Chapter 7. Open Quantum Systems

This chapter discusses the effects of a weak interaction of a quantum system with its environment. Some part of this material is on the fine line between quantum mechanics and (quantum) statistical physics. Here I will only cover those aspects of the latter field[1] that are of key importance for the major goals of this course, including the discussion of quantum measurements in Chapter 10.

7.1. Open systems, and the density matrix

All the way until the last part of the previous chapter, we have discussed quantum systems isolated from their environment. Indeed, from the very beginning, we have assumed that we are dealing with the statistical ensembles of systems as similar to each other as only allowed by the laws of quantum mechanics. Each member of such an ensemble, called *pure* (or *coherent*), may be described by the same state vector $|\alpha\rangle$ – in the wave mechanics case, by the same wavefunction Ψ_α. Even if we deal with a composite system, say, a two-components system like those discussed at the end of the previous chapter, we still can consider its coherent states of the type

$$|\alpha\rangle = \sum_n \alpha_n |n\rangle = \sum_n \alpha_n |n_a\rangle \otimes |n_b\rangle, \tag{7.1}$$

with a *unique* correspondence between the pure states n_a and n_b of the two subsystems.

However, in many important cases, our knowledge of a quantum system's state is less complete.[2] These cases fall into two categories. The first case is when a relatively simple quantum system s of our interest (say, an electron or an atom) is in substantial contact with its environment e – here understood in the most general sense, say, as all the whole Universe less the system s – see Fig. 1. Then there is virtually no chance of making two or more experiments with exactly the same composite system because that would imply a repeated preparation of the whole environment (including the experimenter :-) in a certain quantum state – a rather challenging task, to put it mildly. Then it makes much more sense to consider a statistical ensemble of another kind – a *mixed ensemble*, with *random* states of the environment, though possibly with its macroscopic parameters (e.g., temperature, pressure, etc.) known with high precision. Such ensembles will be the focus of the analysis in this chapter.
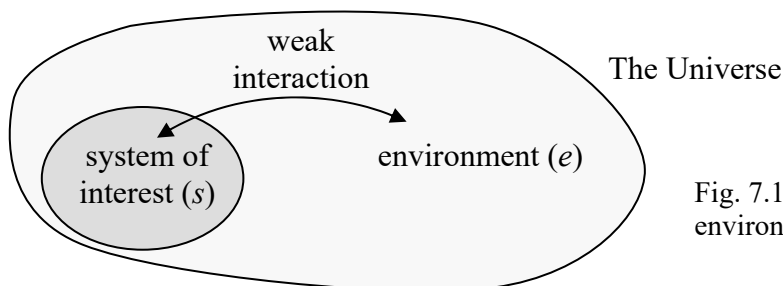

Fig. 7.1. A quantum system and its environment (VERY schematically :-).

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[1] A broader discussion of statistical mechanics and physical kinetics, including those of quantum systems, may be found in the SM part of this series.

[2] Actually, no system, possibly apart from our Universe as a whole (see below), is ever *exactly* coherent, though in many cases, deviations from the coherence may be ignored with acceptable accuracy.

Much of this analysis will also pertain to another category of cases – when the system of our interest is, at present, isolated from its environment with acceptable precision, but our knowledge of its state is still incomplete for some reason. Most typically, the system could be in contact with its environment at earlier times. So, this second category of cases may be considered as a particular case of the first one, and may be described by the results of its analysis, with certain simplifications – which will be spelled out in appropriate places of my narrative.

In classical physics, the analysis of mixed statistical ensembles is based on the notion of the probability W of each detailed ("microscopic") state of the system of interest.[3] Let us see how such an ensemble may be described in quantum mechanics. In the case when the coupling between the system of our interest and its environment is so weak that they may be clearly separated, we can still use state vectors of their states, defined in completely different Hilbert spaces. Then the most general quantum state of the whole Universe, still assumed to be pure,[4] may be described as the following linear superposition:

$$\left|\alpha\right\rangle = \sum_{j,k} \alpha_{jk} \left|s_j\right\rangle \otimes \left|e_k\right\rangle. \tag{7.2}$$

The "only" difference of such a state from the superposition described by Eq. (1), is that there is no one-to-one correspondence between the states of our system and its environment. In other words, a certain quantum state s_j of the system of interest may coexist with different states e_k of its environment. This is the quantum-mechanical description of a *mixed state* of system s.[5]

Of course, the huge size of the Hilbert space of the environment, i.e. of the number of the $\left|e_k\right\rangle$ factors in the superposition (2), strips us of any practical opportunity to make direct calculations using that sum. For example, according to the basic Eq. (4.125), in order to find the expectation value of an arbitrary observable A in the state (2), we would need to calculate all long brackets in the sum

$$\left\langle A\right\rangle = \left\langle\alpha|A|\alpha\right\rangle \equiv \sum_{j,j';k,k'} \alpha_{jk}^* \alpha_{j'k'} \left\langle e_k\right| \otimes \left\langle s_j\left|\hat{A}\right|s_{j'}\right\rangle \otimes \left|e_{k'}\right\rangle. \tag{7.3}$$

Even if we assume that each of the sets $\{s\}$ and $\{e\}$ is full and orthonormal, Eq. (3) still includes a double sum over the enormous basis state set of the environment!

However, let us consider a limited, but the most important subset of all operators – those of *intrinsic* observables, which depend only on the degrees of freedom of the system of our interest (s). These operators do not act upon the environment's degrees of freedom, and hence in Eq. (3), we may move the environment's bra-vectors $\left\langle e_k\right|$ over all the way to the ket-vectors $\left|e_{k'}\right\rangle$. Assuming, again, that the set of environmental eigenstates is full and orthonormal, Eq. (3) is now reduced to

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[3] In systems with a continuum of states, we have to discuss the *probability density w* instead – see below.

[4] Whether this assumption is true is an interesting issue, still being debated (more by philosophers than by physicists), but it is widely believed that its solution is not critical for the validity of the results of this approach to all systems available for our experimentation.

[5] Note also that in this definition, the notion of a mixed state includes pure states as particular cases, while in some texts, this term is limited to states that are *not exactly pure*. Due to the already discussed prevalence of the mixed states (in any definition!) in the world, with the exactly pure states serving only as (sometimes useful and acceptable) abstractions, this is not much of a difference.

$$\langle A \rangle = \sum_{j,j';k,k'} \alpha_{jk}^{*} \alpha_{j'k'} \langle s_j | \hat{A} | s_{j'} \rangle \langle e_k | e_{k'} \rangle = \sum_{jj'} A_{jj'} \sum_{k} \alpha_{jk}^{*} \alpha_{j'k}. \tag{7.4}$$

This is already a big relief because we have "only" a single sum over k, but the main trick is still ahead. After the summation over k, the second sum in the last form of Eq. (4) is some function w of the indices j and j', so according to Eq. (4.96), this relation may be represented as

$$\boxed{\langle A \rangle = \sum_{jj'} A_{jj'} w_{j'j} \equiv \mathrm{Tr}(\mathrm{Aw}),} \tag{7.5}$$

where the matrix w, with the elements

$$\boxed{w_{j'j} \equiv \sum_{k} \alpha_{jk}^{*} \alpha_{j'k}, \quad \text{i.e. } w_{jj'} \equiv \sum_{k} \alpha_{jk} \alpha_{j'k}^{*},} \tag{7.6}$$

is called the *density matrix* of the system.[6] Most importantly, Eq. (5) shows that the knowledge of this matrix allows the calculation of the expectation value of *any* intrinsic observable A (and, according to the general Eqs. (1.33)-(1.34), its r.m.s. fluctuation as well, if needed), even for the very general state (2). This is why let us have a good look at the density matrix.

First of all, we know from the general discussion in Chapter 4, fully applicable to the pure state (2), the expansion coefficients in superpositions of this type may be always expressed as short brackets of the type (4.40); in our current case, we may write

$$\alpha_{jk} = \left(\langle e_k | \otimes \langle s_j | \right) | \alpha \rangle. \tag{7.7}$$

Plugging this expression into Eq. (6), we get

$$w_{jj'} \equiv \sum_{k} \alpha_{jk} \alpha_{j'k}^{*} = \langle s_j | \otimes \left(\sum_{k} \langle e_k | \alpha \rangle \langle \alpha | e_k \rangle \right) \otimes | s_{j'} \rangle = \langle s_j | \hat{w} | s_{j'} \rangle. \tag{7.8}$$

We see that from the point of our system (i.e. in its Hilbert space whose basis states may be numbered by the index j only), the density matrix is indeed just the matrix of some construct,[7]

$$\boxed{\hat{w} \equiv \sum_{k} \langle e_k | \alpha \rangle \langle \alpha | e_k \rangle,} \tag{7.9}$$

which is called the *density* (or "statistical") *operator*. As it follows from the definition (9), in contrast to the density matrix, this operator does not depend on the choice of a particular basis s_j – just as all linear operators considered earlier in this course. However, in contrast to them, the density operator *does* depend on the composite system's state α, including the state of the system s as well. Still, in the j-space, it is mathematically just an operator whose matrix elements obey all relations of the bra-ket formalism.

In particular, due to its definition (6), the density operator is Hermitian:

$$w_{jj'}^{*} = \sum_{k} \alpha_{jk}^{*} \alpha_{j'k} = \sum_{k} \alpha_{j'k} \alpha_{jk}^{*} = w_{j'j}, \tag{7.10}$$

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[6] This notion was introduced in 1927 by John von Neumann.

[7] Note that the "short brackets" in this expression are not c-numbers, because the state α is defined in a larger Hilbert space (of the environment plus the system of interest) than the basis states e_k (of the environment only).

so according to the general analysis of Sec. 4.3, in the Hilbert space of the system s, there should be a certain basis $\{w\}$ in that the matrix of this operator is diagonal:

$$w_{jj'}\big|_{\text{in } w} = w_j \delta_{jj'}. \tag{7.11}$$

Since any operator, in any basis, may be represented in the form (4.59), in the basis $\{w\}$ we may write

$$\hat{w} = \sum_j |w_j\rangle w_j \langle w_j|. \tag{7.12}$$

Density operator in w-basis

This expression reminds but is not equivalent to Eq. (4.44) for the identity operator, that has been used so many times in this course, and in the basis w_j has the form

$$\hat{I} = \sum_j |w_j\rangle\langle w_j|. \tag{7.13}$$

In order to comprehend the meaning of the coefficients w_j participating in Eq. (12), let us use Eq. (5) to calculate the expectation value of any observable A whose eigenstates coincide with those of the special basis $\{w\}$, and whose matrix is, therefore, diagonal in this basis:

$$\langle A \rangle = \text{Tr}(\text{Aw}) = \sum_{jj'} A_{jj'} w_j \delta_{jj'} = \sum_j A_j w_j, \tag{7.14}$$

Expectation value of w_j-compatible variable

where A_j is just the expectation value of the observable A in the state w_j. Hence, to comply with the general Eq. (1.37), the real c-number w_j must have the physical sense of the probability W_j of finding the system in the state j. As the result, we may rewrite Eq. (12) in the form[8]

$$\hat{w} = \sum_j |w_j\rangle W_j \langle w_j|. \tag{7.15}$$

In the ultimate case when only one of the probabilities (say, $W_{j''}$) is different from zero,

$$W_j = \delta_{jj''}, \tag{7.16}$$

the system is in a pure (coherent) state $w_{j''}$. Indeed, it is fully described by one ket-vector $|w_{j''}\rangle$, and we can use the general rule (4.86) to represent it in another (arbitrary) basis $\{s\}$ as a coherent superposition

$$\left|w_{j''}\right\rangle = \sum_{j'} U^{\dagger}_{j''j'} |s_{j'}\rangle = \sum_{j'} U^{*}_{j'j''} |s_{j'}\rangle, \tag{7.17}$$

where U is the unitary matrix of transform from the basis $\{w\}$ to the basis $\{s\}$. According to Eqs. (11) and (16), in such a pure state, the density matrix is diagonal in the $\{w\}$ basis,

$$w_{jj'}\big|_{\text{in } w} = \delta_{j,j''}\delta_{j',j''}, \tag{7.18a}$$

but not in an arbitrary basis. Indeed, using the general rule (4.92), we get

$$w_{jj'}\big|_{\text{in } s} = \sum_{l,l'} U^{\dagger}_{jl} w_{ll'}\big|_{\text{in } w} U_{l'j'} = U^{\dagger}_{jj''} U_{j''j'} = U^{*}_{j''j} U_{j''j'}. \tag{7.18b}$$

To make this result more transparent, let us denote the matrix elements $U_{j''j} \equiv \langle w_{j''}|s_j\rangle$ (which, for a fixed j'', depend on just one index j) as α_j; then

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[8] In some textbooks, this relation is taken for the theory's starting point, leaving the physical sense of the density operator obscure.

$$w_{jj'}\big|_{\text{in } s} = \alpha_j^* \alpha_{j'},$$

(7.19)

so N^2 elements of the whole $N \times N$ matrix are determined by just *one* string of N c-numbers α_j. For example, for a two-level system ($N = 2$),

$$\text{w}\big|_{\text{in } s} = \begin{pmatrix} \alpha_1 \alpha_1^* & \alpha_2 \alpha_1^* \\ \alpha_1 \alpha_2^* & \alpha_2 \alpha_2^* \end{pmatrix}.$$

(7.20)

We see that the off-diagonal terms are, colloquially, "as large as the diagonal ones", in the following sense:

$$w_{12} w_{21} = w_{11} w_{22}.$$

(7.21)

Since the diagonal terms have the sense of the probabilities $W_{1,2}$ to find the system in the corresponding state, we may represent Eq. (20) as

$$\text{w}\big|_{\text{pure state}} = \begin{pmatrix} W_1 & (W_1 W_2)^{1/2} e^{i\varphi} \\ (W_1 W_2)^{1/2} e^{-i\varphi} & W_2 \end{pmatrix}.$$

(7.22)

The physical sense of the (real) constant φ is the phase shift between the coefficients in the linear superposition (17), which represents the pure state $w_{j''}$ in the basis $\{s_{1,2}\}$.

Now let us consider a different statistical ensemble of two-level systems, that includes the member states identical in all aspects (including similar probabilities $W_{1,2}$ in the same basis $s_{1,2}$), besides that the phase shifts φ are random, with the phase's probability uniformly distributed over the trigonometric circle. Then the ensemble averaging is equivalent to the averaging over φ from 0 to 2π,[9] which kills the off-diagonal terms of the density matrix (22), so the matrix becomes diagonal:

$$\text{w}\big|_{\text{classical mixture}} = \begin{pmatrix} W_1 & 0 \\ 0 & W_2 \end{pmatrix}.$$

(7.23)

The mixed statistical ensemble with the density matrix diagonal in the stationary state basis is called the *classical mixture* and represents the limit opposite to the pure state.

After this example, the reader should not be much shocked by the main claim[10] of statistical mechanics that any large ensemble of similar systems in *thermodynamic* (or "thermal") *equilibrium* is exactly such a classical mixture. Moreover, for systems in thermal equilibrium with a much larger environment of a fixed temperature T (such an environment is frequently called either a "heat bath" or a "thermostat"), statistical physics gives a very simple expression, called the *Gibbs distribution*, for the probabilities W_n:

$$W_n = \frac{1}{Z} \exp\left\{-\frac{E_n}{k_B T}\right\}, \qquad \text{with } Z \equiv \sum_n \exp\left\{-\frac{E_n}{k_B T}\right\}.$$

(7.24)

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[9] For a system with a time-independent Hamiltonian, such averaging is especially plausible in the basis of the stationary states n of the system, in which the phase φ is just the difference of integration constants in Eq. (4.158), and its randomness may be naturally produced by minor fluctuations of the energy difference $E_1 - E_2$.
[10] This fact follows from the basic postulate of statistical physics, called the *microcanonical distribution* – see, e.g., SM Sec. 2.2.

where E_n is the eigenenergy of the corresponding stationary state, and the normalization coefficient Z is called the *statistical sum*.[11]

A detailed analysis of classical and quantum ensembles in thermodynamic equilibrium is a major focus of statistical physics courses (such as the SM part of this series) rather than this course of quantum mechanics. However, I would still like to attract the reader's attention to the key fact that, in contrast with the similarly-looking Boltzmann distribution for single particles,[12] the Gibbs distribution is *general*, *not* limited to classical statistics. In particular, for a quantum gas of indistinguishable particles, it is absolutely compatible with the quantum statistics (such as the Bose-Einstein or Fermi-Dirac distributions) of the component particles. For example, if we use Eq. (24) to calculate the average energy of a 1D harmonic oscillator of frequency ω_0 in thermal equilibrium, we easily get[13]

$$W_n = \exp\left\{-n\frac{\hbar\omega_0}{k_B T}\right\}\left(1-\exp\left\{-\frac{\hbar\omega_0}{k_B T}\right\}\right), \qquad Z = \exp\left\{-\frac{\hbar\omega_0}{2k_B T}\right\}\bigg/\left(1-\exp\left\{-\frac{\hbar\omega_0}{k_B T}\right\}\right), \quad (7.25)$$

$$\langle E \rangle \equiv \sum_{n=0}^{\infty} W_n E_n = \frac{\hbar\omega_0}{2}\coth\frac{\hbar\omega_0}{2k_B T} \equiv \frac{\hbar\omega_0}{2} + \frac{\hbar\omega_0}{\exp\{\hbar\omega_0 / k_B T\}-1}. \qquad (7.26a)$$

The final form of the last result,

$$\langle E \rangle = \frac{\hbar\omega_0}{2} + \hbar\omega_0\langle n \rangle, \quad \text{with } \langle n \rangle = \frac{1}{\exp\{\hbar\omega_0 / k_B T\}-1} \to \begin{cases} 0, & \text{for } k_B T \ll \hbar\omega_0, \\ k_B T/\hbar\omega_0, & \text{for } \hbar\omega_0 \ll k_B T, \end{cases} \qquad (7.26b)$$

may be interpreted as an addition, to the ground-state energy $\hbar\omega_0/2$, of the average number $\langle n \rangle$ of thermally-induced excitations, with the energy $\hbar\omega_0$ each. In the harmonic oscillator, whose energy levels are equidistant, such a language is completely appropriate, because the transfer of the system from any level to the one just above it adds the same amount of energy, $\hbar\omega_0$. Note that the above expression for $\langle n \rangle$ is actually the Bose-Einstein distribution (for the particular case of zero chemical potential); we see that it does not contradict the Gibbs distribution (24) of the total energy of the system, but rather immediately follows from it.

Because of the fundamental importance of Eq. (26) for virtually all fields of physics, let me draw the reader's attention to its two main properties. At low temperatures, $k_B T \ll \hbar\omega_0$, there are virtually no excitations, $\langle n \rangle \to 0$, and the average energy of the oscillator is dominated by that of its ground state. In the opposite limit of high temperatures, $\langle n \rangle \to k_B T/\hbar\omega_0 \gg 1$, and $\langle E \rangle$ approaches the classical value $k_B T$.

7.2. Coordinate representation and the Wigner function

For many applications of the density operator, its coordinate representation is convenient. (I will only discuss it for the 1D case; the generalization to multi-dimensional cases is straightforward.)

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[11] See. e.g., SM Sec. 2.4. The Boltzmann constant k_B is only needed if the temperature is measured in non-energy units – say in kelvins.

[12] See, e.g., SM Sec. 2.8.

[13] See, e.g., SM Sec. 2.5 – but mind a different energy reference level, $E_0 = \hbar\omega_0/2$, used for example in SM Eqs. (2.68)-(2.69), affecting the expression for Z. Actually, the calculation, using Eqs. (24) and (5.86), is so straightforward that it is highly recommended to the reader as a simple exercise.

Following Eq. (4.47), it is natural to define the following function of two arguments – traditionally, but a bit misleadingly, also called the *density matrix*:

$$w(x, x') \equiv \langle x|\hat{w}|x'\rangle . \tag{7.27}$$

Inserting, into the right-hand side of this definition, two closure conditions (4.44) for an arbitrary (but full and orthonormal) basis $\{s\}$, and then using Eq. (4.233),[14] we get

$$w(x, x') = \sum_{j,j'} \langle x|s_j\rangle \langle s_j|\hat{w}|s_{j'}\rangle \langle s_{j'}|x'\rangle = \sum_{j,j'} \psi_j(x) w_{jj'}\big|_{\text{in } s} \psi_{j'}^*(x') . \tag{7.28}$$

In the special basis $\{w\}$, in which the density matrix is diagonal, this expression is reduced to

$$w(x, x') = \sum_j \psi_j(x) W_j \psi_j^*(x') . \tag{7.29}$$

Let us discuss the properties of this function. At coinciding arguments, $x' = x$, this is just the probability density:[15]

$$w(x, x) = \sum_j \psi_j(x) W_j \psi_j^*(x) = \sum_j w_j(x) W_j = w(x) . \tag{7.30}$$

However, the density matrix gives more information about the system than just the probability density. As the simplest example, let us consider a pure quantum state, with $W_j = \delta_{j,j'}$, so $\psi(x) = \psi_j(x)$, and

$$w(x, x') = \psi_{j'}(x) \psi_{j'}^*(x') \equiv \psi(x) \psi^*(x') , \tag{7.31}$$

so

$$\left|w(x, x')\right|^2 \equiv w(x, x') w^*(x, x') = \psi(x) \psi^*(x) \psi(x') \psi^*(x') = w(x) w(x') . \tag{7.32}$$

For example, for a simple wave packet with a small spatial extent δx, $w(x, x')$ has an appreciable magnitude only if both points are not farther than $\sim\delta x$ from the packet center, and hence from each other. Note that the density matrix carries information not only about the modulus but also the phase of the wavefunction. However, in the ultimate limit of a pure state, the density-matrix description is redundant because all this information is contained in the wavefunction itself.

The density matrix becomes really invaluable when we deal with an incoherent mixture of several wavefunctions, for example, with the classical mixture describing the thermodynamic equilibrium. In this case, we can use Eq. (24) to rewrite Eq. (29) as follows:

$$w(x, x') = \sum_n \psi_n(x) W_n \psi_n^*(x') = \frac{1}{Z} \sum_n \psi_n(x) \exp\left\{-\frac{E_n}{k_B T}\right\} \psi_n^*(x') . \tag{7.33}$$

As the simplest example, let us see what is the density matrix of a *free* particle in thermal equilibrium. As we know very well by now, in this case, the set of energies $E_p = p^2/2m$ of stationary states (monochromatic waves) forms a continuum, so we need to replace the sum (33) with an integral, using, for example, the "delta-normalized" traveling-wave eigenfunctions (4.264):

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[14] For now, I will focus on a fixed time instant (say, $t = 0$), and hence write $\psi(x)$ instead of $\Psi(x, t)$.
[15] This fact is the origin of the density matrix's name.

$$w(x, x') = \frac{1}{2\pi\hbar Z} \int\limits_{-\infty}^{+\infty} \exp\left\{-\frac{ipx}{\hbar}\right\} \exp\left\{-\frac{p^2}{2mk_BT}\right\} \exp\left\{\frac{ipx'}{\hbar}\right\} dp. \tag{7.34}$$

This is a usual Gaussian integral and may be worked out, as we have done repeatedly in Chapter 2 and beyond, by complementing the exponent to the full square of the momentum p plus a constant. The statistical sum Z may be also readily calculated, [16]

$$Z = (2\pi mk_BT)^{1/2}, \tag{7.35}$$

However, for what follows it is more useful to write the result for the product wZ (the so-called *un-normalized density matrix*):

$$w(x, x')Z = \left(\frac{mk_BT}{2\pi\hbar^2}\right)^{1/2} \exp\left\{-\frac{mk_BT(x-x')^2}{2\hbar^2}\right\}. \tag{7.36}$$

This is a very interesting result: the density matrix depends only on the difference of its arguments, dropping to zero fast as the distance between the points x and x' exceeds the following characteristic scale (sometimes called the *correlation length* or *correlation distance*[17])

$$x_c \equiv \left\langle (x-x')^2 \right\rangle^{1/2} = \frac{\hbar}{(mk_BT)^{1/2}}. \tag{7.37}$$

Some gut feeling of this length may be obtained from the following observation. It is straightforward to use Eq. (24) to verify that the average energy $\langle E \rangle = \langle p^2/2m \rangle$ of a free particle in thermal equilibrium, i.e. in the classical mixture (33), equals $k_BT/2$. (This value agrees with the *equipartition theorem* of classical statistics.[18]) Hence the average magnitude of the particle's momentum may be estimated as

$$p_c \equiv \left\langle p^2 \right\rangle^{1/2} = (2m\langle E \rangle)^{1/2} = (mk_BT)^{1/2}, \tag{7.38}$$

so x_c is of the order of the minimal length allowed by the Heisenberg-like "uncertainty relation":

$$x_c = \frac{\hbar}{p_c}. \tag{7.39}$$

With the growth of temperature, the correlation length (37) goes to zero, and the density matrix (36) tends to a delta function:

$$w(x, x')Z\big|_{T\to\infty} \to \delta(x-x'). \tag{7.40}$$

Since in this limit the average kinetic energy of the particle is not smaller than its potential energy in *any* fixed potential profile, Eq. (40) is the general property of the density matrix (33).

