Chapter 7. Open Quantum Systems

This chapter discusses the effects of interaction of a quantum system with its environment, and in particular, with the instruments used for measurements. 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 this field which are of key importance for the basic goals of this course, in particular for the discussion of quantum measurements in the end of the chapter.¹

7.1. Open systems and the density matrix

All the way until the very end 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 laws of quantum mechanics. Each member of such an ensemble, called pure or coherent, may be described by the same quantum state \( \alpha \)- in the wave mechanics case, by the same wavefunction \( \Psi_\alpha \). Even our discussion of the Golden Rule in the end of the last chapter, in particular its form in which one component system (in Fig. 6.13, system \( b \)) may be used as a model of the environment of another component (\( a \)), was still based on the assumption of a pure initial state (6.146) of the system. Since the interaction of two component systems was described by a certain Hamiltonian (the one given by Eq. (6.145) for example), for the state \( \alpha \) of the system as a whole at arbitrary instant we might write

\[
|\alpha\rangle = \sum_n \alpha_n |n\rangle = \sum_n \alpha_n |n_a\rangle \otimes |n_b\rangle,
\]

with a unique correspondence between eigenstates states \( n_a \) and \( n_b \).

However, in many important cases our knowledge of quantum system’s state is incomplete. This is especially unavoidable² when a relatively simple quantum system \( s \) of our interest (say, an electron or an atom) is in a contact with environment \( e \) – here understood in a most general sense, say, as all the whole Universe less system \( s \) – see Fig. 1. Then there is virtually no chance of making two or more experiments with exactly the same composite system, because it 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. In this case, it makes much more sense to consider a statistical ensemble of another kind, with random quantum states of the environment, though possibly with known macroscopic parameters (e.g., temperature, pressure, etc.).

In classical physics, such mixed ensembles are the subject of statistical (classical) mechanics.³ Let us see how they may be described in quantum mechanics. For the beginning, we need to assume

¹ For a broader discussion of statistical mechanics and physical kinetics, including those of quantum systems, the reader is referred to the SM part of this lecture note series.
² Most of the mixed ensemble analysis in this chapter will pertain also to the cases when the systems of interest are not in a contact with the environment currently, and our knowledge about them is incomplete by some other reason – for example, if they had been in such a contact at some time between their perfect preparation (in a certain quantum state) and the observation, or if such a perfect preparation is impossible (or impracticable, or undesirable :-).
³ See, e.g., SM Sec. 2.1.
again that the coupling between the system of interest and its environment is weak in the sense accepted in the perturbation theory.\textsuperscript{4} In this case we can still use the bra- and ket-vectors of unperturbed states, that depend on different sets of variables (again, “belonging to different Hilbert spaces”). Then the most general quantum state of the whole Universe, still assumed to be pure,\textsuperscript{5} may be described as the following linear superposition:

\[ |\alpha\rangle = \sum_{j,k} \alpha_{jk} |s_j\rangle \otimes |e_k\rangle. \quad (7.2) \]

The “only” difference between the description of such an entangled state and the superposition of separable states, described by Eq. (1), is that coefficients $\alpha_{jk}$ in the right-hand part of Eq. (2) are numbered with two indices: index $j$ listing the quantum states of system $s$, and $k$ numbering the (enormously large) set of quantum states of the environment. So, in a mixed ensemble a certain state $s_j$ of the system of interest may coexist with different states of its environment.\textsuperscript{6} Of course, the enormity of the Hilbert space of the environment, i.e. the number of $k$-components in sum (2), strips us of any 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 state (2), we would need to calculate

\[ \langle A \rangle = \langle \alpha | \hat{A} | \alpha \rangle = \sum_{j,j',k,k'} \alpha_{jk}^* \alpha_{j'k'} \langle s_j | \hat{A} | s_{j'} \rangle \otimes \langle e_k | e_{k'} \rangle. \quad (7.3) \]

Even if we assume that $\{s\}$ and $\{e\}$ are sets of the basis states of, respectively, the system and the environment, and that each 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 operators – those of intrinsic observables, which depend only on the degrees of freedom of the system of interest ($s$). These operators commute do not act on environment’s degrees of freedom, and hence in Eq. (3) we may move the environment bra-vector $\langle e_k |$ over all the way to ket-vector $|e_k\rangle$. Assuming, again, that the set of environmental eigenstates is full and orthonormal, Eq. (3) is now reduced to

\[ \langle A \rangle = \sum_{j,k} \alpha_{jk}^* \alpha_{jk} \langle s_j | \hat{A} | s_j \rangle \otimes \langle e_k | e_k \rangle. \]

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

\textsuperscript{4} In the opposite case, the very partition of the Universe into the system and the environment is impossible.

\textsuperscript{5} 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. In Sec. 6, I will offer a strong argument for this opinion - albeit not its strict proof.

\textsuperscript{6} Actually, such coexistence has been implied (but well hidden :-) in the derivation of the quantum-mechanical Golden Rule, which in all fairness, also belongs to the open systems class.
\[ \langle A \rangle = \sum_{j,k,j',k'} \alpha_{jk}^* \alpha_{j'k'} \langle s_j | A | s_{j'} \rangle \langle e_k | e_{k'} \rangle = \sum_{j,j'} A_{jj'} \sum_{k} \alpha_{jk}^* \alpha_{j'k}, \quad (7.4) \]

This is already some relief, because we have “only” a single sum over \( k \), but the main trick\(^7\) is still ahead. After the summation over \( k \), the second sum in the last form of Eq. (4) is some function \( w \) of indices \( j \) and \( j' \), so that, according to Eq. (4.96), this relation may be presented as

\[ \langle A \rangle = \sum_{j,j'} A_{jj'} w_{jj'} = \text{Tr}(Aw), \quad (7.5) \]

where matrix \( w \), with elements

\[ w_{jj'} = \sum_{k} \alpha_{jk}^* \alpha_{j'k}, \quad \text{i.e.} \, w_{jj'} = \sum_{k} \alpha_{jk} \alpha_{j'k}, \quad (7.6) \]

is called the \textit{density matrix} of the system. 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 Eqs. (1.33)-(1.34), its r.m.s. fluctuation as well if necessary), even for the very general statistical ensemble of states (2). This is why let us have a very good look at the density matrix.

First of all, as we know very well by now that the expansion coefficients in superpositions of the type (2) may be always expressed as bra-kets; in our current case, we may write

\[ \alpha_{jk} = \langle e_k | \otimes | s_j \rangle | \alpha \rangle. \quad (7.7) \]

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

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

We see that from the point of our system (i.e. in its Hilbert space whose basis states may be numbered by indices \( j \) only), the density matrix is indeed just the matrix of some construct,\(^8\)

\[ \hat{w} \equiv \sum_{k} \langle e_k | \alpha \rangle \langle \alpha | e_k \rangle, \quad (7.9) \]

that is called the \textit{statistical (or “density”) operator}. As evident from its 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 previous operators considered in this course, but in contrast to them, the statistical operator \textit{does} depend on composite system’s state \( \alpha \), including the state of system \( s \) as well. However, in the \( j \)-space it is mathematically still an operator whose matrix elements obey all formulas of the bra-ket formalism.

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

\[ w_{jj'} = \sum_{k} \alpha_{jk}^* \alpha_{jk} = \sum_{k} \alpha_{jk} \alpha_{jk}^* = w_{jj'}, \quad (7.10) \]

\(^7\) First suggested in 1927 by J. von Neumann.

\(^8\) Of course the “bra-kets” in this expression are not \( c \)-numbers, because state \( \alpha \) 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 that according to the general analysis of Sec. 4.3, there should be a certain basis \( \{ w \} \) in which the matrix of this operator is diagonal:

\[
| \begin{array}{c} w_{j'} \\ w \end{array} \rangle_{\text{in } w} = w_j \delta_{j'}. \tag{7.11}
\]

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

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

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 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 set \( \{ w \} \):

\[
\langle A \rangle = \text{Tr} (A w) = \sum_{j'} A_{j''} w_j \delta_{j''} = \sum_j A_j w_j . \tag{7.14}
\]

where \( A_j \) is just the expectation value of observable \( A \) in state \( w_j \). Hence, in order to comply with the general Eq. \((1.37)\), real \( c \)-numbers \( w_j \) must have the physical sense of probabilities \( W_j \) of finding the system in state \( j \). As the result, we can rewrite Eq. \((12)\) in the form

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

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

\[
W_j = \delta_{j'}. \tag{7.16}
\]

the system is evidently in a coherent (pure) 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 present it in another (arbitrary) basis \( \{ s \} \) as a coherent superposition

\[
| w_{j''} \rangle = \sum_j U^*_j s_j \rangle = \sum_j U^*_j s_j \rangle , \tag{7.17}
\]

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

\[
| \begin{array}{c} w_{j''} \rangle \langle w_j \end{array} \rangle_{\text{in } w} = \delta_{j, j''} \delta_{j', j''}, \tag{7.18a}
\]

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

\[
| \begin{array}{c} w_{j''} \rangle \langle w_j \end{array} \rangle_{\text{in } s} = \sum_{i, j'} U^*_{ij'} w_i \langle w_j | U_{j'j} = U^*_{ij'} U_{j'j} . \tag{7.18b}
\]

To make this result more transparent, let us denote matrix elements \( U_{j''} = \langle w_{j''} | s_j \rangle \) (that, for fixed \( j'' \), depend on just one index \( j \)) by \( \alpha_j \); then
so that $N^2$ elements of the whole $N \times N$ matrix is determined by just one string of $N$ c-numbers $\alpha_j$. For example, for a two-level system ($N = 2$),

$$w_{|s\rangle} = \begin{pmatrix} \alpha_1 \alpha_1^* & \alpha_2 \alpha_1^* \\ \alpha_1 \alpha_2^* & \alpha_2 \alpha_2^* \end{pmatrix}.$$  

(7.20)

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

$$w_{12} w_{21} = w_{11} w_{22}. \quad (7.21)$$

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

$$w = \begin{pmatrix} W_1 & (W_1 W_2)^{1/2} e^{i\varphi} \\ (W_1 W_2)^{1/2} e^{-i\varphi} & W_2 \end{pmatrix}. \quad (7.22)$$

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

Now let us consider a different statistical ensemble of two-level systems, that includes member states identical in all aspects (including similar probabilities $W_{1,2}$ in the same basis $s_{1,2}$), besides that the phase shifts $\varphi$ are random, with the phase probability uniformly distributed over the trigonometric circle. Then the ensemble averaging is equivalent to averaging over $\varphi$ from 0 to $2\pi$, so that it kills the off-diagonal terms of the density matrix (22), and the matrix becomes diagonal. For a system with a time-independent Hamiltonian, such averaging is especially plausible in the basis of stationary states $n$ of the system, in which phase $\varphi$ is just the difference of integration constants in Eq. (4.158), and randomness is naturally produced by minor fluctuations of the energy difference $E_1 - E_2$. (In Sec. 3 we will study the dynamics of such dephasing process.) The mixed statistical ensemble of systems with the density matrix diagonal in the stationary state basis is called the classical mixture, and presents the limit opposite to the pure (coherent) state.

After that example, the reader should not be much shocked by the main claim$^9$ 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 the thermal equilibrium with a much larger environment with fixed temperature $T$ (such environment is usually called a heat bath or a thermostat) statistical physics gives$^{10}$ a very simple expression, called the Gibbs distribution, for probabilities $W_n$:  

$$W_n = \frac{1}{Z} \exp\left\{ - \frac{E_n}{k_B T} \right\}. \quad (7.23a)$$

$^9$ This is essentially an alternative formulation of the basic postulate of statistical physics, called the microcanonical distribution - see, e.g., SM Sec. 2.2.

$^{10}$ See, e.g., SM Sec. 2.4. The Boltzmann constant $k_B$ is only needed if temperature is measured in non-energy units, say in kelvins.
where \( E_n \) is the eigenenergy of the corresponding stationary state, and \( Z \) is the normalization coefficient called the \textit{statistical sum}

\[
Z \equiv \sum_n \exp \left\{ -\frac{E_n}{k_B T} \right\}. \tag{7.23b}
\]

A detailed analysis of classical and quantum ensembles in thermodynamic equilibrium is the focus of statistical physics courses (such as my SM) rather than this course of quantum mechanics. However, I would still like to attract reader’s attention to the key fact that, in contrast with the similarly-looking Boltzmann distribution for single particles,\(^{11}\) the Gibbs distribution is absolutely general and is \textit{not} limited to classical statistics. In particular, for quantum gases of indistinguishable particles, it is absolutely compatible with quantum statistics (such as the Bose-Einstein or Fermi-Dirac distributions) of the component particles. For example, if we use Eq. (23) to calculate the average energy of a 1D harmonic oscillator of frequency \( \omega_0 \) in thermal equilibrium, we easily get\(^{12}\)

\[
W_n = \exp \left\{ -n \frac{\hbar \omega_0}{k_B T} \right\} \left\{ 1 - \exp \left\{ -\frac{\hbar \omega_0}{k_B T} \right\} \right\}, \tag{7.24}
\]

\[
Z = \exp \left\{ -\frac{\hbar \omega_0}{2k_B T} \right\} \left\{ 1 - \exp \left\{ -\frac{\hbar \omega_0}{k_B T} \right\} \right\}, \tag{7.25}
\]

\[
\langle E \rangle = \sum_{n=0}^{\infty} W_n E_n = \frac{\hbar \omega_0}{2} \coth \frac{\hbar \omega_0}{2k_B T} = \frac{\hbar \omega_0}{2} + \frac{\hbar \omega_0}{\exp \{\hbar \omega_0 / k_B T\} - 1}. \tag{7.26a}
\]

An alternative way to present the last result is to write

\[
\langle E \rangle = \frac{\hbar \omega_0}{2} + \hbar \omega_0 \langle n \rangle, \quad \text{with} \quad \langle n \rangle = \frac{1}{\exp \{\hbar \omega_0 / k_B T\} - 1}, \tag{7.26b}
\]

and to interpret it as the fact that in addition to the so-called \textit{zero-point energy} \( \hbar \omega_0/2 \) of the ground state, the oscillator (on the average) has \( \langle n \rangle \) thermally-induced excitations, with energy \( \hbar \omega_0 \) each. In the harmonic oscillator, whose energy levels are equidistant, such a language is completely appropriate, because the transfer from any level to one just above it adds the same amount of energy, \( \hbar \omega_0 \), to the system. The above expression for \( \langle n \rangle \) is actually the Bose-Einstein distribution (for the particular case of zero chemical potential);\(^ {13}\) we see that it does not only contradict the Gibbs distribution (for the total energy of the system), but immediately follows from it.\(^ {14}\)

\(^{11}\) See, e.g., SM Sec. 2.8.
\(^{12}\) See, e.g., SM Sec. 2.5 - but mind a different energy reference level, \( E_0 = \hbar \omega_0 \) used in Eqs. (2.68)-(2.69), affecting the expression for \( Z \). Actually, the calculation is so straightforward (just the summation of a geometric progression for the enumeration of \( Z \)) that it is highly recommended to the reader as a simple exercise.
\(^{13}\) See, e.g., SM Sec. 2.8.
\(^{14}\) Because of the fundamental importance of Eq. (26) for many fields of physics, let me remind the reader of its main properties. At low temperatures, \( k_B T \ll \hbar \omega_0 \), there are virtually no thermal 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 \( k_B T \) (following, for example, from the \textit{equipartition theorem}, which assigns energy \( k_B T / 2 \) to each quadratic contribution to system’s energy – in the 1D oscillator case, to one potential and one kinetic energy term).
7.2. Coordinate representation and the Wigner function

For many applications of the density matrix to wave mechanics, its coordinate representation is convenient. (I will only discuss it for 1D case; the generalization to multi-dimension case is straightforward.) Following Eq. (4.47), it is natural to define the following function of two arguments (frequently also called the density matrix):

\[ w(x,x') \equiv \langle x| \hat{\rho} |x' \rangle. \]  

(7.27)

Inserting, into the right-hand part of this definition, two closure conditions (4.44) for an arbitrary (full and orthonormal) basis \( \{s\} \), and then using Eq. (5.19), we get\(^\text{15}\)

\[ w(x,x') = \sum_{j,j'} \langle x|s_j\rangle \langle s_j|\hat{\rho}|s_j'\rangle \langle s_j'|x' \rangle = \sum_{j,j'} \psi_j(x) \psi^*_j(x'). \]  

(7.28)

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

\[ w(x,x') = \sum_j \psi_j(x) \psi_j^*(x'). \]  

(7.29)

Let us discuss the properties of this function. At coinciding arguments, \( x = x' \), this is just the probability density:\(^\text{16}\)

\[ w(x,x) = \sum_j \psi_j(x) \psi_j^*(x) = \sum_j w_j(x) = w(x). \]  

(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 \( \psi_j(x) = \delta_{j,j'} \), so that \( \psi(x) = \psi_j(x) \), and

\[ w(x,x') = \psi_j(x) \psi_j^*(x') = \psi(x) \psi^*(x'). \]  

(7.31)

We see that the density matrix carries the information not only about the modulus but also the phase of the wavefunction. (Of course one may argue rather convincingly that in this ultimate limit the density-matrix description is redundant, because all this information is contained in the wavefunction itself.)

How may be the density matrix interpreted? In the simple case (31), we can write

\[ |w(x,x')|^2 = w(x,x') w^*(x,x') = \psi(x) \psi^*(x) \psi(x') \psi^*(x') = w(x) w(x'), \]  

(7.32)

so that the modulus squared of the density matrix may is just as the joint probability density to find the system at point \( x \) and point \( x' \). For example, for a simple wave packet with the spatial extent \( \delta x \), \( w(x,x') \) is appreciable only if the both points are not farther than \( \delta x \) from the packet center, and hence from each other. The interpretation becomes more complex if we deal with an incoherent mixture of several wavefunctions, for example the classical mixture describing the thermodynamic equilibrium. In this case, we can use Eq. (23) to rewrite Eq. (29) as follows:

\(^{15}\) For now, I will focus on a fixed time instant (say, \( t = 0 \)), and hence write \( \psi(x) \) instead of \( \Psi(x, t) \).

