state of the field after the absorption of energy $\hbar\omega$ from the atom is a pure (coherent) Fock state $(n + 1)$. Colloquially, one may say that the new, $(n + 1)^{st}$ photon emitted from the atom is automatically in phase with the n photons that had been in the field mode initially, i.e. joins them coherently.[31] The idea of stimulated emission of coherent radiation using population inversion[32] was first implemented in the early 1950s in the microwave range (*masers*) and in 1960 in the optical range (*lasers*). Nowadays, lasers are ubiquitous components of almost all high-tech systems and constitute one of the cornerstones of our technological civilization.

A quantitative discussion of laser operation is well beyond the framework of this course, and I have to refer the reader to special literature,[33] but still would like to briefly mention two key points:

(i) In a typical laser, each generated electromagnetic field mode is in its Glauber (rather than the Fock) state, so Eqs. (56) and (58) are applicable only for the n averaged over the Fock-state decomposition of the Glauber state – see Eq. (5.134).

(ii) Since in a typical laser $\langle n \rangle >> 1$, its operation may be well described using quasiclassical theories that use Eq. (64) to describe the electromagnetic energy balance (with the addition of a term describing the energy loss due to field absorption in external components of the laser, including the useful load), plus the equation describing the balance of occupancies $W_{1,2}$ due to all interlevel transitions – similar to Eq. (60), but including also the contribution(s) from the particular population inversion mechanism used in the laser. In this approach, the role of quantum mechanics in laser science is essentially reduced to the calculation of the parameter Γ_s for a particular system.

This role becomes more prominent when one needs to describe *fluctuations* of the laser field. Here two approaches are possible, following the two options discussed in Chapter 7. If the fluctuations

[31] It is straightforward to show that this fact is also true if the field is initially in the Glauber state – which is more typical for modes in practical lasers.

[32] This idea has been traced back to an obscure 1939 publication by V. Fabrikant.

[33] I can recommend, for example, P. Milloni and J. Eberly, *Laser Physics*, 2nd ed., Wiley, 2010, and a less technical text by A. Yariv, *Quantum Electronics*, 3rd ed., Wiley, 1989.

are relatively small, one can linearize the Heisenberg equations of motion of the field oscillator operators near their stationary-lasing "values", with the Langevin "forces" (also time-dependent operators) describing the fluctuation sources, and use these Heisenberg-Langevin equations to calculate the radiation fluctuations, just as was described in Sec. 7.5. On the other hand, near the lasing threshold, the field fluctuations are relatively large, smearing the phase transition between the no-lasing and lasing states. Here the linearization is not an option, but one can use the density-matrix approach described in Sec. 7.6, for the fluctuation analysis.[34] Note that while the laser fluctuations may look like a peripheral issue, the pioneering research in that field has led to the development of the general theory of open quantum systems, which was discussed in Chapter 7.

9.4. Cavity QED

Now I have to discuss, at least in passing, the field of *cavity quantum electrodynamics* (usually called *cavity QED* for short) – the art and science of creating and using the entanglement between quantum states of an atomic system (either an atom, or an ion, or a molecule, etc.) and the electromagnetic field in a macroscopic volume called the *resonant cavity* (or just "resonator", or just "cavity"). This field is very popular nowadays, especially in the context of the quantum computation and communication research reviewed in Sec. 8.5.[35]

Our discussion in the previous section was based on the implicit assumption that the energy spectrum of the electromagnetic field interacting with an atomic subsystem is essentially continuous, so its final state is spread among many field modes, effectively losing its coherence with the quantum state of the atomic subsystem. This assumption has justified our use of the quantum-mechanical Golden Rule for the calculation of the spontaneous and stimulated transition rates. However, the assumption becomes invalid if the electromagnetic field is contained inside a relatively small volume, with its linear size comparable with the radiation wavelength. If the walls of such a cavity mostly reflect, rather than absorb, radiation, then in the 0^{th} approximation, the energy dissipation may be disregarded, and the particular solutions $\mathbf{e}_j(\mathbf{r})$ of the Helmholtz equation (5) correspond to discrete, well-separated mode wave numbers k_j and hence well-separated field oscillation frequencies ω_j.[36] Due to the energy conservation, an atomic transition corresponding to the energy $\Delta E = | E_{\text{ini}} - E_{\text{fin}} |$ may be effective only if the corresponding quantum transition frequency $\Omega \equiv \Delta E/\hbar$ is close to one of these resonance frequencies.[37] As a result of such resonant interaction, the quantum states of the atomic system and the resonant electromagnetic mode may become entangled.

A very popular approximation for the quantitative description of this effect is the so-called *Rabi model*,[38] in which the atom is treated as a two-level system interacting with a single electromagnetic field mode of the resonant cavity. (As was shown in Sec. 6.5, this model is justified, e.g., if transitions

[34] This path has been developed (also in the mid-1960s), by several researchers, notably including W. Lamb and M. Sully – see, e.g., M. Sargent III, M. Scully, and W. Lamb, Jr., *Laser Physics,* Westview, 1977.

[35] This popularity was demonstrated, for example, by the award of the 2012 Nobel Prize in Physics to cavity QED experimentalists S. Haroche and D. Wineland.

[36] The calculation of such modes and corresponding frequencies for several simple cavity geometries is the subject of EM Sec. 7.8 of this series.

[37] On the contrary, if Ω is far from any ω_j, the interaction is suppressed; in particular, the spontaneous emission rate may be much lower than that given by Eq. (53) – so this result is not as fundamental as it may look.

[38] After the pioneering work by I. Rabi in 1936-37.

between all other energy level pairs have considerably different frequencies.) As the reader knows well from Chapters 4-6 (see in particular Sec. 5.1), any two-level system may be described, just as a spin-½, by the Hamiltonian $b\hat{I} + \mathbf{c}\cdot\hat{\boldsymbol{\sigma}}$. Since we may always select such energy origin that $b = 0$, and such coordinate system that $\mathbf{c} = c\mathbf{n}_z$, and ignore the atomic subsystem's degrees of freedom that do not participate in the interaction with the field, its Hamiltonian may be taken in the form

$$\hat{H}_{\rm a} = c\hat{\sigma}_z \equiv \frac{\hbar\Omega}{2}\hat{\sigma}_z, \tag{9.65}$$

where $\hbar\Omega \equiv 2c = \Delta E$ is the difference between the energy levels in the absence of interaction with the cavity field. Next, according to Eq. (17), ignoring the constant ground-state energy $\hbar\omega/2$ (which may be always added to the energy at the end – if necessary), the contribution of a single field mode of frequency ω to the total Hamiltonian of the system is

$$\hat{H}_{\rm f} = \hbar\omega\hat{a}^\dagger\hat{a}. \tag{9.66}$$

Finally, according to Eq. (16a), the electric field of the mode may be represented as

$$\hat{\mathscr{E}}(\mathbf{r},t) = \frac{1}{i}\left(\frac{\hbar\omega}{2}\right)^{1/2}\mathbf{e}(\mathbf{r})\left(\hat{a} - \hat{a}^\dagger\right), \tag{9.67}$$

so in the electric-dipole approximation (24), the cavity-atom interaction may be represented as a product of the field by some (say, y-) Cartesian component[39] of the Pauli spin-½ operator:

$$\hat{H}_{\rm int} = {\rm const}\times\hat{\sigma}_y\times\hat{\mathscr{E}} = {\rm const}\times\hat{\sigma}_y\times\left(\frac{\hbar\omega}{2}\right)^{1/2}\frac{1}{i}\left(\hat{a} - \hat{a}^\dagger\right) \equiv i\hbar\kappa\hat{\sigma}_y\left(\hat{a} - \hat{a}^\dagger\right), \tag{9.68}$$

where κ is a coupling constant (with the dimension of frequency). The sum of these three terms,

Rabi Hamiltonian

$$\hat{H} \equiv \hat{H}_{\rm a} + \hat{H}_{\rm f} + \hat{H}_{\rm int} = \frac{\hbar\Omega}{2}\hat{\sigma}_z + \hbar\omega\hat{a}^\dagger\hat{a} + i\hbar\kappa\hat{\sigma}_y\left(\hat{a} - \hat{a}^\dagger\right), \tag{9.69}$$

giving a very reasonable description of the system, is called the *Rabi Hamiltonian*.

Despite the apparent simplicity of Eq. (69), using this Hamiltonian for calculations is not that straightforward.[40] Only in the case when the electromagnetic field is large and hence may be treated classically, the results following from Eq. (69) are reduced to Eqs. (6.94) describing, in particular, the Rabi oscillations discussed in Sec. 6.3. The situation becomes simpler in the most important case when the frequencies Ω and ω are very close, enabling an effective interaction between the cavity field and the atom even if the coupling constant κ is relatively small. Indeed, if both the κ and the so-called *detuning* (defined similarly to the parameter Δ used in Sec. 6.5),

$$\xi \equiv \Omega - \omega, \tag{9.70}$$

[39] The exact component is not important for final results, while intermediate formulas are simpler if the interaction is proportional to either pure $\hat{\sigma}_x$ or pure $\hat{\sigma}_y$.