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[16] Due to the delta-normalization of the eigenfunction, the density matrix (34) for the free particle (and any system with a continuous eigenvalue spectrum) is normalized as

$$\int\limits_{-\infty}^{+\infty} w(x, x')Z dx' = \int\limits_{-\infty}^{+\infty} w(x, x')Z dx = 1.$$

[17] Note that in some other fields of physics, the same term is used for a differently defined notion – see, e.g., SM Eqs. (4.30)-(4.31).
[18] See, e.g., SM Sec. 2.2.

Moreover, as will be shown in a minute (see Eq. (61) below), Eq. (36) may be used to calculate not only the r.m.s. magnitude p_c of the free particle's momentum[19] but also the whole distribution of the momentum's probability density. Thus for mixed states, the density function $w(x, x')$ is indeed much more informative than the probability distribution $w(x)$ – which, in our current case, is flat.

Now note the following important feature of Eq. (36): if we replace $k_B T$ with $\hbar/i(t - t_0)$, and x' with x_0, the un-normalized density matrix wZ for a free particle turns into the particle's propagator – cf. Eq. (2.49). This is not just an occasional coincidence. Indeed, in Chapter 2 we saw that the propagator of a system with an arbitrary stationary Hamiltonian may be expressed via the stationary eigenfunctions as

$$G(x,t;x_0,t_0) = \sum_n \psi_n(x) \exp\left\{-i\frac{E_n}{\hbar}(t - t_0)\right\} \psi_n^*(x_0).$$ (7.41)

Comparing this expression with Eq. (33), we see that the replacement

$$\frac{i(t - t_0)}{\hbar} \to \frac{1}{k_B T},$$ (7.42)

plus the notation replacement $x' \to x_0$, turn the pure-state propagator G into the un-normalized density matrix wZ of the same system in thermodynamic equilibrium. This important fact, rooted in the mathematical similarity of the Gibbs distribution (24) with the Schrödinger equation's solution (1.69), enables a theoretical technique of the so-called *thermodynamic Green's functions*, which is especially productive in condensed matter physics.[20]

For our current purposes, we can employ Eq. (42) to reuse some of the wave mechanics results, in particular, the following formula for the harmonic oscillator's propagator

$$G(x,t;x_0,t_0) = \left(\frac{m\omega_0}{2\pi i\hbar \sin[\omega_0(t - t_0)]}\right)^{1/2} \exp\left\{-\frac{m\omega_0\left[(x^2 + x_0^2)\cos[\omega_0(t - t_0)] - 2xx_0\right]}{2i\hbar \sin[\omega_0(t - t_0)]}\right\}.$$ (7.43)

which may be readily proved to satisfy the Schrödinger equation for the Hamiltonian (5.62), with the appropriate initial condition: $G(x, t_0; x_0, t_0) = \delta(x - x_0)$. Making the substitution (42), we immediately get

Harmonic oscillator in thermal equilibrium

$$w(x, x')Z = \left[\frac{m\omega_0}{2\pi\hbar \sinh(\hbar\omega_0 / k_B T)}\right]^{1/2} \exp\left\{-\frac{m\omega_0\left[(x^2 + x'^2)\cosh(\hbar\omega_0 / k_B T) - 2xx'\right]}{2\hbar \sinh(\hbar\omega_0 / k_B T)}\right\}.$$ (7.44)

As a sanity check, at very low temperatures, $k_B T \ll \hbar\omega_0$, both hyperbolic functions participating in this expression are very large and nearly equal, and it yields

$$w(x, x')Z\big|_{T \to 0} \to \left[\left(\frac{m\omega_0}{\pi\hbar}\right)^{1/4} \exp\left\{-\frac{m\omega_0 x^2}{\hbar}\right\}\right] \times \exp\left\{-\frac{\hbar\omega_0}{2k_B T}\right\} \times \left[\left(\frac{m\omega_0}{\pi\hbar}\right)^{1/4} \exp\left\{-\frac{m\omega_0 x'^2}{\hbar}\right\}\right].$$ (7.45)

---

[19] This is what could be expected from the basic equation (5): the density matrix enables the calculation of the statistical average of any variable pertaining to the system – including its momentum.

[20] I will have no time to discuss this technique and have to refer the interested reader to special literature. Probably, the most famous text of that field is A. Abrikosov, L. Gor'kov, and I. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics*, Prentice-Hall, 1963. (Later reprintings are available from Dover.)

In each of the expressions in square brackets, we can readily recognize the ground state's wavefunction (2.275) of the oscillator, while the middle exponent is just the statistical sum (24) in the low-temperature limit when it is dominated by the ground-level contribution:

$$Z\big|_{T \to 0} \to \exp\left\{-\frac{\hbar\omega_0}{2k_B T}\right\}. \tag{7.46}$$

As a result, Z in both parts of Eq. (45) may be canceled, and the density matrix in this limit is described by Eq. (31), with the ground state as the only state of the oscillator. This is natural when the temperature is too low for the thermal excitation of any other state.

Returning to arbitrary temperatures, Eq. (44) in coinciding arguments gives the following expression for the probability density:[21]

$$w(x,x)Z \equiv w(x)Z = \left[\frac{m\omega_0}{2\pi\hbar \sinh(\hbar\omega_0 / k_B T)}\right]^{1/2} \exp\left\{-\frac{m\omega_0 x^2}{\hbar} \tanh\frac{\hbar\omega_0}{2k_B T}\right\}. \tag{7.47}$$

This is just a Gaussian function of x, with the following variance:

$$\langle x^2 \rangle = \frac{\hbar}{2m\omega_0} \coth\frac{\hbar\omega_0}{2k_B T}. \tag{7.48}$$

To compare this result with our earlier ones, it is useful to recast it as

$$\langle U \rangle = \frac{m\omega_0^2}{2}\langle x^2 \rangle = \frac{\hbar\omega_0}{4} \coth\frac{\hbar\omega_0}{2k_B T}. \tag{7.49}$$

Comparing this expression with Eq. (26), we see that the average value of potential energy is exactly one-half of the total energy – the other half being the average kinetic energy. This is what we could expect, because according to Eqs. (5.96)-(5.97), such relation holds for each Fock state and hence should also hold for their classical mixture.

Unfortunately, besides the trivial case (30) of coinciding arguments, it is hard to give a straightforward interpretation of the density function in terms of the system's measurements. This is a fundamental difficulty, which has been well explored in terms of the *Wigner function* (sometimes called the "Wigner-Ville distribution")[22] defined as

$$W(X,P) \equiv \frac{1}{2\pi\hbar}\int w\left(X + \frac{\tilde{X}}{2}, X - \frac{\tilde{X}}{2}\right) \exp\left\{-\frac{iP\tilde{X}}{\hbar}\right\} d\tilde{X}. \tag{7.50}$$

Wigner function: definition

From the mathematical standpoint, this is just the Fourier transform of the density matrix in one of two new coordinates defined by the following relations (see Fig. 2):

---

[21] I have to confess that this notation is imperfect, because strictly speaking, $w(x, x')$ and $w(x)$ are different functions, and so are the functions $w(p, p')$ and $w(p)$ used below. In a perfect world, I would use different letters for them all, but I desperately want to stay with "w" for all the probability densities, and there are not so many good fonts for this letter. Let me hope that the difference between these functions is clear from their arguments and the context.

[22] It was introduced in 1932 by Eugene Wigner on the basis of a general (*Weyl-Wigner*) transform suggested by Hermann Weyl in 1927 and re-derived in 1948 by Jean Ville on a different mathematical basis.

$$X \equiv \frac{x + x'}{2}, \quad \widetilde{X} \equiv x - x', \quad \text{so that} \quad x \equiv X + \frac{\widetilde{X}}{2}, \quad x' \equiv X - \frac{\widetilde{X}}{2}. \tag{7.51}$$

Physically, the new argument X may be interpreted as the average position of the particle during the time interval $(t - t')$, while $\widetilde{X}$, as the distance passed by it during that time interval, so P characterizes the momentum of the particle during that motion. As a result, the Wigner function may be understood as a mathematical construct intended to characterize the system's probability distribution simultaneously in the coordinate and the momentum space – for 1D systems, on the phase plane $[X, P]$ that was discussed earlier – see Fig. 5.8. Let us see how fruitful this intention is.
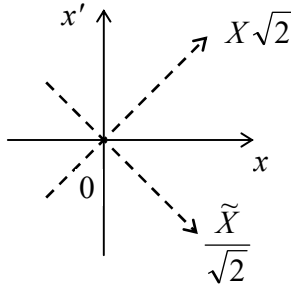

Fig. 7.2. The coordinates X and $\widetilde{X}$ employed in the Weyl-Wigner transform (50). They differ from the coordinates obtained by the rotation of the reference frame by the angle $\pi/4$ only by factors $\sqrt{2}$ and $1/\sqrt{2}$, describing scale stretch.

First of all, we may write the Fourier transform reciprocal to Eq. (50):

$$w\left(X + \frac{\widetilde{X}}{2}, X - \frac{\widetilde{X}}{2} \right) = \int W(X, P) \exp\left\{ \frac{iP\widetilde{X}}{\hbar} \right\} dP. \tag{7.52}$$

For the particular case $\widetilde{X} = 0$, this relation yields

$$w(X) \equiv w(X, X) = \int W(X, P) dP. \tag{7.53}$$

Hence the integral of the Wigner function over the momentum P gives the probability density to find the system at point X – just as it does for a classical distribution function $w_{cl}(X, P)$.[23]

Next, the Wigner function has a similar property for its integration over X. To prove this fact, we may first introduce the momentum representation of the density matrix, in full analogy with its coordinate representation (27):

$$w(p, p') \equiv \langle p | \hat{w} | p' \rangle. \tag{7.54}$$

Inserting, as usual, two identity operators, in the form given by Eq. (4.252), into the right-hand side of this equality, we get the following relation between the momentum and coordinate representations:

$$w(p, p') = \int\int dx dx' \langle p | x \rangle \langle x | \hat{w} | x' \rangle \langle x' | p' \rangle = \frac{1}{2\pi\hbar} \int\int dx dx' \exp\left\{ -\frac{ipx}{\hbar} \right\} w(x, x') \exp\left\{ +\frac{ip'x'}{\hbar} \right\}. \tag{7.55}$$

This is of course nothing else than the unitary transform of an operator from the x-basis to the p-basis, similar to the first form of Eq. (4.272). For coinciding arguments, $p = p'$, Eq. (55) is reduced to

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[23] Such function, used to express the probability dW to find the system in a small area of the phase plane as $dW = w_{cl}(X, P) dX dP$, is a major notion of the (1D) classical statistics – see, e.g., SM Sec. 2.1.

$$w(p) \equiv w(p,p) = \frac{1}{2\pi\hbar} \int\int dxdx' \, w(x,x') \exp\left\{-\frac{ip(x-x')}{\hbar}\right\}. \tag{7.56}$$

Now using Eq. (29) and then Eq. (4.265), this function may be represented as

$$w(p) = \frac{1}{2\pi\hbar} \sum_j W_j \int\int dxdx' \, \psi_j(x)\psi_j^*(x) \exp\left\{-\frac{ip(x-x')}{\hbar}\right\} = \sum_j W_j \varphi_j(p)\varphi_j^*(p), \tag{7.57}$$

and hence interpreted as the probability density of the particle's momentum at value p. Now, in the variables (51), Eq. (56) has the form

$$w(p) = \frac{1}{2\pi\hbar} \int\int w\left(X + \frac{\tilde{X}}{2}, X - \frac{\tilde{X}}{2}\right) \exp\left\{-\frac{ip\tilde{X}}{\hbar}\right\} d\tilde{X}dX. \tag{7.58}$$

Comparing this equality with the definition (50) of the Wigner function, we see that

$$w(P) = \int W(X,P)dX . \tag{7.59}$$

Thus, according to Eqs. (53) and (59), the integrals of the Wigner function over either the coordinate or momentum give the probability densities to find the system at a certain value of the counterpart variable. This is of course the main requirement for any quantum-mechanical candidate for the best analog of the classical probability density, $w_{cl}(X, P)$.

Let us see how the Wigner function looks for the simplest systems at thermodynamic equilibrium. For a free 1D particle, we can use Eq. (34), ignoring for simplicity the normalization issues:

$$W(X,P) \propto \int_{-\infty}^{+\infty} \exp\left\{-\frac{mk_B T\tilde{X}^2}{2\hbar^2}\right\} \exp\left\{-\frac{iP\tilde{X}}{\hbar}\right\} d\tilde{X} . \tag{7.60}$$

The usual Gaussian integration yields

$$W(X,P) = \text{const} \times \exp\left\{-\frac{P^2}{2mk_B T}\right\}. \tag{7.61}$$

We see that the function is independent of X (as it should be for this translational-invariant system), and coincides with the Gibbs distribution (24).[24] We could get the same result directly from classical statistics. This is natural because as we know from Sec. 2.2, the free motion is essentially not quantized – at least in terms of its energy and momentum.

Now let us consider a "more quantum" system, the harmonic oscillator. Plugging Eq. (44) into Eq. (50), for that system in thermal equilibrium it is easy (and hence is left for the reader's exercise) to show that the Wigner function is also Gaussian, now in both its arguments:

$$W(X,P) = \text{const} \times \exp\left\{-C\left[\frac{m\omega_0^2 X^2}{2} + \frac{P^2}{2m}\right]\right\}, \tag{7.62}$$

though the coefficient C is now different from $1/k_B T$, and tends to that limit only at high temperatures, $k_B T \gg \hbar\omega_0$. Moreover, for a Glauber state, the Wigner function also gives a very vivid result – a

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[24] Note also that the width of this Gaussian distribution of momentum is indeed given by Eq. (38).

Gaussian distribution similar to Eq. (62), but properly shifted from the origin to the central point of the state – see Sec. 5.5.

However, for some other possible states of the harmonic oscillator, e.g., any pure Fock state with $n > 0$, the Wigner function takes negative values in some regions of the $[X, P]$ plane – see Fig. 3.[25] (Such plots were the basis of my, admittedly very imperfect, classical images of the Fock states in Fig. 5.8.)
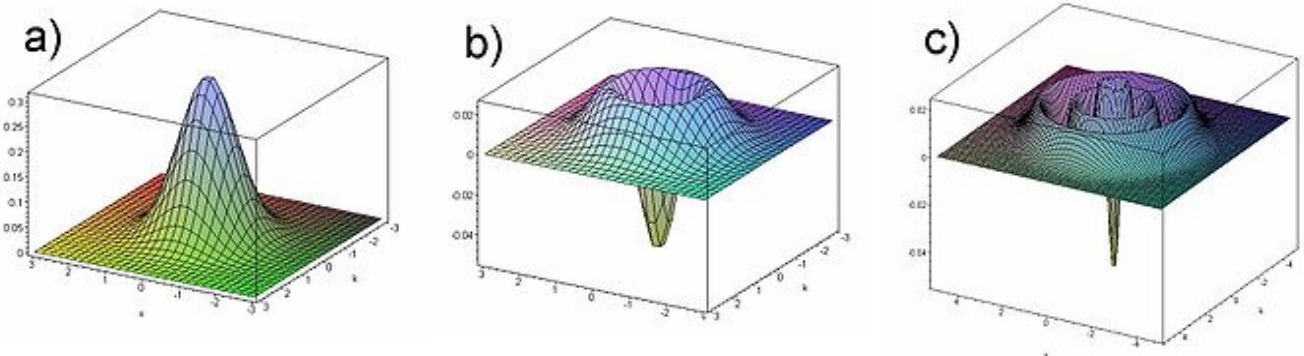

Fig. 7.3. The Wigner functions $W(X, P)$ of a harmonic oscillator, in a few of its stationary (Fock) states n: (a) $n = 0$, (b) $n = 1$; (c) $n = 5$. Graphics by J. S. Lundeen; adapted from http://en.wikipedia.org/wiki/Wigner_function as a public-domain material.

The same is true for most other quantum systems and their states. Indeed, this fact could be predicted just by looking at the definition (50) applied to a pure quantum state, in which the density function may be factored – see Eq. (31):

$$W(X,P) = \frac{1}{2\pi\hbar} \int \psi\left(X + \frac{\widetilde{X}}{2}\right) \psi^*\left(X - \frac{\widetilde{X}}{2}\right) \exp\left\{-\frac{iP\widetilde{X}}{\hbar}\right\} d\widetilde{X}. \tag{7.63}$$

By changing the argument P (say, at fixed X), we are essentially changing the spatial "frequency" (wave number) of the wavefunction product's Fourier component we are calculating, and we know that their Fourier images typically change sign as the frequency is changed. Hence the wavefunctions should have some high-symmetry properties to avoid this effect. Indeed, the Gaussian functions (describing, for example, the Glauber states, the squeezed states, and in their particular case, the ground state of the harmonic oscillator) have such symmetry, but many other functions do not.

Hence the Wigner function cannot serve as a direct quantum-mechanical analog of the classical probability density $w_{cl}(X, P)$. However, the function is useful for semi-quantitative interpretation of complicated mixed states of quantum systems.

7.3. Open system dynamics: Dephasing

So far we have discussed the density operator as something *given* at a particular time instant. Now let us discuss how is it *formed*, i.e. its evolution in time, starting from the simplest case when the probabilities W_j participating in Eq. (15) are *time-independent* – by this or that reason, to be discussed in a moment. In this case, in the Schrödinger picture, we may rewrite Eq. (15) as

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[25] Spectacular experimental measurements of this function (for $n = 0$ and $n = 1$) were carried out recently by E. Bimbard *et al.*, *Phys. Rev. Lett.* **112**, 033601 (2014).

$$\hat{w}(t) = \sum_j \left| w_j(t) \right\rangle W_j \left\langle w_j(t) \right|. \tag{7.64}$$

Taking a time derivative of both sides of this equation, multiplying them by $i\hbar$, and applying Eq. (4.158) to the basis states w_j, with the account of the fact that the Hamiltonian operator is Hermitian, we get

$$
\begin{aligned}
i\hbar \dot{\hat{w}} &= i\hbar \sum_j \left(\left| \dot{w}_j(t) \right\rangle W_j \left\langle w_j(t) \right| + \left| w_j(t) \right\rangle W_j \left\langle \dot{w}_j(t) \right| \right) \\
&= \sum_j \left(\hat{H} \left| w_j(t) \right\rangle W_j \left\langle w_j(t) \right| - \left| w_j(t) \right\rangle W_j \left\langle w_j(t) \right| \hat{H} \right) \\
&\equiv \hat{H} \sum_j \left| w_j(t) \right\rangle W_j \left\langle w_j(t) \right| - \sum_j \left| w_j(t) \right\rangle W_j \left\langle w_j(t) \right| \hat{H}.
\end{aligned}
\tag{7.65}
$$

Now using Eq. (64) again (twice), we get the so-called *von Neumann equation*[26]

$$\boxed{ i\hbar \dot{\hat{w}} = \left[\hat{H}, \hat{w} \right]. } \tag{7.66}$$

Note that this equation is similar in structure to Eq. (4.199) describing the time evolution of time-independent operators in the Heisenberg picture operators:

$$i\hbar \dot{\hat{A}} = \left[\hat{A}, \hat{H} \right], \tag{7.67}$$

besides the opposite order of the operators in the commutator – equivalent to the change of sign on the right-hand side. This should not be too surprising, because Eq. (66) belongs to the Schrödinger picture of quantum dynamics, while Eq. (67), belongs to its Heisenberg picture.

Unfortunately, in most cases when the system is open, i.e. interacts with its environment, Eq. (66) is *not* valid, because the probabilities W_j may change in time.[27] However, the von Neumann equation serves an important role even in this case, provided that the interaction with the environment is so weak that its effect on the system's evolution may be considered as a weak perturbation. The analysis of this situation may be based on the following Hamiltonian:

$$\boxed{ \hat{H} = \hat{H}_s + \hat{H}_e\{\lambda\} + \hat{H}_{\text{int}}, } \tag{7.68}$$

describing the system of our interest (s), its environment as such (e), and their interaction.[28] Here $\{\lambda\}$ denotes the (typically, huge) set of degrees of freedom of the environment. If the energy scale of the interaction Hamiltonian is relatively small, the time evolution of the probabilities W_j is relatively slow, and Eq. (66) may be used, in the 0th approximations of the perturbation theory, for the density matrices of both the system s (with the Hamiltonian $\hat{H}_s$) and the environment (with the Hamiltonian $\hat{H}_e$).

---

[26] In some texts, it is called the "Liouville equation", due to its conceptual proximity to the classical Liouville theorem for the classical distribution function $w_{\text{cl}}(X, P)$ – see, e.g., SM Sec. 6.1 and in particular Eq. (6.5).

[27] Very unfortunately, this fact is not explained in some textbooks, which quote the von Neumann equation without proper qualifications.

[28] Note that by writing Eq. (68), we are treating the whole system, including the environment, as a Hamiltonian one. This can always be done if the accounted part of the environment is large enough so the processes in the system s of our interest do not depend on the type of boundary between this part of the environment and its "external" (even larger) part; in particular, we may assume the total system to be closed, i.e. Hamiltonian.

This approach, which will considered later in this chapter, turns out to be very useful if the elementary act of interaction of the system of interest with the environment is in some sense small. The classical example is the *Brownian particle* interacting with the molecules of the surrounding gas or fluid.[29] (In this example, a single hit by a molecule changes the particle's momentum by a minor fraction.) On the other hand, the model (68) is *not* very productive for a particle interacting with the environment consisting of *similar* particles, when a single collision may change its momentum (or other variables) dramatically. In such cases, the methods discussed in the next chapter are more adequate.

If the interaction with the environment is stronger, the perturbative approach to Eq. (68) also becomes invalid, but in this case, the von Neumann equation may still be used for a discussion of one major effect of the environment, namely *dephasing* (also called "decoherence"). Let us analyze a simple model of an open two-level quantum system, with its intrinsic Hamiltonian having the form

$$\hat{H}_s = c_z \hat{\sigma}_z, \tag{7.69}$$

similar to the Pauli Hamiltonian (4.163),[30] and a factorable interaction with environment – cf. Eq. (6.145) and its discussion:

$$\hat{H}_{\text{int}} = \hat{f}\{\lambda\}\hat{\sigma}_z, \tag{7.70}$$

where $\hat{f}$ is a Hermitian operator depending only on the set $\{\lambda\}$ of environmental degrees of freedom ("coordinates") defined in their Hilbert space – different from that of the two-level system. As a result, the operators $\hat{f}\{\lambda\}$ and $\hat{H}_e\{\lambda\}$ commute with $\hat{\sigma}_z$ – and with any other intrinsic operator of the two-level system. Of course, any realistic $\hat{H}_e\{\lambda\}$ is extremely complex, so how much we will be able to achieve without specifying it, may become a pleasant surprise for the reader.

Before we proceed to the analysis, let us recognize two examples of two-level systems that may be described by this model. The first example is a spin-½ in an external magnetic field of a fixed direction (taken for the z-axis), which includes both an average component $\overline{\mathscr{B}}$ and a random (fluctuating) component $\widetilde{\mathscr{B}}_z(t)$ induced by the environment. As it follows from Eq. (4.163b), it may be described by the Hamiltonian (68)-(70) with

$$c_z = -\frac{\hbar\gamma}{2}\overline{\mathscr{B}_z} \quad \text{and} \quad \hat{f} = -\frac{\hbar\gamma}{2}\hat{\widetilde{\mathscr{B}}}_z(t). \tag{7.71}$$

Another example is a particle in a symmetric double-well potential U_s (Fig. 4), with a barrier between them sufficiently high to be practically impenetrable, and an additional force $F(t)$, exerted by the environment, so the total potential energy is $U(x, t) = U_s(x) - F(t)x$. If the force, including its static

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[29] The theory of the Brownian motion, the effect first observed experimentally by biologist Robert Brown in the 1820s, was pioneered by Albert Einstein in 1905 and developed in detail by Marian Smoluchowski in 1906-1907 and Adriaan Fokker in 1913. Due to this historical background, in some older texts, the approach described in the balance of this chapter is called the "quantum theory of the Brownian motion". Let me, however, emphasize that due to the later progress of experimental techniques, quantum-mechanical behaviors, including the environmental effects in them, have been observed in a rapidly growing number of various quasi-macroscopic systems, for which this approach is quite applicable. In particular, this is true for most systems being explored as possible qubits of prospective quantum computing and encryption systems – see Sec. 8.5 below.