\(^{16}\) This fact is the historic origin of density matrix’ name.
\[ w(x,x') = \sum_n \psi_n(x) W_n \psi_n^*(x') = \frac{1}{Z} \sum_n \psi_n(x) \exp \left\{ -\frac{E_n}{k_B T} \right\} \psi_n^*(x') . \quad (7.33) \]

As the simplest example, let us see what is the density matrix of a free (1D) particle in the thermal equilibrium. As we know very well, in this case, the set of energies \( E_p = \frac{p^2}{2m} \) of stationary states (monochromatic waves) forms a continuum, so that we need to replace sum (33) by an integral, taking “delta-normalized” traveling wavefunctions (5.59) as eigenstates:

\[
w(x,x') = \frac{1}{2\pi \hbar Z} \int_{-\infty}^{+\infty} \exp \left\{ -\frac{i px}{\hbar} \right\} \exp \left\{ -\frac{p^2}{2mk_B T} \right\} \exp \left\{ \frac{ipx'}{\hbar} \right\} dp . \quad (7.34)\]

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 momentum plus a constant. The statistical sum \( Z \) may be also readily calculated,\(^{17}\)

\[
Z = (2\pi nk_B T)^{1/2} , \quad (7.35)
\]

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

\[
w(x,x')Z = \left( \frac{mk_B T}{2\pi \hbar^2} \right)^{1/2} \exp \left\{ -\frac{mk_BT(x-x')^2}{2\hbar^2} \right\} . \quad (7.36)
\]

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 points \( x \) and \( x' \) exceeds the following characteristic scale (called the correlation length)

\[
x_c \equiv \left\langle (x-x')^2 \right\rangle^{1/2} = \frac{\hbar}{(mk_B T)^{1/2}} . \quad (7.37)
\]

This length may be interpreted in the following way. It is straightforward to use Eq. (23) to verify that the average energy \( E_p = \frac{p^2}{2m} \) of a particle in the thermal equilibrium, i.e. the classical mixture (33), equals \( k_B T/2 \) – this is just one more manifestation of the equipartition theorem. Hence the average momentum magnitude may be estimated as

\[
p_c \equiv \left\langle p^2 \right\rangle^{1/2} = \left( 2m \left\langle E \right\rangle \right)^{1/2} = \left( mk_B T \right)^{1/2} , \quad (7.38)
\]

so that \( x_c \) is of the order of the minimal length allowed by the Heisenberg-like “uncertainty relation”:

\[
x_c = \frac{\hbar}{p_c} . \quad (7.39)
\]

\(^{17}\) Due to the delta-normalization of the eigenfunction, the density matrix for the free particle (and any system with continuous eigenvalue spectrum) is normalized as

\[
\int_{-\infty}^{+\infty} w(x,x')Zdx' = \int_{-\infty}^{+\infty} w(x,x')Zdx = 1.
\]
Notice that with the growth of temperature, the correlation length (37) goes to zero, and the density matrix (36) tends to the $\delta$-function:

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

Since in this limit the average kinetic energy of the particle is larger than its potential energy in any fixed potential profile, Eq. (40) is the general property of the density matrix (33).

Let us discuss the following curious 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 – see 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 eigenfunction as

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

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

$$\frac{i(t - t_0)}{\hbar} \to \frac{1}{k_B T}, \quad x_0 \to x',$$

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 formal similarity of the Gibbs distribution (23) with the Schrödinger equation’s solution (1.67), enables a theoretical technique of the so-called thermodynamic Green’s functions, which is especially productive in condensed matter physics.\(^{18}\)

For our purposes, we can use Eq. (42) to recycle some of wave mechanics results, in particular the following formula for the harmonic oscillator’s propagator

$$G(x, t; x_0, t_0) = \left(\frac{m \omega_0}{2\pi\hbar \sin[\omega_0(t - t_0)]}\right)^{1/2} \exp\left\{-m \omega_0 \left(\frac{x^2 + x_0^2}{2\hbar} - 2x_0x_0\right)\right\}. $$

that may be readily proved to satisfy the Schrödinger equation for Hamiltonian (5.95), with the appropriate initial condition, $G(x, t_0; x_0, t_0) = \delta(x - x_0)$. Making substitution (42), we immediately get

$$w(x, x')Z = \left(\frac{m \omega_0}{2\pi\hbar \sinh[\hbar \omega_0 / k_B T]}\right)^{1/2} \exp\left\{-m \omega_0 \left[\frac{x^2 + x'^2}{2\hbar} \cosh[\hbar \omega_0 / k_B T] - 2x_0x_0\right]\right\}. $$

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 Eq. (44) yields

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

\(^{18}\) 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 square brackets we can readily recognize the ground state’s wavefunction (2.269), while the middle exponent is just the statistical sum (24) in the low-temperature limit when it is dominated by the ground-level contribution:

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

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

Returning to arbitrary temperatures, Eq. (44) in coinciding arguments gives the following expression for the probability density:\(^{19}\)

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

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

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

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

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

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. (5.129)-(5.130), 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 system measurements. This is a fundamental difficulty that has been well explored in terms of the Wigner function (sometimes called the “Wigner-Ville distribution”)\(^ {20}\) defined as

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

\(^{19}\) I have to confess that this notation is imperfect, because from the point of view of rigorous mathematics, $w(x, x')$ and $w(x)$ are different functions, and so are $w(p, p')$ and $w(p)$ used below. In the 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 different fonts for this letter. Let me hope that the difference between these functions is clear from their arguments, and from the context.

\(^{20}\) It was introduced in 1932 by E. Wigner on the basis of a general (Weyl-Wigner) transform suggested by H. Weyl in 1927, and re-derived in 1948 by J. Ville on a different mathematical basis.
From the mathematical standpoint, this is just the Fourier expansion of the density matrix in one of two new coordinates (Fig. 2) defined by relations

\[ x = X + \frac{\tilde{X}}{2}, \quad x' = X - \frac{\tilde{X}}{2}. \tag{7.51} \]

Physically, the new argument \( X = (x + x')/2 \) may be understood as the average position of the particle during the time interval \((t - t')\), while \( \tilde{X} = x - x' \) as the distance passed by the particle during that time interval, so that \( P \) may be interpreted as the characteristic momentum of a particle during that motion. As a result, the Wigner function is a construct intended to characterize the system spread simultaneously in the coordinate and momentum space - for 1D systems, on the phase plane \([X, P]\) that we considered before – see Fig. 5.6. Let us see how fruitful these intentions are.

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

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

For the particular case \( \tilde{X} = 0 \), 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 momentum \( P \) gives the probability density to find the system at point \( X \).

Actually, the function has the same property for integration over \( X \). To prove that, we should first introduce the momentum representation of the density matrix, in the full analogy with its coordinate representation (27):

\[
 w(p, p') \equiv \langle p \mid \hat{w} \mid p' \rangle. \tag{7.54}
\]

Inserting, as usual, two identity operators, in the form given by Eq. (5.21), into the right hand part of this equality, we can get the following relation between the momentum and coordinate representations:

\[
 w(p, p') = \int dx dx' \langle p \mid x \rangle \langle x \mid \hat{w} \mid x' \rangle \langle x' \mid p' \rangle = \frac{1}{2\pi\hbar} \int dx dx' \exp \left\{ - \frac{ipx}{\hbar} \right\} w(x, x') \exp \left\{ \frac{ip'x'}{\hbar} \right\}. \tag{7.55}
\]
This is of course nothing else than the unitary transform of an operator from the $x$-basis to $p$-basis, and is similar to the first form of Eq. (5.67).\^\footnote{Note that the last line of Eq. (5.67) is invalid for the density operator $\hat{\rho}$, because it is \textit{not} local!} For coinciding arguments, $p = p'$, Eq. (55) is reduced to

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

Using Eq. (29) and then Eq. (5.60), this function may be presented as

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

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

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

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

$$w(P) = \int W(X, P) dX . \quad (7.59)$$

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 them at certain values of these variables. This is of course the main requirement to any candidate joint probability density, $\rho(X, P)$, to find a classical representation point of a stochastic system on the phase plane $[X, P]$\footnote{Such density, which would express the probability $dW$ to find the system in a small area of the phase plane as $dW = \rho(X, P) dX dP$, is the basic notion of (1D) classical statistics – see, e.g., SM Sec. 2.1.}.

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

$$W(X, P) \propto \int_\infty^{+\infty} \exp \left\{ - \frac{m k_B T \tilde{X}^2}{2 \hbar^2} \right\} \exp \left\{ - \frac{i P \tilde{X}}{\hbar} \right\} d\tilde{X} . \quad (7.60)$$

The usual Gaussian integration yields:

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

We see that the function is independent of $X$ (as it should be for this translational-invariant system), and coincides with the Gibbs distribution (23). 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 substantially quantum system, the harmonic oscillator. Plugging Eq. (44) into Eq. (50), for that system in thermal equilibrium it is easy to show (and hence is left for reader’s exercise) that the Wigner function is also Gaussian, but now in both its arguments:
though 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 the Glauber state it also gives a very plausible result – a Gaussian distribution similar to Eq. (62), but shifted to the central point of the state – see Sec. 5.5.23

Unfortunately, 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 - Fig. 3.24

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

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

Fig. 7.3. The Wigner function of several Fock states of a harmonic oscillator: (a) \( n = 0 \), (b) \( n = 1 \); (c) \( n = 5 \). Adapted from http://en.wikipedia.org/wiki/Wigner_function.

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23 Please note that in notations of that section, arguments \( \{X, P\} \) of the Wigner function should be replaced with \( \{x, p\} \), and capital letters saved for the Cartesian coordinates of the central point (5.133), i.e. the classical complex amplitude of the oscillations.

24 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).
\[ W(X, P) = \frac{1}{2\pi\hbar} \int \psi(X + \frac{\tilde{X}}{2})\psi^*(X - \frac{\tilde{X}}{2}) \exp\left\{-\frac{iP\tilde{X}}{\hbar}\right\} d\tilde{X}. \] (7.63)

Changing argument \( P \) (say, at fixed \( X \)), we are essentially changing the spatial “frequency” (wavenumber) of the wavefunction product’s Fourier component we are calculating, and we know that 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, and as the particular case, the ground state of the harmonic oscillator) have such a symmetry, but many other functions do not.

Hence the Wigner function cannot be used in the role of classical probability density \( \rho(X, P) \), otherwise we would get a negative probability for measurement in certain intervals \( dXdP \) – the notion hard to interpret. However, the Wigner function is still used for a semi-quantitative interpretation of states of open quantum systems.

### 7.3. Open system dynamics: Dephasing

So far we have discussed the density matrix as something given. Now let us discuss the evolution of the matrix in time, starting from the simplest case when the system is in state (15) with \textit{time-independent} probabilities \( W_j \). In the Schrödinger picture we can rewrite Eq. (15) as

\[ \hat{w}(t) = \sum_j w_j(t) |w_j(t)|. \] (7.64)

Differentiating this equation by parts, and using Eqs. (4.157)-(4.158), with the account of the Hermitian nature of the Hamiltonian operator, we get

\[ \dot{\hat{w}} = \sum_j \left[ w_j(t) \dot{w}_j(t) + w_j(t) \dot{\bar{w}}_j(t) \right] = \sum_j \left[ \hat{H} w_j(t) \dot{w}_j(t) - w_j(t) \dot{w}_j(t) \right] = \dot{\hat{H}} \sum_j w_j(t) \dot{w}_j(t) - \dot{w}_j(t) w_j(t) \hat{H}. \] (7.65)

Now using Eq. (64) again (twice), we get the so-called \textit{von Neumann equation}\(^25\)

\[ i\hbar \dot{\hat{w}} = [\hat{H}, \hat{w}]. \] (7.66)

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

\[ i\hbar \dot{\hat{A}} = [\hat{A}, \hat{H}], \] (7.67)

besides the operator order in the commutator, i.e., the sign of the right-hand part. This is quite natural, because Eq. (66) belongs to the Schrödinger picture, while Eq. (67) to the Heisenberg picture of the quantum dynamics.

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\(^25\) In many texts, it is called the “Liouville equation”, due to the philosophical proximity to the classical Liouville theorem for the distribution function \( \rho(X, P) \) or its multi-dimensional analog – see, e.g., SM Sec. 6.1, in particular Eq. (6.5).
In the general case when a system, initially out of equilibrium, comes into a contact with the environment, probabilities \( W_j \) change, and dynamics is described by equations more complex than Eq. (66). However, we still can use this equation to discuss, using a simple model, the second (after the energy relaxation) major effect of the environment, *dephasing* (also called “decoherence”).\(^{26}\) Let us consider the following model of a system interacting (weakly!) with environment:\(^{27}\)

\[
\hat{H} = \hat{H}_s + \hat{H}_e \{ \lambda \} + \hat{H}_{\text{int}} .
\]

(7.68)

Let us consider the simplest, two-level system, taking its Hamiltonian in the simplest form,

\[
\hat{H}_s = a_z \hat{\sigma}_z ,
\]

(7.69)

(as we know from Sec. 4.6, such Hamiltonian is sufficient to avoid the energy level degeneracy), and a factorable (bilinear) interaction - cf. Eq. (6.148) and its discussion:

\[
\hat{H}_{\text{int}} = -\hat{f} \{ \lambda \} \hat{\sigma}_z .
\]

(7.70)

Here \( \hat{f} \) is a Hermitian operator depending only on the set \( \{ \lambda \} \) of environmental degrees of freedom (“coordinates”). These coordinates belong to the Hilbert space different from that of the two-level system, and hence operators \( \hat{f} \{ \lambda \} \) and \( \hat{H}_e \{ \lambda \} \) (that describes the environment) commute with \( \hat{\sigma}_z \) - and any other intrinsic operator of the two-level system. Of course, any realistic \( \hat{H}_e \{ \lambda \} \) is very complex, so that it may be surprising how much we will be able to achieve without specifying it.

Before we proceed to solution, let me remind the reader of the important two-level systems that may be described by this model. The first example is an electron in an external magnetic field of a fixed direction (taken for axis \( z \)), which includes both an average component \( \langle B_z \rangle \) and a random (fluctuating) component \( \tilde{B}_z \). As it follows from the discussion in Chapter 4, it may be described by Hamiltonian (68)-(70) with

\[
a_z = \mu_B \langle B_z \rangle, \quad -\hat{f} = \mu_B \tilde{B}_z .
\]

(7.71)

The second important example is a particle in a double-quantum-well potential (Fig. 4), with a barrier between them sufficiently high to be impenetrable, and an additional force \( F(t) \) exerted by the environment. If the force is sufficiently weak, we can neglect its effects on the shape of quantum wells and hence on the localized wavefunctions \( \psi_{L,R} \), so that the force effect is reduced to the variation of the difference \( E_L - E_R = F(t)\Delta x \) between well eigenenergies. As a result, it may described by Eqs. (608)-(70) with

\[
a_z \approx \langle F \rangle \Delta x / 2; \quad -\hat{f} \approx \tilde{F} \Delta x / 2 .
\]

(7.72)

\(^{26}\) Another example when \( W_j \) are constant in time, and hence Eq. (66) is valid, is the thermodynamic equilibrium. However, in this case the statistical operator is diagonal in the stationary state basis and hence commutes with the Hamiltonian. Hence the right-hand part of Eq. (66) vanishes, and it shows that the density matrix does not evolve in time at all – as it should.

\(^{27}\) Though this model works very well in many cases (see the examples given below), it is not adequate for a particle interacting with the environment of *similar* particles. In this case the methods discussed in the next chapter are more relevant.
Returning to the general model (68)-(70), let us start its analysis from writing the usual equation of motion for the Heisenberg operator $\hat{\sigma}_z$:

$$i\hbar \dot{\hat{\sigma}}_z = [\hat{\sigma}_z, \hat{H}] = (a_z - \hat{f})[\hat{\sigma}_z, \hat{\sigma}_z] = 0,$$

so that operator $\hat{\sigma}_z$ does not evolve in time. What does this mean for the observables? For an arbitrary density matrix of the two-level system,

$$\rho = \begin{pmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{pmatrix},$$

we can readily calculate the trace of operator $\hat{\sigma}_z$ (since operator traces are basis-independent, we can do this in any basis, in particular in the usual $z$-basis):

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

Hence, according to Eq. (5), $\hat{\sigma}_z$ may be considered the operator for observable $W_1 - W_2$, so that in the case (73), the difference $W_1 - W_2$ does not depend on time, and since the sum of the probabilities is also fixed, $W_1 + W_2 = 1$, both of them are constant. (The physics of this result is especially clear for the model shown in Fig. 4: since the potential barrier separating the quantum wells is so high that tunneling through it is negligible, the interaction with environment cannot move the system from well into another one. It may look like nothing interesting may happen in such situation, but in a minute we will see this is not true.) Hence, we may use the von Neumann equation (66) for the density matrix evolution (in the Schrödinger picture). In the usual $z$-basis:

$$i\hbar \dot{\rho} = i\hbar \begin{pmatrix} w_{11} & \dot{w}_{12} \\ \dot{w}_{21} & w_{22} \end{pmatrix} = [H, \rho] = (a_z - \hat{f})[\sigma_z, \rho]$$

$$= (a_z - \hat{f}) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{pmatrix} - \begin{pmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = (a_z - \hat{f}) \begin{pmatrix} 0 & 2w_{12} \\ -2w_{21} & 0 \end{pmatrix}. \tag{7.76}$$

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28 This can be done because we may consider the whole system, including the environment, as a Hamiltonian one – see Eq. (68).
This means that though the diagonal elements, i.e., the probabilities of the states, do not evolve in time (as we already know), the off-diagonal coefficients do change; for example,

$$i\hbar\dot{w}_{12} = 2(a_z - \hat{f})w_{12},$$  \hspace{1cm} (7.77)

with a similar but complex-conjugate equation for $w_{21}$. The solution of the linear differential equation (77) is straightforward, and yields

$$w_{12}(t) = w_{12}(0)\exp\left(-i\frac{2a_z}{\hbar}t\right)\exp\left(i\frac{2}{\hbar}\int_0^t \hat{f}(t')dt'\right).$$ \hspace{1cm} (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, and, from the point of view of the system of our interest, a random function of time.

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

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

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

Here we have used the fact that the first average is equal to zero (it is evident from Eqs. (69)-(70) that if $f$ had any average component, it could be included into parameter $a$), while the second average, called the correlation function, in a statistically- (i.e. macroscopically-) stationary state of environment may only depend on the time difference $\tau \equiv t' - t'':$

$$\langle f(t')f(t'')\rangle \equiv K_f(t' - t'') = K_f(\tau).$$ \hspace{1cm} (7.80)

If this difference is much larger than some time scale $\tau_c$, called the correlation time of the random force, the values $f(t')$ and $f(t'')$ are completely independent (uncorrelated), as illustrated in Fig. 5a, so that 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 $f$: $K_f(0) = \langle f^2 \rangle$, \hspace{1cm} (7.81)

and has to be positive. As a result, the function looks (qualitatively) like the sketch in Fig. 5b.

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29 This assumption is not in any contradiction with the quantum treatment of the two-level system, because a typical environment has very dense energy spectrum, so that the distances between them may be readily bridged by thermal excitations of energies $\sim k_BT << 2a_z$, often making its essentially classical.
Hence, if we are only interested in time differences \( \tau \) much longer than \( \tau_c \), we may approximate \( K(\tau) \) with a delta-function. Let us take it in the following convenient form

\[
K_f(\tau) \approx \hbar^2 D_\phi \delta(\tau), \tag{7.82}
\]

where \( D_\phi \) is a positive constant called the phase diffusion coefficient. The origin of this term stems from the very similar effect of diffusion of atoms or small solid particles in real space – the so-called (the Brownian motion).\(^\text{30}\) Indeed, if a small classical particle moves in a highly viscous medium, its velocity is approximately proportional to the external force. Hence, if the random hits of a 1D particle by the molecules may be described by a force which obeys a law similar to Eq. (82), the velocity (along any Cartesian coordinate) is also delta-correlated:

\[
\langle v(t) \rangle = 0, \quad \langle v(t')v(t'') \rangle = 2D\delta(t'-t''). \tag{7.83}
\]

Now we can integrate the kinematic equation \( \dot{x} = v \), to calculate particle’s deviation from the initial position,

\[
x(t) - x(0) = \int_0^t v(t') dt', \tag{7.84}
\]

and its the variance:

\[
\left\langle (x(t) - x(0))^2 \right\rangle = \int_0^t \int_0^t \langle v(t')v(t'') \rangle dt' dt'' = 2D\int_0^t \int_0^t \delta(t'-t'')dt' dt'' = 2Dt. \tag{7.85}
\]

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 constant \( D \) is called the diffusion coefficient.