[40] For example, an exact quasi-analytical expression for its eigenenergies (as zeros of a Taylor series in the parameter κ, with coefficients determined by a recurrence relation) was found only recently – see D. Braak, *Phys. Rev. Lett.* **107**, 100401 (2011).

are much smaller than $\Omega \approx \omega$, the Rabi Hamiltonian may be simplified using the rotating-wave approximation, already used several times in this course.

For this, it is convenient to use the *spin ladder operators* defined similarly for those of the orbital angular momentum – see Eqs. (5.153):

$$\hat{\sigma}_{\pm} \equiv \hat{\sigma}_x \pm i\hat{\sigma}_y, \qquad \text{so} \quad \hat{\sigma}_y = \frac{\hat{\sigma}_+ - \hat{\sigma}_-}{2i}. \tag{9.71}$$

From Eq. (4.105), it is very easy to find the matrices of these operators in the standard z-basis,

$$\sigma_+ = \begin{pmatrix} 0 & 2 \\ 0 & 0 \end{pmatrix}, \qquad \sigma_- = \begin{pmatrix} 0 & 0 \\ 2 & 0 \end{pmatrix}, \tag{9.72}$$

and their commutation rules – which turn out to be naturally similar to Eqs. (5.154):

$$\left[\hat{\sigma}_+, \hat{\sigma}_-\right] = 4\hat{\sigma}_z, \qquad \left[\hat{\sigma}_z, \hat{\sigma}_\pm\right] = \pm 2\hat{\sigma}_\pm. \tag{9.73}$$

In this notation, the Rabi Hamiltonian becomes

$$\hat{H} = \frac{\hbar\Omega}{2}\hat{\sigma}_z + \hbar\omega\hat{a}^\dagger\hat{a} + \frac{\hbar\kappa}{2}\left(\hat{\sigma}_+ - \hat{\sigma}_-\right)\left(\hat{a} - \hat{a}^\dagger\right), \tag{9.74}$$

and it is straightforward to use Eq. (4.199) and (73) to derive the Heisenberg-picture equations of motion for the involved operators. (Doing this, we have to remember that operators of the "spin" subsystem, on one hand, and of the field mode, on the other hand, are defined in different Hilbert spaces and hence commute – at least at coinciding time moments.) The result (so far, exact!) is

$$\begin{aligned} &\dot{\hat{a}} = -i\omega\hat{a} + \frac{i\kappa}{2}\left(\hat{\sigma}_+ - \hat{\sigma}_-\right), \qquad \dot{\hat{a}}^\dagger = i\omega\hat{a}^\dagger + \frac{i\kappa}{2}\left(\hat{\sigma}_+ - \hat{\sigma}_-\right), \\ &\dot{\hat{\sigma}}_\pm = \pm i\Omega\hat{\sigma}_\pm + 2i\kappa\left(\hat{a} - \hat{a}^\dagger\right)\hat{\sigma}_z, \qquad \dot{\hat{\sigma}}_z = i\kappa\left(\hat{a}^\dagger - \hat{a}\right)\left(\hat{\sigma}_+ + \hat{\sigma}_-\right). \end{aligned} \tag{9.75}$$

At negligible coupling, $\kappa \to 0$, these equations have simple solutions,

$$\hat{a}(t) \propto e^{-i\omega t}, \quad \hat{a}^\dagger(t) \propto e^{i\omega t}, \quad \hat{\sigma}_\pm(t) \propto e^{\pm i\Omega t}, \quad \hat{\sigma}_z(t) \approx \text{const}, \tag{9.76}$$

and the small terms proportional to κ on the right-hand sides of Eqs. (75) cannot affect these time evolution laws dramatically even if κ is not exactly zero. Of those terms, ones with frequencies close to the "basic" frequency of each variable would act in resonance and hence may have a substantial impact on the system's dynamics, while non-resonant terms may be ignored. In this rotating-wave approximation, Eqs. (75) are reduced to a much simpler system of equations:

$$\begin{aligned} &\dot{\hat{a}} = -i\omega\hat{a} - \frac{i\kappa}{2}\hat{\sigma}_-, \qquad \dot{\hat{a}}^\dagger = i\omega\hat{a}^\dagger + \frac{i\kappa}{2}\hat{\sigma}_+, \\ &\dot{\hat{\sigma}}_+ = i\Omega\hat{\sigma}_+ + 2i\kappa\hat{a}^\dagger\hat{\sigma}_z, \qquad \dot{\hat{\sigma}}_- = -i\Omega\hat{\sigma}_- - 2i\kappa\hat{a}\hat{\sigma}_z, \qquad \dot{\hat{\sigma}}_z = i\kappa\left(\hat{a}^\dagger\hat{\sigma}_- - \hat{a}\hat{\sigma}_+\right). \end{aligned} \tag{9.77}$$

Alternatively, these equations of motion may be obtained *exactly* from the Hamiltonian (74) if it is preliminary cleared of the terms proportional to $\hat{\sigma}_+\hat{a}^\dagger$ and $\hat{\sigma}_-\hat{a}$, that oscillate fast and hence self-average to produce virtually zero effect:

Jaynes-Cummings Hamiltonian

$$\hat{H} = \frac{\hbar\Omega}{2}\hat{\sigma}_z + \hbar\omega\hat{a}^\dagger\hat{a} + \frac{\hbar\kappa}{2}\left(\hat{\sigma}_+\hat{a} + \hat{\sigma}_-\hat{a}^\dagger\right), \qquad \text{at } \kappa, |\xi| << \omega, \Omega\,. \tag{9.78}$$

This is the famous *Jaynes-Cummings Hamiltonian*,[41] which is the basic model used in the cavity QED and its applications.[42] To find its eigenstates and eigenenergies, let us note that at negligible interaction ($\kappa \to 0$), the spectrum of the total energy E of the system, which is the sum of two independent contributions from the atomic and cavity-field subsystems, $\pm\hbar\Omega/2$ and $\hbar\Omega n$, forms close pairs (Fig. 5)

$$E\big|_{\kappa=0} = E_n \pm \frac{\hbar\xi}{2}, \tag{9.79}$$

centered to values[43]

$$E_n \equiv \hbar\omega\left(n - \frac{1}{2}\right), \quad \text{with } n = 1, 2, 3\ldots,. \tag{9.80}$$

(At the exact resonance $\omega = \Omega$, i.e. at $\xi = 0$, each pair merges into one double-degenerate level E_n.)

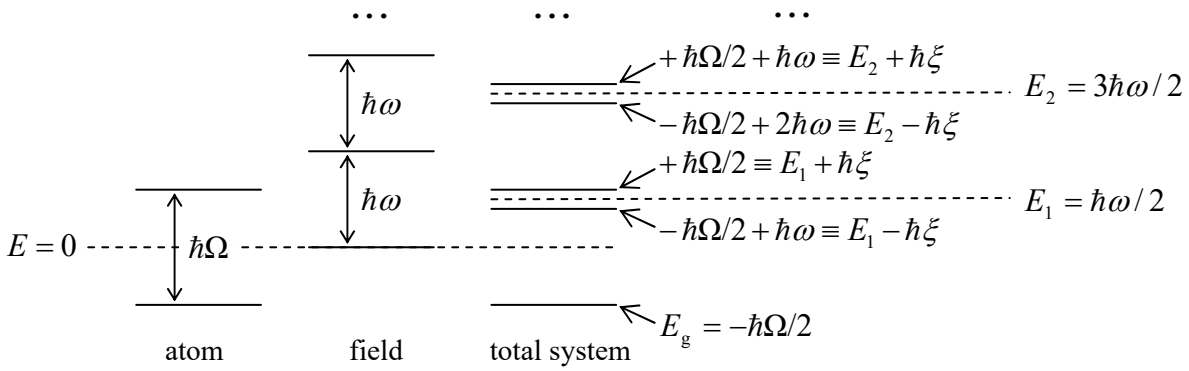

Fig. 9.5. The energy spectrum (79) of the Jaynes-Cummings Hamiltonian in the limit $\kappa << |\xi|$. Note again that the energy is referred to the ground-state energy $\hbar\omega/2$ of the cavity field.

Since at $\kappa \to 0$ the two subsystems do not interact, the eigenstates corresponding to the two levels of the n^{th} pair may be represented by direct products of their independent state vectors:

$$|+\rangle \equiv |\uparrow\rangle \otimes |n-1\rangle \quad \text{and} \quad |-\rangle \equiv |\downarrow\rangle \otimes |n\rangle, \tag{9.81}$$

where the first ket of each product represents the state of the two-level (spin-½-like) atomic subsystem, and the second ket, that of the field oscillator.