[30] As we know from Secs. 4.6 and 5.1, such Hamiltonian is sufficient to lift the energy level degeneracy.

part $\overline{F}$ and fluctuations $\widetilde{F}(t)$, is sufficiently weak, we can neglect its effects on the shape of potential wells and hence on the localized wavefunctions $\psi_{L,R}$, so the force's effect is reduced to the variation of the difference $E_L - E_R = F(t)\Delta x$ between the eigenenergies. As a result, the system may be described by Eqs. (68)-(70) with

$$c_z = -\overline{F}\Delta x/2 \quad \text{and} \quad \hat{f} = -\hat{\widetilde{F}}(t)\Delta x/2. \tag{7.72}$$
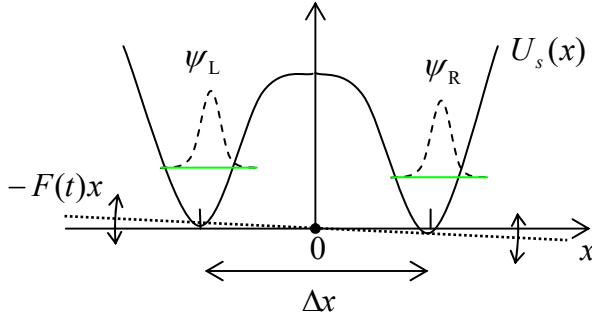

Fig. 7.4. Dephasing in a double-well system.

Now let us start our general analysis of the model described by Eqs. (68)-(70) by writing the equation of motion for the Heisenberg-picture operator $\hat{\sigma}_z(t)$:

$$i\hbar\dot{\hat{\sigma}}_z = \left[\hat{\sigma}_z, \hat{H}\right] = (c_z + \hat{f})\left[\hat{\sigma}_z, \hat{\sigma}_z\right] = 0, \tag{7.73}$$

showing that in our simple model (68)-(70), the operator $\hat{\sigma}_z$ does not evolve in time. What does this mean for the observables? For an arbitrary density matrix of any two-level system,

$$w = \begin{pmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{pmatrix}, \tag{7.74}$$

we can readily calculate the trace of the operator $\hat{\sigma}_z\hat{w}$. Indeed, since the operator traces are basis-independent, we may do this in the usual z-basis:

$$\mathrm{Tr}(\hat{\sigma}_z\hat{w}) = \mathrm{Tr}(\sigma_z w) = \mathrm{Tr}\left[\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{pmatrix}\right] = w_{11} - w_{22} = W_1 - W_2. \tag{7.75}$$

Since, according to Eq. (5), $\hat{\sigma}_z$ may be considered the operator for the difference of the number of particles in the basis states 1 and 2, in the case (73), the difference $W_1 - W_2$ does not depend on time, and since the sum of these probabilities is also fixed, $W_1 + W_2 = 1$, both of them are constant. The physics of this simple result is especially clear for the model shown in Fig. 4: since the potential barrier separating the potential wells is so high that tunneling through it is negligible, the interaction with the environment cannot move the system from one well into another one.

It may look like nothing interesting may happen in such a simple situation, but in a minute we will see that this is not true. Due to the time independence of W_1 and W_2, we may use the von Neumann equation (66) to describe the density matrix evolution. In the z-basis:

$$i\hbar\dot{w} \equiv i\hbar\begin{pmatrix} \dot{w}_{11} & \dot{w}_{12} \\ \dot{w}_{21} & \dot{w}_{22} \end{pmatrix} = [H, w] \equiv \left(c_z + \hat{f}\right)[\sigma_z, w]$$

$$\equiv \left(c_z + \hat{f}\right)\left[\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{pmatrix}\right] = \left(c_z + \hat{f}\right)\begin{pmatrix} 0 & 2w_{12} \\ -2w_{21} & 0 \end{pmatrix}. \tag{7.76}$$

This result means that while the diagonal elements, i.e., the probabilities of the states, do not evolve in time (as we already know), the off-diagonal elements do change; for example,

$$i\hbar\dot{w}_{12} = 2(c_z + \hat{f})w_{12}, \tag{7.77}$$

with a similar but complex conjugate equation for w_{21}. The solution of this linear differential equation is straightforward, and yields

$$w_{12}(t) = w_{12}(0)\exp\left\{-i\frac{2c_z}{\hbar}t\right\}\exp\left\{-i\frac{2}{\hbar}\int_0^t \hat{f}(t')dt'\right\}. \tag{7.78}$$

The first exponent is a deterministic c-number factor, while in the second one $\hat{f}(t) \equiv \hat{f}\{\lambda(t)\}$ is still an operator in the Hilbert space of the environment, but from the point of view of the two-level system of our interest, it is just a random function of time. The time-average part of this function may be included in c_z, so in what follows, we will assume that it equals zero.

   Let us start from the limit when the environment behaves classically.[31] In this case, the operator in Eq. (78) may be considered a *classical* random function $f(t)$, provided that we average its effects over a statistical ensemble of many such functions describing many (macroscopically similar) experiments. For a small time interval $t = dt \to 0$, we can use the Taylor expansion of the exponent, truncating it after the quadratic term:

$$\left\langle\exp\left\{-i\frac{2}{\hbar}\int_0^{dt} f(t')dt'\right\}\right\rangle \approx 1 + \left\langle -i\frac{2}{\hbar}\int_0^{dt} f(t')dt'\right\rangle + \left\langle \frac{1}{2}\left(-i\frac{2}{\hbar}\int_0^{dt} f(t')dt'\right)\left(-i\frac{2}{\hbar}\int_0^{dt} f(t'')dt''\right)\right\rangle$$

$$\equiv 1 - i\frac{2}{\hbar}\int_0^{dt}\langle f(t')\rangle dt' - \frac{2}{\hbar^2}\int_0^{dt} dt'\int_0^{dt} dt''\langle f(t')f(t'')\rangle \equiv 1 - \frac{2}{\hbar^2}\int_0^{dt} dt'\int_0^{dt} dt'' K_f(t' - t''). \tag{7.79}$$

Here we have used the facts that the statistical average of $f(t)$ is equal to zero, while the second average, called the *correlation function*, in a statistically- (i.e. macroscopically-) stationary state of the environment may only depend on the time difference $\tau \equiv t' - t''$:

$$\boxed{\langle f(t')f(t'')\rangle = K_f(t' - t'') \equiv K_f(\tau).} \tag{7.80}$$

If this difference is much larger than some time scale τ_c, called the *correlation time* of the environment, the values $f(t')$ and $f(t'')$ are completely independent (*uncorrelated*), as illustrated in Fig. 5a, so at $\tau \to \infty$, the correlation function has to tend to zero. On the other hand, at $\tau = 0$, i.e. $t' = t''$, the correlation function is just the variance of f:

$$K_f(0) = \langle f^2\rangle, \tag{7.81}$$

and has to be positive. As a result, the function looks approximately as shown in Fig. 5b. (On the way to zero at $\tau \to \pm\infty$, it may or may not change sign.)

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[31] This assumption is not in contradiction with the quantum treatment of the two-level system s, because a typical environment is large, and hence has a very dense energy spectrum, with small adjacent level distances that may be readily bridged by thermal excitations of minor energy, often making it essentially classical.
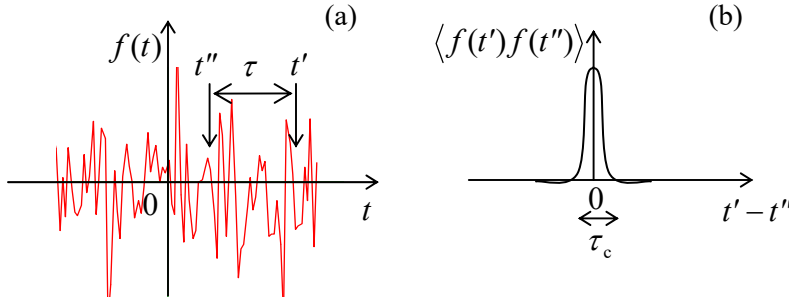
Fig. 7.5. (a) A typical random process and (b) its correlation function – schematically.

Hence, if we are only interested in time differences τ much longer than τ_c, which is typically very short, we may approximate $K_f(\tau)$ well with a delta function of the time difference. Let us take it in the following form, convenient for later discussion:

$$K_f(\tau) \approx \hbar^2 D_\varphi \delta(\tau),$$ (7.82)

Phase diffusion coefficient

where D_φ is a positive constant called the *phase diffusion coefficient*. The origin of this term stems from the very similar effect of classical diffusion of Brownian particles in a highly viscous medium. Indeed, the particle's velocity in such a medium is approximately proportional to the external force. Hence, if the random hits of a particle by the medium's molecules may be described by a force that obeys a law similar to Eq. (82), the velocity (along any Cartesian coordinate) is also *delta-correlated*:

$$\langle v(t) \rangle = 0, \quad \langle v(t')v(t'') \rangle = 2D\delta(t'-t'').$$ (7.83)

Now we can integrate the kinematic relation $\dot{x} = v$, to calculate the particle's displacement from its initial position during a time interval $[0, t]$ and its variance:

$$x(t) - x(0) = \int_0^t v(t')dt',$$ (7.84)

$$\left\langle \left(x(t)-x(0)\right)^2 \right\rangle = \left\langle \int_0^t v(t')dt' \int_0^t v(t'')dt'' \right\rangle = \int_0^t dt' \int_0^t dt'' \langle v(t')v(t'') \rangle = \int_0^t dt' \int_0^t dt'' 2D\delta(t'-t'') = 2Dt.$$ (7.85)

This is the famous law of diffusion, showing that the r.m.s. deviation of the particle from the initial point grows with time as $(2Dt)^{1/2}$, where the constant D is called the *diffusion coefficient*.

Returning to the diffusion of the quantum-mechanical phase, with Eq. (82) the last double integral in Eq. (79) yields $\hbar^2 D_\varphi dt$, so the statistical average of Eq. (78) is

$$\langle w_{12}(dt) \rangle = w_{12}(0)\exp\left\{-i\frac{2c_z}{\hbar}dt\right\}(1-2D_\varphi dt).$$ (7.86)

Applying this formula to sequential time intervals,

$$\langle w_{12}(2dt) \rangle = \langle w_{12}(dt) \rangle \exp\left\{-i\frac{2c_z}{\hbar}dt\right\}(1-2D_\varphi dt) = w_{12}(0)\exp\left\{-i\frac{2c_z}{\hbar}2dt\right\}(1-2D_\varphi dt)^2,$$ (7.87)

etc., for a finite time $t = Ndt$, in the limit $N \to \infty$ and $dt \to 0$ (at fixed t) we get

$$\langle w_{12}(t) \rangle = w_{12}(0)\exp\left\{-i\frac{2c_z}{\hbar}t\right\} \times \lim_{N\to\infty}\left(1-2D_\varphi t\frac{1}{N}\right)^N.$$ (7.88)

By the definition of the natural logarithm base e,[32] this limit is just $\exp\{-2D_\varphi t\}$, so, finally:

$$\langle w_{12}(t)\rangle = w_{12}(0)\exp\left\{-i\frac{2a}{\hbar}t\right\}\exp\left\{-2D_\varphi t\right\} \equiv w_{12}(0)\exp\left\{-i\frac{2a}{\hbar}t\right\}\exp\left\{-\frac{t}{T_2}\right\}. \qquad (7.89)$$

So, due to coupling to the environment, the off-diagonal elements of the density matrix decay with some *dephasing time* $T_2 = 1/2D_\varphi$,[33] providing a natural evolution from the density matrix (22) of a pure state to the diagonal matrix (23), with the same probabilities $W_{1,2}$, describing a fully dephased (incoherent) classical mixture.[34]

This simple model offers a very clear look at the nature of the decoherence: the random "force" $f(t)$ exerted by the environment, "shakes" the energy difference between two eigenstates of the system and hence the instantaneous velocity $2(c_z + f)/\hbar$ of their mutual phase shift $\varphi(t)$ – cf. Eq. (22). Due to the randomness of the force, $\varphi(t)$ performs a random walk around the trigonometric circle, so the average of its trigonometric functions $\exp\{\pm i\varphi\}$ over time gradually tends to zero, killing the off-diagonal elements of the density matrix. Our analysis, however, has left open two important issues:

(i) Is this approach valid for a *quantum* description of a typical environment?
(ii) If yes, what is physically the D_φ that was formally defined by Eq. (82)?

7.4. Fluctuation-dissipation theorem

Similar questions may be asked about a more general situation, when the Hamiltonian $\hat{H}_s$ of the system of interest (s), in the composite Hamiltonian (68), is not specified at all, but the interaction between that system and its environment still has the form similar to Eqs. (70) and (6.130):

$$\hat{H}_{\text{int}} = -\hat{F}\{\lambda\}\,\hat{x}, \qquad (7.90)$$

where x is some observable of our system s – say, one of its generalized coordinates. It may look incredible that in this very general situation, one still can make a very simple and powerful statement about the statistical properties of the generalized force F, under only two (interrelated) conditions – which are satisfied in a huge number of cases of interest:

(i) the coupling of system s of interest to its environment e is not too strong – in the sense that the perturbation theory (see Chapter 6) is applicable, and

(ii) the environment may be considered as staying in thermodynamic equilibrium, with a certain temperature T, regardless of the process in the system of interest.[35]

---

[32] See, e.g., MA Eq. (1.2a) with the substitution $n = -N/2D_\varphi t$.
[33] In context of the spin magnetic resonance (see below), T_2 is frequently called the "spin-spin relaxation time".
[34] Note that this result is valid only if the approximation (82) may be applied at time interval dt which, in turn, should be much smaller than the T_2 in Eq. (88), i.e. if the dephasing time is much longer than the environment's correlation time τ_c. This requirement may be always satisfied by making the coupling to the environment sufficiently weak. In addition, in typical environments, τ_c is very short. For example, in the original Brownian motion experiments with a-few-μm pollen grains in water, it is of the order of the duration of each molecular impact ($\sim 10^{-12}$ s) because the average interval between sequential impacts is even much shorter.
[35] The most frequent example of the violation of this condition is the environment's overheating by the energy flow from system s. Let me leave it to the reader to estimate the overheating of a standard physical laboratory

This famous statement is called the *fluctuation-dissipation theorem* (FDT).[36] Due to the importance of this fundamental result, let me derive it.[37] Since by writing Eq. (68), we treat the whole system ($s + e$) as a Hamiltonian one, we may use the Heisenberg equation (4.199) to write

$$i\hbar\dot{\hat{F}} = \left[\hat{F}, \hat{H}\right] \equiv \left[\hat{F}, \hat{H}_e\right]. \tag{7.91}$$

(The second step uses the fact, discussed in the last section, that $\hat{F}\{\lambda\}$ commutes with both $\hat{H}_s$ and $\hat{x}$.) Generally, very little may be done with this equation, because the time evolution of the environment's Hamiltonian depends, in turn, on that of the force. This is where the perturbation theory becomes indispensable. Let us decompose the force operator into the following sum:

$$\hat{F}\{\lambda\} = \left\langle\hat{F}\right\rangle + \hat{\tilde{F}}(t), \quad \text{with} \quad \left\langle\hat{\tilde{F}}(t)\right\rangle = 0, \tag{7.92}$$

where (here and on, until further notice) the sign $\langle\ldots\rangle$ means the statistical averaging *over the environment alone*, i.e. over an ensemble with absolutely similar evolutions of the system s, but random states of its environment.[38] From the point of view of the system s, the first term of the sum (still an operator!) describes the average response of the environment to the system's dynamics (possibly, including such irreversible effects as friction), and has to be calculated with a proper account of their interaction – as we will do later in this section. On the other hand, the last term in Eq. (92) represents random *fluctuations* of the environment, which exist even in the absence of the system s. Hence, in the first nonvanishing approximation in the interaction strength, the fluctuation part may be calculated ignoring the interaction, i.e. treating the environment as being in thermodynamic equilibrium:

$$i\hbar\dot{\hat{\tilde{F}}} = \left[\hat{\tilde{F}}, \hat{H}_e\big|_{\text{eq}}\right]. \tag{7.93}$$

Since, in this approximation, the environment's Hamiltonian does not have an explicit dependence on time, the solution of this equation may be written by combining Eqs. (4.190) and (4.175):

$$\hat{F}(t) = \exp\left\{+\frac{i}{\hbar}\hat{H}_e\big|_{\text{eq}}t\right\}\hat{F}(0)\exp\left\{-\frac{i}{\hbar}\hat{H}_e\big|_{\text{eq}}t\right\}. \tag{7.94}$$

Let us use this relation to calculate the correlation function of the fluctuations $F(t)$, defined similarly to Eq. (80), but taking care of the order of the time arguments (very soon we will see why):

room by a typical dissipative quantum process – the emission of an optical photon by an atom. (*Hint*: it is extremely small.)

[36] The FDT was first derived by Herbert Callen and Theodore Allen Welton in 1951, on the background of an earlier derivation of its classical limit by Harry Nyquist in 1928 (for a particular case of electric circuits).

[37] The FDT may be proved in several ways that are shorter than the one given below – see, e.g., either the proof in SM Secs. 5.5 and 5.6 (based on H. Nyquist's arguments), or the original paper by H. Callen and T. Welton, *Phys. Rev.* **83**, 34 (1951) – wonderful in its clarity. The longer approach I will describe here, besides giving the important *Green-Kubo formula* (109) as a byproduct, is a very useful exercise in operator manipulation and the perturbation theory in its integral form – different from the differential forms used in Chapter 6. The reader not interested in this exercise may skip the derivation and jump straight to the result expressed by Eq. (134), which uses the notions defined by Eqs. (114) and (123).

[38] For usual ("ergodic") environments, without intrinsic long-term memories, this statistical averaging over an ensemble of environments is equivalent to averaging over intermediate times – much longer than the correlation time τ_c of the environment, but still much shorter than the characteristic time of evolution of the system under analysis, such as the dephasing time T_2 and the energy relaxation time T_1 – both still to be calculated.

$$\left\langle \tilde{F}(t)\tilde{F}(t')\right\rangle = \left\langle \exp\left\{+\frac{i}{\hbar}\hat{H}_e t\right\}\hat{F}(0)\exp\left\{-\frac{i}{\hbar}\hat{H}_e t\right\}\exp\left\{+\frac{i}{\hbar}\hat{H}_e t'\right\}\hat{F}(0)\exp\left\{-\frac{i}{\hbar}\hat{H}_e t'\right\}\right\rangle. \quad (7.95)$$

(Here and in Eq. (96), the thermal equilibrium of the environment is also meant but just implied, for the notation brevity.) We may calculate this expectation value in any basis, and the best choice for it is evident: in the environment's stationary-state basis, the density operator of the environment, its Hamiltonian and hence the exponents in Eq. (95) are all represented by diagonal matrices. Using Eq. (5), the correlation function becomes

$$\begin{aligned}\left\langle \tilde{F}(t)\tilde{F}(t')\right\rangle &= \mathrm{Tr}\left[\hat{w}\exp\left\{+\frac{i}{\hbar}\hat{H}_e t\right\}\hat{F}(0)\exp\left\{-\frac{i}{\hbar}\hat{H}_e t\right\}\exp\left\{+\frac{i}{\hbar}\hat{H}_e t'\right\}\hat{F}(0)\exp\left\{-\frac{i}{\hbar}\hat{H}_e t'\right\}\right]\\[2mm]&\equiv \sum_n\left[\hat{w}\exp\left\{+\frac{i}{\hbar}\hat{H}_e t\right\}\hat{F}(0)\exp\left\{-\frac{i}{\hbar}\hat{H}_e t\right\}\exp\left\{+\frac{i}{\hbar}\hat{H}_e t'\right\}\hat{F}(0)\exp\left\{-\frac{i}{\hbar}\hat{H}_e t'\right\}\right]_{nn}\\[2mm]&= \sum_{n,n'}W_n \exp\left\{+\frac{i}{\hbar}E_n t\right\}\hat{F}_{nn'}\exp\left\{-\frac{i}{\hbar}E_{n'} t\right\}\exp\left\{+\frac{i}{\hbar}E_{n'} t'\right\}\hat{F}_{n'n}\exp\left\{-\frac{i}{\hbar}E_n t'\right\} \quad (7.96)\\[2mm]&\equiv \sum_{n,n'}W_n\left|F_{nn'}\right|^2 \exp\left\{+\frac{i}{\hbar}(E_n - E_{n'})(t - t')\right\}.\end{aligned}$$

Here W_n are the Gibbs-distribution probabilities given by Eq. (24), with the environment's temperature T, and $F_{nn'} \equiv F_{nn'}(0)$ are the Schrödinger-picture matrix elements of the interaction force operator.

We see that though the correlator (96) is a function of the difference $\tau \equiv t - t'$ only (as it should be for fluctuations in a macroscopically stationary system), it may depend on the order of its arguments. This is why let us mark this particular correlation function with the upper index "+",

$$K_F^+(\tau) \equiv \left\langle \tilde{F}(t)\tilde{F}(t')\right\rangle = \sum_{n,n'}W_n\left|F_{nn'}\right|^2 \exp\left\{+\frac{i\tilde{E}\tau}{\hbar}\right\}, \quad \text{where } \tilde{E} \equiv E_n - E_{n'}, \quad (7.97)$$

while its counterpart, with swapped times t and t', with the upper index "–":

$$K_F^-(\tau) \equiv K_F^+(-\tau) = \left\langle \tilde{F}(t')\tilde{F}(t)\right\rangle = \sum_{n,n'}W_n\left|F_{nn'}\right|^2 \exp\left\{-\frac{i\tilde{E}\tau}{\hbar}\right\}. \quad (7.98)$$

So, in contrast with classical processes, in quantum mechanics the correlation function of fluctuations $\tilde{F}$ is not necessarily time-symmetric:

$$K_F^+(\tau) - K_F^-(\tau) \equiv K_F^+(\tau) - K_F^+(-\tau) = \left\langle \tilde{F}(t)\tilde{F}(t') - \tilde{F}(t')\tilde{F}(t)\right\rangle = 2i\sum_{n,n'}W_n\left|F_{nn'}\right|^2 \sin\frac{\tilde{E}\tau}{\hbar} \neq 0, \quad (7.99)$$

so $\hat{F}(t)$ gives one more example of a Heisenberg-picture operator whose "values" at different moments generally do not commute – see Footnote 47 in Chapter 4. (A good sanity check here is that at $\tau = 0$, i.e. at $t = t'$, the difference (99) between K_F^+ and K_F^- vanishes.)

Now let us return to the force operator's decomposition (92), and calculate its first (average) component. To do that, let us write the formal solution of Eq. (91) as follows:

$$\hat{F}(t) = \frac{1}{i\hbar}\int_{-\infty}^{t}\left[\hat{F}(t'),\hat{H}_e(t')\right]dt'. \quad (7.100)$$

On the right-hand side of this relation, we still cannot treat the Hamiltonian of the environment as an unperturbed (equilibrium) one, even if the effect of our system (s) on the environment is very weak, because this would give us zero statistical average of the force $F(t)$. Hence, we should make one more step in our perturbative treatment, taking into account the effect of the force on the environment. To do this, let us use Eqs. (68) and (90) to write the (so far, exact) Heisenberg equation of motion for the environment's Hamiltonian,

$$i\hbar\dot{\hat{H}}_e = \left[\hat{H}_e, \hat{H}\right] \equiv -\hat{x}\left[\hat{H}_e, \hat{F}\right], \tag{7.101}$$

and its formal solution, similar to Eq. (100), but for time t' rather than t:

$$\hat{H}_e(t') = -\frac{1}{i\hbar}\int_{-\infty}^{t'}\hat{x}(t'')\left[\hat{H}_e(t''), \hat{F}(t'')\right]dt''. \tag{7.102}$$

Plugging this equality into the right-hand side of Eq. (100), and averaging the result (again, over the environment only!), we get

$$\left\langle\hat{F}(t)\right\rangle = \frac{1}{\hbar^2}\int_{-\infty}^{t}dt'\int_{-\infty}^{t'}dt''\,\hat{x}(t'')\left\langle\left[\hat{F}(t'), \left[\hat{H}_e(t''), \hat{F}(t'')\right]\right]\right\rangle. \tag{7.103}$$

This is still an exact result, but now it is ready for an approximate treatment, implemented by averaging in its right-hand side over the unperturbed (thermal-equilibrium) state of the environment.[39] This may be done absolutely similarly to that in Eq. (96), at the last step using Eq. (94):

$$\begin{aligned}
\left\langle\left[\hat{F}(t'), \left[\hat{H}_e(t''), \hat{F}(t'')\right]\right]\right\rangle &= \mathrm{Tr}\left\{\mathrm{w}\left[\mathrm{F}(t'), \left[\mathrm{H}_e\mathrm{F}(t'')\right]\right]\right\} \\
&\equiv \mathrm{Tr}\left\{\mathrm{w}\left[\mathrm{F}(t')\mathrm{H}_e\mathrm{F}(t'') - \mathrm{F}(t')\mathrm{F}(t'')\mathrm{H}_e - \mathrm{H}_e\mathrm{F}(t'')\mathrm{F}(t') + \mathrm{F}(t'')\mathrm{H}_e\mathrm{F}(t')\right]\right\} \\
&= \sum_{n,n'}W_n\left[F_{nn'}(t')E_{n'}F_{n'n}(t'') - F_{nn'}(t')F_{n'n}(t'')E_n - E_nF_{nn'}(t'')F_{n'n}(t') + F_{nn'}(t'')E_{n'}F_{n'n}(t'')\right] \\
&\equiv -\sum_{n,n'}W_n\tilde{E}\left|F_{nn'}\right|^2\left[\exp\left\{\frac{i\tilde{E}(t'-t'')}{\hbar}\right\} + \text{c.c.}\right].
\end{aligned} \tag{7.104}$$

Now, if we try to integrate each term of this sum, as Eq. (103) seems to require, we will see that the lower-limit substitution (at t', $t'' \to -\infty$) is uncertain because the exponents oscillate without decay. This mathematical difficulty may be overcome by the following physical reasoning. As illustrated by the example considered in the previous section, coupling to a disordered environment makes the "memory horizon" of the system of our interest (s) finite: its current state does not depend on its history beyond a certain time scale.[40] As a result, the function under the integrals of Eq. (103), i.e. the sum (104), should self-average at a certain finite time. A simplistic technique for expressing this fact mathematically is just dropping the lower-limit substitution; this would give the correct result for Eq. (103). However, a better

---

[39] This is exactly the moment when, in this approach, the reversible quantum dynamics of the formally-Hamiltonian full system ($s + e$) is replaced with irreversible dynamics of the system s. At the conditions formulated at the beginning of this section, this replacement is physically justified – see also the discussions in Secs. 2.5, 6.6, and 6.7.