Returning to the diffusion of the quantum-mechanical phase, using Eq. (82), the last double integral in Eq. (79) yields \( \hbar^2 D_\phi dt \), so that

\[
\langle w_{12}(dt) \rangle = w_{12}(0)\exp\left(-i\frac{2a}{\hbar} dt\right)(1 - 2D_\phi dt). \tag{7.86}
\]

Applying this formula to sequential time intervals,

\(^{30}\) The theory of this phenomenon, first observed experimentally by biologist R. Brown in the early 1800s, was pioneered by A. Einstein in 1905 (see in particular Eq. (206) below) and developed in detail by M. Smoluchowski in 1906-1907, and A. Fokker in 1913.
\[ \langle w_{12}(2dt) \rangle = \langle w_{12}(dt) \rangle \exp \left\{ -i \frac{2a_z}{\hbar} dt \right\} (1 - 2D_\phi dt) = w_{12}(0) \exp \left\{ -i \frac{2a_z}{\hbar} dt \right\} (1 - 2D_\phi dt)^2, \] (7.87)

eq 2, \text{ for a finite time } t = N dt, \text{ in the limit } N \to \infty \text{ and } dt \to 0 \text{ (at fixed } t) \text{ we get,} \quad \lim_{N \to \infty} \langle w_{12}(t) \rangle = w_{12}(0) \exp \left\{ -i \frac{2a_z}{\hbar} t \right\} \left( 1 - 2D_\phi \frac{1}{N} \right)^N. \] (7.88a)

By the definition of the natural logarithm base \( e \), this limit is just \( \exp \{-2D_\phi t\} \), so that, finally:

\[ \langle w_{12}(t) \rangle = w_{12}(0) \exp \left\{ -i \frac{2a_z}{\hbar} t \right\} \exp \left\{ -2D_\phi t \right\} \equiv w_{12}(0) \exp \left\{ -i \frac{2a_z}{\hbar} t \right\} \exp \left\{ -\frac{t}{T_2} \right\}. \] (7.88b)

So, due to coupling to environment, the off-diagonal elements of the density matrix decay with the characteristic dephasing time \( T_2 = 1/2D_\phi \), providing a natural evolution from the density matrix (22) of a pure state, to the diagonal matrix,

\[ w = \begin{pmatrix} W_1 & 0 \\ 0 & W_2 \end{pmatrix}, \] (7.89)

with the same probabilities \( W_{1,2} \), describing a fully dephased (incoherent) classical mixture.

Our simple model offers a very clear look at the nature of decoherence: “force” \( f(t) \), exerted by the environment, “shakes” the energy difference between two eigenstates of the system and hence the instant velocities \( 2(a_z - f)/\hbar \) of their mutual phase shift \( \varphi(t) \) – cf. Eq. (24). Due to randomness of the force, \( \varphi(t) \) performs a random walk around the trigonometric circle, so that eventually, averaging of its trigonometric functions \( \exp \{\pm i\varphi\} \) over the possible states of environment yields zero, killing the off-diagonal elements of the density matrix. Our analysis, however, has left open two important issues:

(i) Is it approach valid for a quantum description of a typical environment?

(ii) If yes, what is \( D_\phi \)?

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 bilinear form similar to Eqs. (70) and (6.130):

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

---

31 This result is valid only if approximation (82) may be applied at time interval \( dt \) which, in turn, should be much smaller than \( T_2 \), i.e. if the dephasing time is much longer that the environment’s correlation time \( \tau_c \). This requirement is usually well satisfied, because in most environments, \( \tau_c \) very short. For example, in the original Brownian motion experiments with few-\( \mu \)m ink particles in water, it is of the order of the average interval between sequential molecular impacts, of the order of \( 10^{-21} \) s.

32 See, e.g., MA Eq. (1.2a).
where $x$ is some observable of the subsystem $s$ (say, a generalized coordinate or a generalized momentum). It may look incredible that in this very general situation one may make a very simple and powerful statement about the statistical properties of the generalized external 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 environment $e$ is weak - in the sense of the perturbation theory (see Chapter 6), and

(ii) the environment may be considered as staying in thermodynamic equilibrium, with certain temperature $T$, regardless of the process in the system of interest.\(^{33}\)

This famous statement is called the *fluctuation-dissipation theorem* (FDT).\(^{34}\) Due to the importance of this fundamental result, let me derive it.\(^{35}\)

Since by writing Eq. (68) we treat the whole system $(s + e)$ as a Hamiltonian one,\(^{36}\) we may use the Heisenberg equation (4.199) to write

$$i\hbar \dot{F} = \left[ \hat{F}, \hat{H} \right] = \left[ \hat{F}, \hat{H}_s \right], \quad (7.91)$$

because, as was discussed in the last section, operator $\hat{F}\{\lambda\}$ commutes with operators $\hat{H}_s$ and $\dot{x}$. 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 external force’s operator into the following sum:

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

where (until further notice) sign $\langle \ldots \rangle$ means the statistical averaging over the environment alone.\(^{37}\) From the point of view of system $s$, the first term of the sum (still an operator!) describes the average response

\(^{33}\) The most frequent example of violation of these conditions is environment’s overheating by the energy flow from the subsystem. I leave it to the reader to estimate the overheating of a standard physical laboratory room by a typical dissipative quantum process – the emission of an optical photon by an atom. *(Hint: extremely small.)*

\(^{34}\) The FDT was first derived by H. Callen and T. Welton in 1951, on the background of an earlier derivation of its classical limit by H. Nyquist in 1928, and the pioneering 1905 work by A. Einstein – see below.

\(^{35}\) The FDT may be proved in several ways which are different from, and shorter than the one given in this section – see, e.g., either 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 describe here, besides giving the important *Kubo formula* (109) as a byproduct, is a very useful exercise in the operator manipulation and the perturbation theory in its integral form, different from the differential form used in Chapter 6. If the reader is not interested in this exercise, he or she may skip the derivation and jump directly to the result expressed by Eq. (134), which uses the notions defined by Eqs. (114) and (123).

\(^{36}\) We can always do that if the local environment is large enough, so that the processes in our subsystem would not depend on the type of boundary between it and the external environment; in particular we may assume the total system closed, i.e. Hamiltonian.

\(^{37}\) For usual (“ergodic”) environments, without intrinsic long-term memories, this statistical averaging over an ensemble of environments is equivalent to averaging over relatively short times - much longer than the correlation time $\tau_c$ 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. As was already mentioned, in most practical environments, $\tau_c$ is very short. Thus, for relatively “massive” (inertial) systems of interest the separation of the averaging into two steps is widely justified.
of the environment to the system dynamics (possibly, including such irreversible effects as friction), and has to be calculated with account of their interaction – as will do later in this section. On the other hand, the second term in Eq. (92) presents fluctuations of the environment, which exist even in the absence of 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 the thermodynamic equilibrium:

\[
i \hbar \dot{\mathcal{F}} = \left[ \mathcal{F}, \hat{H}_{\text{eq}} \right]. \tag{7.93}
\]

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

\[
\mathcal{F}(t) = \exp\left\{ \frac{i}{\hbar} \hat{H}_{\text{eq}} t \right\} \mathcal{F}(0) \exp\left\{ -\frac{i}{\hbar} \hat{H}_{\text{eq}} t \right\}. \tag{7.94}
\]

Let us use this relation to calculate the correlation function of fluctuations, defined similarly to Eq. (80), but paying close attention to the order of the time arguments (very soon we will see why):

\[
\langle \mathcal{F}(t) \mathcal{F}(t') \rangle = \exp\left\{ \frac{i}{\hbar} \hat{H}_{\text{eq}} t \right\} \mathcal{F}(0) \exp\left\{ -\frac{i}{\hbar} \hat{H}_{\text{eq}} t \right\} \mathcal{F}(0) \exp\left\{ -\frac{i}{\hbar} \hat{H}_{\text{eq}} t' \right\} \mathcal{F}(0) \exp\left\{ \frac{i}{\hbar} \hat{H}_{\text{eq}} t' \right\}, \tag{7.95}
\]

where the thermal equilibrium of environment is implied. We are at will to calculate this expectation value in any basis, and the best choice is evident, because in the environment’s stationary state basis, its Hamiltonian, the exponents in Eq. (95), and the density operator of the environment are all represented by diagonal matrices. Using Eq. (5), the correlation function becomes

\[
\langle \mathcal{F}(t) \mathcal{F}(t') \rangle = \text{Tr} \left[ \hat{\mathcal{W}} \exp\left\{ \frac{i}{\hbar} \hat{H}_{\text{eq}} t \right\} \mathcal{F}(0) \exp\left\{ -\frac{i}{\hbar} \hat{H}_{\text{eq}} t \right\} \mathcal{F}(0) \exp\left\{ -\frac{i}{\hbar} \hat{H}_{\text{eq}} t' \right\} \right] = \sum_n \hat{\mathcal{W}} \exp\left\{ \frac{i}{\hbar} \hat{H}_{\text{eq}} t \right\} \mathcal{F}(0) \exp\left\{ -\frac{i}{\hbar} \hat{H}_{\text{eq}} t \right\} \mathcal{F}(0) \exp\left\{ -\frac{i}{\hbar} \hat{H}_{\text{eq}} t' \right\} = \sum_{n,n'} W_n \exp\left\{ \frac{i}{\hbar} E_n t \right\} F_{nn'} \exp\left\{ -\frac{i}{\hbar} E_{n'} t \right\} F_{n'n} \exp\left\{ -\frac{i}{\hbar} E_{n'} t' \right\} = \sum_{n,n'} W_n \left| F_{nn'} \right|^2 \exp\left\{ \frac{i}{\hbar} \frac{(E_n - E_{n'})(t-t')}{\hbar} \right\}, \tag{7.96}
\]

where \( W_n \) are the Gibbs distribution probabilities, given by Eq. (23) with environment’s temperature \( T \), and \( F_{nn'} \) are the Schrödinger-picture matrix elements of the interaction force operator.

We see that correlator (96) is a function of the difference \( \tau = t - t' \) only (as it should be for fluctuations in a macroscopically stationary system), but may depend on the order of the operands. This is why let us denote this particular correlation function by upper index “+”,

\[
K^{+}_F(\tau) \equiv \langle \mathcal{F}(t) \mathcal{F}(t') \rangle = \sum_{n,n'} W_n \left| F_{nn'} \right|^2 \exp\left\{ \frac{i}{\hbar} \frac{\tilde{E} \tau}{\hbar} \right\}, \tag{7.97}
\]

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\[
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\]

Here we assume that for the equilibrium, Eq. (92) has zero average, because if this is not so, this average part of force may be always included into the Hamiltonian of subsystem \( s \).
and its counterpart by upper index “•”:

\[
K_F^\tau(\tau) \equiv K_F^\star(-\tau) = \langle \overline{F}(t)\overline{F}(t) \rangle = \sum_{n,n'} W_n |F_{n\star}|^2 \exp\left\{-\frac{i \overline{E}_\tau}{\hbar}\right\}.
\]  (7.98)

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

\[
K_F^\tau(\tau) - K_F(-\tau) = \langle \overline{F}(t)\overline{F}(t') - \overline{F}(t')\overline{F}(t) \rangle = 2i \sum_{n,n'} W_n |F_{n\star}|^2 \sin \frac{\overline{E}_\tau}{\hbar} \neq 0,
\]  (7.99)

so that \( \overline{F}(t) \) gives a good example of a Heisenberg-picture operator whose “values”, taken in different moments of time, generally do not commute – the opportunity already mentioned in Sec. 4.6.39

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

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

In the right-hand part of this relation, we cannot treat the Hamiltonian of the environment as an unperturbed (equilibrium) one, because the result would have zero statistical average. Hence, we should make one more step in our perturbative treatment, and take into account (in the first nonvanishing approximation) the effect of our system of interest (s) on the environment. To do this, let us write the (so far, exact) Heisenberg equation of motion for the environment’s Hamiltonian,

\[
i\hbar \dot{\hat{H}}_e = \left[ \hat{H}_e, \hat{H} \right] = -\hat{x} \left[ \hat{H}_e, \hat{F} \right],
\]  (7.101)

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

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

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

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

As we will see imminently, this expression gives a nonvanishing result even if the right-hand-part averaging is carried over the unperturbed (thermal-equilibrium) environment, so that unless we are interested in higher-order corrections, there is no need to refine the result any further. This fact enables us to calculate the average in the right-hand part of Eq. (103) absolutely similarly to that in Eq. (96), using Eq. (94):

---

39 A good sanity check here is that at \( \tau = 0 \), the difference (99) between \( K_F(\tau) \) and \( K_F(-\tau) \) vanishes.
\[ \langle [\hat{F}(t'), \hat{H}_c(t'')] \qquad \rangle = \text{Tr} \{ \mathcal{W} [F(t') [H_c F(t'')]] \} \]

\[ = \text{Tr} \{ \mathcal{W} [F(t') H_c F(t'') - F(t') F(t'') H_x - H_x F(t'') F(t') + F(t'') H_x F(t')] \} \]

\[ = \sum_{n,n'} W_n [F_{nn}(t') E_n F_{nn'}(t'') - E_n F_{nn'}(t') F_{nn'}(t'') E_n - E_n F_{nn'}(t') F_{nn'}(t'') E_n + F_{nn'}(t') E_n F_{nn'}(t'')] \]

\[ = -\sum_{n,n'} W_n \bar{E} [F_{nn'}] \left[ \exp \left\{ i \frac{\bar{E}}{\hbar} (t'' - t') \right\} + \text{c.c.} \right]. \] (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 \( t', t'' \rightarrow -\infty \)) is uncertain, because the exponents oscillate without decay. This technical difficulty may be overcome by the following reasoning. As illustrated by the example considered in the previous section, coupling to a disordered environment makes the “memory horizon” of the subsystem of our interest (\( s \)) finite: its current state does not depend on its history beyond certain time scale – in that example, the dephasing time \( T_2 \). (Actually, this is true for virtually all real physical systems, in contrast to the idealized models such as a dissipation-free pendulum that swings for ever and ever with the same amplitude.) As a result, the functions under integrals of Eq. (103), i.e. the sum (104), should self-average at a certain finite time. One simple 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 (mathematically more acceptable) trick is to first multiply the function under each integral by, respectively, \( \exp \{ \epsilon (t - t') \} \) and \( \exp \{ \epsilon (t - t'') \} \), where \( \epsilon \) is a very small positive constant, then carry out the integration, and after that take the limit \( \epsilon \rightarrow 0 \). The physical justification of this procedure may be provided by saying that system’s behavior should not be affected if its interaction with the environment was not kept constant but was turned on gradually – say, exponentially with an infinitesimal rate \( \epsilon \). With this modification, Eq. (103) becomes

\[ \langle \hat{F}(t) \rangle = -\frac{1}{\hbar^2} \sum_{n,n'} W_n \bar{E} [F_{nn'}] \lim_{\epsilon \rightarrow 0} \int_{-\infty}^{t'} \int_{-\infty}^{t''} \int_{-\infty}^{t'} \int_{-\infty}^{t''} \chi(t'') \left[ \exp \left\{ i \frac{\bar{E}}{\hbar} (t'' - t') \right\} + \text{c.c.} \right]. \] (7.105)

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

\[ \int_{-\infty}^{t'} \int_{-\infty}^{t''} \int_{-\infty}^{t'} \int_{-\infty}^{t''} \int_{-\infty}^{t'} \int_{-\infty}^{t''} \int_{-\infty}^{t'} \int_{-\infty}^{t''} \cdots \]

(7.106)

where \( \tau' \equiv t - t' \), and \( \tau \equiv t - t'' \).

Fig. 7.6. 2D integration area in Eqs. (105) and (106).
As a result, Eq. (105) may be rewritten as a single integral,

$$\langle \hat{F}(t) \rangle = \int_{-\infty}^{\infty} G(t-t'') \hat{x}(t'') d\tau'' = \int_{0}^{\infty} G(\tau) \hat{x}(t-\tau) d\tau,$$

(7.107)

whose kernel,

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

(7.108)

$$= \lim_{\varepsilon \to 0} \frac{2}{\hbar} \sum_{n,n'} W_n |F_{nn'}|^2 \sin \frac{\tilde{E} \tau}{\hbar} e^{-\varepsilon \tau} = \frac{2}{\hbar} \sum_{n,n'} W_n |F_{nn'}|^2 \sin \frac{\tilde{E} \tau}{\hbar},$$

does not depend on the particular law of evolution of the subsystem (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.\(^{40}\) Comparing Eq. (108) with Eq. (99), we get a wonderfully simple universal relation,\(^{41}\)

$$\langle \hat{F}(\tau), \hat{F}(0) \rangle = i\hbar G(\tau).$$

(7.109)

that emphasizes once again the quantum nature of the correlation function’s time asymmetry. However, the relation between $G(\tau)$ and the force anti-commutator,

$$\langle \hat{F}(t+\tau), \hat{F}(t) \rangle \equiv \langle \hat{F}(t+\tau) \hat{F}(t) + \hat{F}(t) \hat{F}(t+\tau) \rangle = K^+_f(\tau) + K^-_f(\tau),$$

(7.110)

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

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

(7.111)

that is evidently an even function of time difference $\tau$, looks very similar to the response function (108), “only” with another trigonometric function under the sum. This similarity may be used to obtain an exact algebraic relation between the Fourier images of these two functions of $\tau$. Indeed, function (111) may be represented as the Fourier transform\(^{42}\)

\(^{40}\) For a more detailed discussion of this function and the causality principle, see, e.g., CM Sec. 4.1.

\(^{41}\) This relation, called the Kubo (or “Green-Kubo”) formula, after the works by M. Green (1954) and R. Kubo (1957), does not come up in the easier derivations of the FDT, discussed in the beginning of this section.