As we know from Chapter 6, weak interaction may lead to strong coherent mixing[44] of quantum states with close energies (in this case, the two states (81) within each pair with the same n), even if

[41] It was first proposed and analyzed in 1963 by two engineers, E. Jaynes and F. Cummings, in a paper published in *Proc. IEEE*, and it took the physics community a while to recognize and acknowledge the fundamental importance of that work.

[42] For most applications, the baseline Hamiltonian (78) has to be augmented by additional term(s) describing, for example, the incoming radiation and/or the system's coupling to the environment, for example, due to the electromagnetic energy loss in a finite-Q-factor cavity – see Eq. (7.68).

[43] Only the ground state level $E_g = -\hbar\Omega/2$ is non-degenerate – see Fig. 5.

[44] In some fields, especially chemistry, such mixing is frequently called *hybridization*.

their mixing with the states with farther energies is still negligible. Hence, at $0 < \kappa$, $|\xi| << \omega \approx \Omega$, a good approximation of the eigenstate with $E \approx E_n$ is given by a linear superposition of the states (81):

$$\left|\alpha_n\right\rangle = c_+\left|+\right\rangle + c_-\left|-\right\rangle \equiv c_+\left|\uparrow\right\rangle \otimes \left|n-1\right\rangle + c_-\left|\downarrow\right\rangle \otimes \left|n\right\rangle, \tag{9.82}$$

Jaynes-Cummings eigenstates

with certain c-number coefficients $c_\pm$. This relation describes the entanglement of the atomic eigenstates $\uparrow$ and $\downarrow$ with the Fock states number n and $n - 1$ of the field mode. Let me leave the (straightforward) calculation of the coefficients ($c_\pm$) for the reader's exercise. (The result for the corresponding two eigenenergies $(E_n)_\pm$ may be again represented by the same anticrossing diagram as shown in Figs. 2.29 and 5.1, now with the detuning ξ as the argument.) This calculation shows, in particular, that at $\xi = 0$ (i.e. at $\omega = \Omega$), $|c_+| = |c_-| = 1/\sqrt{2}$ for both states of the pair. This fact may be interpreted as a (coherent!) equal sharing of an energy quantum $\hbar\omega = \hbar\Omega$ by the atom and the cavity field at the exact resonance.

As a (hopefully, self-evident) by-product of the calculation of $c_\pm$ is the fact that the dynamics of the state α_n described by Eq. (82) is similar to that of the generic two-level system that was repeatedly discussed in this course – the first time in Sec. 2.6 and then in Chapters 4-6. In particular, if the composite system had been initially prepared to be in one component state, for example $|\uparrow\rangle\otimes|0\rangle$ (i.e. with the atom excited, while the cavity in its ground state), and then allowed to evolve on its own, after some time interval $\Delta t \sim 1/\kappa$ it may be found definitely in the counterpart state $|\downarrow\rangle\otimes|1\rangle$, including the first excited Fock state $n = 1$ of the field mode. If the process is allowed to continue, after the equal time interval Δt, the system returns to the initial state $|\uparrow\rangle\otimes|0\rangle$, etc. This most striking prediction of the Jaynes-Cummings model was directly observed, by G. Rempe *et al.*, only in 1987, although less directly this model was repeatedly confirmed by numerous experiments carried out in the 1960s and 1970s.

This quantized-field version of the Rabi oscillations can only persist in time if the inevitable electromagnetic energy losses (not described by the basic Jaynes-Cummings Hamiltonian) are somehow compensated – for example, by passing a beam of particles, externally excited into the higher-energy state $\uparrow$, through the cavity. If the losses become higher, the dissipation suppresses quantum coherence, in our case the coherence between two components of each pair (82), as was discussed in Chapter 7. As a result, the transition from the higher-energy atomic state $\uparrow$ to the lower-energy state $\downarrow$, giving the energy quantum $\hbar\omega$ to the cavity ($n - 1 \to n$), which is then rapidly drained into the environment, becomes incoherent, so the system's dynamics is reduced to the Purcell effect mentioned in Sec. 3. A quantitative analysis of this effect is left for the reader's exercise.

The number of interesting games one can play with such systems – say, by adding external sources of radiation at a frequency close to ω and Ω, in particular with manipulated time-dependent amplitude and/or phase, is almost unlimited.[45] Unfortunately, my time/space allowance for the cavity QED is over, and for further discussion, I have to refer the interested reader to special literature.[46]

9.5. The Klein-Gordon and relativistic Schrödinger equations

Now let me switch gears and discuss the basics of relativistic quantum mechanics of particles with a *non-zero* rest mass *m.* In the ultra-relativistic limit $pc >> mc^2$, the quantization scheme of such

[45] Most of them may be described by adding the corresponding terms to the basic Jaynes-Cummings Hamiltonian.
[46] I can recommend, for example, either C. Gerry and P. Knight, *Introductory Quantum Optics*, Cambridge U. Press, 2005, or G. Agarwal, *Quantum Optics*, Cambridge U. Press, 2012.

particles may be essentially the same as for electromagnetic waves, but for the intermediate energy range, $pc \sim mc^2$, a more general approach is necessary. Historically, the first attempts[47] to extend the non-relativistic wave mechanics into the relativistic energy range were based on performing the same transition from the classical observables to their quantum-mechanical operators as in the non-relativistic limit:

$$\mathbf{p} \to \hat{\mathbf{p}} = -i\hbar\nabla, \qquad E \to \hat{H} = i\hbar\frac{\partial}{\partial t}. \tag{9.83}$$

The substitution of these operators, acting on the Schrödinger-picture wavefunction $\Psi(\mathbf{r},t)$, into the classical relation (1) between the energy E and momentum $\mathbf{p}$ (for of a free particle) leads to the following formulas:

Table 9.1. Deriving the Klein-Gordon equation for a free relativistic particle.[48]

	Non-relativistic limit	Relativistic case
Classical mechanics	$E = \frac{1}{2m}p^2$	$E^2 = c^2p^2 + \left(mc^2\right)^2$
Wave mechanics	$i\hbar\frac{\partial}{\partial t}\Psi = \frac{1}{2m}\left(-i\hbar\nabla\right)^2\Psi$	$\left(i\hbar\frac{\partial}{\partial t}\right)^2\Psi = c^2\left(-i\hbar\nabla\right)^2\Psi + (mc^2)^2\Psi$

The resulting equation for the non-relativistic limit, in the left-bottom cell of the table, is just the usual Schrödinger equation (1.28) for a free particle. Its relativistic generalization, in the right-bottom cell, usually rewritten as

Klein-Gordon equation

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2\right)\Psi + \mu^2\Psi = 0, \qquad \text{with } \mu \equiv \frac{mc}{\hbar}, \tag{9.84}$$

is called the *Klein-Gordon* (or sometimes "Klein-Gordon-Fock") *equation*. The fundamental solutions of this equation are the same plane monochromatic waves

$$\Psi(\mathbf{r},t) \propto \exp\left\{i\left(\mathbf{k}\cdot\mathbf{r} - \omega t\right)\right\}. \tag{9.85}$$

as in the non-relativistic case. Indeed, such waves are the eigenstates of the operators (83), with eigenvalues, respectively,

$$\mathbf{p} = \hbar\mathbf{k}, \qquad \text{and } E = \hbar\omega, \tag{9.86}$$

so their substitution into Eq. (84) immediately returns us to Eq. (1) with the replacements (86):

$$E_{\pm} = \hbar\omega_{\pm} = \pm\left[\left(\hbar ck\right)^2 + \left(mc^2\right)^2\right]^{1/2}. \tag{9.87}$$

[47] This approach was suggested in 1926-1927, i.e. virtually simultaneously, by (at least) V. Fock, E. Schrödinger, O. Klein and W. Gordon, J. Kudar, T. de Donder, and F.-H. van der Dungen, and L. de Broglie.

[48] Note that in the left, non-relativistic column of this table, the energy is measured from the rest energy mc^2, while in its right, relativistic column, it is measured from zero – see Eq. (1).

Though one may say that this dispersion relation is just a simple combination of the classical relation (1) and the same basic quantum-mechanical relations (86) as in non-relativistic limit, it attracts our attention to the fact that the energy $\hbar\omega$ as a function of the momentum $\hbar\mathbf{k}$ has two branches, with $E_-(\mathbf{p}) = -E_+(\mathbf{p})$ – see Fig. 6a. Historically, this fact has played a very important role in spurring the fundamental idea of *particle-antiparticle pairs.* In this idea (very similar to the concept of electrons and holes in semiconductors, which was discussed in Sec. 2.8), what we call the "vacuum" actually corresponds to all quantum states of the lower branch, with energies $E_-(\mathbf{p}) < 0$, being completely filled, while the states on the upper branch, with energies $E_+(\mathbf{p}) > 0$, being empty. Then an externally supplied energy,

$$\Delta E = E_+ - E_- \equiv E_+ + \left(-E_-\right) \geq 2mc^2 > 0, \tag{9.88}$$

may bring the system from the lower branch to the upper one (Fig. 6b). The resulting excited state is interpreted as a combination of a particle (formally, of the infinite spatial extension) with an energy $E_+ > 0$ and the corresponding momentum $\mathbf{p}$, and a "hole" (antiparticle), also of a *positive* energy ($-E_-$) and the opposite momentum $-\mathbf{p}$. This idea[49] has led to a search for, and discovery of the positron: the electron's antiparticle with charge $q = +e$, in 1932, and later of the antiproton and other antiparticles.