[40] Indeed, this is true for virtually any real physical system – in contrast to idealized models such as a dissipation-free oscillator that swings for ever and ever with the same amplitude and phase, thus "remembering" the initial conditions.

(mathematically more acceptable) trick is to first multiply the functions under the integrals by, respectively, $\exp\{\varepsilon(t-t')\}$ and $\exp\{\varepsilon(t'-t'')\}$, where ε is a very small positive constant, then carry out the integration, and after that follow the limit $\varepsilon \to 0$. The physical justification of this procedure may be provided by saying that the system's behavior should not be affected if its interaction with the environment was not kept constant but rather turned on gradually and very slowly – say, exponentially with an infinitesimal rate ε. With this modification, Eq. (103) becomes

$$\left\langle \hat{F}(t)\right\rangle = -\frac{1}{\hbar^2}\sum_{n,n'}W_n\widetilde{E}\left|F_{nn'}\right|^2 \lim_{\varepsilon\to 0}\int_{-\infty}^{t}dt'\int_{-\infty}^{t'}dt''\,\hat{x}(t'')\left[\exp\left\{\frac{i\widetilde{E}(t'-t'')}{\hbar}+\varepsilon(t''-t)\right\}+\text{c.c.}\right]. \quad (7.105)$$

This double integration is over the area shaded in Fig. 6, which makes it obvious that the order of integration may be changed to the opposite one as

$$\int_{-\infty}^{t}dt'\int_{-\infty}^{t'}dt''\ldots = \int_{-\infty}^{t}dt''\int_{t''}^{t}dt'\ldots = \int_{-\infty}^{t}dt''\int_{t''-t}^{0}d(t'-t)\ldots \equiv \int_{-\infty}^{t}dt''\int_{0}^{\tau}d\tau'\ldots, \quad (7.106)$$

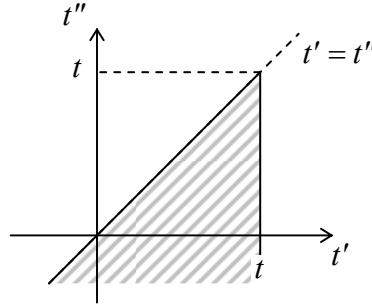where $\tau' \equiv t - t'$, and $\tau \equiv t - t''$.

Fig. 7.6. The 2D integration area in Eqs. (105) and (106).

As a result, Eq. (105) may be rewritten as a single integral,

$$\left\langle \hat{F}(t)\right\rangle = \int_{-\infty}^{t}G(t-t'')\,\hat{x}(t'')dt'' \equiv \int_{0}^{\infty}G(\tau)\,\hat{x}(t-\tau)d\tau, \quad (7.107)$$

whose kernel,

$$G(\tau>0)\equiv -\frac{1}{\hbar^2}\sum_{n,n'}W_n\widetilde{E}\left|F_{nn'}\right|^2\lim_{\varepsilon\to 0}\int_{0}^{\tau}\left[\exp\left\{\frac{i\widetilde{E}(\tau-\tau')}{\hbar}-\varepsilon\tau\right\}+\text{c.c.}\right]d\tau'$$
$$= \lim_{\varepsilon\to 0}\frac{2}{\hbar}\sum_{n,n'}W_n\left|F_{nn'}\right|^2\sin\frac{\widetilde{E}\tau}{\hbar}e^{-\varepsilon\tau} \equiv \frac{2}{\hbar}\sum_{n,n'}W_n\left|F_{nn'}\right|^2\sin\frac{\widetilde{E}\tau}{\hbar}, \quad (7.108)$$

does not depend on the particular law of evolution of the system (s) under study, i.e. provides a general characterization of its coupling to the environment.

In Eq. (107) we may readily recognize the most general form of the linear response of a system (in our case, the environment), taking into account the causality principle, where $G(\tau)$ is the *response function* (also called the "temporal Green's function") of the environment. Now comparing Eq. (108) with Eq. (99), we get a wonderfully simple universal relation,

$$\left\langle\left[\hat{\widetilde{F}}(\tau),\hat{\widetilde{F}}(0)\right]\right\rangle = i\hbar G(\tau). \quad (7.109)$$

that emphasizes once again the quantum nature of the correlation function's time asymmetry. (This relation, called the *Green-Kubo* (or just "Kubo") *formula* after the works by Melville Green in 1954 and Ryogo Kubo in 1957, did not come up in the easier derivations of the FDT, mentioned in the beginning of this section.)

However, for us the relation between the function $G(\tau)$ and the force's *anti*-commutator,

$$\left\langle \left\{ \hat{\tilde{F}}(t+\tau), \hat{\tilde{F}}(t) \right\} \right\rangle \equiv \left\langle \hat{\tilde{F}}(t+\tau)\hat{\tilde{F}}(t) + \hat{\tilde{F}}(t)\hat{\tilde{F}}(t+\tau) \right\rangle \equiv K_F^+(\tau) + K_F^-(\tau), \qquad (7.110)$$

is much more important, because of the following reason. Eqs. (97)-(98) show that the so-called *symmetrized correlation function*,

$$K_F(\tau) \equiv \frac{K_F^+(\tau) + K_F^-(\tau)}{2} = \frac{1}{2}\left\langle \left\{ \hat{\tilde{F}}(\tau), \hat{\tilde{F}}(0) \right\} \right\rangle = \lim_{\varepsilon \to 0} \sum_{n,n'} W_n \left| F_{nn'} \right|^2 \cos\frac{\tilde{E}\tau}{\hbar} e^{-2\varepsilon|\tau|}$$
$$\equiv \sum_{n,n'} W_n \left| F_{nn'} \right|^2 \cos\frac{\tilde{E}\tau}{\hbar}, \qquad (7.111)$$

Symmetrized correlation function

which is an even function of the time difference τ, looks very similar to the response function (108), "only" with another trigonometric function under the sum, and a different constant front factor.[41] This similarity may be used to obtain a direct algebraic relation between the Fourier images of these two functions of τ. Indeed, the function (111) may be represented as the Fourier integral[42]

$$K_F(\tau) = \int_{-\infty}^{+\infty} S_F(\omega)e^{-i\omega\tau}\,d\omega = 2\int_0^{+\infty} S_F(\omega)\cos\omega\tau\,d\omega, \qquad (7.112)$$

with the reciprocal transform

$$S_F(\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} K_F(\tau)e^{i\omega\tau}\,d\tau = \frac{1}{\pi}\int_0^{+\infty} K_F(\tau)\cos\omega\tau\,d\tau, \qquad (7.113)$$

of the *symmetrized spectral density* of the variable F, defined as

$$S_F(\omega)\delta(\omega - \omega') \equiv \frac{1}{2}\left\langle \hat{F}_\omega \hat{F}_{-\omega'} + \hat{F}_{-\omega'}\hat{F}_\omega \right\rangle \equiv \frac{1}{2}\left\langle \left\{ \hat{F}_\omega, \hat{F}_{-\omega'} \right\} \right\rangle, \qquad (7.114)$$

Symmetrized spectral density

where the function $\hat{F}_\omega$ (also a Heisenberg-picture operator rather than a *c*-number!) is defined as

$$\hat{F}_\omega \equiv \frac{1}{2\pi}\int_{-\infty}^{+\infty} \hat{\tilde{F}}(t)e^{i\omega t}\,dt, \qquad \text{so that } \hat{\tilde{F}}(t) = \int_{-\infty}^{+\infty} \hat{F}_\omega e^{-i\omega t}\,d\omega. \qquad (7.115)$$

The physical meaning of the function $S_F(\omega)$ becomes clear if we write Eq. (112) for the particular case $\tau = 0$:

$$K_F(0) \equiv \left\langle \hat{\tilde{F}}^2 \right\rangle = \int_{-\infty}^{+\infty} S_F(\omega)\,d\omega = 2\int_0^{+\infty} S_F(\omega)\,d\omega. \qquad (7.116)$$

---

[41] For the heroic reader who has suffered through the calculations up to this point: our conceptual work is done! What remains is just some simple math to bring the relation between Eqs. (108) and (111) to an explicit form.

[42] Due to their practical importance, and certain mathematical issues of their justification for random functions, Eqs. (112)-(113) have their own grand name, the *Wiener-Khinchin theorem*, though the math rigor aside, they are just a straightforward corollary of the standard Fourier integral transform (115).

This formula infers that if we pass the function $F(t)$ through a linear filter cutting from its frequency spectrum a narrow band $d\omega$ of physical (positive) frequencies, then the variance $\langle F_f^2 \rangle$ of the filtered signal $F_f(t)$ would be equal to $2 S_F(\omega) d\omega$ – hence the name "spectral density".[43]

Let us use Eqs. (111) and (113) to calculate the spectral density of fluctuations $\widetilde{F}(t)$ in our model, using the same ε-trick as at the deviation of Eq. (108), to quench the upper-limit substitution:

$$
\begin{aligned}
S_F(\omega) &= \sum_{n,n'} W_n |F_{nn'}|^2 \frac{1}{2\pi} \lim_{\varepsilon \to 0} \int_{-\infty}^{+\infty} \cos\frac{\widetilde{E}\tau}{\hbar} e^{-\varepsilon|\tau|} e^{i\omega\tau} d\tau \\
&\equiv \frac{1}{2\pi} \sum_{n,n'} W_n |F_{nn'}|^2 \lim_{\varepsilon \to 0} \int_{0}^{+\infty} \left[\exp\left\{ \frac{i\widetilde{E}\tau}{\hbar} \right\} + \text{c.c.} \right] e^{-\varepsilon\tau} e^{i\omega\tau} d\tau \qquad (7.117) \\
&= \frac{1}{2\pi} \sum_{n,n'} W_n |F_{nn'}|^2 \lim_{\varepsilon \to 0} \left[\frac{1}{i(\widetilde{E}/\hbar + \omega) - \varepsilon} + \frac{1}{i(-\widetilde{E}/\hbar + \omega) - \varepsilon} \right].
\end{aligned}
$$

Now it is a convenient time to recall that each of the two summations here is over the eigenenergies of the environment, whose spectrum is virtually continuous because of its large size, so we may transform each sum into an integral – just as this was done in Sec. 6.6:

$$
\sum_{n} \ldots \to \int \ldots dn = \int \ldots \rho(E_n)\, dE_n, \qquad (7.118)
$$

where $\rho(E) \equiv dn/dE$ is the environment's density of states at a given energy. This transformation yields

$$
S_F(\omega) = \frac{1}{2\pi} \lim_{\varepsilon \to 0} \int dE_n W(E_n) \rho(E_n) \int dE_{n'} \rho(E_{n'}) |F_{nn'}|^2 \left[\frac{1}{i(\widetilde{E}/\hbar - \omega) - \varepsilon} + \frac{1}{i(-\widetilde{E}/\hbar - \omega) - \varepsilon} \right]. \quad (7.119)
$$

Since the expression inside the square bracket depends only on a specific linear combination of two energies, namely on $\widetilde{E} \equiv E_n - E_{n'}$, it is convenient to introduce another, linearly independent combination of the energies, for example, the average energy $\overline{E} \equiv (E_n + E_{n'})/2$, so the state energies may be represented as

$$
E_n = \overline{E} + \frac{\widetilde{E}}{2}, \quad E_{n'} = \overline{E} - \frac{\widetilde{E}}{2}. \qquad (7.120)
$$

With this notation, Eq. (119) becomes

$$
\begin{aligned}
S_F(\omega) = -\frac{\hbar}{2\pi} \lim_{\varepsilon \to 0} \int d\overline{E} &\left[\int d\widetilde{E}\, W\left(\overline{E} + \frac{\widetilde{E}}{2} \right) \rho\left(\overline{E} + \frac{\widetilde{E}}{2} \right) \rho\left(\overline{E} - \frac{\widetilde{E}}{2} \right) |F_{nn'}|^2 \frac{1}{i(\widetilde{E} - \hbar\omega) - \hbar\varepsilon} \right. \\
&\left. + \int d\widetilde{E}\, W\left(\overline{E} + \frac{\widetilde{E}}{2} \right) \rho\left(\overline{E} + \frac{\widetilde{E}}{2} \right) \rho\left(\overline{E} - \frac{\widetilde{E}}{2} \right) |F_{nn'}|^2 \frac{1}{i(-\widetilde{E} - \hbar\omega) - \hbar\varepsilon} \right]. \quad (7.121)
\end{aligned}
$$

Due to the smallness of the parameter $\hbar\varepsilon$ (which should be much smaller than all genuine energies of the problem, including $k_B T$, $\hbar\omega$, E_n, and $E_{n'}$), each of the internal integrals in Eq. (121) is dominated by

---

[43] An alternative popular measure of the spectral density of a process $F(t)$ is $S_F(\nu) \equiv \langle F_f^2 \rangle / d\nu = 4\pi S_F(\omega)$, where $\nu = \omega/2\pi$ is the "cyclic" frequency (measured in Hz).

an infinitesimal vicinity of one point, $\widetilde{E}_\pm = \pm\hbar\omega$. In these vicinities, the state densities, the matrix elements, and the Gibbs probabilities do not change considerably and may be taken out of the integral, which may be then worked out explicitly:[44]

$$S_F(\omega) = -\frac{\hbar}{2\pi}\lim_{\varepsilon\to 0}\int d\overline{E}\,\rho_+\rho_-\left[W_+|F_+|^2\int_{-\infty}^{+\infty}\frac{d\widetilde{E}}{i(\widetilde{E}-\hbar\omega)-\hbar\varepsilon}+W_-|F_-|^2\int_{-\infty}^{+\infty}\frac{d\widetilde{E}}{i(-\widetilde{E}-\hbar\omega)-\hbar\varepsilon}\right]$$

$$\equiv -\frac{\hbar}{2\pi}\lim_{\varepsilon\to 0}\int d\overline{E}\,\rho_+\rho_-\left[W_+|F_+|^2\int_{-\infty}^{+\infty}\frac{-i(\widetilde{E}-\hbar\omega)-\hbar\varepsilon}{(\widetilde{E}-\hbar\omega)^2+(\hbar\varepsilon)^2}d\widetilde{E}+W_-|F_-|^2\int_{-\infty}^{+\infty}\frac{i(\widetilde{E}+\hbar\omega)-\hbar\varepsilon}{(\widetilde{E}+\hbar\omega)^2+(\hbar\varepsilon)^2}d\widetilde{E}\right]$$

$$= \frac{\hbar}{2}\int\rho_+\rho_-\left[W_+|F_+|^2+W_-|F_-|^2\right]d\overline{E}\,, \qquad (7.122)$$

where the indices $\pm$ mark the functions' values at the special points $\widetilde{E}_\pm = \pm\hbar\omega$, i.e. $E_n = E_{n'} \pm \hbar\omega$. The physics of these points becomes simple if we interpret the state n, for which the equilibrium Gibbs distribution function equals W_n, as the initial state of the environment, and n' as its final state. Then the top-sign point corresponds to $E_{n'} = E_n - \hbar\omega$, i.e. to the result of emission of one energy quantum $\hbar\omega$ of the "observation" frequency ω by the environment to the system s of our interest, while the bottom-sign point $E_{n'} = E_n + \hbar\omega$, corresponds to the absorption of such quantum by the environment. As Eq. (122) shows, both processes give similar, positive contributions to the force fluctuations.

The situation is different for the Fourier image of the response function $G(\tau)$,[45]

$$\boxed{\chi(\omega) \equiv \int_0^{+\infty}G(\tau)e^{i\omega\tau}d\tau\,,} \qquad (7.123)$$

Generalized susceptibility

that is usually called *generalized susceptibility* – in our case, of the environment. Its physical meaning is that according to Eq. (107), the complex function $\chi(\omega) = \chi'(\omega) + i\chi''(\omega)$ relates the Fourier amplitudes of the generalized coordinate and the generalized force: [46]

$$\left\langle\hat{F}_\omega\right\rangle = \chi(\omega)\hat{x}_\omega\,. \qquad (7.124)$$

The physics of its imaginary part $\chi''(\omega)$ is especially clear. Indeed, if x_ω represents a sinusoidal *classical* oscillation waveform, say

$$x(t) = x_0\cos\omega t \equiv \frac{x_0}{2}e^{-i\omega t}+\frac{x_0}{2}e^{+i\omega t}\,, \quad\text{i.e. } x_\omega = x_{-\omega} = \frac{x_0}{2}\,, \qquad (7.125)$$

---

[44] Using, e.g., MA Eq. (6.5a). (The imaginary parts of the integrals vanish, because the integration in infinite limits may be always re-centered to the finite points $\pm\hbar\omega$.) A math-enlightened reader may have noticed that the integrals might be taken without the introduction of small ε, by using the Cauchy theorem – see MA Eq. (15.1).

[45] The integration in Eq. (123) may be extended to the whole time axis, $-\infty < \tau < +\infty$, if we complement the definition (107) of the function $G(\tau)$ for $\tau > 0$ with its definition as $G(\tau) = 0$ for $\tau < 0$, in correspondence with the causality principle.

[46] To prove this relation, it is sufficient to plug the expression $\hat{x}_s = \hat{x}_\omega e^{-i\omega t}$, or any sum of such exponents, into Eqs. (107) and then use the definition (123). This (simple) exercise is highly recommended to the reader.

then, in accordance with the correspondence principle, Eq. (124) should hold for the *c*-number complex amplitudes F_ω and x_ω, enabling us to calculate the time dependence of the force as

$$
\begin{aligned}
F(t) &= F_\omega e^{-i\omega t} + F_{-\omega} e^{+i\omega t} = \chi(\omega) x_\omega e^{-i\omega t} + \chi(-\omega) x_{-\omega} e^{+i\omega t} = \frac{x_0}{2}\left[\chi(\omega)e^{-i\omega t} + \chi^*(\omega)e^{+i\omega t}\right] \\
&= \frac{x_0}{2}\left[(\chi' + i\chi'')e^{-i\omega t} + (\chi' - i\chi'')e^{+i\omega t}\right] \equiv x_0\left[\chi'(\omega)\cos\omega t + \chi''(\omega)\sin\omega t\right].
\end{aligned}
\tag{7.126}
$$

We see that $\chi''(\omega)$ weighs the force's part (frequently called *quadrature*) that is $\pi/2$-shifted from the coordinate x, i.e. is in phase with its velocity and hence characterizes the time-average power flow from the system into its environment, i.e. the *energy dissipation* rate:[47]

$$
\overline{\mathscr{P}} = \overline{-F(t)\dot{x}(t)} = \overline{-x_0\left[\chi'(\omega)\cos\omega t + \chi''(\omega)\sin\omega t\right](-\omega x_0 \sin\omega t)} = \frac{x_0^2}{2}\omega\chi''(\omega).
\tag{7.127}
$$

Let us calculate this function from Eqs. (108) and (123), just as we have done for the spectral density of fluctuations:

$$
\begin{aligned}
\chi''(\omega) &= \mathrm{Im}\int_0^{+\infty} G(\tau)e^{i\omega\tau}d\tau = \frac{2}{\hbar}\sum_{n,n'} W_n |F_{nn'}|^2 \lim_{\varepsilon\to 0} \mathrm{Im}\int_0^{+\infty} \frac{1}{2i}\left(\exp\left\{i\frac{\tilde{E}\tau}{\hbar}\right\} - \mathrm{c.c.}\right)e^{i\omega\tau}e^{-\varepsilon\tau}d\tau \\
&= \sum_{n,n'} W_n |F_{nn'}|^2 \lim_{\varepsilon\to 0} \mathrm{Im}\left(\frac{1}{-\tilde{E}-\hbar\omega-i\hbar\varepsilon} - \frac{1}{\tilde{E}-\hbar\omega-i\hbar\varepsilon}\right) \\
&\equiv \sum_{n,n'} W_n |F_{nn'}|^2 \lim_{\varepsilon\to 0}\left(\frac{\hbar\varepsilon}{(\tilde{E}+\hbar\omega)^2 + (\hbar\varepsilon)^2} - \frac{\hbar\varepsilon}{(\tilde{E}-\hbar\omega)^2 + (\hbar\varepsilon)^2}\right).
\end{aligned}
\tag{7.128}
$$

Making the transfer (118) from the double sum to the double integral, and then the integration variable transfer (120), we get

$$
\begin{aligned}
\chi''(\omega) = \lim_{\varepsilon\to 0}\int d\overline{E}\Bigg[&\int_{-\infty}^{+\infty} W\left(\overline{E}+\frac{\tilde{E}}{2}\right)\rho\left(\overline{E}+\frac{\tilde{E}}{2}\right)\rho\left(\overline{E}-\frac{\tilde{E}}{2}\right)|F_{nn'}|^2 \frac{\hbar\varepsilon}{(\tilde{E}+\hbar\omega)^2+(\hbar\varepsilon)^2}d\tilde{E} \\
&-\int_{-\infty}^{+\infty} W\left(\overline{E}+\frac{\tilde{E}}{2}\right)\rho\left(\overline{E}+\frac{\tilde{E}}{2}\right)\rho\left(\overline{E}-\frac{\tilde{E}}{2}\right)|F_{nn'}|^2 \frac{\hbar\varepsilon}{(\tilde{E}-\hbar\omega)^2+(\hbar\varepsilon)^2}d\tilde{E}\Bigg].
\end{aligned}
\tag{7.129}
$$

Now using the same argument about the smallness of parameter ε as above, we may take the spectral densities, the matrix elements of force, and the Gibbs probabilities out of the integrals, and work out the remaining integrals, getting a result very similar to Eq. (122):

$$
\chi''(\omega) = \pi\int \rho_+ \rho_-\left[W_- |F_-|^2 - W_+ |F_+|^2\right]d\overline{E}.
\tag{7.130}
$$

To relate these results, it is sufficient to notice that according to Eq. (24), the Gibbs probabilities $W_\pm$ are related by a coefficient depending on only the temperature T and observation frequency ω:

---

[47] The sign minus in Eq. (127) is due to the fact that according to Eq. (90), F is the force exerted *on* our system (*s*) by the environment, so the force exerted *by* our system on the environment is $-F$. With this sign clarification, the expression $\mathscr{P} = -F\dot{x} = -Fv$ for the instant power flow is evident if x is the usual Cartesian coordinate of a 1D particle. However, according to analytical mechanics (see, e.g., CM Chapters 2 and 10), it is also valid for any {generalized coordinate, generalized force} pair that forms the interaction Hamiltonian (90).

$$W_{\pm} \equiv W\left(\overline{E} + \frac{\tilde{E}_{\pm}}{2}\right) \equiv W\left(\overline{E} \pm \frac{\hbar\omega}{2}\right) = \frac{1}{Z}\exp\left\{-\frac{\overline{E} \pm \hbar\omega/2}{k_{\mathrm{B}}T}\right\} = W(\overline{E})\exp\left\{\mp\frac{\hbar\omega}{2k_{\mathrm{B}}T}\right\}, \qquad (7.131)$$

so both the spectral density (122) and the dissipative part (130) of the generalized susceptibility may be expressed via the same integral over the environment energies:

$$S_F(\omega) = \hbar\cosh\left(\frac{\hbar\omega}{2k_{\mathrm{B}}T}\right)\int \rho_+\rho_- W(\overline{E})\left[\left|F_+\right|^2 + \left|F_-\right|^2\right]d\overline{E}, \qquad (7.132)$$

$$\chi''(\omega) = 2\pi\sinh\left(\frac{\hbar\omega}{2k_{\mathrm{B}}T}\right)\int \rho_+\rho_- W(\overline{E})\left[\left|F_+\right|^2 + \left|F_-\right|^2\right]d\overline{E}, \qquad (7.133)$$

and hence are universally related as

$$S_F(\omega) = \frac{\hbar}{2\pi}\chi''(\omega)\coth\frac{\hbar\omega}{2k_{\mathrm{B}}T}. \qquad (7.134)$$

<div style="text-align:right">Fluctuation-dissipation theorem</div>

This is, finally, the much-celebrated Callen-Welton's fluctuation-dissipation theorem (FDT). It reveals a fundamental, intimate relationship between these two effects of the environment ("no dissipation without fluctuation") – hence the name. A curious feature of the FDT is that Eq. (134) includes the same function of temperature as the average energy (26) of a quantum oscillator of frequency ω, though, as the reader could witness, the notion of the oscillator was by no means used in its derivation. As we will see in the next section, this fact leads to rather interesting consequences and even conceptual opportunities.