\(^{42}\) Due to their practical importance, and certain mathematical issues with 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 Fourier integral transform (115) – see, e.g., SM Sec. 5.4.
\[ K_F(\tau) = \int_{-\infty}^{+\infty} S_F(\omega) e^{-i\omega\tau} d\omega = 2 \int_{0}^{+\infty} S_F(\omega) \cos \omega\tau \, d\omega, \]  
(7.112)

with the reciprocal transform
\[ S_F(\omega) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} K_F(\tau) e^{i\omega\tau} d\tau = \frac{1}{\pi} \int_{0}^{+\infty} K_F(\tau) \cos \omega\tau \, d\tau. \]  
(7.113)

via the symmetrized spectral density of variable \( F \), defined as
\[ S_F(\omega) \delta(\omega - \omega') \equiv \frac{1}{2} \left< \hat{F}_\omega \hat{F}_{-\omega'} + \hat{F}_{-\omega'} \hat{F}_\omega \right> = \frac{1}{2} \left< \left[ \hat{F}_\omega, \hat{F}_{-\omega'} \right] \right>. \]  
(7.114)

where \( \hat{F}_\omega \) (also an operator rather than a \( c \)-number!) is defined as
\[ \hat{F}_\omega \equiv \frac{1}{2\pi} \int_{-\infty}^{+\infty} \hat{F}(t) e^{i\omega t} \, dt, \quad \text{so that} \quad \hat{F}(t) = \int_{-\infty}^{+\infty} \hat{F}_\omega e^{-i\omega t} d\omega. \]  
(7.115)

The physical meaning of function \( S_F(\omega) \) becomes evident if we write Eq. (112) for the particular case \( \tau = 0 \):
\[ K_F(0) \equiv \left< \hat{F}^2 \right> = \int_{-\infty}^{+\infty} S_F(\omega) \, d\omega = 2 \int_{0}^{+\infty} S_F(\omega) \, d\omega. \]  
(7.116)

This formula implies that if we pass function \( F(t) \) through a linear filter cutting from its frequency spectrum a narrow band \( d\omega \) of real (positive) frequencies, then variance \( \left< F^2 \right> \) of the filtered signal \( F(t) \) would be equal to \( 2S_F(\omega) \, d\omega \) – hence the name “spectral density”.43

Let us use Eqs. (111) and (113) to calculate the spectral density for our model:
\[ S_F(\omega) = \sum_{\eta, \eta'} \left| F_{\eta\eta'} \right|^2 \lim_{\epsilon \to 0} \left[ \frac{\tilde{E}}{\hbar} e^{-\epsilon} \right] \int_{-\infty}^{+\infty} e^{i\omega \tau} d\tau \]  
(7.117)

Thus it is a convenient time to recall that each of the two summations here is over the eigenenergy spectrum of the environment whose spectrum is virtually continuous because of its large size, so that we may transform each sum into an integral just as this was done in Sec. 6.6:
\[ \sum_{n} \rightarrow \int \ldots \rho(E_n) \, dE_n, \]  
(7.118)

43 An alternative popular measure of spectral density is \( S_F(\nu) \equiv \left< F^2 \right>/\nu = 4\pi S_F(\omega), \) where \( \nu = \omega/2\pi \) is the “cyclic” frequency (measured in Hz).
where $\rho(E)$ is the density of environment’s states at a given energy. This transformation yields

$$S_F(\omega) = \frac{1}{2\pi} \lim_{\varepsilon \to 0} \int dE_n W(E_n) \rho(E_n) \int dE' \rho(E') \left\{ \frac{1}{i(E/h - \omega) - \varepsilon} + \frac{1}{i(-E/h - \omega) - \varepsilon} \right\}.$$  

(7.119)

Since the square bracket depends only on a specific linear combination of two energies, $E \equiv E_n - E_n'$, it is convenient to introduce also another, linearly-independent combination of the energies, for example, the average energy $\bar{E} = (E_n + E_n')/2$, so that the state energies may be presented as

$$E_n = \bar{E} + \frac{E}{2}, \quad E_n' = \bar{E} - \frac{E}{2}. \quad (7.120)$$

With this notation, Eq. (119) becomes

$$S_F(\omega) = -\frac{\hbar}{2\pi} \lim_{\varepsilon \to 0} \int dE \left\{ \int W \left| F_{nm} \right|^2 \rho \left( \frac{E}{2} + \bar{E} \right) \rho \left( \frac{E}{2} - \bar{E} \right) \frac{dE}{i(E/h - \omega) - \varepsilon} + \int W \left| F_{nm} \right|^2 \rho \left( \frac{E}{2} + \bar{E} \right) \rho \left( \frac{E}{2} - \bar{E} \right) \frac{dE}{i(-E/h - \omega) - \varepsilon} \right\}. \quad (7.121)$$

Due to the smallness of parameter $\hbar \varepsilon$ (which should be much less than all real energies, including $k_B T$, $\hbar \omega$, $E_n$, and $E_{n'}$), each of the internal integrals is dominated by an infinitesimal vicinity of one point, $\bar{E}_\pm = \pm \hbar \omega$, in which the spectral density, matrix elements, and the Gibbs probabilities do not change considerably, and may be taken out of the integrals, so that they may be worked out explicitly:\footnote{Using, e.g., MA Eq. (6.5a). (The imaginary parts of the integrals vanish, because integration in infinite limits may be always re-centered to finite points $\pm \hbar \omega$.) A mathematically enlightened reader may have noticed that the integrals might be taken without the introduction of small $\varepsilon$, using the Cauchy theorem – see MA Eq. (15.1).}

$$S_F(\omega) = -\frac{\hbar}{2\pi} \lim_{\varepsilon \to 0} \int d\varepsilon \rho, \rho \left[ W_+ |F_{i+}|^2 \int_{-\infty}^{+\infty} \frac{d\bar{E}}{i(\bar{E} - \hbar \omega) - \hbar \varepsilon} + W_- |F_{i-}|^2 \int_{-\infty}^{+\infty} \frac{d\bar{E}}{i(-\bar{E} - \hbar \omega) - \hbar \varepsilon} \right] = -\frac{\hbar}{2\pi} \lim_{\varepsilon \to 0} \int d\varepsilon \rho, \rho \left[ W_+ |F_{i+}|^2 \int_{-\infty}^{+\infty} \frac{d\bar{E}}{i(\bar{E} - \hbar \omega) + \hbar \varepsilon} \right] + W_- |F_{i-}|^2 \int_{-\infty}^{+\infty} \frac{d\bar{E}}{i(-\bar{E} + \hbar \omega) + \hbar \varepsilon} \right] \quad (7.122)$$

where indices $\pm$ mark function values at the special points $\bar{E}_\pm = \pm \hbar \omega$, i.e. $E_n = E_{n'} \pm \hbar \omega$. The physics of these points becomes simple if we interpret state $n$, that is the argument of the equilibrium Gibbs distribution function $W_n$, 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 emission of one energy quantum $\hbar \omega$ of the “observation” frequency $\omega$ by the environment into subsystem $s$ of 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 into force fluctuations.
The situation is different for the Fourier image of the response function $G(\tau)$\textsuperscript{45}

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

that is frequently called either the \textit{generalized susceptibility} or the \textit{response function} - in our case, of the environment. Its physical meaning is that the complex function $\chi(\omega) = \chi'(\omega) + i\chi''(\omega)$ relates the Fourier amplitudes of the generalized coordinate and generalized force:\textsuperscript{46}

$$\langle \hat{F}_\omega \rangle = \chi(\omega)\hat{x}_\omega. \quad (7.124)$$

The physics of its imaginary part $\chi''(\omega)$ is especially clear. Indeed, if both $F_\omega$ and $x_\omega$ represent a sinusoidal classical process, say

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

Then, in accordance with the correspondence principle, Eq. (124) should hold for the $c$-number complex amplitudes $F_\omega$ and $x_\omega$, enabling us to calculate the time dependence of force,

$$F(t) = F_\omega e^{-i\omega t} + F_{-\omega} e^{+i\omega t} = \chi(\omega) x_\omega e^{-i\omega t} + \chi(-\omega) x_{-\omega} e^{+i\omega t} = \frac{x_0}{2} \left[ \chi(\omega) e^{-i\omega t} + \chi(-\omega) e^{+i\omega t} \right]$$

$$= \frac{x_0}{2} \left[ \chi' + \chi'' \right] e^{-i\omega t} + \left[ \chi' - i\chi'' \right] e^{+i\omega t} = x_0 \left[ \chi'(\omega) \cos \omega t + \chi''(\omega) \sin \omega t \right]. \quad (7.126)$$

We see that $\chi''(\omega)$ scales the part of the force that is $\pi/2$-shifted from the coordinate oscillations, i.e. is in phase with those of velocity, and hence characterizes the time-average power flow from the system into the environment, i.e. the \textit{energy dissipation} rate:\textsuperscript{47}

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

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

$$\chi''(\omega) = \operatorname{Im} \int_0^{+\infty} G(\tau) e^{i\omega \tau} d\tau = \frac{2}{\hbar} \sum_{n,n'} W_n |F_{nn'}|^2 \lim_{\epsilon \to 0} \operatorname{Im} \int_0^{+\infty} \left( \exp \left\{ \frac{i\tilde{E}\tau}{\hbar} \right\} - \text{c.c.} \right) e^{i\omega \tau} e^{-\epsilon \tau} d\tau$$

$$= \sum_{n,n'} W_n |F_{nn'}|^2 \lim_{\epsilon \to 0} \operatorname{Im} \left( \frac{1}{-\tilde{E} - \hbar \omega - i\hbar \epsilon} - \frac{1}{\tilde{E} - \hbar \omega - i\hbar \epsilon} \right) \quad (7.128)$$

\textsuperscript{45} Integration in Eq. may be extended to the whole time axis, $-\infty < \tau < +\infty$, if we complement definition (107) of $G(\tau)$ for $\tau > 0$ with its definition as $G(\tau) = 0$ for $\tau < 0$, in correspondence with the causality principle.

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

\textsuperscript{47} The expression $P = F\dot{x} = Fv$ used for the instant power flow is evident if $x$ is the usual Cartesian coordinate of a mechanical system. According to analytical mechanics (see, e.g., CM Chapters 2 and 10), it is valid for any generalized coordinate – generalized force pair which forms the interaction Hamiltonian (90).
\[ = \sum_{n,m} W_n |F_{nn'}|^2 \lim_{\varepsilon \to 0} \left( \frac{\hbar \varepsilon}{(E + \hbar \omega)^2 + (\hbar \varepsilon)^2} - \frac{\hbar \varepsilon}{(E - \hbar \omega)^2 + (\hbar \varepsilon)^2} \right). \quad (7.128) \]

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

\[ \chi''(\omega) = \lim_{\varepsilon \to 0} \int dE \int_{-\infty}^{+\infty} W(E + \frac{\hbar \omega}{2}) \rho(E + \frac{\hbar \omega}{2}) \rho(E - \frac{\hbar \omega}{2}) |F_{nn'}|^2 \frac{\hbar \varepsilon}{(E + \hbar \omega)^2 + (\hbar \varepsilon)^2} dE \]

\[ - \int_{-\infty}^{+\infty} W(E + \frac{\hbar \omega}{2}) \rho(E + \frac{\hbar \omega}{2}) \rho(E - \frac{\hbar \omega}{2}) |F_{nn'}|^2 \frac{\hbar \varepsilon}{(E - \hbar \omega)^2 + (\hbar \varepsilon)^2} dE \] \quad (7.129)

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

\[ \chi''(\omega) = \pi \int \rho_+ \rho_- \left[ W_+ |F_+|^2 - W_- |F_-|^2 \right] dE. \quad (7.130) \]

In order to relate these results, it is sufficient to notice that according to Eq. (23), the Gibbs probabilities \( W_\pm \) are related by coefficients dependent on only the temperature \( T \) and observation frequency \( \omega \):

\[ W_\pm \equiv W\left(E + \frac{\hbar \omega}{2}\right) = \frac{1}{Z} \exp \left\{ - \frac{E \mp \hbar \omega/2}{k_B T} \right\} = W(E) \exp \left\{ \mp \frac{\hbar \omega}{2k_B T} \right\}, \quad (7.131) \]

so that both the spectral density and the dissipative part of susceptibility may expressed via the same integral over environment energies:

\[ S_F(\omega) = \hbar \cosh \left( \frac{\hbar \omega}{2k_B T} \right) \int \rho_+ \rho_- W(E) \left[ |F_+|^2 + |F_-|^2 \right] dE, \quad (7.132) \]

\[ \chi''(\omega) = 2\pi \sinh \left( \frac{\hbar \omega}{2k_B T} \right) \int \rho_+ \rho_- W(E) \left[ |F_+|^2 + |F_-|^2 \right] dE, \quad (7.133) \]

and hence are universally related as

\[ S_F(\omega) = \frac{\hbar}{2\pi} \chi''(\omega) \coth \frac{\hbar \omega}{2k_B T}. \quad (7.134) \]

This is the Callen-Welton's fluctuation-dissipation theorem (FDT). It reveals the fundamental, intimate relation between dissipation and fluctuations induced by environment ("no dissipation without fluctuations") – hence the name.\(^*\) In the classical limit, \( \hbar \omega \ll k_B T \), the FDT is reduced to

\(^*\) A curious feature of the FDT is that Eq. (134) includes the exactly same function of temperature as the average energy (26) of a quantum oscillator of frequency \( \omega \), though, as the reader could witness, the notion of the
\[
S_\omega (\omega) = \frac{\hbar}{2\pi} \chi''(\omega) \frac{2k_B T}{\hbar \omega} \frac{k_B T}{\pi} \frac{\text{Im} \chi(\omega)}{\omega}.
\] (7.135)

In most systems of interest the last fraction tends to a finite (positive) constant in a substantial range of relatively low frequencies. Indeed, expanding Eq. (123) in the Taylor series in small \( \omega \), we get

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

Since the temporal Green’s function is real by definition, the Taylor expansion of \( \chi''(\omega) \equiv \text{Im} \chi(\omega) \) starts with the linear term \( i\omega \eta \), where \( \eta \) is a certain real coefficient, and unless \( \eta = 0 \), is dominated by this term at small \( \omega \). (The physical sense of constant \( \eta \) becomes clear if we consider an environment that provides viscous friction with the simple law

\[
\left\langle \dot{F} \right\rangle = -\eta \dot{x}, \quad \eta \geq 0.
\] (7.137)

For the Fourier images of coordinate and force this gives the relation \( F_\omega = i\omega \chi_0 \), so that according to Eq. (124),

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

Hence, even in the general case, coefficient \( \eta \) describes an effective low-speed drag (kinematic friction) provided by the environment.)

In this case Eq. (134) turns into the Nyquist formula:\(^49\)

\[
S_\omega (\omega) = \frac{k_B T}{\pi} \eta, \quad \text{i.e. } \left\langle F_j^2 \right\rangle = 4k_B T \eta d\nu.
\] (7.139)

According to Eq. (112), if such a constant spectral density\(^50\) persisted at all frequencies, it would correspond to a delta-correlated process \( F(t) \), with

\[
K_\omega (\tau) = 2\pi S_\omega (0) \delta(\tau) = 2k_B T \eta \delta(\tau),
\] (7.140)

similar to already discussed above – see Eq. (82).

oscillator was by no means used in its derivation. As will see in the next section, this fact leads to rather interesting consequences and even conceptual opportunities.

\(^49\) Actually, the 1928 work by H. Nyquist was about electronic noise in resistors, just discovered experimentally by his Bell Labs colleague J. Johnson. For an Ohmic resistor, as a dissipative “environment” of the electric circuit it is connected with, Eq. (137) is just the Ohm’s law, and may be recast as either \( \left\langle V \right\rangle = -R(dQ/dt) = RI, \) or \( \left\langle I \right\rangle = -G(d\Phi/dt) = GV. \) Thus for voltage \( V \) in an open circuit, \( \eta \) corresponds to resistance \( R \), while for current \( I \) in the short circuit, to 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 Eqs. (136)-(137) is frequently referred to as Ohmic dissipation, even if the physical nature of variables \( x \) and \( F \) is quite different.)\(^50\) Another note: the Nyquist formula (139) should not be confused with the Nyquist-Shannon theorem describing the minimum sampling rate of an analog signal.

\(^50\) A random process whose properties may be reasonably approximated by constant spectral density is frequently called the white noise, because then it is a random mixture of all possible sinusoidal components with equal weights, reminding natural white light’s composition.
Since in the classical limit the right-hand part 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 low observation frequencies (in the sense that \( \omega \) is much smaller than not only the quantum frontier \( k_B T/\hbar \), but also the frequency scale of function \( \chi''(\omega)/\omega \), Eq. (138) may be used to recast Eq. (135) in the form

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

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 \( T_2 = 1/2D_\phi \). Hence the classical approach to the environment, used in Sec. 3, is adequate if \( \hbar D_\phi << k_B T \). Next, we may identify operators \( \hat{F} \) and \( \hat{\sigma}_z \) participating in Eq. (70) with, respectively, operators \( \hat{F} \) and \( \hat{x} \) of the general Eq. (90). Then the comparison of Eqs. (82), (88) and (140) yields

\[
\frac{1}{T_2} = 2D_\phi = \frac{4k_B T}{\hbar^2} \eta , \tag{7.142}
\]

so that, for the model described by Eq. (137) with temperature-independent drag coefficient \( \eta \), the dephasing rate is proportional to temperature.

### 7.5. The Heisenberg-Langevin approach

The fluctuation-dissipation theorem opens a very simple and efficient way for analysis of the system of interest (s in Fig. 1). It is to write its Heisenberg equations (4.199) of motion for 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). Such approach to classical equations of motion is commonly associated with the name of Langevin,\(^{52}\) so that its extension to dynamics of Heisenberg-picture operators is frequently referred to as the Heisenberg-Langevin (or "quantum Langevin") approach to open system analysis.\(^{53}\)

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 that 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 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 external force, are

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51 In some fields (especially in physical kinetics and chemical physics), this particular limit of the Nyquist formula, is called the Green-Kubo (or just “Kubo”) formula. As was discussed above, these names may be more reasonably associated with Eq. (109).

52 After P. Langevin, whose 1908 work was the first systematic development of Einstein’s ideas (1905) of the Brownian motion theory in the random force language, as an alternative to M. Smoluchowski’s approach using the probability density language – see Sec. 6 below.

53 Perhaps the largest credit for this extension belongs to M. 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.
\[
\dot{x} = \frac{\hat{p}}{m}, \quad \dot{p} = -m\omega_0^2 x + \hat{F}, \tag{7.143}
\]
so that using Eqs. (92) and (137), we get
\[
\dot{x} = \frac{\hat{p}}{m}, \quad \dot{p} = -m\omega_0^2 x - \eta \dot{x} + \hat{F}(t). \tag{7.144}
\]
Combining Eqs. (144), we may write their system as a single differential equation
\[
m\ddot{x} + \eta \dot{x} + m\omega_0^2 x = \hat{F}(t), \tag{7.145}
\]
that is absolutely similar to the classical equation of motion.\(^{54}\) (In the view of Eqs. (5.42) and (5.48), whose corollary the Ehrenfest theorem (5.49) is, this should be by no means surprising.) For the Fourier images of the operators, defined similarly to Eq. (115), Eq. (145) gives the following relation,
\[
\hat{x}_{\omega} = \frac{\hat{F}_{\omega}}{m(\omega_0^2 - \omega^2) - i\eta\omega}, \tag{7.146}
\]
that should be also well known to the reader from the classical theory of forced oscillations. However, since the Fourier components are still Heisenberg-picture operators, and their “values” for different \(\omega\) 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 that used in Eq. (114). The result is
\[
\frac{1}{2} \left\{ \hat{x}_{\omega - \omega'} + \hat{x}_{-\omega + \omega'} \right\} = \frac{1}{\left| m(\omega_0^2 - \omega^2) - i\eta\omega \right|^2} \frac{1}{2} \left\{ \hat{F}_{\omega} \hat{F}_{-\omega} + \hat{F}_{-\omega'} \hat{F}_{\omega'} \right\}. \tag{7.147}
\]
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:
\[
S_x(\omega) = \frac{S_F(\omega)}{\left| m(\omega_0^2 - \omega^2) - i\eta\omega \right|^2} = \frac{S_F(\omega)}{m^2 (\omega_0^2 - \omega^2)^2 + (\eta\omega)^2}. \tag{7.148}
\]
Now using an analog of Eq. (116) for \(x\), we can calculate coordinate’s variance:
\[
\langle x^2 \rangle = K_x(0) = \int_{-\infty}^{+\infty} S_x(\omega) d\omega = 2 \int_{0}^{\infty} \frac{S_F(\omega) d\omega}{m^2 (\omega_0^2 - \omega^2)^2 + (\eta\omega)^2}, \tag{7.149}
\]
where now, in contrast to the notation used in Sec. 4, sign \(\langle \ldots \rangle\) means the averaging over the usual statistical ensemble of many systems of interest – in our current case, of many harmonic oscillators.