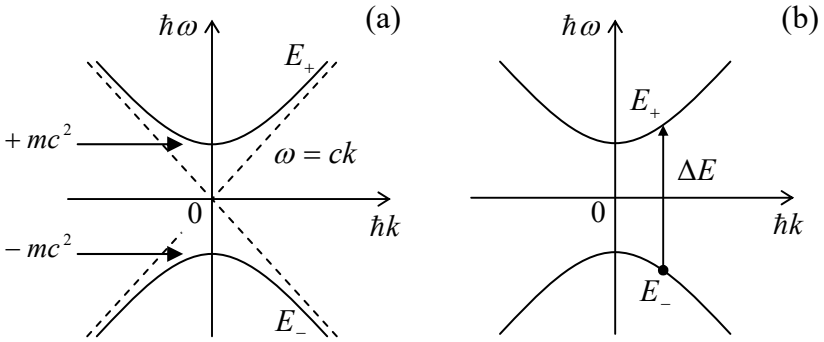

Fig. 9.6. (a) The free-particle dispersion relation resulting from the Klein-Gordon and Dirac equations, and (b) the scheme of creation of a particle-antiparticle pair from the vacuum.

Free particles of a finite spatial extension may be described, in this approach, just as in the non-relativistic Schrödinger equation, by wave packets, i.e. linear superpositions of the de Broglie waves (85) with close wave vectors $\mathbf{k}$, and the corresponding values of ω given by Eq. (87), with the positive sign for the "usual" particles, and negative sign for antiparticles – see Fig. 6a above. Note that to form, from a particle's wave packet, a similar wave packet for the antiparticle, with the same phase and group velocities (2.33a) in each direction, we need to change the sign not only before ω, but also before $\mathbf{k}$, i.e. to replace all component wavefunctions (85), and hence the full wavefunction, with their complex conjugates.

Of more formal properties of Eq. (84), it is straightforward (and hence left for the reader's exercise) to prove that its solutions satisfy the same continuity equation (1.52), with the probability current density $\mathbf{j}$ still given by Eq. (1.47), but a different expression for the probability density w – which becomes very similar to that for $\mathbf{j}$:

$$w = \frac{i\hbar}{2mc^2}\left(\Psi^* \frac{\partial \Psi}{\partial t} - \text{c.c.}\right), \qquad \mathbf{j} = \frac{i\hbar}{2m}\left(\Psi \nabla \Psi^* - \text{c.c.}\right) \tag{9.89}$$

[49] Due to the same P. A. M. Dirac!

– very much in the spirit of the relativity theory, which treats space and time on equal footing. (In the non-relativistic limit $p/mc \to 0$, Eq. (84) allows the reduction of this expression for w to the non-relativistic Eq. (1.22): $w \to \Psi\Psi^*$.)

The Klein-Gordon equation may be readily generalized to describe a particle moving in external fields; for example, the electromagnetic field effects on a particle with charge q may be described by the same replacement as in the non-relativistic limit (see Sec. 3.1):

$$\hat{\mathbf{p}} \to \hat{\mathbf{P}} - q\mathbf{A}(\mathbf{r},t), \qquad \hat{H} \to \hat{H} - q\phi(\mathbf{r},t), \tag{9.90}$$

where $\hat{\mathbf{P}} = -i\hbar\nabla$ is the canonical momentum operator (3.25), and the vector- and scalar potentials, $\mathbf{A}$ and ϕ, should be treated appropriately – either as c-number functions if the electromagnetic field quantization is not important for a particular problem, or as operators (see Secs. 1-4 above) if it is.

However, the practical value of the resulting *relativistic Schrödinger equation* is rather limited, for two main reasons. First of all, it does not give the correct description of particles with spin. For example, for the hydrogen-like atom/ion problem, i.e. the motion of an electron with the electric charge $-e$, in the Coulomb central field of an immobile nucleus with charge $+Ze$, the equation may be readily solved exactly[50] and yields the following spectrum of (doubly degenerate) energy levels:

$$E = mc^2\left(1+\frac{Z^2\alpha^2}{\lambda^2}\right)^{-1/2}, \quad \text{with } \lambda \equiv n + \left[\left(l+\tfrac{1}{2}\right)^2 - Z^2\alpha^2\right]^{1/2} - \left(l+\tfrac{1}{2}\right), \tag{9.91}$$

where $n = 1, 2, \ldots$ and $l = 0, 1, \ldots, n-1$ are the same quantum numbers as in the non-relativistic theory (see Sec. 3.6), and $\alpha \approx 1/137$ is the fine structure constant (6.62). The three leading terms of the Taylor expansion of this result in the small parameter $Z\alpha$ are as follows:

$$E \approx mc^2\left[1 - \frac{Z^2\alpha^2}{2n^2} - \frac{Z^4\alpha^4}{2n^4}\left(\frac{n}{l+\tfrac{1}{2}} - \frac{3}{4}\right)\right]. \tag{9.92}$$

The first of these terms is just the rest energy of the particle. The second term,

$$E_n = -mc^2\frac{Z^2\alpha^2}{2n^2} \equiv -\frac{mZ^2e^4}{(4\pi\varepsilon_0)^2\hbar^2}\frac{1}{2n^2} \equiv -\frac{E_0}{2n^2}, \quad \text{with } E_0 = Z^2E_{\rm H}, \tag{9.93}$$

reproduces the non-relativistic Bohr's formula (3.201). Finally, the third term,

$$-mc^2\frac{Z^4\alpha^4}{2n^4}\left(\frac{n}{l+\tfrac{1}{2}} - \frac{3}{4}\right) \equiv -\frac{2E_n^2}{mc^2}\left(\frac{n}{l+\tfrac{1}{2}} - \frac{3}{4}\right), \tag{9.94}$$

is just the perturbative kinetic-relativistic contribution (6.51) to the fine structure of the Bohr levels (93). However, as we already know from Sec. 6.3, for a spin-½ particle such as the electron, the spin-orbit interaction (6.55) gives an additional contribution to the fine structure, of the same order, so the net result, confirmed by experiment, is given by Eq. (6.60), i.e. is different from Eq. (94). This is very natural because the relativistic Schrödinger equation does not have the very notion of spin.

Second, even for massive spinless particles (such as the Z^0 bosons), for which this equation is believed to be valid, the most important problems are related to particle interactions at high energies of

[50] This task is left for the reader's exercise.

the order of $\Delta E \sim 2mc^2$ and beyond – see Eq. (88). Due to the possibility of creation and annihilation of particle-antiparticle pairs at such energies, the number of particles participating in such interactions is typically considerable (and variable), and the adequate description of the system is given not by the relativistic Schrödinger equation (which is formulated in single-particle terms), but by the quantum field theory – to which I will devote only a few sentences at the very end of this chapter.

9.6. Dirac's theory

The real breakthrough toward the quantum relativistic theory of electrons (and other spin-½ fermions) was achieved in 1928 by P. A. M. Dirac. For that time, the structure of his theory was highly nontrivial. Namely, while formally preserving, in the coordinate representation, the same Schrödinger-picture equation of quantum dynamics as in the non-relativistic quantum mechanics,[51]

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi , \tag{9.95}$$

it postulates that the wavefunction Ψ it describes is not a scalar complex function of time and coordinates, but a *four-component* column-vector (sometimes called the *bispinor*) of such functions, its Hermitian-conjugate bispinor $\Psi^\dagger$ being a four-component row-vector of their complex conjugates:

$$\Psi = \begin{pmatrix} \Psi_1(\mathbf{r},t) \\ \Psi_2(\mathbf{r},t) \\ \Psi_3(\mathbf{r},t) \\ \Psi_4(\mathbf{r},t) \end{pmatrix}, \qquad \Psi^\dagger = \left(\Psi_1^*(\mathbf{r},t), \quad \Psi_2^*(\mathbf{r},t), \quad \Psi_3^*(\mathbf{r},t), \quad \Psi_4^*(\mathbf{r},t)\right), \tag{9.96}$$

and that the Hamiltonian participating in Eq. (95) is a 4×4 matrix defined in the Hilbert space of bispinors Ψ. For a free particle, the postulated Hamiltonian looks amazingly simple:[52]

$$\boxed{\hat{H} = c\hat{\boldsymbol{\alpha}} \cdot \hat{\mathbf{p}} + \hat{\beta} mc^2 .} \tag{9.97}$$

Free-particle's Hamiltonian

[51] After the "naturally-relativistic" form of the Klein-Gordon equation (84), this apparent return to the non-relativistic Schrödinger equation may look very counter-intuitive. However, it becomes a bit less surprising taking into account the fact (whose proof is left for the reader's exercise) that Eq. (84) may be also recast into the form (95) for a *two-component* column-vector Ψ (sometimes called *spinor*), with a Hamiltonian which may be represented by a 2×2 matrix – and hence expressed via the Pauli matrices (4.105) and the identity matrix I.