In the classical limit, $\hbar\omega \ll k_{\mathrm{B}}T$, the FDT is reduced to

$$S_F(\omega) = \frac{\hbar}{2\pi}\chi''(\omega)\frac{2k_{\mathrm{B}}T}{\hbar\omega} = \frac{k_{\mathrm{B}}T}{\pi}\frac{\mathrm{Im}\,\chi(\omega)}{\omega}. \qquad (7.135)$$

In most systems of interest, the last fraction is close to a finite (positive) constant within a substantial range of relatively low frequencies. Indeed, expanding the right-hand side of Eq. (123) into the Taylor series in small ω, we get

$$\chi(\omega) = \chi(0) + i\omega\eta + \ldots, \quad \text{with} \quad \chi(0) = \int_0^\infty G(\tau)d\tau, \quad \text{and} \quad \eta \equiv \int_0^\infty G(\tau)\tau d\tau. \qquad (7.136)$$

Since the temporal Green's function G is real by definition, the Taylor expansion of $\chi''(\omega) \equiv \mathrm{Im}\chi(\omega)$ at $\omega = 0$ starts with the linear term $\omega\eta$, where η is a certain real coefficient, and unless $\eta = 0$, is dominated by this term at small ω. The physical sense of the constant η becomes clear if we consider an environment that provides a force described by a simple, well-known kinematic friction law

$$\left\langle \hat{F} \right\rangle = -\eta\dot{x}, \qquad \text{with} \quad \eta \geq 0, \qquad (7.137)$$

where η is usually called the *drag coefficient*. For the Fourier images of coordinate and force, this gives the relation $F_\omega = i\omega\eta x_\omega$, so according to Eq. (124),

$$\chi(\omega) = i\omega\eta, \qquad \text{i.e.} \quad \frac{\chi''(\omega)}{\omega} \equiv \frac{\mathrm{Im}\,\chi(\omega)}{\omega} = \eta \geq 0. \qquad (7.138)$$

<div style="text-align:right">Ohmic dissipation</div>

With this approximation, and in the classical limit, Eq. (135) is reduced to the well-known *Nyquist formula*:[48]

$$S_F(\omega) = \frac{k_B T}{\pi}\eta, \qquad \text{i.e.} \ \left\langle F_f^2 \right\rangle = 4k_B T \eta d\nu. \tag{7.139}$$

According to Eq. (112), if such a constant spectral density[49] persisted at all frequencies, it would correspond to a delta-correlated process $F(t)$, with

$$K_F(\tau) = 2\pi S_F(0)\delta(\tau) = 2k_B T \eta \delta(\tau) \tag{7.140}$$

– cf. Eqs. (82) and (83). Since in the classical limit, the right-hand side of Eq. (109) is negligible, and the correlation function may be considered an even function of time, the symmetrized function under the integral in Eq. (113) may be rewritten just as $\langle F(\tau)F(0)\rangle$. In the limit of relatively low observation frequencies (in the sense that ω is much smaller than not only the quantum frontier $k_B T/\hbar$ but also the frequency scale of the function $\chi''(\omega)/\omega$), Eq. (138) may be used to recast Eq. (135) in the form[50]

$$\eta \equiv \lim_{\omega\to 0}\frac{\chi''(\omega)}{\omega} = \frac{1}{k_B T}\int_0^\infty \langle F(\tau)F(0)\rangle d\tau. \tag{7.141}$$

To conclude this section, let me return for a minute to the questions formulated in our earlier discussion of dephasing in the two-level model. In that problem, the dephasing time scale is $T_2 = 1/2D_\varphi$. Hence the classical approach to the dephasing, used in Sec. 3, is adequate if $\hbar D_\varphi \ll k_B T$. Next, we may identify the operators $\hat{f}$ and $\hat{\sigma}_z$ participating in Eq. (70) with, respectively, $\left(-\hat{F}\right)$ and $\hat{x}$ participating in the general Eq. (90). Then the comparison of Eqs. (82), (89), and (140) yields

$$\frac{1}{T_2} \equiv 2D_\varphi = \frac{4k_B T}{\hbar^2}\eta, \tag{7.142}$$

so, for the model described by Eq. (137) with a temperature-independent drag coefficient η, the rate of dephasing by a classical environment is proportional to its temperature.

---

[48] Actually, the 1928 work by H. Nyquist was about the electronic noise in resistors, just discovered experimentally by his Bell Labs colleague John Bertrand Johnson. For an Ohmic resistor, as the dissipative "environment" of the electric circuit it is connected with, Eq. (137) is just the Ohm's law, and may be recast as either $\langle V\rangle = -R(dQ/dt) = RI$, or $\langle I\rangle = -G(d\Phi/dt) = GV$. Thus for the voltage V across an open circuit, η corresponds to its resistance R, while for current I in a short circuit, to its conductance $G = 1/R$. In this case, the fluctuations described by Eq. (139) are referred to as the *Johnson-Nyquist noise*. (Because of this important application, any model leading to Eq. (138) is commonly referred to as the *Ohmic dissipation*, even if the physical nature of the variables x and F is quite different from voltage and current.)

[49] A random process whose spectral density may be reasonably approximated by a constant is frequently called *white noise*, because it is a random mixture of all possible sinusoidal components with equal weights, reminding the spectral composition of natural white light.

[50] Note that in some fields (especially in physical kinetics and chemical physics), this particular limit of the Nyquist formula is called the Green-Kubo (or just the "Kubo") formula. However, in view of the FDT development history (described above), it is much more reasonable to associate these names with Eq. (109) – as it is done in most fields of physics.

7.5. The Heisenberg-Langevin approach

The fluctuation-dissipation theorem offers a very simple and efficient though limited approach to the analysis of the system of interest (s in Fig. 1). It is to write its Heisenberg equations (4.199) of motion of the relevant operators, which would now include the environmental force operator, and explore these equations using the Fourier transform and the Wiener-Khinchin theorem (112)-(113). This approach to classical equations of motion is commonly associated with the name Langevin,[51] so its extension to dynamics of Heisenberg-picture operators is frequently referred to as the *Heisenberg-Langevin* (or "quantum Langevin", or "Langevin-Lax"[52]) *approach* to open system analysis.

Perhaps the best way to describe this method is to demonstrate how it works for the very important case of a 1D harmonic oscillator, so the generalized coordinate x of Sec. 4 is just the oscillator's coordinate. For the sake of simplicity, let us assume that the environment provides the simple Ohmic dissipation described by Eq. (137) – which is a very good approximation in many cases. As we already know from Chapter 5, the Heisenberg equations of motion for operators of coordinate and momentum of the oscillator, in the presence of an external force $F(t)$, are

$$\dot{\hat{x}} = \frac{\hat{p}}{m}, \qquad \dot{\hat{p}} = -m\omega_0^2 \hat{x} + \hat{F}, \tag{7.143}$$

so using Eqs. (92) and (137), we get

$$\dot{\hat{x}} = \frac{\hat{p}}{m}, \qquad \dot{\hat{p}} = -m\omega_0^2 \hat{x} - \eta\dot{\hat{x}} + \tilde{\hat{F}}(t). \tag{7.144}$$

Combining both Eqs. (144), we may write their system as a single differential equation

$$m\ddot{\hat{x}} + \eta\dot{\hat{x}} + m\omega_0^2 \hat{x} = \tilde{\hat{F}}(t), \tag{7.145}$$

which is similar to the well-known classical equation of motion of a damped oscillator under the effect of an external force. In the view of Eqs. (5.29) and (5.35), whose corollary the Ehrenfest theorem (5.36) is, this may look not surprising, but please note again that the approach discussed in the previous section justifies such quantitative description of the drag force in quantum mechanics – necessarily in parallel with the accompanying fluctuation force.

For the Fourier images of the operators, defined similarly to Eq. (115), Eq. (145) gives the following relation,

$$\hat{x}_\omega = \frac{\hat{F}_\omega}{m\left(\omega_0^2 - \omega^2\right) - i\eta\omega}, \tag{7.146}$$

which should be also well-known to the reader from the classical theory of forced oscillations.[53] However, since these Fourier components are still Heisenberg-picture operators and their "values" for

---

[51] A 1908 work by Paul Langevin was the first systematic development of Einstein's ideas (1905) on the Brownian motion, using the random force language, as an alternative to M. Smoluchowski's approach using the probability density language – see Sec. 6 below.

[52] Indeed, perhaps the largest credit for the extension of the Langevin approach to quantum systems belongs to Melvin J. Lax, whose work in the early 1960s was motivated mostly by quantum electronics applications – see, e.g., his monograph M. Lax, *Fluctuation and Coherent Phenomena in Classical and Quantum Physics*, Gordon and Breach, 1968, and references therein.

[53] If necessary, see CM Sec. 5.1.

different ω generally do not commute, we have to tread carefully. The best way to proceed is to write a copy of Eq. (146) for frequency $(-\omega')$, and then combine these equations to form a symmetrical combination similar to that used in Eq. (114). The result is

$$\frac{1}{2}\left\langle \hat{x}_\omega \hat{x}_{-\omega'} + \hat{x}_{-\omega'}\hat{x}_\omega \right\rangle = \frac{1}{\left| m\left(\omega_0^2 - \omega^2\right) - i\eta\omega \right|^2} \frac{1}{2}\left\langle \hat{F}_\omega \hat{F}_{-\omega'} + \hat{F}_{-\omega'}\hat{F}_\omega \right\rangle. \tag{7.147}$$

Since the spectral density definition similar to Eq. (114) is valid for any observable, in particular for x, Eq. (147) allows us to relate the symmetrized spectral densities of coordinate and force:

$$S_x(\omega) = \frac{S_F(\omega)}{\left| m\left(\omega_0^2 - \omega^2\right) - i\eta\omega \right|^2} \equiv \frac{S_F(\omega)}{m^2\left(\omega_0^2 - \omega^2\right)^2 + \left(\eta\omega\right)^2}. \tag{7.148}$$

Now using an analog of Eq. (116) for x, we can calculate the coordinate's variance:

$$\left\langle x^2 \right\rangle = K_x(0) = \int_{-\infty}^{+\infty} S_x(\omega)d\omega = 2\int_0^{+\infty} \frac{S_F(\omega)d\omega}{m^2\left(\omega_0^2 - \omega^2\right)^2 + \left(\eta\omega\right)^2}, \tag{7.149}$$

where now, in contrast to the notation used in Sec. 4, the sign $\langle \dots \rangle$ means averaging over the usual statistical ensemble of many systems of interest – in our current case, of many harmonic oscillators.

If the coupling to the environment is so weak that the drag coefficient η is small (in the sense that the oscillator's dimensionless Q-factor is large, $Q \equiv m\omega_0/\eta \gg 1$), this integral is dominated by the resonance peak in a narrow vicinity, $|\omega - \omega_0| \equiv |\xi| \ll \omega_0$, of its resonance frequency, and we can take the relatively smooth function $S_F(\omega)$ out of the integral, thus reducing it to a table form:[54]

$$\left\langle x^2 \right\rangle \approx 2S_F(\omega_0)\int_0^{+\infty} \frac{d\omega}{m^2\left(\omega_0^2 - \omega^2\right)^2 + \left(\eta\omega\right)^2} \approx 2S_F(\omega_0)\int_{-\infty}^{+\infty} \frac{d\xi}{\left(2m\omega_0\xi\right)^2 + \left(\eta\omega_0\right)^2}$$

$$\equiv 2S_F(\omega_0)\frac{1}{\left(\eta\omega_0\right)^2}\int_{-\infty}^{+\infty} \frac{d\xi}{\left(2m\xi/\eta\right)^2 + 1} = 2S_F(\omega_0)\frac{1}{\left(\eta\omega_0\right)^2}\frac{\pi\eta}{2m} = \frac{\pi S_F(\omega_0)}{\eta m\omega_0^2}. \tag{7.150}$$

With the account of the FDT (134) and of Eq. (138), this gives[55]

$$\left\langle x^2 \right\rangle = \frac{\pi}{\eta m\omega_0^2}\frac{\hbar}{2\pi}\eta\omega_0 \coth\frac{\hbar\omega_0}{2k_B T} \equiv \frac{\hbar}{2m\omega_0}\coth\frac{\hbar\omega_0}{2k_B T}. \tag{7.151}$$

But this is exactly Eq. (48), which was derived in Sec. 2 from the Gibbs distribution, without any explicit account of the environment – though implying it by using the notion of the thermally-equilibrium ensemble.[56]

---

[54] See, e.g., MA Eq. (6.5a).

[55] Note that this calculation remains correct even if the dissipation's dispersion law deviates from the Ohmic model (138), provided that the drag coefficient η is replaced with its effective value $\text{Im}\chi(\omega_0)/\omega_0$.

[56] By the way, the simplest way to calculate $S_F(\omega)$, i.e. to derive the FDT, is to *require* that Eqs. (48) and (150) give the same result for an oscillator with any eigenfrequency ω. This was exactly the approach used by H. Nyquist (for the classical case) – see also SM Sec. 5.5.

Notice that in the final form of Eq. (151), the coefficient η, which characterizes the oscillator-to-environment interaction strength, has canceled! Does this mean that in Sec. 4 we toiled in vain? By no means. First of all, the result (150), augmented by the FDT (134), has an important conceptual value. For example, let us consider the low-temperature limit $k_B T << \hbar\omega_0$ where Eq. (151) is reduced to

$$\left\langle x^2 \right\rangle = \frac{\hbar}{2m\omega_0} \equiv \frac{x_0^2}{2}. \tag{7.152}$$

Let us ask a naïve question: what exactly is the origin of this coordinate's uncertainty? From the point of view of the usual quantum mechanics of absolutely closed (Hamiltonian) systems, there is no doubt: this non-vanishing variance of the coordinate is the result of the final spatial extension of the ground-state wavefunction (2.275), reflecting Heisenberg's uncertainty relation – which in turn results from the fact that the operators of coordinate and momentum do not commute. However, from the point of view of the Heisenberg-Langevin equation (145), the variance (152) is an inalienable part of the oscillator's response to the fluctuation force $\widetilde{F}(t)$ *exerted by the environment* at frequencies $\omega \approx \omega_0$. Though it is impossible to refute the former, absolutely legitimate point of view, in many applications it is easier to subscribe to the latter standpoint and treat the coordinate's uncertainty as the result of the so-called *quantum noise* of the environment, which, in equilibrium, obeys the FTD (134). This notion has received numerous confirmations in experiments that did not include *any* oscillators with their own frequencies ω_0 close to the noise measurement frequency ω.[57]

The second advantage of the Heisenberg-Langevin approach is that it is possible to use Eq. (148) to calculate the (experimentally measurable!) distribution $S_x(\omega)$, i.e. decompose the fluctuations into their spectral components. This procedure is not restricted to the limit of small η (i.e. of large Q); for any damping, we may just plug the FDT (134) into Eq. (148). For example, let us have a look at the so-called *quantum diffusion*. A free 1D particle, moving in a viscous medium providing it with the Ohmic damping (137), may be considered as a particular case of a 1D harmonic oscillator (145), but with $\omega_0 = 0$, so combining Eqs. (134) and (149), we get

$$\left\langle x^2 \right\rangle = 2\int_0^{+\infty} \frac{S_F(\omega)d\omega}{(m\omega^2)^2 + (\eta\omega)^2} = 2\eta \int_0^{+\infty} \frac{1}{(m\omega^2)^2 + (\eta\omega)^2} \frac{\hbar\omega}{2\pi} \coth\frac{\hbar\omega}{2k_B T} d\omega. \tag{7.153}$$

This integral has two divergences. The first one, of the type $\int d\omega/\omega^2$ at the lower limit, is just a classical effect: according to Eq. (85), the particle's displacement variance grows with time, so it cannot have a finite time-independent value that Eq. (153) tries to calculate. However, we still can use that result to single out the quantum effects on diffusion – say, by comparing it with a similar but purely classical case. These effects are prominent at high frequencies, especially if the quantum noise overcomes the thermal noise before the dynamic cut-off, i.e. if

$$\frac{k_B T}{\hbar} << \frac{\eta}{m}. \tag{7.154}$$

In this case, there is a broad range of frequencies where the quantum noise gives a substantial contribution to the integral:

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[57] See, for example, R. Koch *et al.*, *Phys. Lev. B* **26**, 74 (1982).

<div style="text-align:right">Quantum diffusion</div>

$$\left\langle x^2 \right\rangle_Q \approx 2\eta \int\limits_{k_B T/\hbar}^{\eta/m} \frac{1}{(\eta\omega)^2} \frac{\hbar\omega}{2\pi} d\omega \equiv \frac{\hbar}{\pi\eta} \int\limits_{k_B T/\hbar}^{\eta/m} \frac{d\omega}{\omega} = \frac{\hbar}{\pi\eta} \ln \frac{\hbar\eta}{mk_B T} \sim \frac{\hbar}{\eta}. \qquad (7.155)$$

Formally, this contribution diverges at either $m \to 0$ or $T \to 0$, but this logarithmic (i.e. extremely weak) divergence is readily quenched by almost any change of the environment model at very high frequencies, where the "Ohmic" approximation (136) becomes unrealistic.

The Heisenberg-Langevin approach is very powerful because its straightforward generalizations enable analyses of fluctuations in virtually arbitrary linear systems, i.e. the systems described by linear differential (or integro-differential) equations of motion, including those with many degrees of freedom, and distributed systems (*continua*), and such systems dominate many fields of physics. However, this approach also has a major limitation: if the equations of motion of the Heisenberg operators are *not* linear, then there is no linear relation, such as Eq. (146), between the Fourier images of the generalized forces and the generalized coordinates, and as the result, there is no simple relation, such as Eq. (148), between their spectral densities. In other words, if the Heisenberg equations of motion are nonlinear, there is no regular simple way to use them to calculate the statistical properties of the observables.

For example, let us return for a second to the dephasing problem described by Eqs. (68)-(70), and assume that the deterministic and fluctuating parts of the effective force $-f$ exerted by the environment, are characterized by relations similar, respectively, to Eqs. (124) and (134). Now writing the Heisenberg equations of motion for the two remaining spin operators, and using the commutation relations between them, we get

$$\dot{\hat{\sigma}}_x = \frac{1}{i\hbar}\left[\hat{\sigma}_x, \hat{H}\right] = \frac{1}{i\hbar}\left[\hat{\sigma}_x, \left(c_z + \hat{f}\right)\hat{\sigma}_z\right] = -\frac{2}{\hbar}\hat{\sigma}_y\left(c_z + \hat{f}\right) = -\frac{2}{\hbar}\hat{\sigma}_y\left(c_z + \eta\hat{\sigma}_z + \hat{\tilde{f}}\right), \qquad (7.156)$$

and a similar equation for $\dot{\hat{\sigma}}_y$. Such nonlinear equations cannot be used to calculate the statistical properties of the Pauli operators in this system exactly – at least analytically.

For some calculations, this problem may be circumvented by *linearization*: if we are only interested in small fluctuations of the observables, their nonlinear Heisenberg equations of motion, such as Eq. (156), may be linearized with respect to small deviations of the operators from their (generally, deterministic "values", and then the resulting linear equations for the operator variations may be solved either as has been demonstrated above, or (if the deterministic "values" evolve in time) using their Fourier expansions. Sometimes this approach gives relatively simple and important results,[58] but for many other problems, this approach is insufficient, leaving a lot of space for alternative methods.

7.6. Density matrix approach

The main alternative approach to the dynamics of open quantum systems, which is essentially a generalization of the one discussed in Sec. 2, is to extract the final results of interest from the dynamics of the density operator of our system *s*. Let us discuss this approach in detail.[59]

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[58] For example, the formula used for processing the experimental results by R. Koch *et al*. (mentioned above), had been derived in this way. (This derivation will be suggested to the reader as an exercise.)

[59] As in Sec. 4, the reader not interested in the derivation of the basic equation (181) of the density matrix evolution may immediately jump to the discussion of this equation and its applications.

We already know that the density matrix allows the calculation of the expectation value of any observable of the system s – see Eq. (5). However, our initial recipe (6) for the density matrix element calculation, which requires the knowledge of the exact state (2) of the whole Universe, is not too practicable, while the von Neumann equation (66) for the density matrix evolution is limited to cases in which probabilities W_j of the system states are fixed – thus excluding such important effects as the energy relaxation. However, such effects may be analyzed using a different assumption – that the system of interest interacts only with a *local environment* that is very close to its thermally-equilibrium state described, in the stationary-state basis, by a diagonal density matrix with the elements (24).

This calculation is facilitated by the following general observation. Let us number the basis states of the full local system (the system of our interest plus its local environment) by l, and use Eq. (5) to write

$$\langle A \rangle = \mathrm{Tr}\left(\hat{A}\hat{w}_l\right) \equiv \sum_{l,l'} A_{ll'} w_{l'l} = \sum_{l,l'} \langle l|\hat{A}|l'\rangle \langle l'|\hat{w}_l|l\rangle, \tag{7.157}$$

where $\hat{w}_l$ is the full density operator of this local system. At a weak interaction between the system s and the local environment e, their states reside in different Hilbert spaces, so we can write[60]

$$|l\rangle = |s_j\rangle \otimes |e_k\rangle, \tag{7.158}$$

and if the observable A depends only on the coordinates of the system s of our interest, we may reduce Eq. (157) to the form similar to Eq. (5):

$$\langle A \rangle = \sum_{j,j';k,k'} \langle e_k|\otimes\langle s_j|\hat{A}|s_{j'}\rangle\otimes|e_{k'}\rangle\langle e_{k'}|\otimes\langle s_{j'}|\hat{w}_l|s_j\rangle\otimes|e_k\rangle$$
$$= \sum_{j,j'} A_{jj'}\langle s_{j'}|\otimes\left(\sum_k \langle e_k|\hat{w}_l|e_k\rangle\right)\otimes|s_j\rangle = \mathrm{Tr}_j\left(\hat{A}\hat{w}\right), \tag{7.159}$$

where

$$\hat{w} \equiv \sum_k \langle e_k|\hat{w}_l|e_k\rangle = \mathrm{Tr}_k\,\hat{w}_l, \tag{7.160}$$

showing how the density operator $\hat{w}$ of the system s (sometimes called the *reduced density operator*) may be calculated from the full operator $\hat{w}_l$.

Now comes the key physical assumption of this approach: since we may select the local environment e to be much larger than the system s of our interest, we may consider the composite system l as a Hamiltonian one, with time-independent probabilities of its stationary states, so for the description of the evolution in time of *its* full density operator $\hat{w}_l$ (again, in contrast to that, $\hat{w}$, of the system of our interest) we *may* use the von Neumann equation (66). Partitioning its right-hand side in accordance with Eq. (68), we get:

$$i\hbar\dot{\hat{w}}_l = \left[\hat{H}_s,\hat{w}_l\right] + \left[\hat{H}_e,\hat{w}_l\right] + \left[\hat{H}_{\mathrm{int}},\hat{w}_l\right]. \tag{7.161}$$

The next step is to use the perturbation theory to solve this equation in the lowest order in $\hat{H}_{\mathrm{int}}$, that would yield a non-vanishing contribution due to the interaction. For that, Eq. (161) is not very

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[60] Let me emphasize that this simple representation is valid only for the *basis states* of our local system but, generally, not for its *quantum state*! Indeed, the calculation we are performing is valid (and is most relevant) even when the local system is not in *any* definite quantum state, and may be only described by the density matrix $w_{ll'}$.

convenient, because its right-hand side contains two other terms, of a much larger scale than the interaction Hamiltonian. To mitigate this technical difficulty, the interaction picture that was discussed at the end of Sec. 4.6, is very natural. (It is not necessary though, and I will use this picture mostly as an exercise of its application – unfortunately, the only example I can afford to give in this course.)