If the coupling to environment is so weak that the drag coefficient \(\eta\) is small (in the sense that the oscillator’s dimensionless \textit{Q-factor}\(^{48}\) 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 integral.\(^{55}\)

\(^{54}\) See, e.g., CM Sec. 4.1.

\(^{55}\) See, e.g., MA Eq. (6.5a).
\[
\langle x^2 \rangle \approx 2S_F(\omega_0) \int_0^\infty \frac{d\omega}{m^2(\omega_0^2 - \omega^2)^2 + (\eta \omega)^2} \approx 2S_F(\omega_0) \int_0^\infty \frac{d\xi}{2m\omega_0 \xi^2 + (\eta \omega_0)^2} \\
= 2S_F(\omega_0) \frac{1}{(\eta \omega_0)^2} \int_0^\infty \frac{d\xi}{(2m \xi / \eta)^2 + 1} = 2S_F(\omega_0) \frac{1}{(\eta \omega_0)^2} \frac{\pi \eta}{2m} = \frac{\pi}{\eta m \omega_0^2} S_F(\omega_0).
\]  

(7.150)

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

\[
\langle x^2 \rangle = \frac{\pi}{\eta m \omega_0^2} \frac{\hbar}{2\pi} \eta \omega_0 \coth \frac{\hbar \omega_0}{2k_B T} = \frac{\hbar}{2m \omega_0} \coth \frac{\hbar \omega_0}{2k_B T}.
\]

(7.151)

But this is exactly Eq. (48) that was obtained from the Gibbs distribution, without any explicit account of the environment - though keeping it in mind by using the notion of the thermally-equilibrium ensemble.56 (Notice that the drag coefficient \(\eta\), which characterizes the oscillator-to-environment interaction strength, has cancelled!) Does this mean that we have toiled in vain?

By no means. First of all, the FDT result has an important conceptual value. For example, let us consider the low-temperature limit \(k_B T << \hbar \omega_0\), when Eq. (151) is reduced to

\[
\langle x^2 \rangle = \frac{x_0^2}{2} = \frac{\hbar}{2m \omega_0}.
\]

(7.152)

Let us ask a naïve question: What exactly is the origin of this coordinate uncertainty? From the point of view of the usual quantum mechanics of closed (Hamiltonian) systems, there is no doubt: this nonvanishing variance of coordinate is the result of the final spatial extension of the ground-state wavefunction, reflecting the Heisenberg’s uncertainty relation (that in turn results from the fact that the operators of coordinate and momentum do not commute) – see Eq. (2.271). However, from the point of view of the Heisenberg-Langevin equation (145), variance (152) is an unalienable part of the oscillator’s response to the fluctuation force \(\tilde{F}(t)\) 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 much easier to subscribe to the latter standpoint, and treat the coordinate uncertainty as the result of the so-called quantum noise of the environment. This notion has received numerous confirmations in experiments that did not include any oscillators with the eigenfrequencies \(\omega_0\) close to the noise measurement frequency \(\omega\).57

The advantage of the Heisenberg-Langevin approach is that for any \(\eta > 0\) it is possible to calculate the (experimentally measurable!) distribution \(S_x(\omega)\), i.e. decompose the fluctuations into spectral components. This procedure is not restricted to the limit of small \(\eta\) (large \(Q\) factors); for any damping we may just plug the FDT (134) into Eq. (149) and integrate. As an example, let us have a look at the so-called quantum diffusion. A free 1D particle may be considered as the particular case of a 1D harmonic oscillator with \(\omega_0 = 0\), so that combining Eqs. (134) and (149), we get

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 \(\omega\). This is exactly the approach used by H. Nyquist (for the classical case) – see also SM Sec. 5.5.

57 See, for example, R. Koch et al., Phys. Lev. B 26, 74 (1982).
\[
\langle x^2 \rangle = 2 \int_{0}^{\infty} \frac{S_{F}(\omega) d\omega}{(m \omega^2)^2 + (\eta \omega)^2} = 2\eta \int_{0}^{\infty} \frac{1}{(m \omega^2)^2 + (\eta \omega)^2} \frac{h \omega}{2\pi} \coth \frac{h \omega}{2k_{B}T} d\omega. \quad (7.153)
\]

This integral has two divergences. The first one, of the type \( \int \frac{d\omega}{\omega^2} \) at the lower limit, is just a classical effect: according to Eq. (85), 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 noise effect 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

\[
\frac{k_{B}T}{\hbar} < \frac{\eta}{m}. \quad (7.154)
\]

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

\[
\langle x^2 \rangle \approx 2\eta \int_{k_{B}T/\hbar}^{\eta/m} \frac{1}{(m \omega^2)^2 + (\eta \omega)^2} \frac{h \omega}{2\pi} d\omega = \frac{h}{\pi \eta} \int_{k_{B}T/\hbar}^{\eta/m} \frac{d\omega}{\omega} = \frac{h \eta}{\pi k_{B}T m} \ln \frac{h \eta}{m k_{B}T} \sim \frac{h}{\eta}. \quad (7.155)
\]

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

The Heisenberg-Langevin approach is extremely simple and powerful, but it has its limitations. The main one is that if the equations of motion for the Heisenberg operators are not linear, there is no linear relation, such as Eq. (146), between the Fourier images of the generalized force and generalized coordinate, and as the result there is no simple relation, such as Eq. (148), between their spectral densities. In other words, if the Heisenberg equation of motion are nonlinear, there is no regular simple way to use them to calculate statistical properties of the observables. For example, let us return to the dephasing problem described by Eqs. (68)-(70), and assume that the generalized force is characterized by relations similar to (93) and (134). Now writing the Heisenberg equations of motion for the two remaining spin operators, and using the commutation relations between them, we get

\[
\dot{\hat{\sigma}}_x = -2 \frac{a - \hat{f}(t)}{\hbar} \hat{\sigma}_y, \quad \dot{\hat{\sigma}}_y = 2 \frac{a - \hat{f}(t)}{\hbar} \hat{\sigma}_x. \quad (7.156)
\]

These equations do not provide a linear relation between the Pauli operators and the fluctuation force, so even if we know spectral properties of the latter from the FDT, this does not help too much - unless we return to the approximate, classical approach described in Sec. 3 above.\footnote{\textsuperscript{59}}

\footnote{\textsuperscript{58} Its natural generalizations enable analyses of fluctuations in 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).}

\footnote{\textsuperscript{59} For some calculations, this problem may be avoided by linearization: if we are only interested in small fluctuations, the Heisenberg equations of motion may be linearized about their expectation values (see, e.g., CM Sec. 4.2), and the linear equations for variations solved either as has been shown above, or (if the expectation values evolve in time) by their Fourier expansions.}
7.6. Density matrix approach

The main alternative approach, that is essentially a generalization of that used in Sec. 2, is to extract the final results from the dynamics of the density matrix of our subsystem $s$ of interest (which, from this point on, will be called $w_s$). I will discuss this approach in detail, cutting just a few technical corners, in each case referring the reader to special literature.

We already know that the density matrix allows the calculation of the expectation value of any observable of system $s$ – see Eq. (5). However, our initial recipe (6) for the density matrix 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 some local environment (say, with the lab room) that is in the thermally-equilibrium state described by a diagonal density matrix – see Eqs. (15) and (23).

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

$$\langle A \rangle = \text{Tr}(\hat{A}\hat{w}) = \sum_{l,l'} A_{ll'} w_{ll'} = \sum_{l,l'} \langle l|\hat{A}|l'\rangle \langle l'|\hat{w}|l \rangle,$$

where $\hat{w}$ is the statistical operator of this full composite system. At weak interaction between the system $s$ and local environment $e$, their variables reside in different Hilbert spaces, so that we can write

$$|l \rangle = |s_j \rangle \otimes |e_k \rangle,$$

and if the observable $A$ depends only on the coordinates of system $s$, Eq. (157) yields

$$\langle A \rangle = \sum_{l,l'} \langle e_k | \otimes \langle s_j | \hat{A} | s_{j'} \rangle \otimes | e_{k'} \rangle \langle s_{j'} | \hat{w} | s_j \rangle \otimes | e_k \rangle = \sum_{j,j'} A_{jj'} \langle s_{j'} | \left( \sum_k \langle e_k | \hat{w} | e_k \rangle \otimes | e_k \rangle \right) |s_j \rangle = \text{Tr}_j (\hat{A} \hat{w}_s),$$

where $\hat{w}_s$ is defined as

$$\hat{w}_s \equiv \sum_k \langle e_k | \hat{w} | e_k \rangle = \text{Tr}_k \hat{w}.$$

Since Eq. (159) is similar to Eq. (5), $\hat{w}_s$ may serve as the statistical operator defined in the Hilbert space of the system of our interest. The huge advantage of Eqs. (159)-(160) is that they are valid for an arbitrary state of the local environment, including the case when it is in the thermodynamic equilibrium. By the way, the similarity of Eqs. (5) and (159) may serve as the strong argument, promised in Sec. 1, for the validity of the former relation even if the Universe as a whole is not in a pure state. (The argument is, however, imperfect, because the latter relation has been derived from the former one.)

---

60 As in Sec. 4, the reader not interested in the derivation of the basic equation (181) for the density matrix evolution may immediately jump to the discussion of this equation and its applications.
Now, since at a sufficiently large size of the local environment \( e \), the composite system \((s + e)\) may be considered Hamiltonian, with fixed probabilities of its states, for the description of time evolution of its statistical operator \( \hat{w} \) (again, in contrast to that, \( \hat{w}_s \), of the system of our interest) we may use the von Neumann equation (66). Partitioning its right-hand part in accordance with Eq. (68), we get:

\[
i \hbar \dot{\hat{w}} = \left[ \hat{H}_s, \hat{w} \right] + \left[ \hat{H}_e, \hat{w} \right] + \left[ \hat{H}_{\text{int}}, \hat{w} \right].
\]  

(7.161)

The next step is to use the perturbation theory to solve this equation in the lowest order in \( \hat{H}_{\text{int}} \) that yields nonvanishing results due to the interaction. For that, Eq. (161) is not very convenient, because its right-hand part contains two other terms, which are much larger than the interaction Hamiltonian. To mitigate this technical difficulty, the interaction picture (which was discussed in the end of Sec. 4.6), is very handy - though not absolutely necessary.

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 matrix) depend on time. However, the time evolution of the operator of any observable \( A \) is described by Eq. (67) with the unperturbed part of the Hamiltonian only – see Eq. (4.214). In our current case (68), this means

\[
i \hbar \dot{\hat{A}}_I = \left[ \hat{A}_I, \hat{H}_0 \right].
\]  

(7.162)

where the unperturbed Hamiltonian consists of two independent parts:

\[
\hat{H}_0 \equiv \hat{H}_s + \hat{H}_e.
\]  

(7.163)

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

\[
\hat{H}_I \equiv \hat{u}_0^\dagger \hat{H}_{\text{int}} \hat{u}_0
\]  

(7.164)

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

\[
i \hbar \dot{\hat{w}}_I = \left[ \hat{H}_I, \hat{w}_I \right].
\]  

(7.165)

Since this equation is similar in structure (with the opposite sign) to the Heisenberg equation (66), we may use solution Eq. (4.190) of the latter equation to write its analog:\footnote{Notice the opposite order of the unitary operators, which results from the already mentioned sign difference. Note also that we could write a similar expression in the Schrödinger picture: \( \hat{w}(t) = \hat{u}(0)\hat{w}(0)\hat{u}^\dagger(t) \), where \( \hat{u} \) is the full time-evolution operator.}

\[
\hat{w}_I(t) = \hat{u}_I(t,0)\hat{w}(0)\hat{u}_I^\dagger(t,0).
\]  

(7.166)

It is also straightforward to verify that in this picture, the expectation value of any observable \( A \) may be found from the expression similar to the basic Eq. (5):
\[ \langle A \rangle = \text{Tr}(\hat{A}, \hat{\psi}), \]  

so that the interaction and Schrödinger pictures give the same final results.

In the most frequent case of bilinear interaction (90), Eq. (162) is readily simplified, in different ways, for the both operators participating in the product. In particular, for \( \hat{A} = \hat{x} \), it yields

\[ i\hbar \dot{\hat{x}} = [\hat{x}, \hat{H}_0] = [\hat{x}, \hat{H}_s] + [\hat{x}, \hat{H}_e]. \]  

(7.168)

Since operator of coordinate is defined in the Hilbert space of system \( s \), it commutes with the Hamiltonian of the environment, so that we finally get

\[ i\hbar \dot{\hat{x}} = [\hat{x}, \hat{H}_s]. \]  

(7.169)

On the other hand, taking \( \hat{A} = \hat{F} \), we should take into account that the last 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

\[ i\hbar \dot{\hat{F}} = [\hat{F}, \hat{H}_e]. \]  

(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):

\[ \hat{F}_i(t) = \exp \left\{ \frac{i}{\hbar} \hat{H}_s t \right\} \hat{F}(0) \exp \left\{ -\frac{i}{\hbar} \hat{H}_e t \right\}, \]  

(7.171)

so that in the stationary (eigenstate) basis of the environment,

\[ \langle \hat{F}_i \rangle_{nm'}(t) = \exp \left\{ \frac{i}{\hbar} E_n t \right\} F_{nm'}(0) \exp \left\{ -\frac{i}{\hbar} E_{n'} t \right\} = F_{nm'}(0) \exp \left\{ -i \frac{E_n - E_{n'}}{\hbar} t \right\}, \]  

(7.172)

and similarly (but in the basis of the eigenstates of system \( s \)) for operator \( \hat{x} \). As a result, Eq. (164) may be also factored:

\[ \hat{H}_f(t) = \hat{u}^\dagger_0(t,0) \hat{H}_i \hat{u}_0(t,0) = \exp \left\{ \frac{i}{\hbar} (\hat{H}_s + \hat{H}_e) t \right\} \hat{x} \exp \left\{ -\frac{i}{\hbar} (\hat{H}_s + \hat{H}_e) t \right\} \]  

\[ = \left\{ \exp \left\{ \frac{i}{\hbar} \hat{H}_s t \right\} \hat{x} \exp \left\{ -\frac{i}{\hbar} \hat{H}_s t \right\} \right\} \left\{ \exp \left\{ \frac{i}{\hbar} \hat{H}_e t \right\} \hat{F}(0) \exp \left\{ -\frac{i}{\hbar} \hat{H}_e t \right\} \right\} = -\hat{x}_i(t) \hat{F}_i(t). \]  

(7.173)

Now, as in Sec. 4, we may rewrite Eq. (165) in the integral form:

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

(7.174)

62 A similar analysis of a more general case, when the interaction with environment may be represented as a sum of products of the type (90), may be found in a monograph by K. Blum, *Density Matrix Theory and Applications*, 3rd ed., Springer, 2012.
plugging this result, for time $t'$, into the right-hand part of Eq. (174) again, we get

$$\hat{\dot{\mathcal{W}}}_I(t) = -\frac{1}{\hbar^2} \int_{-\infty}^{t} [\hat{H}_I(t), [\hat{H}_I(t'), \hat{\dot{\mathcal{W}}}_I(t')]] dt' = -\frac{1}{\hbar^2} \int_{-\infty}^{t} [\hat{x}(t)\hat{F}(t), [\hat{x}(t')\hat{F}(t'), \hat{\dot{\mathcal{W}}}_I(t')]] dt', \quad (7.175)$$

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

So far, this equation is exact (and cannot be solved analytically), but this is the right time to notice that even if we take the density matrix in its right-hand part equal to its unperturbed value (corresponding to no interaction between system $s$ and its thermally-equilibrium environment $e$),

$$\hat{\mathcal{W}}_I(t') \rightarrow \hat{\mathcal{W}}_s(t')\hat{\mathcal{W}}_e, \quad \text{with} \quad \langle e_n | \hat{\mathcal{W}}_s | e_{n'} \rangle = W_n \delta_{nn'}, \quad (7.176)$$

where $e_n$ are the stationary states of the environment and $W_n$ are the Gibbs probabilities (23), Eq. (175) would still provide some nonvanishing time evolution of the density operator. This is exactly the first nonvanishing perturbation we have been looking for. Now using Eq. (160), we find the equation of evolution of the density operator of our system of interest:

$$\hat{\dot{\mathcal{W}}}_s(t) = -\frac{1}{\hbar^2} \int_{-\infty}^{t} \text{Tr}_n [\hat{x}(t)\hat{F}(t), [\hat{x}(t')\hat{F}(t'), \hat{\mathcal{W}}_s(t')\hat{\mathcal{W}}_e]] dt', \quad (7.177)$$

where the trace is over the stationary states of the environment. In order to spell out the right-hand part 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, so that we may write

$$\text{Tr}_n [\ldots, \ldots ] = \hat{x}(t)\hat{x}(t')\hat{\mathcal{W}}_s(t')\hat{\mathcal{W}}_e - \hat{x}(t)\hat{\mathcal{W}}_s(t')\hat{x}(t')\hat{\mathcal{W}}_e - \hat{\mathcal{W}}_s(t')\hat{x}(t)\hat{x}(t') - \hat{x}(t')\hat{\mathcal{W}}_e\hat{x}(t)\hat{x}(t') + \hat{\mathcal{W}}_s(t')\hat{x}(t)\hat{x}(t')\sum_{n,n'} F_{nm}(t)F_{n'm'}(t')W_n W_{n'}(t) - \hat{\mathcal{W}}_s(t')\hat{x}(t)\hat{x}(t')\sum_{n,n'} F_{nm}(t)W_n F_{n'm'}(t')$$

$$- \hat{x}(t')\hat{\mathcal{W}}_e\hat{x}(t) - \hat{x}(t)\hat{x}(t')\sum_{n,n'} F_{nm}(t)W_n F_{n'm'}(t) - \hat{x}(t')\hat{\mathcal{W}}_e\hat{x}(t) - \hat{x}(t)\hat{x}(t')\sum_{n,n'} W_n F_{nm}(t)F_{n'm'}(t')$$

$$= \hat{x}(t)\hat{x}(t')\sum_{n,n'} F_{nm}(t)F_{n'm'}(t')W_n W_{n'}(t) - \hat{x}(t)\hat{\mathcal{W}}_s(t')\hat{x}(t')\sum_{n,n'} F_{nm}(t)W_n F_{n'm'}(t')$$

$$- \hat{x}(t')\hat{\mathcal{W}}_e\hat{x}(t) - \hat{x}(t)\hat{x}(t')\sum_{n,n'} W_n F_{nm}(t)F_{n'm'}(t) - \hat{x}(t')\hat{\mathcal{W}}_e\hat{x}(t) - \hat{x}(t)\hat{x}(t')\sum_{n,n'} W_n F_{nm}(t)F_{n'm'}(t')$$