[52] Moreover, if the time derivative participating in Eq. (95), and the three coordinate derivatives participating (via the momentum operator) in Eq. (97), are merged into one 4-vector operator $\partial/\partial x_k \equiv \{\nabla, \partial/\partial(ct)\}$, the Dirac equation (95) may be rewritten in an even simpler, manifestly Lorentz-invariant 4-vector form (with the implied summation over the repeated index $k = 1, ..., 4$ – see, e.g., EM Sec. 9.4):

$$\left(\hat{\gamma}_k \frac{\partial}{\partial x_k} + \mu\right)\Psi = 0, \quad \text{where } \hat{\boldsymbol{\gamma}} \equiv \{\hat{\gamma}_1, \hat{\gamma}_2, \hat{\gamma}_3\} = \begin{pmatrix} 0 & -i\hat{\boldsymbol{\sigma}} \\ i\hat{\boldsymbol{\sigma}} & 0 \end{pmatrix}, \quad \hat{\gamma}_4 = \hat{\beta},$$

where $\mu \equiv mc/\hbar$ – just as in Eq. (84). Note also that, very counter-intuitively, the Dirac Hamiltonian (97) is *linear* with respect to the momentum, while the non-relativistic Hamiltonian of a particle, as well as the relativistic Schrödinger equation, are *quadratic* in $\mathbf{p}$. In my humble opinion, Dirac's theory (including the concept of antiparticles it has inspired) may compete for the title of the most revolutionary theoretical idea in physics of all times, despite such strong contenders as Newton's laws, Maxwell's equations, Gibbs' statistical distribution, Bohr's theory of the hydrogen atom, and Einstein's general relativity.

where $\hat{\mathbf{p}} = -i\hbar\nabla$ is the same 3D vector operator of momentum as in the non-relativistic case, while the operators $\hat{\boldsymbol{\alpha}}$ and $\hat{\beta}$ may be represented in the following shorthand 2×2 form:

Dirac operators

$$\hat{\boldsymbol{\alpha}} \equiv \begin{pmatrix} \hat{0} & \hat{\boldsymbol{\sigma}} \\ \hat{\boldsymbol{\sigma}} & \hat{0} \end{pmatrix}, \qquad \hat{\beta} \equiv \begin{pmatrix} \hat{I} & \hat{0} \\ \hat{0} & -\hat{I} \end{pmatrix}. \tag{9.98a}$$

The operator $\hat{\boldsymbol{\alpha}}$, composed of the Pauli vector operators $\hat{\boldsymbol{\sigma}}$, is also a vector in the usual 3D space, with each of its 3 Cartesian components being a 4×4 matrix. The particular form of the 2×2 matrices corresponding to the operators $\hat{\boldsymbol{\sigma}}$ and $\hat{I}$ in Eq. (98a) depends on the basis selected for the spin state representation; for example, in the standard z-basis, in which the Cartesian components of $\hat{\boldsymbol{\sigma}}$ are represented by the Pauli matrices (4.105), the 4×4 matrix form of Eq. (98a) is

$$\alpha_x = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \quad \alpha_y = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}, \quad \alpha_z = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \tag{9.98b}$$

It is straightforward to use Eqs. (98) to verify that the matrices α_x, α_y, α_z and β satisfy the following relations:

$$\alpha_x^2 = \alpha_y^2 = \alpha_z^2 = \beta^2 = \mathrm{I}, \tag{9.99}$$

$$\alpha_x\alpha_y + \alpha_y\alpha_x = \alpha_y\alpha_z + \alpha_z\alpha_y = \alpha_z\alpha_x + \alpha_x\alpha_z = \alpha_x\beta + \beta\alpha_x = \alpha_y\beta + \beta\alpha_y = \alpha_z\beta + \beta\alpha_z = 0, \tag{9.100}$$

i.e. anticommute.

Using these commutation relations, and acting essentially as in Sec. 1.4, it is straightforward to show that any solution to the Dirac equation obeys the probability conservation law, i.e. the continuity equation (1.52), with the probability density:

$$w = \Psi^\dagger\Psi, \tag{9.101}$$

and the probability current,

$$\mathbf{j} = \Psi^\dagger c\hat{\boldsymbol{\alpha}}\Psi, \tag{9.102}$$

looking *almost* as in the non-relativistic wave mechanics – cf. Eqs. (1.22) and (1.47). Note, however, the Hermitian conjugation used in these formulas instead of the complex conjugation, in order to form the scalars w, j_x, j_y, and j_z from the 4-component state vectors (96).

This close similarity is extended to the fundamental plane-wave solutions of the Dirac equations in free space. Indeed, plugging such a solution, in the form

$$\Psi = \mathrm{u}e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} \equiv \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}, \tag{9.103}$$

into Eqs. (95) and (97), we see that they are indeed satisfied, provided that a system of four coupled linear algebraic equations for four complex c-number amplitudes $u_{1,2,3,4}$ is satisfied. The condition of its

consistency yields the same dispersion relation (87), i.e. the same two-branch diagram shown in Fig. 6, as follows from the Klein-Gordon equation. The difference is that plugging each value of ω, given by Eq. (87), back into the system of the linear equations for the four amplitudes u, we get two solutions for their vector $\mathbf{u} \equiv (u_1, u_2, u_3, u_4)$ for each of the two energy branches – see Fig. 6 again. In the standard z-basis of spin operators, they may be represented as follows:

$$\text{for } E = E_+ > 0: \quad \mathrm{u}_{+\uparrow} = c_{+\uparrow}\begin{pmatrix} 1 \\ 0 \\ \dfrac{cp_z}{E_+ + mc^2} \\ \dfrac{cp_+}{E_+ + mc^2} \end{pmatrix}, \quad \mathrm{u}_{+\downarrow} = c_{+\downarrow}\begin{pmatrix} 0 \\ 1 \\ \dfrac{cp_-}{E_+ + mc^2} \\ \dfrac{-cp_z}{E_+ + mc^2} \end{pmatrix}, \tag{9.104a}$$

$$\text{for } E = E_- < 0: \quad \mathrm{u}_{-\uparrow} = c_{-\uparrow}\begin{pmatrix} \dfrac{cp_z}{E_- - mc^2} \\ \dfrac{cp_+}{E_- - mc^2} \\ 1 \\ 0 \end{pmatrix}, \quad \mathrm{u}_{-\downarrow} = c_{-\downarrow}\begin{pmatrix} \dfrac{cp_-}{E_- - mc^2} \\ \dfrac{-cp_z}{E_- - mc^2} \\ 0 \\ 1 \end{pmatrix}, \tag{9.104b}$$

where $p_\pm \equiv p_x \pm ip_y$, and $c_\pm$ are the normalization coefficients determined by initial conditions.

The simplest interpretation of these solutions is that Eq. (103), with the vectors $\mathbf{u}_+$ given by Eq. (104a), represents a spin-½ particle (say, an electron), while with the vectors $\mathbf{u}_-$ given by Eq. (104b), it represents an antiparticle (a positron), and the two solutions for each particle, indexed with opposite arrows, correspond to two possible directions of the spin: $\sigma_z = \pm 1$, i.e. $S_z = \pm\hbar/2$. This interpretation is indeed solid in the non-relativistic limit, when the two last components of the vector (104a), and two first components of the vector (104b) are negligibly small:

$$\mathrm{u}_{+\uparrow} \to \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad \mathrm{u}_{+\downarrow} \to \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad \mathrm{u}_{-\uparrow} \to \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad \mathrm{u}_{-\downarrow} \to \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \qquad \text{for } \frac{p_{x,y,z}}{mc} \to 0. \tag{9.105}$$

However, at arbitrary energies, the physical picture is more complex. To show this, let us use the Dirac equation to calculate the Heisenberg-picture law of time evolution of the operator of some Cartesian component of the orbital angular momentum $\mathbf{L} \equiv \mathbf{r}\times\mathbf{p}$, for example of $L_x = yp_z - zp_y$, taking into account the fact that the Dirac operators (98a) commute with those of $\mathbf{r}$ and $\mathbf{p}$, and also the Heisenberg commutation relations (2.14):

$$i\hbar\frac{\partial \hat{L}_x}{\partial t} = \left[\hat{L}_x, \hat{H}\right] = c\hat{\boldsymbol{\alpha}}\cdot\left[\left(\hat{y}\hat{p}_z - \hat{z}\hat{p}_y\right), \hat{\mathbf{p}}\right] = -i\hbar c\left(\hat{\alpha}_z\hat{p}_y - \hat{\alpha}_y\hat{p}_z\right), \tag{9.106}$$

with similar relations for two other Cartesian components. Since the right-hand side of these equations is different from zero, the orbital momentum is generally *not* conserved – even for a free particle! Let us, however, consider the following vector operator,