As a reminder, in that picture (whose entities will be marked with index "I", with the unmarked operators assumed to be in the Schrödinger picture), both the operators *and* the state vectors (and hence the density operator) depend on time. However, the time evolution of the operator of any observable *A* is described by an equation similar to Eq. (67), but with the *unperturbed* part of the Hamiltonian only – see Eq. (4.214). In the model (68), this means

$$i\hbar\dot{\hat{A}}_{\mathrm{I}} = \left[\hat{A}_{\mathrm{I}}, \hat{H}_0\right].$$
(7.162)

where the unperturbed Hamiltonian consists of two parts defined in different Hilbert spaces:

$$\hat{H}_0 \equiv \hat{H}_s + \hat{H}_e.$$
(7.163)

On the other hand, the state vector's dynamics is governed by the interaction evolution operator $\hat{u}_{\mathrm{I}}$ that obeys Eqs. (4.215). Since this equation, using the interaction-picture Hamiltonian (4.216),

$$\hat{H}_{\mathrm{I}} \equiv \hat{u}_0^{\dagger} \hat{H}_{\mathrm{int}} \hat{u}_0,$$
(7.164)

is absolutely similar to the ordinary Schrödinger equation using the full Hamiltonian, we may repeat all arguments given at the beginning of Sec. 3 to prove that the dynamics of the density operator in the interaction picture of a Hamiltonian system is governed by the following analog of the von Neumann equation (66):

$$i\hbar\dot{\hat{w}}_{\mathrm{I}} = \left[\hat{H}_{\mathrm{I}}, \hat{w}_{\mathrm{I}}\right],$$
(7.165)

where the index *l* is dropped for the notation simplicity. Since this equation is similar in structure (with the opposite sign) to the Heisenberg equation (67), we may use the solution Eq. (4.190) of the latter equation to write its analog:

$$\hat{w}_{\mathrm{I}}(t) = \hat{u}_{\mathrm{I}}(t,0)\hat{w}_l(0)\hat{u}_{\mathrm{I}}^{\dagger}(t,0).$$
(7.166)

It is also straightforward (and hence is left for the reader) to verify that in this picture, the expectation value of any observable *A* may be found from an expression similar to the basic Eq. (5):

$$\langle A \rangle = \mathrm{Tr}\left(\hat{A}_{\mathrm{I}}\hat{w}_{\mathrm{I}}\right),$$
(7.167)

showing again that the interaction and Schrödinger pictures give the same final results.

In the case of the factorable interaction (90),[61] Eq. (162) is simplified for both operators participating in that product – for each one in its own way. In particular, for $\hat{A} = \hat{x}$, it yields

$$i\hbar\dot{\hat{x}}_{\mathrm{I}} = \left[\hat{x}_{\mathrm{I}}, \hat{H}_0\right] \equiv \left[\hat{x}_{\mathrm{I}}, \hat{H}_s\right] + \left[\hat{x}_{\mathrm{I}}, \hat{H}_e\right].$$
(7.168)

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[61] An analysis of a much more general case when the interaction with the environment is represented as a sum of several/many products of the type (90), may be found, for example, in the monograph by K. Blum, *Density Matrix Theory and Applications*, 3rd ed., Springer, 2012.

Since the coordinate operator is defined in the Hilbert space of our system s, it commutes with the Hamiltonian of the environment, so we get

$$i\hbar\dot{\hat{x}}_\mathrm{I} = \left[\hat{x}_\mathrm{I}, \hat{H}_s\right].$$
(7.169)

On the other hand, if $\hat{A} = \hat{F}$, this operator is defined in the Hilbert space of the environment, and commutes with the Hamiltonian of the unperturbed system s. As a result, we get

$$i\hbar\dot{\hat{F}}_\mathrm{I} = \left[\hat{F}_\mathrm{I}, \hat{H}_e\right].$$
(7.170)

This means that with our time-independent unperturbed Hamiltonians, $\hat{H}_s$ and $\hat{H}_e$, the time evolution of the interaction-picture operators is rather simple. In particular, the analogy between Eq. (170) and Eq. (93) allows us to immediately write the following analog of Eq. (94):

$$\hat{F}_\mathrm{I}(t) = \exp\left\{+\frac{i}{\hbar}\hat{H}_e t\right\}\hat{F}(0)\exp\left\{-\frac{i}{\hbar}\hat{H}_e t\right\},$$
(7.171)

so in the stationary-state basis n of the environment,

$$\left(\hat{F}_\mathrm{I}\right)_{nn'}(t) = \exp\left\{+\frac{i}{\hbar}E_n t\right\}F_{nn'}(0)\exp\left\{-\frac{i}{\hbar}E_n t\right\} \equiv F_{nn'}(0)\exp\left\{-i\frac{E_n - E_{n'}}{\hbar}t\right\},$$
(7.172)

and similarly (but in the basis of the stationary states of system s) for the operator $\hat{x}$. As a result, the right-hand side of Eq. (164) may be also factored:

$$\hat{H}_\mathrm{I}(t) \equiv \hat{u}_0^\dagger(t,0)\hat{H}_\mathrm{int}\hat{u}_0(t,0) = \exp\left\{\frac{i}{\hbar}\left(\hat{H}_s + \hat{H}_e\right)t\right\}\left(-\hat{x}\hat{F}\right)\exp\left\{-\frac{i}{\hbar}\left(\hat{H}_s + \hat{H}_e\right)t\right\}$$

$$= -\left(\exp\left\{+\frac{i}{\hbar}\hat{H}_s t\right\}\hat{x}\exp\left\{-\frac{i}{\hbar}\hat{H}_s t\right\}\right)\left(\exp\left\{+\frac{i}{\hbar}\hat{H}_e t\right\}\hat{F}(0)\exp\left\{-\frac{i}{\hbar}\hat{H}_e t\right\}\right) \equiv -\hat{x}_\mathrm{I}(t)\hat{F}_\mathrm{I}(t).$$
(7.173)

So, the transfer to the interaction picture has taken some time, but now it enables a smooth ride.[62] Indeed, just as in Sec. 4, we may rewrite Eq. (165) in the integral form:

$$\hat{w}_\mathrm{I}(t) = \frac{1}{i\hbar}\int_{-\infty}^{t}\left[\hat{H}_\mathrm{I}(t'), \hat{w}_\mathrm{I}(t')\right]dt';$$
(7.174)

plugging this result into the right-hand side of Eq. (165), we get

$$\dot{\hat{w}}_\mathrm{I}(t) = -\frac{1}{\hbar^2}\int_{-\infty}^{t}\left[\hat{H}_\mathrm{I}(t), \left[\hat{H}_\mathrm{I}(t'), \hat{w}_\mathrm{I}(t')\right]\right]dt' = -\frac{1}{\hbar^2}\int_{-\infty}^{t}\left[\hat{x}(t)\hat{F}(t), \left[\hat{x}(t')\hat{F}(t'), \hat{w}_\mathrm{I}(t')\right]\right]dt',$$
(7.175)

where, for the notation's brevity, from this point on I will strip the operators $\hat{x}$ and $\hat{F}$ of their index "I". (I hope their time dependence indicates the interaction picture clearly enough.)

So far, this equation is exact (and cannot be solved analytically), but this is a good time to notice that even if we approximate the density operator on its right-hand side by its unperturbed, factorable "value"

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[62] If we used either the Schrödinger or the Heisenberg picture instead, the forthcoming Eq. (175) would pick up a rather annoying multitude of fast-oscillating exponents, of different time arguments, on its right-hand side.

$$\hat{w}_I(t') \rightarrow \hat{w}(t')\hat{w}_e, \qquad \text{with } \langle e_n | \hat{w}_e | e_{n'} \rangle = W_n \delta_{nn'}, \tag{7.176}$$

corresponding to no interaction between the system s and its thermally-equilibrium environment e, where e_n are the stationary states of the environment and W_n are the Gibbs probabilities (24), Eq. (175) still describes a nontrivial time evolution of the density operator.[63] This is exactly the first non-vanishing approximation (in the weak interaction) we have been looking for. Now using Eq. (160), we find the equation of evolution of the density operator of the system of our interest: [64]

$$\dot{w}(t) = -\frac{1}{\hbar^2} \int_{-\infty}^{t} \mathrm{Tr}_n \left[\hat{x}(t)\hat{F}(t), \left[\hat{x}(t')\hat{F}(t'), \hat{w}(t')\hat{w}_e \right] \right] dt', \tag{7.177}$$

where the trace is over the stationary states of the environment. To spell out the right-hand side of Eq. (177), note again that the coordinate and force operators commute with each other (but not with themselves at different time moments!) and hence may be swapped at will, so we may write

$$\begin{aligned}
\mathrm{Tr}_n\left[\ldots,\left[\ldots,\ldots\right]\right] &= \hat{x}(t)\hat{x}(t')\hat{w}(t')\mathrm{Tr}_n\left[\hat{F}(t)\hat{F}(t')\hat{w}_e\right] - \hat{x}(t)\hat{w}(t')\hat{x}(t')\mathrm{Tr}_n\left[\hat{F}(t)\hat{w}_e\hat{F}(t')\right] \\
&\quad - \hat{x}(t')\hat{w}(t')\hat{x}(t)\mathrm{Tr}_n\left[\hat{F}(t')\hat{w}_e\hat{F}(t)\right] + \hat{w}(t')\hat{x}(t')\hat{x}(t)\mathrm{Tr}_n\left[\hat{w}_e\hat{F}(t')\hat{F}(t)\right] \\
&= \hat{x}(t)\hat{x}(t')\hat{w}(t')\sum_{n,n'} F_{nn'}(t)F_{n'n}(t')W_n - \hat{x}(t)\hat{w}(t')\hat{x}(t')\sum_{n,n'} F_{nn'}(t)W_{n'}F_{n'n}(t') \\
&\quad - \hat{x}(t')\hat{w}(t')\hat{x}(t)\sum_{n,n'} F_{nn'}(t')W_{n'}F_{n'n}(t) + \hat{w}(t')\hat{x}(t')\hat{x}(t)\sum_{n,n'} W_n F_{nn'}(t')F_{n'n}(t).
\end{aligned} \tag{7.178}$$

Since the summation over both indices n and n' in this expression is over the same energy level set (of all stationary states of the environment), we may swap these indices in any of the sums. Doing this only in the terms including the factors $W_{n'}$, we turn them into W_n, so this factor becomes common:

$$\begin{aligned}
\mathrm{Tr}_n\left[\ldots,\left[\ldots,\ldots\right]\right] &= \sum_{n,n'} W_n \left[\hat{x}(t)\hat{x}(t')\hat{w}(t')F_{nn'}(t)F_{n'n}(t') - \hat{x}(t)\hat{w}(t')\hat{x}(t')F_{n'n}(t)F_{nn'}(t') \right. \\
&\quad \left. - \hat{x}(t')\hat{w}\hat{x}(t)F_{n'n}(t')F_{nn'}(t) + \hat{w}\hat{x}(t')\hat{x}(t)F_{nn'}(t')F_{n'n}(t)\right].
\end{aligned} \tag{7.179}$$

Now using Eq. (172), we get

$$\begin{aligned}
\mathrm{Tr}_n\left[\ldots,\left[\ldots,\ldots\right]\right] &= \sum_{n,n'} W_n |F_{nn'}|^2 \times \left[\begin{array}{l} \hat{x}(t)\hat{x}(t')\hat{w}(t')\exp\left\{+\dfrac{i\widetilde{E}(t-t')}{\hbar}\right\} - \hat{x}(t)\hat{w}(t')\hat{x}(t')\exp\left\{-\dfrac{i\widetilde{E}(t-t')}{\hbar}\right\} \\[2ex] - \hat{x}(t')\hat{w}(t')\hat{x}(t)\exp\left\{+\dfrac{i\widetilde{E}(t-t')}{\hbar}\right\} + \hat{w}(t')\hat{x}(t')\hat{x}(t)\exp\left\{-\dfrac{i\widetilde{E}(t-t')}{\hbar}\right\} \end{array} \right] \\[2ex]
&\equiv \sum_{n,n'} W_n |F_{nn'}|^2 \cos\frac{\widetilde{E}(t-t')}{\hbar}\left[\hat{x}(t),\left[\hat{x}(t'),\hat{w}(t')\right]\right] + i\sum_{n,n'} W_n |F_{nn'}|^2 \sin\frac{\widetilde{E}(t-t')}{\hbar}\left[\hat{x}(t),\{\hat{x}(t'),\hat{w}(t')\}\right].
\end{aligned} \tag{7.180}$$

Comparing the two double sums participating in this expression with Eqs. (108) and (111), we see that they are nothing else than, respectively, the symmetrized correlation function and the temporal Green's

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[63] This is exactly the moment of transition from the reversible quantum dynamics to irreversible one, in this approach.

[64] For the notation simplicity, the fact that here (and in all following formulas) the density operator $\hat{w}$ of the system s of our interest is taken in the interaction picture, is just implied.

function (multiplied by $\hbar/2$) of the time-difference argument $\tau = t - t' \geq 0$. As a result, Eq. (177) takes a compact form:

$$\dot{\hat{w}}(t) = -\frac{1}{\hbar^2}\int_{-\infty}^{t} K_F(t-t')\left[\hat{x}(t),\left[\hat{x}(t'),\hat{w}(t')\right]\right]dt' - \frac{i}{2\hbar}\int_{-\infty}^{t} G(t-t')\left[\hat{x}(t),\left\{\hat{x}(t'),\hat{w}(t')\right\}\right]dt'. \quad (7.181)$$

Density matrix: time evolution

Let me hope that the readers (especially the ones who have braved this derivation) enjoy this beautiful result as much as I do. It gives an equation for the time evolution of the density operator of the system of our interest (s), with the effects of its environment represented only by two real, c-number functions of τ: one (K_F) describing the fluctuation force exerted by the environment, and the other one (G) representing its ensemble-averaged environment's response to the system's evolution. And most spectacularly, these are exactly the same functions that participate in the alternative, Heisenberg-Langevin approach to the problem, and hence related to each other by the fluctuation-dissipation theorem (134).

After a short celebration, let us acknowledge that Eq. (181) is still an integro-differential equation, and needs to be solved together with Eq. (169) for the system coordinate's evolution. Such equations do not allow explicit analytical solutions, besides a few very simple (and not very interesting) cases. For most applications, further simplifications should be made. One of them is based on the fact (which was already discussed in Sec. 3) that both environmental functions participating in Eq. (181) tend to zero when their argument $\tau \equiv t - t'$ becomes much larger than the environment's correlation time τ_c, which is independent of the system-to-environment coupling strength. If the coupling is sufficiently weak, the time scales $T_{nn'}$ of the evolution of the density matrix elements, following from Eq. (181), are much longer than this correlation time, and also than the characteristic time scale of the coordinate operator's evolution. In this limit, all arguments t' of the density operator, giving substantial contributions to the right-hand side of Eq. (181), are so close to t that it does not matter whether its argument is t' or just t. This simplification, $w(t') \approx w(t)$, is known as the *Markov approximation*.[65]

However, this approximation alone is still insufficient for finding the general solution of Eq. (181). Substantial further progress is possible in two important cases. The most important of them is when the intrinsic Hamiltonian $\hat{H}_s$ of the system s of our of interest does not depend on time explicitly and has a *discrete* eigenenergy spectrum E_n,[66] with well-separated levels:

$$\left|E_n - E_{n'}\right| >> \frac{\hbar}{T_{nn'}}. \quad (7.182)$$

Let us see what this condition yields for Eq. (181) rewritten for the matrix elements in the stationary state basis, in the Markov approximation:

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[65] Named after A. A. Markov (1856-1922; in older Western literature, "Markoff"), a mathematician famous for his general theory of the so-called *Markov processes*, whose future development is completely determined by its present state, but not its pre-history.

[66] Here, rather reluctantly, I will use this standard notation, E_n, for the eigenenergies of our system of interest (s), in the hope that the reader would not confuse these discrete energy levels with the quasi-continuous energy levels of its environment (e), participating in particular in Eqs. (108) and (111). As a reminder, by this stage of our calculations, the environment's levels have disappeared from our formulas, leaving behind their functionals $K_F(\tau)$ and $G(\tau)$.

$$\dot{w}_{nn'} = -\frac{1}{\hbar^2} \int_{-\infty}^{t} K_F(t-t') \left[\hat{x}(t), [\hat{x}(t'), \hat{w}]\right]_{nn'} dt' - \frac{i}{2\hbar} \int_{-\infty}^{t} G(t-t') \left[\hat{x}(t), \{\hat{x}(t'), \hat{w}\}\right]_{nn'} dt'. \quad (7.183)$$

After spelling out the commutators, the right-hand side of this expression includes four operator products, which differ "only" by the operator order. Let us first have a look at one of these products,

$$\left[\hat{x}(t)\hat{x}(t')\hat{w}\right]_{nn'} \equiv \sum_{m,m'} x_{nm}(t) x_{mm'}(t') w_{m'n'}, \quad (7.184)$$

where the indices m and m' run over the same set of stationary states of the system s of our interest as the indices n and n'. According to Eq. (169) with a time-independent H_s, the matrix elements $x_{nn'}$ (in the stationary state basis) oscillate in time as $\exp\{i\omega_{nn'}t\}$, so

$$\left[\hat{x}(t)\hat{x}(t')\hat{w}\right]_{nn'} = \sum_{m,m'} x_{nm} x_{mm'} \exp\{i(\omega_{nm}t + \omega_{mm'}t')\} w_{m'n'}, \quad (7.185)$$

where on the right-hand side, the coordinate matrix elements are in the Schrödinger picture, and the usual notation (6.85) is used for the quantum transition frequencies:

$$\hbar\omega_{nn'} \equiv E_n - E_{n'}. \quad (7.186)$$

According to condition (182), frequencies $\omega_{nn'}$ with $n \neq n'$ are much higher than the speed of evolution of the density matrix elements (in the interaction picture!) – on both the left-hand and right-hand sides of Eq. (183). Hence, on the right-hand side of Eq. (183), we may keep only the terms that do not oscillate with these frequencies $\omega_{nn'}$, because rapidly-oscillating terms would give negligible contributions to the density matrix dynamics.[67] For that, in the double sum (185) we should save only the terms proportional to the difference $(t - t')$ because they will give (after the integration over t') a slowly changing contribution to the right-hand side.[68] These terms should have $\omega_{nm} + \omega_{mm'} = 0$, i.e. $(E_n - E_m) + (E_m - E_{m'}) \equiv E_n - E_{m'} = 0$. For a non-degenerate energy spectrum, this requirement means $m' = n$; as a result, the double sum is reduced to a single one:

$$\left[\hat{x}(t)\hat{x}(t')\hat{w}\right]_{nn'} \approx w_{nn'} \sum_{m} x_{nm} x_{mn} \exp\{i\omega_{nm}(t-t')\} \equiv w_{nn'} \sum_{m} |x_{nm}|^2 \exp\{i\omega_{nm}(t-t')\}. \quad (7.187)$$

Another product, $\left[\hat{w}\hat{x}(t')\hat{x}(t)\right]_{nn'}$, which appears on the right-hand side of Eq. (183) may be simplified absolutely similarly, giving

$$\left[\hat{w}\hat{x}(t')\hat{x}(t)\right]_{nn'} \approx \sum_{m} |x_{n'm}|^2 \exp\{i\omega_{n'm}(t'-t)\} w_{nn'}. \quad (7.188)$$

These expressions hold whether n and n' are equal or not. The situation is different for two other products on the right-hand side of Eq. (183), with w sandwiched between $x(t)$ and $x(t')$. For example,

$$\left[\hat{x}(t)\hat{w}\hat{x}(t')\right]_{nn'} = \sum_{m,m'} x_{nm}(t) w_{mm'} x_{m'n'}(t') = \sum_{m,m'} x_{nm} w_{mm'} x_{m'n'} \exp\{i(\omega_{nm}t + \omega_{m'n'}t')\}. \quad (7.189)$$

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[67] This is essentially the same rotating-wave approximation (RWA) as was used in Sec. 6.5.

[68] As was already discussed in Sec. 4, the lower-limit substitution ($t' = -\infty$) in the integrals participating in Eq. (183) gives zero, due to the finite-time "memory" of the system, expressed by the decay of the correlation and response functions at large values of the time delay $\tau = t - t'$.

For this term, the same requirement of keeping an oscillating function of $(t - t')$ only, yields a different condition: $\omega_{nm} + \omega_{m'n'} = 0$, i.e.

$$(E_n - E_m) + (E_{m'} - E_{n'}) = 0. \tag{7.190}$$

Here the double sum's reduction is possible only if we make an additional assumption that all interlevel energy distances are unique, i.e. our system of interest has no equidistant levels (such as in the harmonic oscillator). For the diagonal elements ($n = n'$), the RWA requirement is reduced to $m = m'$, giving sums over all diagonal elements of the density matrix:

$$[\hat{x}(t)\hat{w}\hat{x}(t')]_{nn} = \sum_m |x_{nm}|^2 \exp\{i\omega_{nm}(t - t')\}w_{mm}. \tag{7.191}$$

(Another similar term, $[\hat{x}(t')\hat{w}\hat{x}(t)]_{nn}$, is just a complex conjugate of this one.) However, for off-diagonal matrix elements ($n \neq n'$), the situation is different: Eq. (190) may be satisfied only if $m = n$ and $m' = n'$, so the double sum is reduced to just one, non-oscillating term:

$$[\hat{x}(t)\hat{w}\hat{x}(t')]_{nn'} = x_{nn}w_{nn'}x_{n'n'}, \quad \text{for } n \neq n'. \tag{7.192}$$

The second similar term, $[\hat{x}(t')\hat{w}\hat{x}(t)]_{nn}$, is exactly the same, so in the first of the integrals in Eq. (183), these terms add up, while in the second one, they cancel.

This is why the final equations of evolution look differently for diagonal and off-diagonal elements of the density matrix. For the former case ($n = n'$), Eq. (183) is reduced to the so-called *master equation*[69] relating diagonal elements w_{nn} of the density matrix, i.e. the energy level occupancies W_n:[70]

$$\dot{W}_n = \sum_{m \neq n} |x_{nm}|^2 \int_0^\infty \left[-\frac{1}{\hbar^2} K_F(\tau)(W_n - W_m)(\exp\{i\omega_{nm}\tau\} + \exp\{-i\omega_{nm}\tau\}) \right. \\ \left. -\frac{i}{2\hbar} G(\tau)(-W_n - W_m)(\exp\{i\omega_{nm}\tau\} - \exp\{-i\omega_{nm}\tau\}) \right]d\tau, \tag{7.193}$$

where $\tau \equiv t - t'$. Changing the summation index notation from m to n', we may rewrite the master equation in its canonical form

$$\boxed{\dot{W}_n = \sum_{n' \neq n}(\Gamma_{n' \to n}W_{n'} - \Gamma_{n \to n'}W_n),} \tag{7.194}$$

where the coefficients

$$\boxed{\Gamma_{n' \to n} \equiv |x_{nn'}|^2 \int_0^\infty \left[\frac{2}{\hbar^2} K_F(\tau)\cos\omega_{nn'}\tau - \frac{1}{\hbar}G(\tau)\sin\omega_{nn'}\tau \right]dt',} \tag{7.195}$$

are called the *interlevel transition rates*.[71] Formula (194) has a very clear physical meaning of the level occupancy dynamics (i.e. the balance of the probability flows ΓW) due to quantum transitions between

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[69] The master equations, which were first introduced to quantum mechanics in 1928 by W. Pauli, are sometimes called the "Pauli master equations", or "kinetic equations", or "rate equations".

[70] As Eq. (193) shows, the term with $m = n$ would vanish and thus may be legitimately excluded from the sum.

[71] As Eq. (193) shows, the result for $\Gamma_{n \to n'}$ is described by Eq. (195) as well, provided that the indices n and n' are swapped in all components of its right-hand side, including the swap $\omega_{nn'} \to \omega_{n'n} = -\omega_{nn'}$.

the energy levels (see Fig. 7), in our current case caused by the interaction between the system of our interest and its environment.
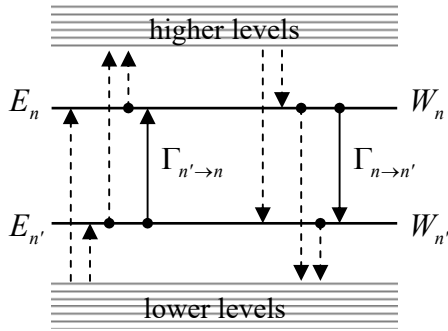

Fig. 7.7. Probability flows in a discrete-spectrum system. Solid arrows: the exchange between the two energy levels, n and n', described by one term in the master equation (194); dashed arrows: other transitions to/from these two levels.