Since the summation on both indices $n$ and $n'$ in this expression is over the same energy level set (of all eigenstates of the environment), we may swap the indices in any of the sums. Doing that in the terms with factors $W_n$, we turn them into $W_n$, so that this factor becomes common:

$$\text{Tr}_n [\ldots, \ldots ] = \sum_{n,n'} W_n \hat{x}(t)\hat{x}(t')\hat{\mathcal{W}}_s(t')F_{nm}(t)F_{n'm'}(t') - \hat{x}(t)\hat{\mathcal{W}}_s(t')\hat{x}(t')\hat{\mathcal{W}}_e\hat{\mathcal{W}}_s(t')F_{nm}(t)F_{n'm'}(t')$$

$$- \hat{x}(t')\hat{\mathcal{W}}_e\hat{\mathcal{W}}_s(t')F_{nm}(t)F_{n'm'}(t') + \hat{\mathcal{W}}_s(t')\hat{\mathcal{W}}_e\hat{x}(t)F_{nm}(t)F_{n'm'}(t') - \hat{x}(t')\hat{\mathcal{W}}_e\hat{\mathcal{W}}_s(t')F_{nm}(t)F_{n'm'}(t') \quad (7.179)$$

Now using Eq. (172), we get
\[ \text{Tr}_n [... \ldots \ldots] = \sum_{n,n'} W_n |F_{nn'}|^2 \left[ \hat{x}(t) \hat{\tilde{x}}(t') \hat{w}_s(t') \exp \left\{ i \frac{\tilde{E}(t-t')}{\hbar} \right\} - \hat{x}(t) \hat{\tilde{w}}_s(t') \hat{\tilde{x}}(t') \exp \left\{ -i \frac{\tilde{E}(t-t')}{\hbar} \right\} \right. \\
\left. - \hat{x}(t) \hat{\tilde{w}}_s(t') \hat{\tilde{x}}(t') \exp \left\{ -i \frac{\tilde{E}(t-t')}{\hbar} \right\} \right] \]

(7.180)

where \{ \ldots \ldots \} means the anticommutator – see Eq. (4.34). 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 Green’s function (multiplied by \( \hbar/2 \)) of the time-difference argument \( \tau = t - t' \geq 0 \). As the result, Eq. (177) takes a very simple form:

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

(7.181)

Let me hope that the reader enjoys this beautiful result as much as I do, and that it is a sufficient intellectual award for his or her effort of following its derivation. It gives a self-sufficient equation for time evolution of the density matrix of the system of our interest (s), with the effects of its environment represented only by two real algebraic functions of \( \tau \) – one \( K_F \) describing environment’s fluctuations and another one \( G \) representing the average response to system’s dynamics. And most spectacularly, these are exactly the same functions as participate in the 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 that needs to be solved together with Eq. (169). Such equations do not allow explicit analytical solutions except for 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 \( \tau \) becomes larger than a certain environment correlation time \( \tau_\text{e} \), which is frequently much shorter than the time scales \( T_{nn'} \) of the evolution of the density matrix elements. Moreover, the characteristic time scale of the coordinate operator evolution may be also short on the scale of \( T_{nn'} \). In this limit, all arguments \( t' \) of the density operator giving substantial contributions to the right-hand part of Eq. (172) are so close to \( t \) that it does not matter whether its argument is \( t' \) or just \( t \). This simplification \( (t' \to t) \) is known as the Markov approximation.\(^{63}\) 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 our system of interest is time-independent and has a very discrete eigenenergy spectrum \( E_{nn'} \), with well-separated levels:

\(^{63}\) Named after A. Markov (1856-1922; in older literature, “Markoff”), because the result of this approximation is a particular case of the Markov process whose future development is completely determined by its present state.

\(^{64}\) Rather reluctantly, I will use this standard notation, \( E_{nn'} \), for the eigenenergies of our system of interest (s), in hope that the reader would not confuse these discrete energy levels with the quasi-continuous energy levels of its environment, participating in particular in Eqs. (108) and (111). As a reminder, by this stage of our calculations the environment levels have disappeared, leaving behind their “trace functions” \( K_F(\tau) \) and \( G(\tau) \).
\[ |E_n - E_{n'}| >> \frac{\hbar}{\mathcal{I}_{nn'}}. \] (7.182)

Let us see what does this condition yield for Eq. (181) rewritten for the matrix elements in the stationary state basis (from this point on, I will drop index \( s \) for brevity):

\[ \dot{w}_{nn'} = -\frac{i}{\hbar^2} \int_{-\infty}^{\infty} K_F(t-t') \{ [\hat{x}(t), \hat{\omega}(t')] w \}_{nn'} dt' - \frac{i}{2\hbar} \int_{-\infty}^{t'} G(t-t') \{ [\hat{x}(t), \hat{\omega}(t')] w \}_{nn'} dt'; \] (7.183)

after spelling out the commutators, it includes 4 operator products, which differ “only” by the operator order. Let us have a good look at the first product,

\[ (\hat{x}(t)\hat{x}(t')\hat{w})_{nn'} = \sum_{m,m'} x_{nm}(t)x_{nm'}(t')w_{nm'}, \] (7.184)

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

\[ (\hat{x}(t)\hat{x}(t')\hat{w})_{nm} = \sum_{m,m'} x_{nm}x_{nm'} \exp\{i(\omega_{mn}t + \omega_{nm'}t')\}w_{nm'}, \] (7.185)

where the coordinate matrix elements are in the Schrödinger picture now, and I have used the natural notation (6.85) for the quantum transition frequencies:

\[ \hbar \omega_{mn} \equiv E_n - E_{n'}. \] (7.186)

According to condition (182), frequencies \( \omega_{mn} \) with \( n \neq n' \) are much higher than the speed of evolution of the density matrix elements (in the interaction picture!) – in both the left-hand and right-hand parts of Eq. (183). As we already know from Sec. 6.5, this means that in the right-hand part of Eq. (183) we may keep only the terms that do not oscillate with frequencies \( \omega_{mn} \), because they would give negligible contribution to the density matrix dynamics.\(^{65}\) For that, in the double sum (185) we may keep only the terms proportional to difference \( (t - t') \), because they will give (after integration over \( t' \)) a slowly changing contribution to the right-hand part.\(^{66}\) These terms should have \( \omega_{mn} + \omega_{nm} = 0 \), i.e. \( (E_n - E_m) + (E_m - E_{m'}) \equiv E_n - E_{n'} = 0 \). For a non-degenerate energy spectrum, this requirement means \( m' = n \); as a result, the double sum is reduced to a single one:

\[ (\hat{x}(t)\hat{x}(t')\hat{w})_{nn'} \approx \sum_m x_{nm}x_{nm} \exp\{i\omega_{nm}(t-t')\}w_{nn'} = \sum_m |x_{nm}|^2 \exp\{i\omega_{nm}(t-t')\}w_{nn'}. \] (7.187)

Another product, \( (\hat{\omega}\hat{x}(t')\hat{x})_{m'n'} \), that appears in the right-hand part of Eq. (183), may be simplified absolutely similarly, giving

\[ (\hat{\omega}\hat{x}(t')\hat{x})_{m'n'} \approx \sum_m |x_{m'n'}|^2 \exp\{i\omega_{m'n}(t'-t')\}w_{m'n'}. \] (7.188)

\(^{65}\) This is essentially the same rotating-wave approximation (RWA) that is so instrumental in other fields of not only quantum mechanics, but classical physics as well – see, e.g., CM Secs. 4.2-4.5.

\(^{66}\) As was already discussed in Sec. 4, the lower-limit substitution \( (t' = -\infty) \) in integrals (174) 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 \( \tau = t - t' \).
These expressions hold true whether \( n \) and \( n' \) are equal or not. The situation is different for two other products in the right-hand part of Eq. (183), with \( w \) sandwiched between \( x \) and \( x' \). For example,

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

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

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

Here the double sum 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 diagonal elements \((n = n')\), the RWA requirement is reduced to \( m = m' \), giving sums over all diagonal elements of the density matrix:

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

(Another similar term \((\hat{x}(t')\hat{w}(t))_{nn'}\), is just a complex conjugate of Eq. (191).) However, for off-diagonal matrix elements \((n \neq n')\), the situation is different: Eq. (190) may be satisfied only if \( m = n \) and also \( m' = n' \), so that the double sum is reduced to just one, non-oscillating term:

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

The second similar term, \((\hat{x}(t')\hat{w}(t))_{nn'}\), is exactly the same, so that in one of the integrals of 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\(^67\) relating diagonal elements \( w_{nn} \) of the density matrix, i.e. the energy level occupancies \( W_n \): \(^68\)

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

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

\[
\dot{W}_n = \sum_{n' \neq n} (\Gamma_{n \rightarrow n'} W_{n'} - \Gamma_{n' \rightarrow n} W_n), \tag{7.194}
\]

where coefficients

\[
\Gamma_{n' \rightarrow n} = |x_{nn'}|^2 \int_0^\infty \frac{2}{\hbar^2} K_F(\tau) \cos \omega_{nn'} \tau - \frac{1}{\hbar} G(\tau) \sin \omega_{nn'} \tau \ d\tau', \tag{7.195}
\]

\(^67\) The master equations, first introduced to quantum mechanics in 1928 by W. Pauli, are sometimes called the “Pauli master equations”, or “kinetic equations”, or “rate equations”.

\(^68\) As Eq. (193) shows, the term with \( m = n \) would vanish, and thus may be legitimately excluded from the sum.
are called the \textit{interlevel transition rates}.\textsuperscript{69} Equation (194) has a very clear physical meaning of the level occupancy dynamics (i.e. the balance of probability flows $\Gamma W$) due to the quantum transitions between the energy levels (Fig. 6), in our current case caused by the interaction between the system of our interest and its environment.\textsuperscript{70}

\begin{equation}
\Gamma_{n\rightarrow n'} = \frac{1}{\hbar} |\chi''(\omega_{mn})| \left( \coth \frac{\hbar \omega_{mn}}{2k_B T} - 1 \right) = \frac{2}{\hbar} |\chi''(\omega_{mn})| \frac{\chi''(\omega_{n'n'})}{\exp\left(\frac{(E_n - E_{n'})}{k_B T}\right) - 1}.
\end{equation}

\textsuperscript{69} As Eq. (193) shows, the result for $\Gamma_{n\rightarrow n'}$ is described by Eq. (195) as well, provided that indices $n$ and $n'$ are swapped in all components of its right-hand part, including the swap $\omega_{nn'} \rightarrow \omega_{n'n} = -\omega_{nn'}$.

\textsuperscript{70} It is straightforward to show that at relatively low temperatures ($k_B T \ll |E_{n'} - E_n|$), Eq. (196) gives the same result as the Golden Rate formula (6.134) – see Exercise 2. (The low temperature limit is necessary to ensure that the initial occupancy of the excited level is negligible, as was assumed at the derivation of Eq. (6.134).)
systems including quantum generators (masers and lasers). It is important to remember that it is strictly valid only in the rotating-wave approximation, i.e. if Eq. (182) is well satisfied for all \( n \) and \( n' \).

For a particular but very important case of a two-level system (with, say, \( E_1 > E_2 \)), the rate \( \Gamma_{1 \rightarrow 2} \) may be interpreted (especially in the low-temperature limit \( k_B T \ll \hbar \omega_{12} = E_1 - E_2 \), when \( \Gamma_{1 \rightarrow 2} \gg \Gamma_{2 \rightarrow 1} \)) as the reciprocal characteristic time \( 1/T_1 \equiv \Gamma_{1 \rightarrow 2} \) of the energy relaxation process that brings the diagonal elements of the density matrix to their thermally-equilibrium values (24). For the Ohmic dissipation described by Eqs. (137)-(138), Eq. (196) yields

\[
\frac{1}{T_1} \equiv \Gamma_{1 \rightarrow 2} = \frac{2}{\hbar^2} |x_{12}|^2 \eta \times \begin{cases} \hbar \omega_{12}, & \text{for } k_B T \ll \hbar \omega_{12}, \\ k_B T, & \text{for } \hbar \omega_{12} \ll k_B T. \end{cases}
\]  

(7.199)

Of course, time \( T_1 \) should not be confused with the characteristic time \( T_2 \) of relaxation of the off-diagonal elements, i.e. dephasing, which was already discussed in Sec. 3. By the way, let us see what do Eqs. (183) say about the dephasing rate. Taking into account our intermediate results (187)-(192), and merging the non-oscillating components (with \( m = n \) and \( m = n' \)) of sums Eq. (187) and (188) with the terms (192), that also do not oscillate in time, we get the following equation:71

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

(7.200)

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

\[
\dot{w}_{nn'} = -(1/T_{nn'} + i \Delta_{nn'}) w_{nn'},
\]  

(7.201)

where both factors \( 1/T_{nn'} \) and \( \Delta_{nn'} \) are real.72 As should be clear from Eq. (201), the second term in the right-hand part of this equation causes slow oscillations of the matrix elements \( w_{nn'} \); that, after returning to the Schrödinger picture, add just small corrections73 to the unperturbed frequencies (186) of their oscillations, and are hence are not important for most applications. More important is the first term,

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71 Because of the reason explained above, this (relatively :-) simple result is not valid for systems with equidistant energy spectra, most importantly, for the harmonic oscillator (while Eq. (7.194) is). For the oscillator, with its simple matrix elements \( x_{nn'} \), it is straightforward to repeat the above calculations, starting from (7.183), to obtain an equation similar to Eq. (7.200), but with two other terms, proportional to \( w_{nn' \pm 1 \pm 1} \), in its right-hand part. Since for the harmonic oscillator the Heisenberg-Langevin approach allows obtaining most results in a much simpler way, I will skip the derivation of this equation and the discussion of its solutions. The interested reader may find such a discussion, for example, in a paper by B. Zeldovich et al., Sov. Phys. JETP 28, 308 (1969).

72 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 several other authors, notably including (in the alphabetical order) H. Haken, W. Lamb, M. Lax, W. Louisell, and M. Scully, also made key contributions into the very fast development of the density-matrix approach to open quantum systems in the mid-1960s.

73 This correction is frequently called the Lamb shift, because it was first observed experimentally in 1947 by W. Lamb and R. Retherford, as a minor, \( \sim 1 \) GHz shift between energy levels of \( 2s \) and \( 2p \) states of hydrogen, due to the electric-dipole coupling of hydrogen atoms to the free-space electromagnetic environment. (These levels are equal not only in the non-relativistic theory (Sec. 3.6), but also in the relativistic, Dirac theory (Sec. 9.7), if the
\[ \frac{1}{T_{nn'}} = \frac{1}{\hbar} \int_0^\infty K_F(\tau) \left( \sum_{m \neq n} |x_{nm}|^2 \cos \omega_{nm} \tau + \sum_{m \neq n'} |x_{nm'}|^2 \cos \omega_{nm'} \tau + (x_{nn'} - x_{n'n'})^2 \right) \]
\[ - \frac{1}{2\hbar} G(\tau) \left( \sum_{m \neq n} |x_{nm}|^2 \sin \omega_{nm} \tau + \sum_{m \neq n'} |x_{nm'}|^2 \sin \omega_{nm'} \tau \right) \]  
\( d\tau, \) for \( n \neq n', \)  
\( (7.202) \)

because it describes the effect absent without the environment: an exponential decay of the off-diagonal matrix elements, i.e. dephasing. Comparing the first 2 terms of Eq. (202) with Eq. (195), we see that the dephasing rates may be described by a very simple formula:
\[
\frac{1}{T_{nn'}} = \frac{1}{2} \left( \sum_{m \neq n} \Gamma_{n \rightarrow m} + \sum_{m \neq n'} \Gamma_{n' \rightarrow m} \right) + \frac{\pi}{\hbar^2} (x_{nn'} - x_{n'n'})^2 S_F(0) 
\]
\[ = \frac{1}{2} \left( \sum_{m \neq n} \Gamma_{n \rightarrow m} + \sum_{m \neq n'} \Gamma_{n' \rightarrow m} \right) + \frac{k_B T}{h^2} \eta (x_{nn'} - x_{n'n'})^2, \quad \text{for} \ n \neq n', 
\]
\[ (7.203) \]
where the low-frequency drag coefficient \( \eta \) is again defined as \( \lim_{\omega \rightarrow 0} \chi''(\omega)/\omega \) - see Eq. (138).

This result shows that two effects yield independent contributions into dephasing. The first of them may be interpreted as a result of the “virtual” transitions of the system to other energy levels \( m; \) according to Eq. (187), it is proportional to the strength of coupling to environment at relatively high frequencies \( \omega_{nm} \) and \( \omega_{nm'}. \) (If the energy quanta \( \hbar \omega \) of these frequencies are much larger than the thermal fluctuation scale \( k_B T, \) only the lower levels, with \( E_m < \max[E_n, E_n'] \) are important.) 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. If the susceptibility (more exactly, the ratio \( \eta = \chi''(\omega)/\omega \) is frequency-independent, both contributions are of the same order, but their exact relation depends on the relation between the matrix elements \( x_{nn'} \) of a particular system.

Returning again to the two-level system discussed in Sec. 3, the high-frequency contributions vanish because of the absence of transitions between its energy levels, while the low-frequency contribution yields
\[
\frac{1}{T_2} = \frac{1}{T_{12}} = \frac{k_B T}{h^2} \eta (x_{nn'} - x_{n'n'})^2 \rightarrow \frac{k_B T}{h^2} \eta \left[ (\sigma_z)_{11} - (\sigma_z)_{22} \right] \frac{3}{2} = \frac{4k_B T}{h^2} \eta, 
\]
\[ (7.204) \]
thus exactly reproducing the result (142) of the Heisenberg-Langevin approach.\(^74\) Note also that Eq. (204) for \( T_2 \) is very close in structure to Eq. (199) for \( T_1. \) For our simple interaction model (70), the off-diagonal elements of operator \( \hat{x} = \hat{\sigma}_z \) in the stationary-state \( z \)-basis vanish, so that \( T_1 \to \infty. \) For the two-well implementation of the model (see Fig. 4 and its discussion), this result corresponds to a very high energy barrier between the wells, that inhibits tunneling, and hence any change of well occupancies \( W_L \)
electromagnetic environment is ignored.) The explanation of the shift, by H. Bethe in the same 1947, has launched the whole field of quantum electrodynamics – to be briefly discussed in Chapter 9.\(^74\) The first form of Eq. (203), as well as the analysis of Sec. 3, imply that low-frequency fluctuations of any other origin, not taken into account in own current calculations (say, unintentional noise from experimental equipment), may also cause dephasing; such “technical fluctuations” are indeed a serious challenge at the experimental implementation of coherent qubit systems – see Sec. 8.5 below.
and $W_R$. However, $T_1$ may become finite, and comparable with $T_2$, if tunneling between the wells is substantial.\textsuperscript{75}

Now let us briefly discuss dissipative systems with \textit{continuous} spectrum. Unfortunately, for them the only (relatively :-) simple results that may be obtained from Eq. (181) are essentially classical in nature. As an illustration, let us consider the simplest example of a 1D particle that interacts with a thermally-equilibrium environment, but otherwise is free to move (unconfined). As we know from Chapters 2 and 5, in this case the most convenient basis is that of momentum eigenstates $p$. In the momentum representation, the density matrix is just the $c$-number function $w(p, p')$, defined by Eq. (54), that has already been discussed in brief in Sec. 2. On the other hand, the coordinate operator, that also participates in the right-hand part of Eq. (181), has the form given by the first of Eqs. (5.64),

\[
\hat{x} = i\hbar \frac{\partial}{\partial p},
\]

dual to the coordinate representation formula (5.29). As we already know, such operators are local – see, e.g., Eq. (5.28b). Due to this locality, the whole right-hand part of Eq. (181) is local as well, and hence (within the framework of our perturbative treatment) the interaction with environment affects essentially only the diagonal values $w(p, p)$ of the density matrix, i.e. the momentum probability density $w(p)$. Let us find the equation governing the evolution of this function in time.