Spin operator in Dirac's theory

$$\hat{\mathbf{S}} \equiv \frac{\hbar}{2}\begin{pmatrix} \hat{\boldsymbol{\sigma}} & \hat{0} \\ \hat{0} & \hat{\boldsymbol{\sigma}} \end{pmatrix}. \tag{9.107a}$$

According to Eqs. (4.105), its Cartesian components, in the z-basis, are represented by the 4×4 matrices

$$\mathrm{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad \mathrm{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix}, \quad \mathrm{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \tag{9.107b}$$

Let us calculate the Heisenberg-picture law of time evolution of these components, for example

$$i\hbar \frac{\partial \hat{S}_x}{\partial t} = \left[\hat{S}_x, \hat{H}\right] = c\left[\hat{S}_x, \left(\hat{\alpha}_x \hat{p}_x + \hat{\alpha}_y \hat{p}_y + \hat{\alpha}_z \hat{p}_z\right)\right]. \tag{9.108}$$

A direct calculation of the commutators of the matrices (98) and (107) yields

$$\left[\hat{S}_x, \hat{\alpha}_x\right] = 0, \quad \left[\hat{S}_x, \hat{\alpha}_y\right] = i\hbar\hat{\alpha}_z, \quad \left[\hat{S}_x, \hat{\alpha}_z\right] = -i\hbar\hat{\alpha}_y, \tag{9.109}$$

so we finally get

$$i\hbar \frac{\partial \hat{S}_x}{\partial t} = i\hbar c\left(\hat{\alpha}_z \hat{p}_y - \hat{\alpha}_y \hat{p}_z\right), \tag{9.110}$$

with similar expressions for the other two components of the operator. Comparing this result with Eq. (106), we see that any Cartesian component of the operator defined similarly to Eq. (5.170),

$$\hat{\mathbf{J}} \equiv \hat{\mathbf{L}} + \hat{\mathbf{S}}, \tag{9.111}$$

is an integral of motion,[53] so this operator may be interpreted as the one representing the total angular momentum of the particle. Hence, the operator (107) *may* be interpreted as the spin operator of a spin-½ particle (e.g., electron). As it follows from the last of Eq. (107b), in the non-relativistic limit, the columns (105) represent the eigenkets of the z-component of that operator, with eigenvalues $S_z = \pm\hbar/2$, the sign corresponding to the arrow index. So, the Dirac theory provides a justification for spin-½ – or, somewhat more humbly, replaces the Pauli Hamiltonian postulate (4.163) with that of a simpler (and hence more plausible) Lorentz-invariant Hamiltonian (97).

Note, however, that this simple interpretation, fully separating a particle from its antiparticle, is not valid for the exact solutions (103)-(104), so generally the eigenstates of the Dirac Hamiltonian are certain linear (coherent) superpositions of the components describing the particle and its antiparticle – each with both directions of spin. This fact leads to several interesting effects, including the so-called *Klien paradox* at the reflection of a relativistic electron from a potential barrier.[54]

[53] It is straightforward to show that this result remains valid for a particle in any central field $U(r)$.

[54] See, e.g., A. Calogeracos and N. Dombey, *Contemp. Phys.* **40**, 313 (1999).

9.7. Low-energy limit

The generalization of Dirac's theory to the case of a (spin-½) particle with an electric charge q, moving in a classically-described electromagnetic field, may be obtained using the same replacement (90). As a result, Eq. (95) turns into

$$\left[c\hat{\boldsymbol{\alpha}}\cdot\left(-i\hbar\nabla-q\mathbf{A}\right)+mc^2\hat{\beta}+\left(q\phi-\hat{H}\right)\right]\Psi=0\,, \tag{9.112}$$

Dirac equation in EM field

where the Hamiltonian operator $\hat{H}$ is understood in the sense of Eq. (95), i.e. as the partial time derivative with the multiplier $i\hbar$. Let us prepare this equation for a low-energy approximation by acting on its left-hand side by a similar square bracket but with the opposite sign before the last parentheses – also an operator! Using Eqs. (99) and (100), and the fact that the space- and time-independent operators $\hat{\boldsymbol{\alpha}}$ and $\hat{\beta}$ commute with the spin-independent c-number functions $\mathbf{A}(\mathbf{r},t)$ and $\phi(\mathbf{r},t)$, as well as with the Hamiltonian operator $i\hbar\partial/\partial t$, the result is

$$\left\{c^2\left[\hat{\boldsymbol{\alpha}}\cdot\left(-i\hbar\nabla-q\mathbf{A}\right)\right]^2+\left(mc^2\right)^2-c\left[\hat{\boldsymbol{\alpha}}\cdot\left(-i\hbar\nabla-q\mathbf{A}\right),\left(q\phi-\hat{H}\right)\right]-\left(q\phi-\hat{H}\right)^2\right\}\Psi=0\,. \tag{9.113}$$

A direct calculation of the first square bracket, using Eqs. (98) and (107), yields

$$\left[\hat{\boldsymbol{\alpha}}\cdot\left(-i\hbar\nabla-q\mathbf{A}\right)\right]^2\equiv\left(-i\hbar\nabla-q\mathbf{A}\right)^2-2q\hat{\mathbf{S}}\cdot\nabla\times\mathbf{A}\,. \tag{9.114}$$

But the last vector product on the right-hand side is just the magnetic field – see, e.g., Eqs. (3.21):

$$\mathscr{B}=\nabla\times\mathbf{A}\,. \tag{9.115}$$

Similarly, we may use the first of Eqs. (3.21), for the electric field,

$$\mathscr{E}=-\nabla\phi-\frac{\partial\mathbf{A}}{\partial t}, \tag{9.116}$$

to simplify the commutator participating in Eq. (9.113):

$$\left[\hat{\boldsymbol{\alpha}}\cdot\left(-i\hbar\nabla-q\mathbf{A}\right),\left(q\phi-\hat{H}\right)\right]\equiv-q\hat{\boldsymbol{\alpha}}\cdot\left[\hat{H},\mathbf{A}\right]-i\hbar q\hat{\boldsymbol{\alpha}}\cdot\left[\nabla,\phi\right]\equiv-i\hbar q\frac{\partial\mathbf{A}}{\partial t}-i\hbar\hat{\boldsymbol{\alpha}}\cdot\nabla\phi\equiv i\hbar q\hat{\boldsymbol{\alpha}}\cdot\mathscr{E}\,. \tag{9.117}$$

As a result, Eq. (113) becomes

$$\left\{c^2\left(-i\hbar\nabla-q\mathbf{A}\right)^2+\left(q\phi-\hat{H}\right)^2-\left(mc^2\right)^2-2qc^2\hat{\mathbf{S}}\cdot\mathscr{B}+i\hbar cq\hat{\boldsymbol{\alpha}}\cdot\mathscr{E}\right\}\Psi=0\,. \tag{9.118}$$

So far, this is an exact result equivalent to Eq. (112), but it is more convenient for an analysis of the low-energy limit, in which not only the energy offset $E-mc^2$ (which is just the energy used in the non-relativistic mechanics), but also the electrostatic energy of the particle, $|q\langle\phi\rangle|$, are much smaller than the rest energy mc^2. In this limit, the second and third terms of Eq. (118) almost cancel, and introducing the rest-energy-offset Hamiltonian

$$\hat{\tilde{H}}\equiv\hat{H}-mc^2\hat{I}\,. \tag{9.119}$$

we may approximate their difference, up to the first non-zero term, as

$$\left(q\phi\hat{I}-\hat{H}\right)^2-\left(mc^2\right)^2\hat{I}\equiv\left(q\phi\hat{I}-mc^2\hat{I}-\hat{\tilde{H}}\right)^2-\left(mc^2\right)^2\hat{I}\approx 2mc^2\left(\hat{\tilde{H}}-q\phi\hat{I}\right). \tag{9.120}$$

As a result, after the division of all terms by $2mc^2$, Eq. (118) may be approximated as

Low-energy Hamiltonian

$$\hat{\tilde{H}}\Psi = \left[\frac{1}{2m}\left(-i\hbar\nabla - q\mathbf{A}\right)^2 + q\phi - \frac{q}{m}\hat{\mathbf{S}}\cdot\mathscr{B} + \frac{i\hbar q}{2mc}\hat{\boldsymbol{\alpha}}\cdot\mathscr{E}\right]\Psi . \tag{9.121}$$

Let us discuss this important result. The first two terms in the square brackets give the non-relativistic Hamiltonian (3.26), which was extensively used in Chapter 3 for the discussion of charged particle motion. Note again that the contribution of the vector potential **A** into that Hamiltonian is essentially relativistic, in the following sense: the magnetic interaction of two charged particles, due to their *orbital* motion with speed $v << c$, is a factor of $(v/c)^2$ smaller than the electrostatic interaction of the particles.[55] The reason why we did discuss the effects of **A** in Chapter 3 was that is was used there to describe *external* magnetic fields, keeping our analysis valid even for the cases when that field is strong because of being produced by relativistic effects – such as aligned spins of a permanent magnet.