The Fourier transforms (113) and (123) enable us to express the two integrals in Eq. (195) via, respectively, the symmetrized spectral density $S_F(\omega)$ of environment force fluctuations and the imaginary part $\chi''(\omega)$ of the generalized susceptibility, both at frequency $\omega = \omega_{nn'}$. After that we may use the fluctuation-dissipation theorem (134) to exclude the former function, getting finally[72]

$$\Gamma_{n' \to n} = \frac{1}{\hbar}|x_{nn'}|^2 \chi''(\omega_{nn'})\left(\coth\frac{\hbar\omega_{nn'}}{2k_BT} - 1\right) \equiv \frac{2}{\hbar}|x_{nn'}|^2 \frac{\chi''(\omega_{nn'})}{\exp\{(E_n - E_{n'})/k_BT\} - 1}.$$ (7.196)

Note that since the imaginary part χ'' of the generalized susceptibility is an odd function of frequency, Eq. (196) is in compliance with the Gibbs distribution for arbitrary temperature. Indeed, according to this formula, the ratio of the "up" and "down" rates for each pair of levels equals

$$\frac{\Gamma_{n' \to n}}{\Gamma_{n \to n'}} = \frac{\chi''(\omega_{nn'})}{\exp\{(E_n - E_{n'})/k_BT\} - 1}\bigg/\frac{\chi''(\omega_{n'n})}{\exp\{(E_{n'} - E_n)/k_BT\} - 1} \equiv \exp\left\{-\frac{E_n - E_{n'}}{k_BT}\right\}.$$ (7.197)

On the other hand, according to the Gibbs distribution (24), in thermal equilibrium the level populations should be in the same proportion. Hence, Eq. (196) complies with the so-called *detailed balance equation*,

$$W_n\Gamma_{n \to n'} = W_{n'}\Gamma_{n' \to n},$$ (7.198)

valid in the equilibrium for each pair $\{n, n'\}$, so all right-hand sides of all Eqs. (194), and hence the time derivatives of all W_n vanish – as they should. Thus, the stationary solution of the master equations indeed describes the thermal equilibrium correctly. As will be shown in the next section, the speed of reaching this equilibrium, within each pair of levels, is determined by the sum of these two rates:

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[72] It is straightforward (and highly recommended to the reader as an exercise) to show that at low temperatures ($k_BT \ll |E_{n'} - E_n|$), Eq. (196) gives the same result as the Golden Rate formula (6.111), with $A = x$. (The low-temperature condition ensures that the initial occupancy of the excited level n is negligible, as was assumed at the derivation of Eq. (6.111).)

$$\left(\Gamma_{\Sigma}\right)_{nn'} \equiv \Gamma_{n \to n'} + \Gamma_{n' \to n} = \Gamma_{nn'} \coth \frac{\hbar \omega_{nn'}}{2 k_{\mathrm{B}} T} \to \Gamma_{nn'} \times \begin{cases} 1, & \text{for } k_{\mathrm{B}} T \ll \hbar \omega_{nn'}, \\ 2 k_{\mathrm{B}} T / \hbar \omega_{nn'}, & \text{for } k_{\mathrm{B}} T \gg \hbar \omega_{nn'}, \end{cases} \quad (7.199)$$

$$\text{with} \quad \Gamma_{nn'} \equiv \frac{2}{\hbar} \left| x_{nn'} \right|^2 \chi''(\omega_{nn'}).$$

In situations when the level specification is obvious, the rate Γ_{Σ} is frequently denoted as the reciprocal *energy relaxation time* $1/T_1$.

The system of master equations (194), frequently complemented by additional right-hand-side terms describing interlevel transitions due to other factors (e.g., by an external ac force with a frequency close to one of $\omega_{nn'}$), is the key starting point for practical analyses of many applied quantum systems, notably including optical quantum amplifiers and generators (lasers). It is important to remember that they are strictly valid only in the rotating-wave approximation, i.e. if the condition (182) is satisfied for all n and n' of substance.

The relaxation times T_1, characterizing the dynamics of the *diagonal* elements of the density matrix, should not be confused with the characteristic times T_2 of the *off-diagonal* element decay, i.e. of the dephasing, which was preliminary discussed in Sec. 3. Now let us see what Eqs. (183) have to say about the dephasing rates. Taking into account our intermediate results (187)-(192), and merging the non-oscillating components (with $m = n$ and $m = n'$) of the sums Eq. (187) and (188) with the terms (192), which also do not oscillate in time, we get the following equation:[73]

$$\dot{w}_{nn'} = -\left\{ \int_0^\infty \left[\frac{1}{\hbar^2} K_F(\tau) \left(\sum_{m \neq n} \left| x_{nm} \right|^2 \exp\{i \omega_{nm} \tau\} + \sum_{m \neq n'} \left| x_{n'm} \right|^2 \exp\{-i \omega_{n'm} \tau\} + \left(x_{nn} - x_{n'n'} \right)^2 \right) \right. \right.$$
$$\left. \left. + \frac{i}{2\hbar} G(\tau) \left(\sum_{m \neq n} \left| x_{nm} \right|^2 \exp\{i \omega_{nm} \tau\} - \sum_{m \neq n'} \left| x_{n'm} \right|^2 \exp\{-i \omega_{n'm} \tau\} \right) \right] d\tau \right\} w_{nn'}, \text{ for } n \neq n'. \quad (7.200)$$

In contrast with Eq. (194), the right-hand side of this equation includes both a real and an imaginary part, and hence may be represented as

$$\dot{w}_{nn'} = -\left(1/T_{nn'} + i \Delta_{nn'}\right) w_{nn'}, \quad (7.201)$$

where both factors $1/T_{nn'}$ and $\Delta_{nn'}$ are real. As Eq. (201) shows, the second term in the right-hand side of this equation causes slow oscillations of the matrix elements $w_{nn'}$, which, after returning to the Schrödinger picture, add just small corrections[74] to the unperturbed frequencies (186) of their oscillations, and are not important for most applications. More important is the first term, proportional to

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[73] Sometimes Eq. (200) (in any of its numerous alternative forms) is called the *Redfield equation*, after the 1965 work by A. Redfield. Note, however, that in the mid-1960s, several other authors, notably including (in the alphabetical order) H. Haken, W. Lamb, M. Lax, W. Louisell, and M. Scully, also made major contributions to the very fast development of the density-matrix approach to open quantum systems.

[74] Such corrections are sometimes called *Lamb shifts*, because they are the generic form of the particular effect more commonly called the Lamb shift: a minute (~1 GHz) difference between the frequencies of transitions $2s \leftrightarrow 1s$ and $2p \leftrightarrow 1s$ (with all states having $j = \frac{1}{2}$) of hydrogen, due to the electric-dipole coupling to the free-space electromagnetic environment, first observed experimentally in 1947 by Willis Lamb and Robert Retherford. (These frequencies have to be equal not only in the non-relativistic theory described in Sec. 3.6 but also in the relativistic quantum theory (see Secs. 6.3, 9.7), if the electromagnetic environment is ignored.) The explanation of

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$$\frac{1}{T_{nn'}} = \int_0^\infty \left[\frac{1}{\hbar^2} K_F(\tau) \left(\sum_{m \neq n} |x_{nm}|^2 \cos\omega_{nm}\tau + \sum_{m \neq n'} |x_{n'm}|^2 \cos\omega_{n'm}\tau + (x_{nn} - x_{n'n'})^2 \right) \right.$$
$$\left. - \frac{1}{2\hbar} G(\tau) \left(\sum_{m \neq n} |x_{nm}|^2 \sin\omega_{nm}\tau + \sum_{m \neq n'} |x_{n'm}|^2 \sin\omega_{n'm}\tau \right) \right] d\tau, \quad \text{for } n \neq n', \qquad (7.202)$$

because it describes the effect completely absent without the environment coupling: exponential decay of the off-diagonal matrix elements, i.e. the dephasing. Comparing the first two terms of Eq. (202) with Eq. (195), we see that the dephasing rates may be described by a very simple formula:

$$\frac{1}{T_{nn'}} = \frac{1}{2} \left(\sum_{m \neq n} \Gamma_{n \to m} + \sum_{m \neq n'} \Gamma_{n' \to m} \right) + \frac{\pi}{\hbar^2} (x_{nn} - x_{n'n'})^2 S_F(0). \qquad (7.203a)$$

Moreover, since at low frequencies, the dissipation provided by most real environments is Ohmic (138), this expression may be further simplified:

<div style="border:1px solid blue;">

Dephasing rate

$$\frac{1}{T_{nn'}} \equiv \frac{1}{2} \left(\sum_{m \neq n} \Gamma_{n \to m} + \sum_{m \neq n'} \Gamma_{n' \to m} \right) + \frac{k_B T}{\hbar^2} \eta (x_{nn} - x_{n'n'})^2, \quad \text{for } n \neq n'. \qquad (7.203b)$$

</div>

This result shows that two effects yield independent contributions to the dephasing. The first of them may be interpreted as a result of "virtual" transitions of the system from the levels n and n' of our interest to other energy levels m; according to Eq. (196), this contribution is proportional to the strength of coupling to the environment at relatively high frequencies ω_{nm} and $\omega_{n'm}$. On the contrary, the second contribution is due to low-frequency, essentially classical fluctuations of the environment, and hence to the low-frequency dissipative susceptibility. In the Ohmic dissipation case, when the ratio $\eta \equiv \chi''(\omega)/\omega$ is frequency-independent, both contributions are of the same order, but their exact relation depends on the matrix elements $x_{nn'}$ of a particular system. Note also that Eq. (203a), as well as the analysis carried out in Sec. 3, implies that low-frequency fluctuations of any other origin, not taken into account in our analysis (say, an unintentional noise from experimental equipment), may also contribute to dephasing. Such "technical fluctuations" are indeed a very serious challenge for the experimental implementation of coherent qubit systems – see Sec. 8.5 below. On the other hand, in optical systems, the low-frequency contribution to dephasing is usually negligible.

7.7. Application to two-level systems

Let us see what these results mean for the particular but very important case of a two-level system, with just two relevant states. As was discussed in Sec. 3, it may be described by the Hamiltonian (7.68), with the interaction term in the form (7.70) which coincides with Eq. (7.90) used for the calculations in the previous section, at the replacement $\hat{x} \to \hat{\sigma}_z$. However, instead of the simple intrinsic Hamiltonian (7.69) excluding interstate transitions, which was discussed in Sec. 3, the theory described above is valid for the most general Hamiltonian (5.3) in the two-function Hilbert space. As was discussed in Sec. 5.1, after dropping just the trivial term $b\mathrm{I}$, which may be always removed by selecting the proper energy reference, this Hamiltonian, in the usual z-representation, is described by the following matrix

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the Lamb shift by H. Bethe, in the same 1947, essentially launched the whole field of quantum electrodynamics – to be briefly discussed in Chapter 9.

$$H_s = \mathbf{c} \cdot \hat{\boldsymbol{\sigma}} \equiv \begin{pmatrix} c_z & c_x - ic_y \\ c_x + ic_y & -c_z \end{pmatrix} \equiv c \begin{pmatrix} \cos\theta & \sin\theta\, e^{-i\varphi} \\ \sin\theta\, e^{i\varphi} & -\cos\theta \end{pmatrix}, \tag{7.204}$$

where θ and φ are the angles describing the direction of the c-number "field vector" $\mathbf{c}$:

$$\mathbf{c} \equiv c_x \mathbf{n}_x + c_y \mathbf{n}_y + c_z \mathbf{n}_z \equiv c\left(\mathbf{n}_x \sin\theta \cos\varphi + \mathbf{n}_y \sin\theta \sin\varphi + \mathbf{n}_z \cos\theta\right). \tag{7.205}$$

As was discussed in Sec. 5.1, this Hamiltonian may describe a large variety of two-level quantum systems, from spin-½ in a magnetic field, where it is just the Pauli Hamiltonian (4.163), to a particle placed into a system of two coupled quantum wells – see Figs. 2.19 and 2.21.

First, let us consider the case when the field vector $\mathbf{c}$ is time-independent. The two stationary states of the system (let us call them + and –), or rather the coefficients $\langle\uparrow\downarrow|\pm\rangle$ of their expansion in the z-basis, and their energies $E_\pm$ may be easily found from the corresponding system of equations (4.102):[75]

$$\begin{aligned} \left(c\cos\theta - E_\pm\right)\langle\uparrow|\pm\rangle + c\sin\theta\, e^{-i\varphi}\langle\downarrow|\pm\rangle = 0, \\ c\sin\theta\, e^{i\varphi}\langle\uparrow|\pm\rangle + \left(-c\cos\theta - E_\pm\right)\langle\downarrow|\pm\rangle = 0. \end{aligned} \tag{7.206}$$

The results are $E_\pm = \pm c$ (so that $E_+ - E_- = 2c$), and (up to an arbitrary common phase multiplier):

$$\langle\uparrow|+\rangle = \langle\downarrow|-\rangle = \cos\frac{\theta}{2}, \qquad \langle\downarrow|+\rangle = -\langle\uparrow|-\rangle^* = \sin\frac{\theta}{2}e^{i\varphi}. \tag{7.207}$$

Now we may readily calculate the matrix elements that participate (after the replacement $\hat{x} \to \hat{\sigma}_z$) in Eqs. (196) and (203):

$$\begin{aligned} (\sigma_z)_{\pm\pm} &\equiv \langle\pm|\hat{\sigma}_z|\pm\rangle = \left(\langle\uparrow|\pm\rangle^*, \langle\downarrow|\pm\rangle^*\right)\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} \langle\uparrow|\pm\rangle \\ \langle\downarrow|\pm\rangle \end{pmatrix} = \pm\cos\theta, \\ (\sigma_z)_{\pm\mp} &\equiv \langle\pm|\hat{\sigma}_z|\mp\rangle = \left(\langle\uparrow|\pm\rangle^*, \langle\downarrow|\pm\rangle^*\right)\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} \langle\uparrow|\mp\rangle \\ \langle\downarrow|\mp\rangle \end{pmatrix} = -\sin\theta\, e^{\mp i\varphi}. \end{aligned} \tag{7.208}$$

With these substitutions, Eq. (199) with $\omega_{nn'} = \Omega \equiv 2c/\hbar$ gives

$$\frac{1}{T_1} \equiv \Gamma_\Sigma = \frac{2}{\hbar}\chi''(\Omega)\coth\left(\frac{\hbar\Omega}{k_B T}\right)\sin^2\theta = \frac{4\Omega}{\hbar}\eta\coth\left(\frac{\hbar\Omega}{k_B T}\right)\sin^2\theta, \tag{7.209}$$

where the last expression is valid only for the Ohmic dissipation (138), while Eq. (203) yields

$$\frac{1}{T_2} \equiv \frac{1}{T_{+-}} = \frac{1}{2T_1} + \frac{4k_B T}{\hbar^2}\eta\cos^2\theta. \tag{7.210}$$

So, the relaxation (T_1) and dephasing (T_2) times generally depend on the angle θ between the z-axis (i.e., with our assumption (70), the Bloch-sphere direction of the system's dissipative coupling to the environment) and the dc "field" $\mathbf{c}$ that determines the position of the stationary states on the sphere –

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[75] Since particular cases of this procedure were repeatedly performed in Chapter 4 (see also the solutions of Problems 4.27-4.29 and 5.2-5.4), I hope that more detailed explanations are not needed.

see Fig. 5.2.[76] In particular, at $\theta = 0$, i.e. in the absence of interlevel transitions, Eq. (210) reduces to the result (142) obtained under the same assumption, by using the Heisenberg-Langevin approach.

Now let us have a brief look at what the master equations (194), now taking the form

$$\dot{W}_+ = \Gamma_\uparrow W_- - \Gamma_\downarrow W_+, \qquad \dot{W}_- = \Gamma_\downarrow W_+ - \Gamma_\uparrow W_-, \tag{7.211}$$

say about the environment's effects on the two-level system's dynamics. Since the total probability $W_+ + W_-$ of finding the system on some energy level has to equal 1, we can eliminate one of these probabilities from these (compatible) equations, and readily integrate the remaining linear equation, for arbitrary initial conditions, getting

$$W_\pm(t) = W_\pm(0)\exp\left\{-\frac{t}{T_1}\right\} + W_\pm(\infty)\left(1 - \exp\left\{-\frac{t}{T_1}\right\}\right), \tag{7.212}$$

where

$$W_+(\infty) = \frac{\Gamma_\uparrow}{\Gamma_\Sigma} = \frac{1}{\exp\{\hbar\Omega/k_B T\}+1}, \qquad W_-(\infty) = \frac{\Gamma_\downarrow}{\Gamma_\Sigma} = \frac{1}{\exp\{-\hbar\Omega/k_B T\}+1}. \tag{7.213}$$

If the system was initially incoherent (i.e. was a classical mixture of two states), then this result, describing the exponential transient of both probabilities from their initial values $W_\pm(0)$ to the final (stationary) values, would be all we could say about its dynamics. However, if the initial state is pure, there is more to the story, and we also need to use the dephasing equation (201) for the off-diagonal matrix element w_{+-}. (According to Eq. (6), $w_{-+} = w_{+-}{}^*$.) Using the relation reciprocal to Eq. (166) to transfer from the interaction picture back to the Schrödinger one, and neglecting the small Lamb-shift correction due to the environment, we get a simple equation:

$$\dot{w}_{+-} = \left(-\frac{1}{T_2} + i\Omega\right)w_{+-}, \tag{7.214}$$

with the obvious solution

$$w_{+-}(t) = w_{+-}(0)\exp\left\{\left(-\frac{1}{T_2} + i\Omega\right)t\right\}, \quad \text{so } w_{-+}(t) = w_{-+}(0)\exp\left\{\left(-\frac{1}{T_2} - i\Omega\right)t\right\}. \tag{7.215}$$

For example, let the system be initially in a pure state ↑. (For a spin-½, this would mean that it is z-polarized, while for the two-well implementation shown in Fig. 4, this is the state with the particle is definitely in the right well.) Then, according to Eqs. (18b) or (20),

$$W_+(0) \equiv w_{++}(0) = \left|\langle+|\uparrow\rangle\right|^2 = \cos^2\frac{\theta}{2}, \qquad W_-(0) \equiv w_{--}(0) = \left|\langle-|\uparrow\rangle\right|^2 = \sin^2\frac{\theta}{2},$$

$$w_{+-}(0) = \langle-|\uparrow\rangle^*\langle+|\uparrow\rangle = -\sin\frac{\theta}{2}\cos\frac{\theta}{2}e^{i\varphi}, \qquad w_{-+}(0) = w_{+-}^*(0) = -\sin\frac{\theta}{2}\cos\frac{\theta}{2}e^{-i\varphi}, \tag{7.216}$$

where Eqs. (207) were used. Formally, Eqs. (212)-(216) give the full solution of the problem, but in order to comprehend its meaning, let us have a look at the probability $W_\uparrow(t)$ to find our system in the initial state ↑ at an arbitrary moment t. Since $t > 0$, due to dephasing, the system's state is no longer pure, in order to recalculate the density matrix elements (216) calculated in the stationary-state basis,

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[76] Since in most optical systems, where the low-frequency contribution to dephasing is small, Eq. (210) gives a very simple (and frequently used) relation $T_2 \approx 2T_1$.

into $W_\uparrow(t)$, i.e. one of the elements of the density matrix in the z-basis, we need to use the general Eq. (4.93), which is valid for any operator, in particular for the density operator:

$$W_\uparrow(t) \equiv \langle \uparrow | + \rangle w_{++}(t) \langle \uparrow | + \rangle^* + \langle \uparrow | + \rangle w_{+-}(t) \langle \uparrow | - \rangle^* + \langle \uparrow | - \rangle w_{-+}(t) \langle \uparrow | + \rangle^* + \langle \uparrow | - \rangle w_{--}(t) \langle \uparrow | - \rangle^*. \quad (7.217)$$

Plugging in Eqs. (207), (212), (213), (215), and (216), we finally get

$$W_\uparrow(t) \equiv \left(\sin^4 \frac{\theta}{2} + \cos^4 \frac{\theta}{2} \right) \exp\left\{ -\frac{t}{T_1} \right\} + W_\uparrow(\infty) \left(1 - \exp\left\{ -\frac{t}{T_1} \right\} \right)$$
$$+ 2 \sin^2 \frac{\theta}{2} \cos^2 \frac{\theta}{2} \cos \Omega t \, \exp\left\{ -\frac{t}{T_2} \right\}, \quad (7.218)$$

where

$$W_\uparrow(\infty) = \frac{\Gamma_\uparrow}{\Gamma_\Sigma} \cos^2 \frac{\theta}{2} + \frac{\Gamma_\downarrow}{\Gamma_\Sigma} \sin^2 \frac{\theta}{2} \equiv \frac{1}{2} \left(1 - \frac{\Gamma_\downarrow - \Gamma_\uparrow}{\Gamma_\Sigma} \cos \theta \right) \equiv \frac{1}{2} \left[1 - \tanh\left(\frac{\hbar\Omega}{2k_B T} \right) \cos \theta \right]. \quad (7.219)$$

So, the probability of the initial state of the system not only relaxes with the time constant T_1 to its final, thermal-equilibrium values $W_\uparrow(\infty)$ and $W_\downarrow(\infty) = 1 - W_\uparrow(\infty)$, but also performs the quantum oscillations with frequency $\Omega \equiv 2c/\hbar = (E_+ - E_-)/\hbar$ between these two states, decaying with the time constant T_2. (For spin-½ implementations of the two-level system, this means that the spin's precession about the field's direction decays, with the expectation values $\langle S_{x,y} \rangle$ tending to zero at $t \sim T_2$, and $\langle S_z \rangle$ tending to its thermally-equilibrium value $\hbar[W_\uparrow(\infty) - ½]$ at $t \sim T_1$.) In many experimental situations when Eqs. (211) and (214) are valid but the constants T_1 and T_2 cannot be reliably calculated,[77] they may be measured by observation of these two relaxation effects.

More complex problems of this type, for example those described by time-dependent Hamiltonians, may evade such simple analytical solutions because the very notions of stationary state and energy levels cannot be used. However, if the time-dependent part of a Hamiltonian is small and may be considered a perturbation, the two-level system may be still described by Eqs. (211) and (214), with additional terms describing this perturbation. In some of these cases, the Bloch equation (5.22), also with additional terms on its right-hand side, may be very useful for analysis. In Sec. 10, one of such problems is offered to the reader as an exercise.

7.8. Damped harmonic oscillator

As was explained in Section 6, the performed calculations starting from Eq. (191) are not valid for systems with equidistant energy spectra – for example, the harmonic oscillator. For this particular but very important system, with its simple matrix elements $x_{nn'}$ given by Eqs. (5.92), it is longish but straightforward to perform similar calculations, starting from (183), to obtain an equation similar in structure to Eq. (200), but with two other terms, proportional to $w_{n\pm1,n'\pm1}$, on its right-hand side. Neglecting the minor Lamb-shift term, the equation reads

$$\dot{w}_{nn'} = -\delta \left\{ \left[(n_e + 1)(n + n') + n_e(n + n' + 2) \right] w_{nn'} \right.$$
$$\left. - 2(n_e + 1)[(n+1)(n'+1)]^{1/2} w_{n+1,n'+1} - 2n_e (nn')^{1/2} w_{n-1,n'-1} \right\}. \quad (7.220)$$

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[77] For example, in systems whose coupling to the environment cannot be expressed as a single product (46).

Here δ is the effective damping coefficient,[78]

$$\delta \equiv \frac{x_0^2}{2\hbar} \operatorname{Im} \chi(\omega_0) \equiv \frac{\operatorname{Im} \chi(\omega_0)}{2m\omega_0}, \tag{7.221}$$

equal to just $\eta/2m$ for the Ohmic dissipation, and n_e is the equilibrium number of oscillator's excitations, given by Eq. (26b), with the environment's temperature T. (I am using this new notation because in dynamics, the instant expectation value $\langle n \rangle$ may be time-dependent, and is generally different from its equilibrium value n_e.)

Alternatively, the derivation of Eq. (220) may be started at a bit earlier point, from the Markov approximation applied to Eq. (181), by expressing the coordinate operator via the creation-annihilation operators (5.65). This procedure gives the result in the operator (i.e. basis-independent) form:[79]

$$\dot{w} = -\delta \left[(n_\mathrm{e}+1) \left(\left\{ \hat{a}^\dagger \hat{a}, \hat{w} \right\} - 2\hat{a}\hat{w}\hat{a}^\dagger \right) + n_\mathrm{e} \left(\left\{ \hat{a}\hat{a}^\dagger, \hat{w} \right\} - 2\hat{a}^\dagger \hat{w}\hat{a} \right) \right]. \tag{7.222}$$

In the Fock state basis, this equation immediately reduces to Eq. (220); however, Eq. (222) may be more convenient for some applications.