Generally, in the interaction picture, matrix elements of operators $\hat{x}$ and $\hat{w}$ acquire some time dependence, but in the limit $p' \to p$, this dynamics lacks the high frequencies (186) that have been so helpful for the derivation of master equations. As a result, the only serious simplification of Eq. (181) is possible in the Markov approximation, when the time scale of the density matrix evolution is much longer than the correlation time $\tau_c$ of the environment, i.e. the time scale of functions $K_F(\tau)$ and $G(\tau)$. In this approximation, we may take the matrix elements out of the first integral of Eq. (181),

\[
-\frac{1}{\hbar^2} \int_0^\infty K_F(t-t')dt' [\hat{x}(t), [\hat{x}(t'), \hat{w}(t')]] \approx -\frac{1}{\hbar^2} \int_0^\infty K_F(\tau)d\tau [\hat{x}, [\hat{x}, \hat{w}]]
\]

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

and calculate the double commutator in the Schrödinger picture. This may be done either using an explicit expression for the matrix elements of the coordinate operator, dual to Eq. (5.28b), 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 one of its arguments (say, $p$),

\[
f(p) = \sum_{k=0}^\infty \frac{1}{k!} \frac{\partial^k f}{\partial p^k} p^k,
\]

and applying Eq. (205) to each term, we can prove the following simple commutation relation:

\textsuperscript{75} The tunneling may be described without altering Eq. (70), just by adding, to the unperturbed Hamiltonian (69), terms proportional to other Pauli matrices. The reader is encouraged to spell out the equations for the time evolution of the density matrix elements of this system, and analyze their main properties – at least in the low-temperature limit.
\[
[\hat{x}, f] = \sum_{k=0}^{\infty} \frac{1}{k!} \frac{\partial^k f}{\partial p^k} [\hat{x}, p^k] = \sum_{k=0}^{\infty} \frac{1}{k!} \frac{\partial^k f}{\partial p^k} (ihkp^{k-1}) = i\hbar \sum_{k=1}^{\infty} \frac{1}{(k-1)!} \frac{\partial^{k-1} f}{\partial p^{k-1}} \left( \frac{\partial}{\partial p} \right)^{k-1} p^{k-1} = i\hbar \frac{\partial f}{\partial p}.
\] (7.208)

Now applying this result sequentially, first to \( w(p, p') \) and then to the resulting commutator, we get

\[
[\hat{x}, [\hat{x}, w]] = \left[ \hat{x}, i\hbar \frac{\partial w}{\partial p} \right] = i\hbar \frac{\partial}{\partial p} \left( i\hbar \frac{\partial w}{\partial p} \right) = -\hbar^2 \frac{\partial^2 w}{\partial p^2}.
\] (7.209)

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 that in order to calculate the first nonvanishing 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 Hamiltonian consisting of the kinetic-energy contribution alone:

\[
\hat{x}(t') - \hat{x}(t) \approx -\tau \frac{1}{i\hbar} [\hat{x}, \hat{H}_x] = -\tau \frac{1}{i\hbar} \left[ \hat{x}, \frac{\hat{p}^2}{2m} \right] = -\tau \frac{\hat{p}}{m},
\] (7.210)

where the exact argument of the operator in the right-hand part 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 in the right-hand part of Eq. (181) to

\[
-\frac{i}{2\hbar} \int_{-\infty}^{t} G(t - t') \left[ \hat{x}(t'), \{\hat{x}(t'), \hat{w}(t')\} \right] dt' \approx \frac{i}{2\hbar} \int_{0}^{\infty} G(\tau) \tau d\tau \left[ \hat{x}, \{\hat{p}, \hat{w}\} \right] = \frac{\eta}{2i\hbar} \left[ \hat{x}, \{\hat{P}, \hat{W}\} \right].
\] (7.211)

In the momentum representation, the momentum operator and the density matrix \( w \) are just c-numbers and commute, so that, applying Eq. (208) to product \( pw \), we get

\[
\left[ \hat{x}, \left\{ \hat{P}, \hat{W} \right\} \right] = \left[ \hat{x}, 2 \frac{\hat{P}}{m} w \right] = 2i\hbar \frac{\partial}{\partial p} \left( \frac{P}{m} w \right),
\] (7.212)

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

\[
\frac{\partial w}{\partial t} = \frac{\partial}{\partial p} \left( \eta \frac{P}{m} w \right) + k_BT \eta \frac{\partial^2 w}{\partial p^2}.
\] (7.213)

This is the 1D form of the famous **Fokker-Planck equation** describing the classical statistics of motion of a free 1D particle in a medium with a linear drag characterized by the coefficient \( \eta \). The first, **drift** term in the right-hand part of Eq. (213) describes particle’s deceleration due to the average viscous force (137), \( \langle F \rangle = -\eta v = -\eta \hat{p}/m \), provided by the environment, while the second, **diffusion** term describes the effect of fluctuations: particle’s random walk that obeys Eq. (85) with the diffusion coefficient

\[
D = \eta k_B T.
\] (7.214)

This fundamental **Einstein relation**,\(^76\) shows again the intimate connection between the dissipation (friction) and fluctuations, in this classical limit represented by their thermal energy scale \( k_B T \).\(^77\)

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\(^76\) It was the main result of A. Einstein’s pioneering analysis of such **Brownian motion** in 1905. (The development of this analysis in 1906-1908 by M. Smoluchowski has led in 1912 to the Fokker-Planck theory.)
Just for reader’s reference, let me note that the Fokker-Planck equation (213) may be readily generalized to the 3D motion of a particle under the effect of an additional external force $F_{\text{ext}}(r, t)$:

$$\frac{\partial w}{\partial t} = -\nabla \left( \frac{p}{m} w \right) - \nabla_p \cdot (F w) + D \nabla^2 p w, \quad \text{with } F = F_{\text{ext}} - \eta \frac{p}{m},$$

(7.215)

where $w = w(r, p, t)$ is the time-dependent probability density in the 6D phase space, and $\nabla_p$ is the nabla/del operator of differentiation over the momentum components, defined similarly to its coordinate counterpart $\nabla$. The Fokker-Planck equation in this form is the basis for many important applications; however, due to its classical character, its discussion is left for the SM part of my lecture notes.

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 three sections, let me emphasize that they give descriptions of the same phenomena, and are characterized by the same two functions $G(\tau)$ and $K_{\text{F}}(\tau)$, but from two different points of view. Namely, in the Heisenberg-Langevin approach we describe the system by operators that change (fluctuate) in time, even in thermal equilibrium, while in the density-matrix approach the system is described by non-fluctuating probability functions, such as $W_n(t)$ or $w(p)$, that are stationary in equilibrium. In the (relatively rare) cases when a problem may be solved by either method, they give identical results for all observables.

### 7.7. Quantum measurements

Now we have got a sufficient quantum mechanics background for a brief discussion of quantum measurements. Let me start with reminding the reader the only postulate of quantum mechanics that relates this theory with experiment. In Chapter 4 it was formulated for a pure state described with ket-vector

$$|\alpha\rangle = \sum_j \alpha_j |a_j\rangle,$$

(7.216)

---

77 This classical relation may be derived using several other ways – including those much simpler than used above. For example, since the Brownian particle’s motion may be described by a linear Langevin equation, Eq. (214) may be readily obtained from the Nyquist formula (139) – see, e.g., SM Sec. 5.5.

78 Moreover, Eq. (213) may be generalized to the motion in an additional periodic potential $U(r)$. In this case, an analog of Eq. (215) for the probability density of quasi-momentum $\hbar \mathbf{q}$ (rather than the genuine momentum $\mathbf{p}$) includes an additional energy band index (say, $n$), an additional force $F_{\text{an}} = -\nabla E_n$ (where $E_n(\mathbf{q})$ is the energy band structure that was discussed in Secs. 2.7 and 3.4), and an additional term similar to the right-hand part of Eq. (194), describing interband transitions with quasi-momentum-dependent rates $\Gamma_{n\rightarrow n'}(\mathbf{q})$. These rates are still expressed by Eq. (196), but with the matrix elements $x_{nm}$ replaced by those of the vector operator $\hat{\Omega} \equiv \hat{r} - i \hat{\nabla}_q$ of interband transitions, which was discussed in Chapter 5. For details and a particular example of a sinusoidal potential see, e.g., K. Likharev and A. Zorin, *J. Low Temp. Phys.*, 59, 347 (1985).


80 “Quantum measurements” is a very unfortunate term; it would be more sensible to speak about “measurements of quantum mechanical observables”. However, the former term is so common and compact that I will use it.
where $a_j$ and $A_j$ are, respectively, the eigenstates of the operator of observable $A$, defined by Eq. (4.68). According to the postulate, the outcome of each particular measurement of observable $A$ may be uncertain, but is restricted to the set of eigenstates $A_j$, with the probability of outcome $A_j$ equal to

$$W_j = |\alpha_j|^2.$$  

(7.217)

Since we know now that the state of the system (or rather of the statistical ensemble of similar systems we are using for measurements) is generally not pure, this postulate should be re-worded as follows: even if the system is in the least uncertain state (216), the measurement outcomes are still probabilistic, and obey Eq. (133).  

Quantum measurement may be understood as a procedure of transferring the “microscopic” information contained in coefficients $\alpha_j$ into “macroscopically” available information about the outcomes of particular experiments, that may be recorded and reliably stored – say, on paper, or in a computer, or in our minds. If we believe that such transfer may be always done well enough, and do not worry too much how exactly, we are subscribing to the mathematical notion of measurement, that was (rather reluctantly) used in these notes – up to this point. However, every physicist should understand that measurements are performed by physical devices that also should obey the laws of quantum mechanics, and it is important to understand the basic laws of their operation.

The founding fathers of quantum mechanics have not paid much attention to these issues, probably because of the following two reasons. First, at that time it looked like the experimental instruments (at least the best of them :-) were doing exactly what postulate (217) was telling. For example, had not the $z$-oriented Stern-Gerlach experiment turned two complex coefficients $\alpha_\uparrow$ and $\alpha_\downarrow$, describing the incoming electron beam, into particle counter clicks with rates proportional to, respectively, $|\alpha_\uparrow|^2$ and $|\alpha_\downarrow|^2$? Also, the crude internal nature of these instruments made more detailed questions unnatural. For example, the electron rate counting with a Geiger counter involves an effective disappearance of each incoming electron inside a zillion-particle electric discharge avalanche. Thinking about such devices, it was hard to even imagine measurements that would not disturb the quantum state of the particle being measured.

However, since that time the experimental techniques, notably including high vacuum, low temperatures, and low-noise electronics, have much improved, and eventually more inquisitive questions started to look not so hopeless. In my scheme of things, these questions may be grouped as follows:

(i) What are the main laws of a quantum measurement as a physical process? In particular, should it always involve time irreversibility? a human/intelligent observer? (The last question is not as laughable as it may look – see below.)

(ii) What is the state of the measured system just after a single-shot measurement - meaning the measurement process limited to a time interval much shorter that the time scale of measured system’s evolution? This question is naturally related to the issues of repeated measurements and continuous monitoring of system’s state.

81 Besides the trivial case $\alpha_j = \delta_{jj'}$ (so that $W_j = \delta_{jj'}$), when the system is in a certain eigenstate ($a_j$) of operator $\hat{A}$ .

82 The reader in doubt is invited to compare entropy $\mathcal{S} = -\sum W_j \ln W_j$, the measure of system’s disorder (see, e.g., SM Sec. 2.2) of the pure state ($\mathcal{S} = 0$) with that in any state with several nonvanishing values of $W_j$ ($\mathcal{S} > 0$).
(iii) If a measurement of observable $A$ produced a certain outcome $A_j$, can we believe that the system had been in the corresponding state $\alpha_j$ just before the measurement?

The last question is most closely related to various interpretations of quantum mechanics, and will be discussed in the concluding Chapter 10, and now let me provide some input on the first two groups of issues.

First of all, I am happy to report that there is a virtual consensus of physicists on the two first questions of series (i). According to this consensus, any quantum measurement needs to result in a certain, distinguishable state of a macroscopic output component of the measurement instrument - see Fig. 7. (Traditionally, its component is called a pointer, though its role may be played by a printer or a plotter, an electronic circuit sending out the result as a number, etc.).

This requirement implies that the measurement process should have the following features:

- be time-irreversible,
- provide large “signal gain”, i.e. mapping the quantum process with its $\hbar$-scale of action (i.e. of the energy-by-time product) onto a macroscopic motion of the pointer with a much larger action scale, and
- if we want high measurement fidelity, the process should introduce as little additional uncertainty as permitted by the law of physics.

All these requirements are fulfilled in a good Stern-Gerlach experiment. However, since the internal physics of the particle detector at this measurement is rather complex, let me give an example of a different, more simple single-shot scheme capable of measuring the instant state of a typical two-level system, for example, a particle in a double quantum well potential (Fig. 8). Let the system be, at $t = 0$, in a pure quantum state described by ket-vector

$$\alpha = \alpha_+ |\rightarrow\rangle + \alpha_- |\leftarrow\rangle,$$  \hspace{1cm} (7.218)

83 This scheme may be implemented, for example, using a simple Josephson-junction circuit called the balanced comparator - see, e.g., T. Walls et al., IEEE Trans. on Appl. Supercond. 17, 136 (2007), and references therein. Experiments by V. Semenov et al., IEEE Trans. Appl. Supercond. 7, 3617 (1997) have demonstrated that this system may have measurement accuracy dominated by quantum-mechanical uncertainty at relatively modest cooling (to ~ 1K). One of advantages of such implementation of this measurement scheme is that it is based on externally-shunted Josephson junctions – devices whose quantum-mechanical model is in a quantitative agreement with experiment - see, e.g., D. Schwartz et al., Phys. Rev. Lett. 55, 1547 (1985). Colloquially, the balanced comparator is an instrument with a “well-documented Hamiltonian” including its part describing coupling to environment.

84 As a reminder, dynamics of this system was discussed in Sec. 2.6 and then again in Sec. 6.1.
where the component states $\rightarrow$ and $\leftarrow$ may be described by wavefunctions localized near the potential well bottoms at $x_s \sim \pm x_0$ – see the blue lines in Fig. 8b. Let us rapidly change the potential profile of the system at $t = 0$, so that at $t > 0$, and near the origin, it may be well approximated by an inverted parabola (see the red line in Fig. 8b):

$$U(x_s) \approx -\frac{m\lambda^2}{2}x_s^2, \quad \text{at } t > 0, \quad |x_s| \ll x_f. \quad (7.219)$$

![Diagram of potential inversion](image)

It is straightforward to verify that the Heisenberg equations of motion in such inverted potential describe an exponential growth of operator $\hat{x}_s$ in time (proportional to $\exp\{\lambda t\}$ and hence a similar growth of the expectation value $\langle x_s \rangle$ and its r.m.s. uncertainty $\delta x_s$. At this “inflation” stage, the coherence between the two component states $\rightarrow$ and $\leftarrow$ is still preserved, i.e. the time evolution is reversible.

Now let the system be weakly coupled to a dissipative (e.g., Ohmic) environment. As we already know, the environment performs two functions. First, it provides motion with the drag coefficient $\eta$ (141), so that the system would eventually come to rest at one of the relatively distant minima, $\pm x_0$, of the inverted potential (Fig. 8a). Second, the dissipative environment ensures state’s dephasing on some time scale $T_2$. If we select the measurement system parameters in such a way that

$$x_0 \ll x_f \exp\{\lambda T_2\} \ll x_f, \quad (7.220)$$

then the process, after the potential inversion, consists of the following stages, well separated in time:

- the “inflation” stage, preserving the component state coherence but providing an exponential increase of its energy,

---

85 Somewhat counter-intuitively, the latter growth plays a positive role for measurement fidelity. Indeed, it does not affect the intrinsic “signal-to-noise ratio” $\delta x_s/\langle x_s \rangle$, while making the intrinsic (say, quantum-mechanical) uncertainty much larger that possible noise contribution by the latter measurement stage(s).
- the dephasing stage, at which the coherence is suppressed, and the density matrix of the system is reduced to a diagonal form describing the classical mixture of the probability packets propagating to the left and to the right, and

- the stage of settling to a new stationary state – a classical mixture of two states located near points $x_s = \pm x_f$, with probabilities (217) equal to, respectively, $W_\rightarrow = |\alpha_\rightarrow|^2$ and $W_\leftarrow = |\alpha_\leftarrow|^2 = 1 - |\alpha_\rightarrow|^2$.

If the final states are macroscopically distinguishable (i.e. may play the role of a bistable pointer), as they are in the balanced-comparator implementation, there is absolutely no need, at any of these stages, to involve any mysterious “another mechanism of wavefunction change” (different from the regular, Schrödinger evolution) for the measurement process description.

This may be the only appropriate time to mention, very briefly, the famous - or rather infamous *Schrödinger cat paradox* so much overplayed in popular press. (The only good aspect of this popularity is that the formulation of this paradox is certainly so well known to the reader, that I do not need to repeat it.) In this thought experiment, there is no need to discuss the (rather complex :-) physics of the cat. As soon as the charged particle, produced at the radioactive decay, reaches the Geiger counter, the process rapidly becomes irreversible, so that the coherent state of the system is reduced to a classical mixture of two possible states: “decay” – “no decay”, leading, correspondingly, to the “cat alive” – “cat dead” states. So, despite attempts by numerous authors, typically without proper physics background, to present this situation as a mystery whose discussion needs the involvement of professional philosophers, hopefully by this point the reader knows enough about dephasing to pay any attention. Let me, however, note the two non-trivial features of this gedanken experiment, that are met in most real experiments as well, including that with the potential inversion (Fig. 8).

First, the role of the measured coordinate of the system under observation ($s$) may be played not by a coordinate of a single fundamental particle, but a certain combination of coordinates of many microscopic components of a macroscopic body. In particular, in Josephson junction systems such as the balanced comparator we essentially measure the persistent electric current (“supercurrent”) - a certain linear combination of Cartesian components of the momenta of the electrons that constitute the Bose-Einstein condensate of Cooper pairs. At that, the role of the local environment (that contributes significantly to dissipative phenomena) is played by the same electrons, with other linear combinations of electron momenta playing the role of environmental degrees of freedom - which were called \{λ\} in the last few sections. This makes the coupling to environment somewhat less apparent (at least for the people who do not know what a linear combination is :-).  