The next, third term in the square brackets of Eq. (121) should be also familiar to the reader: this is the Pauli Hamiltonian – see Eqs. (4.3), (4.5), and (4.163). When justifying this form of interaction in Chapter 4, I referred mostly to the results of Stern-Gerlach-type experiments, but it is extremely pleasing that this result[56] follows from such a fundamental relativistic treatment as Dirac's theory. As we already know from the discussion of the Zeeman effect in Sec. 6.4, the magnetic field effects on the orbital motion of an electron (described by the orbital angular momentum **L**) and its spin **S** are of the same order, though quantitatively different.

Finally, the last term in the square brackets of Eq. (121) is also not quite new for us: in particular, it describes the spin-orbit interaction. Indeed, in the case of a classical, spherical-symmetric electric field $\mathscr{E}$ corresponding to the potential $\phi(r) = U(r)/q$, this term may be reduced to Eq. (6.56):

Spin-orbit coupling

$$\hat{H}_{so} = \frac{1}{2m^2c^2}\hat{\mathbf{S}}\cdot\hat{\mathbf{L}}\frac{1}{r}\frac{dU}{dr} \equiv -\frac{q}{2m^2c^2}\hat{\mathbf{S}}\cdot\hat{\mathbf{L}}\frac{1}{r}\mathscr{E} . \tag{9.122}$$

The proof of this correspondence requires a bit of additional work.[57] Indeed, in Eq. (121), the term responsible for the spin-orbit interaction acts on 4-component wavefunctions, while the Hamiltonian (122) is supposed to act on non-relativistic state vectors with an account of spin, whose coordinate representation may be given by 2-component spinors:[58]

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[55] This difference may be traced by classical means – see, e.g., EM Sec. 5.1.

[56] Note that in this result, the *g*-factor of the particle is still equal to exactly 2 – see Eq. (4.115) and its discussion in Sec. 4.4. In order to describe the small deviation of g_e from 2, the electromagnetic field should be quantized (just as this was discussed in Secs. 1-4 of this chapter), and its potentials **A** and ϕ, participating in Eq. (121), should be treated as operators – rather than as *c*-number functions as was assumed above.

[57] The only facts immediately evident from Eq. (121) are that the term we are discussing is proportional to the electric field, as required by Eq. (122), and that it is of the proper order of magnitude. Indeed, Eqs. (101)-(102) imply that in the Dirac theory, $c\hat{\boldsymbol{\alpha}}$ plays the role of the velocity operator, so the expectation values of the term are of the order of $\hbar qv\mathscr{E}/2mc^2$. Since the expectation values of the operators participating in the Hamiltonian (122) scale as $S \sim \hbar/2$ and $L \sim mvr$, the spin-orbit interaction energy has the same order of magnitude.

[58] In this course, the notion of spinor (popular in some textbooks) was not used much; it was introduced earlier only for two-particle states – see Eq. (8.13). For a single particle, such definition is reduced to $\psi(\mathbf{r})|s\rangle$, whose representation in a particular spin-½ basis is the column (123). Note that such spinors may be used as a basis for an expansion of the spin-orbitals $\psi_j(\mathbf{r})$ defined by Eq. (8.125), where the index *j* is used for numbering both the spin's orientation (i.e. the particular component of the spinor's column) and the orbital eigenfunction.

$$\psi = \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix}. \tag{9.123}$$

The simplest way to prove the equivalence of these two expressions is not to use Eq. (121) directly, but to return to the Dirac equation (112), for the particular case of motion in a static electric field but no magnetic field, when Dirac's Hamiltonian is reduced to

$$\hat{H} = c\hat{\boldsymbol{\alpha}} \cdot \hat{\mathbf{p}} + \hat{\beta} mc^2 + U(\mathbf{r}), \qquad \text{with } U = q\phi. \tag{9.124}$$

Since this Hamiltonian is time-independent, we may look for its 4-component eigenfunctions in the form

$$\Psi(\mathbf{r},t) = \begin{pmatrix} \psi_+(\mathbf{r}) \\ \psi_-(\mathbf{r}) \end{pmatrix} \exp\left(-i\frac{E}{\hbar}t\right), \tag{9.125}$$

where each of $\psi_\pm$ is a 2-component column of the type (123), representing two spin states of the particle (index +) and its antiparticle (index –). Plugging Eq. (125) into Eq. (95) with the Hamiltonian (124), and using Eq. (98a), we get the following system of two linear equations:

$$\left[E - mc^2 - U(\mathbf{r})\right]\psi_+ - c\hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{p}}\,\psi_- = 0, \qquad \left[E + mc^2 - U(\mathbf{r})\right]\psi_- - c\hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{p}}\,\psi_+ = 0. \tag{9.126}$$

Expressing ψ_- from the latter equation, and plugging the result into the former one, we get the following single equation for the particle's spinor:

$$\left[E - mc^2 - U(\mathbf{r}) - c^2\hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{p}} \frac{1}{E + mc^2 - U(\mathbf{r})} \hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{p}}\right]\psi_+ = 0. \tag{9.127}$$

So far, this is an exact equation for eigenstates and eigenvalues of the Hamiltonian (124), but it may be substantially simplified in the low-energy limit when both the potential energy[59] and the non-relativistic eigenenergy

$$\widetilde{E} \equiv E - mc^2 \tag{9.128}$$

are much lower than mc^2. Indeed, in this case, the expression in the denominator of the last term in the brackets of Eq. (127) is very close to $2mc^2$. Since $\boldsymbol{\sigma}^2 = 1$, with that replacement, Eq. (127) is reduced to the non-relativistic Schrödinger equation, similar for both spin components of ψ_+, and hence giving spin-degenerate energy levels. To recover small relativistic and spin-orbit effects, we need a slightly more accurate approximation:

$$\frac{1}{E + mc^2 - U(\mathbf{r})} \equiv \frac{1}{2mc^2 + \widetilde{E} - U(\mathbf{r})} \equiv \frac{1}{2mc^2}\left[1 + \frac{\widetilde{E} - U(\mathbf{r})}{2mc^2}\right]^{-1} \approx \frac{1}{2mc^2}\left[1 - \frac{\widetilde{E} - U(\mathbf{r})}{2mc^2}\right], \tag{9.129}$$

in which Eq. (127) is reduced to

$$\left[\widetilde{E} - U(\mathbf{r}) - \frac{\hat{p}^2}{2m} + \hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{p}} \frac{\widetilde{E} - U(\mathbf{r})}{(2mc^2)^2} \hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{p}}\right]\psi_+ = 0. \tag{9.130}$$

As Eqs. (5.34) shows, the operators of the momentum and of a function of coordinates commute as

$$\left[\hat{\mathbf{p}}, U(\mathbf{r})\right] = -i\hbar\nabla U, \tag{9.131}$$

[59] Strictly speaking, this requirement is imposed on the expectation values of $U(\mathbf{r})$ in the eigenstates to be found.

so the last term in the square brackets of Eq. (130) may be rewritten as

$$\hat{\boldsymbol{\sigma}}\cdot\hat{\mathbf{p}}\,\frac{\widetilde{E}-U(\mathbf{r})}{(2mc)^2}\,\hat{\boldsymbol{\sigma}}\cdot\hat{\mathbf{p}}\equiv\frac{\widetilde{E}-U(\mathbf{r})}{(2mc)^2}\,\hat{p}^2-\frac{i\hbar}{(2mc)^2}(\hat{\boldsymbol{\sigma}}\cdot\nabla U)(\hat{\boldsymbol{\sigma}}\cdot\hat{\mathbf{p}}). \tag{9.132}$$

Since in the low-energy limit, both terms on the right-hand side of this relation are much smaller than the three leading terms of Eq. (130), we may replace the first term's numerator with its non-relativistic approximation $\hat{p}^2/2m$. With this replacement, the term coincides with the first relativistic correction to the kinetic energy operator – see Eq. (6.47). The second term, proportional to the electric field $\mathscr{E}=-\nabla\phi=-\nabla U/q$, may be transformed further on, using a readily verifiable identity

$$(\hat{\boldsymbol{\sigma}}\cdot\nabla U)(\hat{\boldsymbol{\sigma}}\cdot\hat{\mathbf{p}})\equiv(\nabla U)\cdot\hat{\mathbf{p}}+i\hat{\boldsymbol{\sigma}}\cdot[(\nabla U)\times\hat{\mathbf{p}}]. \tag{9.133}$$

Of the two terms on the right-hand side of this relation, only the second one depends on the spin,[60] giving the following spin-orbital interaction contribution to the Hamiltonian,

$$\hat{H}_{\rm so}=\frac{\hbar}{(2mc)^2}\hat{\boldsymbol{\sigma}}\cdot[(\nabla U)\times\hat{\mathbf{p}}]\equiv\frac{q}{2m^2c^2}\hat{\mathbf{S}}\cdot[(\nabla\phi)\times\hat{\mathbf{p}}]. \tag{9.134}$$

For a central potential $\phi(r)$, its gradient has only the radial component: $\nabla\phi=(d\phi/dr)\mathbf{r}/r=-\mathscr{E}\mathbf{r}/r$, and with the angular momentum definition (5.147), Eq. (134) is (finally!) reduced to Eq. (122).