Returning to Eq. (220), we see that it inter-relates only the elements $w_{nn'}$ located at the same distance $(n - n')$ from the principal diagonal of the density matrix. This means, in particular, that the dynamics of the diagonal elements w_{nn} of the matrix, i.e. the Fock state probabilities W_n, is independent of the off-diagonal elements, and may be represented in the form (194) truncated to the transitions between the adjacent energy levels only ($n' = n \pm 1$):

$$\dot{W}_n = \left(\Gamma_{n+1 \to n} W_{n+1} - \Gamma_{n \to n+1} W_n \right) + \left(\Gamma_{n-1 \to n} W_{n-1} - \Gamma_{n \to n-1} W_n \right), \tag{7.223}$$

with the following rates:

$$\begin{aligned} \Gamma_{n+1 \to n} &= 2\delta(n+1)(n_\mathrm{e}+1), & \Gamma_{n \to n+1} &= 2\delta(n+1)n_\mathrm{e}, \\ \Gamma_{n-1 \to n} &= 2\delta\, n\, n_\mathrm{e}, & \Gamma_{n \to n-1} &= 2\delta\, n(n_\mathrm{e}+1). \end{aligned} \tag{7.224}$$

According to the definition of n_e, given by Eq. (26b),

$$n_\mathrm{e} = \frac{1}{\exp\{\hbar\omega_0 / k_\mathrm{B}T\} - 1}, \qquad \text{so } n_\mathrm{e} + 1 = \frac{1}{1 - \exp\{-\hbar\omega_0 / k_\mathrm{B}T\}}, \tag{7.225}$$

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[78] This coefficient participates prominently in the classical theory of damped oscillations (see, e.g., CM Sec. 5.1), in particular defining the oscillator's Q-factor as $Q \equiv \omega_0/2\delta$, and the decay time of the amplitude A and the energy E of free oscillations: $A(t) = A(0)\exp\{-\delta t\}$, $E(t) = E(0)\exp\{-2\delta t\}$.

[79] Sometimes Eq. (222) is called the *Lindblad equation*, but I believe this terminology is inappropriate. It is true that its structure falls into a general category of equations suggested by G. Lindblad in 1976 for the density operators in the Markov approximation, whose diagonalized form in the interaction picture is

$$\dot{w} = \sum_j \gamma_j \left(2\hat{L}_j \hat{w}\hat{L}_j^\dagger - \left\{ \hat{L}_j \hat{L}_j^\dagger, \hat{w} \right\} \right).$$

However, Eq. (222) was derived much earlier (by L. Landau in 1927 for zero temperature, and by M. Lax in 1960 for an arbitrary temperature), and in contrast to the general Lindblad equation, spells out the participating operators $\hat{L}_j$ and coefficients γ_j for a particular physical system – the harmonic oscillator.

so taking into account Eqs. (5.92), (186), and (221), and the asymmetry of the function $\chi''(\omega)$, we see that these rates are again described by Eq. (196), even though the last formula was derived for non-equidistant energy spectra.

Hence the only substantial new feature of the master equation for the harmonic oscillator is that the decay of the off-diagonal elements of its density matrix is scaled by the same parameter (2δ) as that of the decay of its diagonal elements, i.e. there is no radical difference between the dephasing and energy-relaxation times T_2 and T_1. This fact may be interpreted as the result of the independence of the energy level distances, $\hbar\omega_0$, of the fluctuations $F(t)$ exerted on the oscillator by the environment, so their low-frequency density, $S_F(0)$, does not contribute to dephasing. (This fact formally follows also from Eq. (203) as well, taking into account that for the oscillator, $x_{nn} = x_{n'n'} = 0$.)

The simple equidistant structure of the oscillator's spectrum makes it possible to readily solve the system of Eqs. (223), with $n = 0, 1, 2, \ldots$, for some important cases. In particular, if the initial state of the oscillator is a classical mixture, with no off-diagonal elements, its further relaxation proceeds as such a mixture: $w_{nn'}(t) = 0$ for all $n' \neq n$.[80] In particular, it is straightforward to use Eq. (208) to verify that if the initial classical mixture obeys the Gibbs distribution (25), but with a temperature T_i different from that of the environment (T_e), then the relaxation process is reduced to a simple exponential transient of the effective temperature from T_i to T_e:

$$W_n(t) = \exp\left\{-n\frac{\hbar\omega_0}{k_B T_{ef}(t)}\right\}\left(1 - \exp\left\{-\frac{\hbar\omega_0}{k_B T_{ef}(t)}\right\}\right), \qquad \text{with } T_{ef}(t) = T_i e^{-2\delta t} + T_e\left(1 - e^{-2\delta t}\right), \quad (7.226)$$

with the corresponding evolution of the expectation value of the full energy E – cf. Eq. (26b):

$$\langle E \rangle(t) = \frac{\hbar\omega_0}{2} + \hbar\omega_0 \langle n \rangle(t), \qquad \langle n \rangle(t) = \frac{1}{\exp\{\hbar\omega_0/k_B T_{ef}(t)\} - 1} \xrightarrow{t\to\infty} n_e. \qquad (7.227)$$

However, if the initial state of the oscillator is different (say, corresponds to some excited Fock state), the relaxation process described by Eqs. (223)-(224), is more complex – see, e.g., Fig. 8.

At low temperatures (Fig. 8a), it may be interpreted as a gradual "roll" of the probability distribution down the energy staircase, with a gradually decreasing velocity $d\langle n \rangle/dt \propto \langle n \rangle$. However, at substantial temperatures, with $k_B T \sim \hbar\omega_0$, i.e. $n_e \sim 1$ (Fig. 8b), this "roll-down" is saturated when the level occupancies $W_n(t)$ approach their equilibrium values (25).[81]

The analysis of this process may be simplified in the case when $W(n, t) \equiv W_n(t)$ is a smooth function of the energy level number n, limited to high levels: $n \gg 1$. In this limit, we may use the Taylor expansion of this function (written for the points $\Delta n = \pm 1$), truncated to three leading terms:

$$W_{n\pm1}(t) \equiv W(n\pm1, t) \approx W(n,t) \pm \frac{\partial W(n,t)}{\partial n} + \frac{1}{2}\frac{\partial^2 W(n,t)}{\partial n^2}. \qquad (7.228)$$

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[80] Note, however, that this is not true for many applications, in which a damped oscillator is also under the effect of an external time-dependent field, which may be described by additional, typically off-diagonal terms on the right-hand side of Eqs. (220).

[81] The reader may like to have a look at the results of very nice measurements of such functions $W_n(t)$ in microwave oscillators, performed using their coupling with Josephson-junction circuits: H. Wang *et al.*, *Phys. Rev. Lett.* **101**, 240401 (2008), and with Rydberg atoms: M. Brune *et al.*, *Phys. Rev. Lett.* **101**, 240402 (2008).
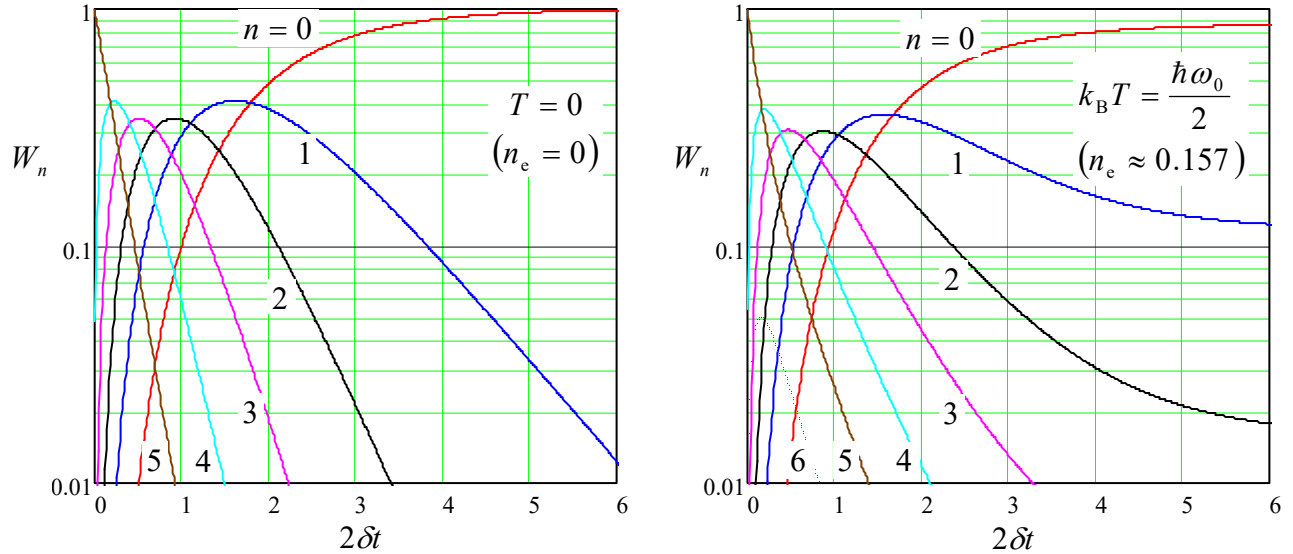
Fig. 7.8. Relaxation of a harmonic oscillator, initially in its 5th Fock state, at: (a) $T = 0$, and (b) $T > 0$. Note that in the latter case, even the energy levels with $n > 5$ get populated, due to their thermal excitation.

Plugging this expression into Eqs. (223)-(224), we get for the function $W(n, t)$ a partial differential equation, which may be recast in the following form:

$$\frac{\partial W}{\partial t} = -\frac{\partial}{\partial n}[f(n)W] + \frac{\partial^2}{\partial n^2}[d(n)W], \quad \text{with } f(n) \equiv 2\delta(n_e - n), \quad d(n) \equiv 2\delta(n_e + \tfrac{1}{2})n. \quad (7.229)$$

Since the energy E of an oscillator with $n \gg 1$ is close to $\hbar\omega_0 n$, this *energy diffusion equation* essentially describes the time evolution of the continuous probability density $w(E, t)$ that in this case, may be defined as $w(E, t) \equiv W(E/\hbar\omega_0, t)/\hbar\omega_0$. In the classical limit $n_e \gg 1$, Eq. (229) is analytically solvable for arbitrary initial conditions.[82] Note, however, that the most important properties of the damped harmonic oscillator (including its relaxation dynamics) may be analyzed much simpler by using the Heisenberg-Langevin approach which was discussed in Section 5.

7.9. Continuous-spectrum systems

The continuous approximation explored at the end of the last section naturally reminds us of the need to discuss dissipative systems with *continuous* spectra. Unfortunately, for such systems the few (relatively :-) simple results that may be obtained from the basic Eq. (181), are essentially classical in nature and are discussed in detail in the SM part of this series. Here, I will give only a simple illustration.

Let us consider a 1D particle that interacts weakly with a thermally-equilibrium environment, but otherwise is free to move along the x-axis. As we know from Chapters 2 and 5, in this case, the most convenient basis is that of the momentum eigenstates p. In the momentum representation, the density matrix is just the c-number function $w(p, p')$ defined by Eq. (54), which was already discussed in brief

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[82] See, e.g., the paper by B. Zeldovich *et al.*, *Sov. Phys. JETP* **28**, 308 (1969), which also gives some more intricate solutions of Eqs. (223)-(224).

in Sec. 2. On the other hand, the coordinate operator, which participates on the right-hand side of Eq. (181), has the form given by the first of Eqs. (4.269),

$$\hat{x} = i\hbar \frac{\partial}{\partial p}, \tag{7.230}$$

dual to the coordinate-representation formula (4.268). As we already know, such operators are local – see, e.g., Eq. (4.244). Due to this locality, the whole right-hand side of Eq. (181) is local as well, and hence (within the framework of our perturbative treatment) the interaction with the environment affects only the diagonal values $w(p, p)$ of the density matrix, i.e. the momentum's probability density $w(p)$.

Let us find the equation governing the evolution of this function in time in the Markov approximation, when the time scale of the density matrix evolution is much longer than the correlation time τ_c of the environment, i.e. the time scale of the functions $K_F(\tau)$ and $G(\tau)$. In this approximation, we may take the matrix elements out of the first integral of Eq. (181),

$$-\frac{1}{\hbar^2} \int_{-\infty}^{t} K_F(t - t') dt' \left[\hat{x}(t), [\hat{x}(t'), \hat{w}(t')]\right] \approx -\frac{1}{\hbar^2} \int_{0}^{\infty} K_F(\tau) d\tau \left[\hat{x}, [\hat{x}, \hat{w}]\right]$$

$$= -\frac{\pi}{\hbar^2} S_F(0) \left[\hat{x}, [\hat{x}, \hat{w}]\right] = -\frac{k_B T}{\hbar^2} \eta \left[\hat{x}, [\hat{x}, \hat{w}]\right], \tag{7.231}$$

and calculate the last double commutator in the Schrödinger picture. This may be done either using an explicit expression for the matrix elements of the coordinate operator or in a simpler way – using the same trick as at the derivation of the Ehrenfest theorem in Sec. 5.2. Namely, expanding an arbitrary function $f(p)$ into the Taylor series in p,

$$f(p) = \sum_{k=0}^{\infty} \frac{1}{k!} \frac{\partial^k f}{\partial p^k} p^k, \tag{7.232}$$

and using Eq. (240), we can write

$$[\hat{x}, f] = \sum_{k=0}^{\infty} \frac{1}{k!} \frac{\partial^k f}{\partial p^k} [\hat{x}, p^k] = \sum_{k=0}^{\infty} \frac{1}{k!} \frac{\partial^k f}{\partial p^k} \left(i\hbar k p^{k-1}\right) = i\hbar \sum_{k=1}^{\infty} \frac{1}{(k-1)!} \frac{\partial^{k-1}}{\partial p^{k-1}} \left(\frac{\partial f}{\partial p}\right) p^{k-1} = i\hbar \frac{\partial f}{\partial p}. \tag{7.233}$$

Now applying this result sequentially, first to w and then to the resulting commutator, we get

$$[\hat{x}, [\hat{x}, w]] = \left[\hat{x}, i\hbar \frac{\partial w}{\partial p}\right] = i\hbar \frac{\partial}{\partial p}\left(i\hbar \frac{\partial w}{\partial p}\right) = -\hbar^2 \frac{\partial^2 w}{\partial p^2}. \tag{7.234}$$

It may look like the second integral in Eq. (181) might be simplified similarly. However, it vanishes at $p' \to p$, and $t' \to t$, so in order to calculate the first non-vanishing contribution from that integral for $p = p'$, we have to take into account the small difference $\tau \equiv t - t' \sim \tau_c$ between the arguments of the coordinate operators under that integral. This may be done using Eq. (169) with the free particle's Hamiltonian consisting of the kinetic-energy contribution alone:

$$\hat{x}(t') - \hat{x}(t) \approx -\tau \dot{\hat{x}} = -\tau \frac{1}{i\hbar}\left[\hat{x}, \hat{H}_s\right] = -\tau \frac{1}{i\hbar}\left[\hat{x}, \frac{\hat{p}^2}{2m}\right] = -\tau \frac{\hat{p}}{m}, \tag{7.235}$$

where the exact argument of the operator on the right-hand side is already unimportant and may be taken for t. As a result, we may use the last of Eqs. (136) to reduce the second term on the right-hand side of Eq. (181) to

$$-\frac{i}{2\hbar}\int_{-\infty}^{t}G(t-t')[\hat{x}(t),\{\hat{x}(t'),\hat{w}(t')\}]dt' \approx \frac{i}{2\hbar}\int_{0}^{\infty}G(\tau)\tau d\tau\left[\hat{x},\left\{\frac{\hat{p}}{m},\hat{w}\right\}\right] = \frac{\eta}{2i\hbar}\left[\hat{x},\left\{\frac{\hat{p}}{m},\hat{w}\right\}\right]. \quad (7.236)$$

In the momentum representation, the momentum operator and the density matrix w are just c-numbers and commute, so by applying Eq. (233) to the product pw, we get

$$\left[\hat{x},\left\{\frac{\hat{p}}{m},\hat{w}\right\}\right] = \left[\hat{x},2\frac{p}{m}w\right] = 2i\hbar\frac{\partial}{\partial p}\left(\frac{p}{m}w\right), \quad (7.237)$$

and may finally reduce the integro-differential equation Eq. (181) to a partial differential equation:

$$\boxed{\frac{\partial w}{\partial t} = -\frac{\partial}{\partial p}(Fw) + \eta k_{\text{B}}T\frac{\partial^2 w}{\partial p^2}, \qquad \text{with } F \equiv -\eta\frac{p}{m}.} \quad (7.238)$$

This is the 1D form of the famous *Fokker-Planck equation* describing the classical statistics of motion of a particle (in our particular case, of a free particle) in an environment providing a linear drag characterized by the coefficient η; it belongs to the same drift-diffusion type as Eq. (229). The first, *drift* term on its right-hand side describes the particle's deceleration due to the drag force (137), $F = -\eta p/m = -\eta v$, provided by the environment. The second, *diffusion* term on the right-hand side of Eq. (238) describes the effect of fluctuations: the particle momentum's random walk around its average (drift-affected, and hence time-dependent) value. The walk obeys the law similar to Eq. (85), but with the *momentum-space* diffusion coefficient

$$D_p = \eta k_{\text{B}}T. \quad (7.239)$$

This is the reciprocal-space version of the fundamental Einstein relation between the dissipation (friction) and fluctuations, in this classical limit represented by their thermal energy scale $k_{\text{B}}T$.[83]

The Fokker-Planck equation (238) may be readily generalized to the 3D motion of a particle under the effect of an additional external force,[84] and in this more general form is the basis for many important applications; however, due to its classical character, its discussion is also left for the SM part of this series.[85]

To summarize our discussion of the two alternative approaches to the analysis of quantum systems interacting with a thermally-equilibrium environment, described in the last five sections, let me emphasize again that they give different descriptions of the same phenomena, and are characterized by the same two functions $G(\tau)$ and $K_F(\tau)$. Namely, in the Heisenberg-Langevin approach, we describe the

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[83] Note that Eq. (224), as well as the original Einstein's relation between the diffusion coefficient D in the direct space and temperature, may be derived much simpler by other means – for example, from the Nyquist formula (139). These issues are discussed in detail in SM Chapter 5.

[84] Moreover, Eq. (223) may be generalized to the motion of a *quantum* particle in an additional periodic potential $U(\mathbf{r})$. In this case, due to the band structure of the energy spectrum (which was discussed in Secs. 2.7 and 3.4), the coupling to the environment produces not only a continuous drift-diffusion of the probability density in the space of the quasimomentum $\hbar\mathbf{q}$ but also quantum transitions between different energy bands at the same $\hbar\mathbf{q}$ – see, e.g., K. Likharev and A. Zorin, *J. Low Temp. Phys.* **59**, 347 (1985).

[85] See SM Secs. 5.6-5.7. Some examples of *quantum* effects in dissipative systems with continuous spectra, mostly for particular models of the environment, may be found, e.g., in the monographs by U. Weiss, *Quantum Dissipative Systems*, 2nd ed., World Scientific, 1999, and H.-P. Breuer and F. Petruccione, *The Theory of Open Quantum Systems*, Oxford U. Press, 2007, and in references therein.

system by operators that change (fluctuate) in time, even in thermal equilibrium, while in the density-matrix approach, the system is described by deterministic probability functions, such as $W_n(t)$ or $w(p, t)$, which are stationary in equilibrium. In all cases when a problem may be solved analytically to the end by both methods (for example, for a harmonic oscillator), they give identical results.

7.10. Exercise problems

7.1. Calculate the density matrix of a two-level system whose Hamiltonian is described, in a certain basis, by the following matrix:

$$\mathrm{H} = \mathbf{c} \cdot \boldsymbol{\sigma} \equiv c_x \sigma_x + c_y \sigma_y + c_z \sigma_z,$$

where σ_k are the Pauli matrices and c_j are c-numbers, in thermal equilibrium at temperature T.

7.2. In the usual z-basis, spell out the density matrix of a spin-½ with gyromagnetic ratio γ:

(i) in a pure state with the spin definitely directed along the z-axis,
(ii) in a pure state with the spin definitely directed along the x-axis,
(iii) in thermal equilibrium at temperature T, in a magnetic field directed along the z-axis, and
(iv) in thermal equilibrium at temperature T, in a magnetic field directed along the x-axis.

7.3. Calculate the Wigner function of a harmonic oscillator, with mass m and frequency ω_0, in thermodynamic equilibrium at temperature T. Discuss the relation between the result and the Gibbs distribution.

7.4. Calculate the Wigner function of a harmonic oscillator, with mass m and frequency ω_0:

(i) in the ground state,
(ii) in the first excited stationary state ($n = 1$),
(iii) in the Glauber state with an arbitrary dimensionless complex amplitude α, and
(iv) in the so-called *cat state*:[86] a linear superposition of two Glauber states with equal and opposite values of α.

In the last case, explore and interpret the behavior of the function near the origin at $|\alpha| \gg 1$.

7.5.[*] A harmonic oscillator is weakly coupled to an Ohmic environment that is in thermal equilibrium at temperature T.

(i) Use the rotating-wave approximation to write the reduced equations of motion for the Heisenberg operators of the complex amplitude of oscillations.
(ii) Calculate the expectation values of the correlators of the fluctuation force operators participating in these equations, and express them via the average number n_e of thermally-induced excitations in equilibrium, given by the second of Eqs. (26b).

7.6. Calculate the average potential energy of the long-range electrostatic interaction between two similar isotropic 3D harmonic oscillators, each with the electric dipole moment $\mathbf{d} = q\mathbf{s}$, where $\mathbf{s}$ is the oscillator's displacement from its equilibrium position, at arbitrary temperature T.

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[86] This state is frequently used to discuss the well-known *Schrödinger cat paradox* – see Sec. 10.1 below.

7.7. A semi-infinite string with mass μ per unit length is attached to a wall and stretched with a constant force (tension) $\mathcal{T}$. Calculate the spectral density of the transverse force exerted on the wall, in thermal equilibrium at temperature T.

7.8.[*] Calculate the low-frequency spectral density of small fluctuations of the voltage V across a Josephson junction shunted with an Ohmic conductor and biased with a dc external current $\bar{I} > I_c$.

Hint: You may use Eqs. (1.73)-(1.74) to describe the junction's dynamics, and assume that the shunting conductor remains in thermal equilibrium.

7.9. Prove that in the interaction picture of quantum dynamics, the expectation value of an arbitrary observable A may be indeed calculated using Eq. (167).

7.10. Show that the quantum-mechanical Golden Rule (6.149) and the master equation (196) give the same results for the rate of spontaneous quantum transitions $n' \rightarrow n$ in a system with a discrete energy spectrum, which is weakly coupled to a low-temperature heat bath (with $k_B T \ll \hbar \omega_{nn'}$).

Hint: You may establish the relation between the function $\chi''(\omega_{nn'})$ that participates in Eq. (196) and the density of states ρ_n that participates in the Golden Rule, by considering the particular case of sinusoidal classical oscillations in the system of interest.

7.11. A spin-½ with gyromagnetic ratio γ had been placed into a constant magnetic field with magnitude $\mathcal{B} \gg k_B T/\hbar\gamma$, and let relax into its ground state. Then the direction of the field was suddenly changed by $\pi/2$ and kept constant after that. Taking into account the spin's weak coupling to a dissipative environment:
    (i) calculate the time evolution of the spin's density matrix (in any basis you like), and
    (ii) calculate the time evolution of the spin vector's expectation value $\langle \mathbf{S} \rangle$ and sketch its trajectory.

7.12. A spin-½ with gyromagnetic ratio γ is placed into the magnetic field $\mathscr{B}(t) = \mathscr{B}_0 + \widetilde{\mathscr{B}}(t)$ with an arbitrary but relatively small time-dependent component, and is also weakly coupled to a dissipative environment in thermal equilibrium at temperature T. Derive the differential equations describing the time evolution of the expectation values of the spin's Cartesian components.

7.13. Use the Bloch equations derived in the previous problem to analyze the magnetic resonance[87] in a spin-½ which is weakly connected to a dissipative environment in thermal equilibrium. Use the result for a semi-quantitative discussion of the environmental broadening of arbitrary quantum transitions in systems with discrete energy spectra.

Hint: You may use the same rotating field model as in Problem 5.5.

7.14. Use the Bloch equations (see the solution of Problem 12) to analyze the dynamics of spin-½ with gyromagnetic ratio γ under the effect of an external ac magnetic field with a relatively low

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[87] See the discussion in Sec. 5.2 and the solution of Problem 5.5.

frequency ω and/or large amplitude $\mathscr{B}_{max}$ (so that $|\gamma\mathscr{B}_{max}| \gg \omega, 1/T_{1,2}$), assuming that the constants $T_{1,2}$ are field-independent.

7.15. Derive Eq. (220) from Eq. (222).

7.16. For a harmonic oscillator with weak Ohmic dissipation, use Eq. (220) to find the time evolution of the expectation value $\langle E \rangle$ of oscillator's energy for an arbitrary initial state, and compare the result with that following from the Heisenberg-Langevin approach.

7.17. Derive Eq. (234) in an alternative way – by using an expression dual to Eq. (4.244).