Second, one may argue that even after the balanced comparator (in our first example) or the cat (in the second example) has reached its final macroscopic state, human observer’s realization that in this particular experiment the bistable pointer is in a certain state instantly decreases the probability (for the same observer!) of its being in the opposite state to zero. However, as was already discussed in Sec. 2.5, this is a very classical problem of the statistical ensemble redefinition that may be (or may be not) performed at observer’s will. Such redefinition, if performed, is the only possible role of a human (or otherwise intelligent :-) observer in the measurement process; if we are only interested in an objective recording of results of a pre-fixed sequence of experiments, there is no need to include such observer into any discussion.
The ensemble redefinition at measurement leads to several other paradoxes, of which the so-called quantum Zeno paradox is perhaps most spectacular. Let us return to a two-level system with the unperturbed Hamiltonian given by Eq. (4.166), with \(2\pi/\Omega\) much longer than the single-shot measurement time, in which the system initially (at \(t = 0\)) is in a certain quantum well. Then, as we know from Secs. 2.6 and 4.6, before the first measurement, the probability to find state in the initial state at time \(t\) is

\[
W(t) = \cos^2 \frac{\Omega t}{2}.
\]  

(7.221)

If the time is small enough (\(t = dt \ll 1/\Omega\)), we may use the Taylor expansion to write

\[
W(dt) \approx 1 - \frac{\Omega^2 dt^2}{4}.
\]  

(7.222)

Now, let us return the two-level system, after its measurement, into the same quantum well, and let it evolve with the same Hamiltonian. Since the occupation of the opposite state is very small, the evolution of \(W\) will closely follow the same law as in Eq. (221), but with the initial value given by Eq. (222) Thus, when the system is measured again at time \(2dt\),

\[
W(2dt) \approx W(dt) \left(1 - \frac{\Omega^2 dt^2}{4}\right) = \left(1 - \frac{\Omega^2 dt^2}{4}\right)^2.
\]  

(7.223)

After repeating this cycle \(N\) times (with the total time \(t = Nd\) still much less than \(N^{1/2}/\Omega\)), the probability that the system is still in the initial state is

\[
W(Nd) \equiv W(t) \approx \left(1 - \frac{\Omega^2 dt^2}{4}\right)^N = \left(1 - \frac{\Omega^2 t^2}{4N^2}\right)^N \approx 1 - \frac{\Omega^2 t^2}{4N}.
\]  

(7.224)

Comparing this result with Eq. (222), we see that the process of system transfer to the opposite quantum well has been slowed down rather dramatically, and in the limit \(N \to \infty\) (at fixed \(t\)), its evolution is completely stopped by the measurement process. There is of course nothing mysterious here; the evolution slowdown is due to statistical ensemble’s redefinition.

Now let me proceed to question group (ii), in particular to the general issue of the back action of the instrument upon the system under measurement (symbolized with the back arrow in Fig. 7). In instruments like the Geiger counter or the balanced comparator, such back action is very large, because the instrument essentially destroys (“demolishes”) the initial state of the system under measurement.

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86 This name, coined by E. Sudarshan and B. Mishra in 1997 (though the paradox had been discussed in detail by A. Turing in 1954); is due to the apparent similarity of this paradox to classical paradoxes by ancient Greek philosopher Zeno of Elea. By the way, just to have a minute of fun, let us have a look what happens when Mother Nature is discussed by people to do not understand math and physics. The most famous of the classical Zeno paradoxes is the Achilles and Tortoise case: a fast runner Achilles can apparently never overtake a slower Tortoise, because (in the words by Aristotle) “the pursuer must first reach the point whence the pursued started, so that the slower must always hold a lead”. For a physicist, the paradox has a trivial resolution, but let us listen what a philosopher (D. Burton) writes about it - not in some year BC, but in 2010 AD: "Given the history of 'final resolutions', from Aristotle onwards, it's probably foolhardy to think we've reached the end.” For me, this is a sad symbol of modern philosophy.
However, in the 1970s it was realized that this is not really necessary. In Sec. 3, we have already discussed an example of a two-level system coupled with environment (in our current context, with measurement instrument) and described by Hamiltonian
\[
\hat{H} = \hat{H}_s + \hat{H}_{\text{int}} + \hat{H}_c \{ \lambda \}, \quad \text{with} \quad \hat{H}_s = a \hat{\sigma}_z, \quad \hat{H}_{\text{int}} = -f(\lambda) \hat{\sigma}_z,
\]
so that
\[
\left[ \hat{H}_s, \hat{H}_{\text{int}} \right] = 0. \tag{7.226}
\]
Comparing this equality with Eq. (67) we see that in the Heisenberg picture, the Hamiltonian operator (and hence the energy) of the system of our interest does not change with time. On the other hand, the interaction can change the state of the instrument, so it may be used to measure its energy – or another observable whose operator commutes with the interaction Hamiltonian. Such trick is called either the quantum non-demolition (QND) or back-action-evading (BAE) measurements.\(^87\) Let me present a fine example of a real measurement of this kind - see Fig. 9.\(^88\)

[Image of a Penning trap]

Fig. 7.9. QND measurement of single electron’s energy by Peil and Gabrielse: (a) the core of experimental setup, and (b) a record of the thermal excitation and spontaneous relaxation of Fock states. © 1999 APS.

In this experiment, a single electron is captured in a Penning trap – a combination of a (virtually) uniform magnetic field \(\mathbf{B}\) and a quadrupole electric field.\(^89\) Such electric field stabilizes cyclotron orbits but does not have any noticeable effect on electron motion in the plane perpendicular to the magnetic field, and hence on its Landau level energies (see Sec. 3.2):

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\(^{89}\) Similar to the one discussed in EM Sec. 2.4 (see in particular Eq. (2.77) and Fig. 2.7), but with additional rotation about one of the axes – either \(x\) or \(y\).
\[ E_n = \hbar \omega_c \left( n + \frac{1}{2} \right), \quad \text{with} \quad \omega_c = \frac{eB}{m_e}. \]  

(7.227)

(In the cited work, at \( B \approx 5.3 \) T, the cyclic frequency \( \omega_c/2\pi \) was about 147 GHz, so that the level splitting \( \hbar \omega_c \) was close to \( 10^{-22} \) J, i.e. corresponded to temperature \( \sim 10 \) K, while the physical temperature of the system might be reduced well below that, down to \( \sim 80 \) mK). Now note that the analogy between a particle on a Landau levels and a harmonic oscillator goes beyond the energy spectrum. Indeed, since the Hamiltonian of a 2D particle in a perpendicular magnetic field may be reduced to that of a 1D oscillator, we may repeat all procedures of Sec. 5.4 and rewrite it in the terms of creation-annihilation operators:

\[ \hat{H}_s = \hbar \omega_c \left( \hat{a}^\dagger \hat{a} + \frac{1}{2} \right). \]  

(7.228)

In the Peil and Gabrielse experiment, the electron had one more degree of freedom – along the magnetic field. The electric field of the Penning trap creates a soft confining potential along this direction (vertical in Fig. 9a; let us take it for axis \( z \)), so that small electron oscillations along that axis could be well described as a 1D harmonic oscillator of much lower eigenfrequency, in that particular experiment with \( \omega_z/2\pi \approx 64 \) MHz. This frequency could be measured very accurately (with error \( \sim 1 \) Hz) by sensitive electronics whose electric field affects \( z \)-motion of the electron, but not its motion in the perpendicular plane. In an exactly uniform magnetic field, the two modes of electron motion would be completely uncoupled. However, the experimental setup included two special superconducting rings made of niobium (Fig. 9a), which slightly distorted the magnetic field and created an interaction between the modes, which might be well approximated by Hamiltonian\(^90\)

\[ \hat{H}_{\text{int}} = \text{const} \times \left( \hat{a}^\dagger \hat{a} + \frac{1}{2} \right)^2, \]  

(7.228)

so that the main condition (226) of a QND measurement was well satisfied. At the same time, coupling (228) ensured that a change of the Fock state number \( n \) by 1 changed the \( z \)-oscillation eigenfrequency by \( \sim 12.4 \) Hz. Since this shift was substantially larger than electronics noise, spontaneous changes of \( n \) (due to an uncontrolled coupling of the electron to environment) could be readily observed – moreover, continuously monitored – see Fig. 9b. (These data imply that there is virtually no effect of the measuring instrument on the statistics on \( n \) – at least on the scale of minutes, i.e. as many as \( \sim 10^{13} \) cyclotron orbit periods.) Of course, any measurement – QND or not - cannot avoid the Heisenberg uncertainty relations; in this particular case, a permanent monitoring of the Fock state number \( n \) keeps its quantum phase fully uncertain.

It is natural to wonder whether the QND measurement concept may be extended from quadratic forms like the energy to “usual” observables such as coordinates and momenta whose uncertainties are bound by the fundamental Heisenberg’s relation. The answer is yes, but the required methods are a bit more tricky. For example, let us place an electrically charged particle into a uniform electric field \( \mathcal{E} = n_s \mathcal{E}(t) \) of the instrument, so that their interaction Hamiltonian is

\(^90\) I am simplifying the real situation a bit. Actually, in the experiment there was an electron spin’s contribution to the interaction Hamiltonian as well, but since the large magnetic field polarized the spins quite reliably, their only role was a constant shift of frequency \( \omega_z \).
\[ \hat{H}_{\text{int}} = -q \hat{E}(t) \hat{x}. \]  

(7.229)

Such interaction certainly passes the information on the time evolution of coordinate \( x \) to the instrument. However, since Eq. (226) is not satisfied - at least for the kinetic-energy part of system's Hamiltonian; as a result the interaction simultaneously distorts the time evolution of particle’s momentum. Indeed, writing the Heisenberg equation of motion (4.199) for the \( x \)-component of momentum, we get

\[ \dot{\hat{p}} - \hat{p} \bigg|_{\varepsilon=0} = q \hat{E}(t). \]  

(7.230)

Integrating Eq. (5.139) for the coordinate operator evolution, \(^91\) we get expression,

\[ \hat{x}(t) = \hat{x}(0) + \frac{1}{m} \int_0^t \hat{p}(t')dt', \]  

(7.231)

that shows that the perturbations (230) of the momentum would eventually find their way to the coordinate evolution.

However, for such an important particular system as a harmonic oscillator, the following trick is possible. For this system, Eqs. (5.170) and (230) may be readily combined to give a second-order differential equation for the coordinate operator, that is absolutely similar to the classical equation of motion, and has a similar solution: \(^92\)

\[ \hat{x}(t) = \hat{x}(0) + \frac{q}{m \omega_0} \int_0^t \hat{E}(t') \sin \omega_0 (t - t') dt'. \]  

(7.232)

This formula confirms that generally the external field \( \mathcal{A}(t) \) (in our case, the sensing field of the measurement instrument) affects the time evolution law. Note, however, that if the field is applied only at moments \( t_n' \) separated by intervals \( T/2 \), where \( T = 2\pi/\omega_0 \) is the oscillation period, its effect on coordinate vanishes at similarly spaced observation instants \( t_n = t_n' + (m +1/2)T \). This the idea of stroboscopic QND measurements. Of course, according to Eq. (230), even such measurement strongly perturbs the oscillator momentum, so that even if values \( x_n \) are measured with high accuracy, the Heisenberg’s uncertainty relation is not violated.

Experimental implementation of such measurements is not simple (and to the best of my knowledge they have never been successfully demonstrated), but this initial idea has opened a way to more practicable solutions. For example, it straightforward to use the Heisenberg equations of motion to show that if coupling of two harmonic oscillators, with coordinates \( x \) and \( X \), and unperturbed eigenfrequencies \( \omega \) and \( \Omega \), is modulated in time as

\[ \hat{H}_{\text{int}} \propto \hat{x} \hat{X} \cos \omega t \cos \Omega t, \]  

(7.233)

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\(^91\) This simple equation is limited to 1D systems with Hamiltonians of the type (2.50), but the reader should agree that this is a pretty general form.

\(^92\) See, e.g., CM Sec. 4.1. Note in particular that function \( \sin \omega_0 \tau \) (with \( \tau \equiv t - t' \)) under the integral, divided by \( \omega_0 \), is nothing more than the temporal Green’s function \( G(\tau) \), of a loss-free harmonic oscillator.
then the process in one of oscillators (say, that with frequency $\Omega$) does not affect dynamics of one of the 
quadrature components of another oscillator, defined by relations\[^{93}\]

$$
\hat{x}_1 = \hat{x}\cos\alpha - \frac{\hat{p}}{m\omega}\sin\alpha, \quad \hat{x}_2 = \hat{x}\sin\alpha + \frac{\hat{p}}{m\omega}\cos\alpha,
$$

(7.234)

while this component’s motion does affect the dynamics of one of quadrature components of the counterpart oscillator. (For the counterpart couple of quadrature components, the information transfer goes in the opposite direction.) This scheme has been successfully used for QND measurements in the optical range, with coupling (233) provided by the optical Kerr effect.\[^{94}\]

Please note that the last two QND measurement examples are based on the idea of modulation of a certain parameter in time – either in a short-pulse or sinusoidal form. So, the reader should not be surprised that if the only role of a QND measurement is a sensitive measurement of a weak classical force acting on a quantum probe system,\[^{95}\] i.e. a 1D oscillator of eigenfrequency $\omega_0$, it may be implemented much simpler – just by modulating the oscillator parameter with frequency $\omega \approx 2\omega_0$. From classical dynamics, we know that if the depth of such modulation exceeds a certain threshold value, it results in excitation of the so-called parametric oscillations with frequency $\omega/2$, and one of two opposite phases.\[^{96}\] In the language of Eq. (234), parametric excitation means an exponential growth of one of the quadrature components, with the sign depending on initial conditions, while the counterpart component is suppressed. Close to, but below the excitation threshold, the parameter modulation boosts all perturbations of the almost-excited component (including its quantum-mechanical uncertainty), and suppresses (squeezes) those of the counterpart component. The result is a squeezed state, already discussed in Sec. 5.5 above (see in particular Fig. 5.6), that allows one to notice the effect of external force on the oscillator on the backdrop of a quantum uncertainty smaller that the standard quantum limit (5.138) – see the first of Eqs. (5.174).

In electrical engineering, this fact may be conveniently formulated in terms of noise parameter $\Theta_N$ of a linear amplifier – the instrument for continuous monitoring of an input “signal” – e.g., a microwave or optical waveform.\[^{97}\] Namely, $\Theta_N$ of “usual” (say, transistor or maser) amplifiers which are equally sensitive to both quadrature components of the signal, $\Theta_N$ has a minimum value $\hbar\omega/2$, due to the quantum uncertainty pertinent to the quantum state of the amplifier itself (which therefore plays the role

\[^{93}\] The physical sense of these relations should be clear from Fig. 5.6: they define a system of coordinates rotating clockwise with angular velocity $\omega$, so that the point representing unperturbed classical oscillations with that frequency is at rest in that rotating frame. (The “probability cloud” presenting a Glauber state is also stationary in coordinates $[x_1, x_2]$.) The reader familiar with the classical theory oscillations may notice that $x_1$ and $x_2$ are essentially the RWA variables $u$ and $v$, i.e. the Poincaré plane coordinates – see, e.g., CM Sec. 4.3-4.6, and especially Fig. 4.9.

\[^{94}\] See, e.g., P. Grangier et al., Nature 396, 537 (1998), and references therein. This was, however, not the first QND implementation in optics – for a review see J. Roch et al., Appl. Phys. B 55, 291 (1992).

\[^{95}\] As it is, for example, for gravitational wave detectors – see the discussion and references in Sec. 2.10.

\[^{96}\] See, e.g., CM Sec. 4.5.

\[^{97}\] For the exact definition of the latter parameter, suitable for the quantum sensitivity range ($\Theta_N \sim \hbar\omega$) as well, see, e.g., I. Devyatov et al., J. Appl. Phys. 60, 1808 (1986). In the classical noise limit ($\Theta_N \gg \hbar\omega$), it coincides with $k_B T_N$, where $T_N$ is a more popular measure of electronics noise, called the noise temperature.
of its “quantum noise”). On the other hand, a degenerate parametric amplifier, sensitive to just one quadrature component, may have $\Theta_N$ well below $\hbar \omega/2$, due to the squeezing of its ground state.

Finally, let me note that the parameter-modulation schemes of the QND measurements are not limited to harmonic oscillators, and may be applied to other important quantum systems, notably including two-level (i.e. spin-$\frac{1}{2}$-like) systems.

7.8. Exercise problems

7.1. Calculate the density matrix of a two-level system described by Hamiltonian with matrix

$$H = a \cdot \sigma = a_x \sigma_x + a_y \sigma_y + a_z \sigma_z,$$

where $\sigma_k$ are the Pauli matrices, and $a_k$ are $c$-numbers, in thermodynamic equilibrium.

7.2. Find the Wigner function of a harmonic oscillator in:

(i) at the thermodynamic equilibrium at temperature $T$,
(ii) in the ground state, and
(ii) in the Glauber state with dimensionless complex amplitude $\alpha$.

Discuss the relation between the first of the results and the Gibbs distribution.

7.3. Calculate the Wigner function of a harmonic oscillator, with mass $m$ and frequency $\omega_0$, in its first excited stationary state ($n = 1$).

7.4. Show that the quantum-mechanical Golden Rule (6.111) and the master equation (196) give the same results for the rate of spontaneous quantum transitions $n' \rightarrow n$ in a system with discrete energy spectrum, weakly coupled to a low-temperature heat bath ($k_B T << \hbar \omega_{nm}$).

Hint: Try to establish a relation between function $\Im \chi(\omega_{nm})$ that participates in Eq. (196), and the density of states $\rho_n$ that participates in the Golden Rule formulas, by considering a particular case of sinusoidal oscillations in the system of interest.

7.5. A harmonic oscillator is weakly coupled to an Ohmic environment.

(i) Use the rotating-wave approximation to write 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 $\langle n \rangle$ of thermally-induced excitations in equilibrium, given by the second of Eqs. (26b).

7.6. For a harmonic oscillator with weak Ohmic dissipation:

(i) Spell out the system of differential equations for the energy level occupancies $W_n$.

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98 This fact was recognized very early – see, e.g., H. Haus and J. Mullen, *Phys. Rev.* 128, 2407 (1962).


(ii) Use this system to find the time evolution of the expectation value $\langle E \rangle$ of oscillator’s energy.
(iii) Compare the last result with that following from the Heisenberg-Langevin approach.

7.7. Derive Eq. (209) in an alternative way, using an expression dual to Eq. (5.28b).

7.8. A particle in a system of two coupled quantum wells (see, e.g., Fig. 4) is weakly coupled to an Ohmic environment.

(i) Derive the equations of time evolution of the density matrix elements.
(ii) Solve these equations in the low-temperature limit, when the energy level splitting is much larger than $k_B T$, to calculate the time evolution of the probability $W_L(t)$ of finding the particle one of the wells, after it had been placed there at $t = 0$.

7.9. A spin-$\frac{1}{2}$ particle is placed into magnetic field $\mathcal{B}(t) = \mathcal{B}_0 + \mathcal{B}(t)$ with an arbitrary but small time-dependent component ($|\mathcal{B}| \ll |\mathcal{B}_0|$), and is also weakly coupled to dissipative environment. Derive the differential equations describing the time evolution of the expectation values ($\langle S_x \rangle$, etc.) of spin’s Cartesian components.