As was shown in Sec. 6.3, the perturbative treatment of Eq. (122), together with the kinetic-relativistic correction (6.47), in the hydrogen-like atom/ion problem, leads to the fine structure of each Bohr level E_n, given by Eq. (6.60):

$$\Delta E_{\rm fine}=\frac{E_n}{2mc^2}\left(3-\frac{4n}{j+1/2}\right)\equiv-mc^2\frac{Z^4\alpha^4}{2n^4}\left(\frac{n}{j+1/2}-\frac{3}{4}\right). \tag{9.135}$$

This result receives a confirmation from the surprising fact that for the hydrogen-like atom/ion problem, the Dirac equation may be solved *exactly* – without any assumptions. I would not have time/space to reproduce the solution,[61] and will only list the final result for the energy spectrum:

H-like atom/ion: energies

$$\frac{E}{mc^2}=\left(1+\frac{Z^2\alpha^2}{\left\{n+\left[(j+1/2)^2-Z^2\alpha^2\right]^{1/2}-(j+1/2)\right\}^2}\right)^{-1/2}. \tag{9.136}$$

Here n = 1, 2, … is the same principal quantum number as in Bohr's theory, while j is the quantum number specifying the eigenvalues (5.175) of J^2, in our case of a spin-½ particle taking half-integer values: $j = l \pm 1/2$ = 1/2, 3/2, 5/2, … – see Eq. (5.189). This is natural because due to the spin-orbit interaction, the orbital momentum and spin are not conserved, while their vector sum, $\mathbf{J}=\mathbf{L}+\mathbf{S}$, is. Each energy level (136), besides that of the ground state with n = 1 and j + ½ = 1,[62] is doubly degenerate, with two eigenstates representing two directions of the spin. (In the low-energy limit, we may say: corresponding to two values of $l = j \mp 1/2$, at fixed j.)

[60] The first term gives a small spin-independent energy shift, which is very difficult to verify experimentally.

[61] Good descriptions of the solution are available in several textbooks – see, e.g., Sec. 24.9 in E. Merzbacher, *Quantum Mechanics*, 3rd ed., Wiley (1998).

[62] Note that for that level, the theory yields $E_g/mc^2=(1-Z^2\alpha^2)^{1/2}$, so it is consistent only for $Z<1/\alpha\approx137$.

Speaking of that limit (when $E - mc^2 \sim E_H << mc^2$): since according to Eq. (1.13) for E_H, the square of the fine-structure constant $\alpha \equiv e^2/4\pi\varepsilon_0\hbar c$ may be represented as the ratio E_H/mc^2, we may follow this limit by expanding Eq. (136) into the Taylor series in $(Z\alpha)^2 << 1$. The result,

$$E \approx mc^2\left[1-\frac{Z^2\alpha^2}{2n^2}-\frac{Z^4\alpha^4}{2n^4}\left(\frac{n}{j+½}-\frac{3}{4}\right)\right], \tag{9.137}$$

has the same structure, and allows the same interpretation as Eq. (92), but with the last term coinciding with Eq. (135) – and with experimental results. Historically, this correct description of the fine structure of the atomic levels provided decisive proof of Dirac's theory.

However, even such an impressive theory does not have too many direct applications. The main reason for that was already mentioned at the end of Sec. 5: due to the possibility of creation and annihilation of particle-antiparticle pairs by an energy influx higher than $2mc^2$, the number of particles participating in high-energy interactions is not fixed. An adequate general description of such situations is given by the quantum field theory, in which the particle's wavefunction is treated as a field to be quantized, using so-called *field operators* $\hat{\Psi}(\mathbf{r},t)$– very much similar to the electromagnetic field operators (16). The Dirac equation follows from such a theory in the single-particle approximation.

As was mentioned earlier on several occasions, the quantum field theory is beyond the time/space limits of this course, and I have to stop here, referring the interested reader to one of several excellent textbooks on this discipline.[63] However, I would strongly encourage the students going in this direction to start by playing with the field operators on their own, taking clues from Eqs. (16) but replacing the creation/annihilation operators $\hat{a}_j^\dagger$ and $\hat{a}_j$ of the electromagnetic field oscillators with those of the general second quantization formalism outlined in Sec. 8.3.

9.8. Exercise problems

9.1. Prove the Casimir formula (23) 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 by a free-space gap of width $t << A^{1/2}$.

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[64] to the difference between these two results.

9.2. Electromagnetic radiation by 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. (29) to this case.

(ii) Use this generalized expression to show that incident waves in different Fock states do not create an interference pattern.

[63] For a gradual introduction see, e.g., either L. Brown, *Quantum Field Theory*, Cambridge U. Press (1994) or R. Klauber, *Student Friendly Quantum Field Theory*, Sandtrove (2013). On the other hand, M. Srednicki, *Quantum Field Theory*, Cambridge U. Press (2007) and A. Zee, *Quantum Field Theory in a Nutshell*, 2nd ed., Princeton (2010), among others, offer steeper learning curves.

[64] See, e.g., MA Eq. (2.12a).

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 α and a certain phase shift between them.

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 ζ defined by Eq. (5.142).

9.5. Calculate the rate of spontaneous photon emission (into unrestricted free space) by a hydrogen atom, initially in the 2*p* state ($n = 2$, $l = 1$) with $m = 0$. Would the result be different for $m = \pm 1$? for the 2*s* 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.

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.

9.7. Derive an analog of Eq. (53) for the spontaneous photon emission (into free space) due to a change of the *magnetic* dipole moment **m** of a small-size system.

9.8. A spin-½ particle with a gyromagnetic ratio γ is in its orbital ground state in a static magnetic field $\mathscr{B}_0$. Calculate the rate of its spontaneous transition from the higher to the lower 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.

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.

9.10. Find the eigenstates and eigenvalues of the Jaynes-Cummings Hamiltonian (78), and discuss their behavior near the resonance point $\omega = \Omega$.

9.11. Analyze the Purcell effect, mentioned in Secs. 3 and 4, quantitatively. In particular, calculate the so-called *Purcell factor* F_P defined as the ratio of the rate Γ_s of an atom's spontaneous emission into a resonant cavity tuned exactly to the quantum transition frequency, to that into free space.

9.12. Use Eq. (84) to prove the continuity relation (1.52) with the probability density w and current density **j** given by Eqs. (89).

9.13. Prove that the Klein-Gordon equation (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 2×2-matrix:

$$\mathrm{H} = -\left(\sigma_z + i\sigma_y\right)\frac{\hbar^2}{2m}\nabla^2 + mc^2\sigma_z .$$

Use your solution to discuss the physical meaning of the wavefunction's components.

9.14. Calculate and discuss the energy spectrum of a relativistic, spinless, charged particle placed into an external uniform, time-independent magnetic field $\mathscr{B}$. Use the result to formulate the condition of validity of the non-relativistic theory for this case.

9.15. Prove Eq. (91) 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 given by Eq. (3.201), $\varepsilon_n = -1/2n^2$, with $n = l + 1 + n_r$, where $n_r = 0, 1, 2, \ldots$, even if the parameter l is not an integer.

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 $\phi(\mathbf{r}) = Ze/4\pi\varepsilon_0 r$.

9.17. Starting from Eqs. (95)-(98), prove that the probability density w given by Eq. (101) and the probability current density $\mathbf{j}$ defined by Eq. (102) do indeed satisfy the continuity equation (1.52): $\partial w/\partial t + \nabla\cdot\mathbf{j} = 0$.

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.

9.19. Calculate commutators of the operators $\hat{S}^2$ and $\hat{J}^2$ with the Dirac Hamiltonian (97) and give an interpretation of the results.

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.

9.21. Calculate the energy spectrum of a relativistic spin-½ particle with an electric charge q, placed into a time-independent uniform external magnetic field $\mathscr{B}$. Compare the calculated spectrum with that following from the non-relativistic theory and the relativistic Schrödinger equation.

9.22.* Following the discussion at the end of Section 7, introduce quantum field operators $\hat{\psi}$ that would be related to the usual wavefunctions ψ just as the electromagnetic field operators (16) are related to the classical electromagnetic fields, and explore the basic properties of these operators. (For this preliminary study, consider the fixed-time situation.)