Path, motive, guide, original, and end
SAMUEL JOHNSON (1709-1784), The Rambler

18

Nonequilibrium Quantum Statistics

Quantum statistics described by the theoretical tools of the previous chapters is quite limited. The physical system under consideration must be in thermodynamic equilibrium, with a constant temperature enforced by a thermal reservoir. In this situation, partition function and the density matrix can be calculated from an analytic continuation of quantum-mechanical time evolution amplitudes to an imaginary time $t_b - t_a = -i\hbar/k_BT$. In this chapter we want to go beyond such equilibrium physics and extend the path integral formalism to nonequilibrium time-dependent phenomena. The tunneling processes discussed in Chapter 17 belong really to this class of phenomena, and their full understanding requires the theoretical framework of this chapter. In the earlier treatment this was circumvented by addressing only certain quasi-equilibrium questions. These were answered by applying the equilibrium formalism to the quantum system at positive coupling constant, which guaranteed perfect equilibrium, and extending the results to the quasi-equilibrium situation analytic continuation to small negative coupling constants.

Before we can set up a path integral formulation capable of dealing with true nonequilibrium phenomena, some preparatory work is useful based on the traditional tools of operator quantum mechanics.

18.1 Linear Response and Time-Dependent Green Functions for $T \neq 0$

If the deviations of a quantum system from thermal equilibrium are small, the easiest description of nonequilibrium phenomena proceeds via the *theory of linear response*. In operator quantum mechanics, this theory is introduced as follows. First, the system is assumed to have a time-independent Hamiltonian operator $\hat{H}$. The ground state is determined by the Schrödinger equation, evolving as a function of time according to the equation

$$|\Psi_S(t)\rangle = e^{-i\hat{H}t}|\Psi_S(0)\rangle \tag{18.1}$$

(in natural units with $\hbar = 1$, $k_B = 1$). The subscript S denotes the Schrödinger picture.

Next, the system is slightly disturbed by adding to $\hat{H}$ a time-dependent external interaction,

$$\hat{H} \to \hat{H} + \hat{H}^{\rm ext}(t), \tag{18.2}$$

where $\hat{H}^{\rm ext}(t)$ is assumed to set in at some time t_0, i.e., $\hat{H}^{\rm ext}(t)$ vanishes identically for $t < t_0$. The disturbed Schrödinger ground state has the time dependence

$$|\Psi_S^{\rm dist}(t)\rangle = e^{-i\hat{H}t}\hat{U}_H(t)|\Psi_S(0)\rangle, \tag{18.3}$$

where $\hat{U}_H(t)$ is the time translation operator in the Heisenberg picture. It satisfies the equation of motion

$$i\dot{\hat{U}}_H(t) = \hat{H}_H^{\rm ext}(t)\hat{U}_H(t), \tag{18.4}$$

with[1]

$$\hat{H}_H^{\rm ext}(t) \equiv e^{i\hat{H}t}\hat{H}^{\rm ext}(t)e^{-i\hat{H}t}. \tag{18.5}$$

To lowest-order perturbation theory, the operator $\hat{U}_H(t)$ is given by

$$\hat{U}_H(t) = 1 - i\int_{t_0}^{t} dt'\, \hat{H}_H^{\rm ext}(t') + \cdots\ . \tag{18.6}$$

In the sequel, we shall assume the onset of the disturbance to lie at $t_0 = -\infty$. Consider an arbitrary time-independent Schrödinger observable $\hat{O}$ whose Heisenberg representation has the time dependence

$$\hat{O}_H(t) = e^{i\hat{H}t}\hat{O}e^{-i\hat{H}t}. \tag{18.7}$$

Its time-dependent expectation value in the disturbed state $|\Psi_S^{\rm dist}(t)\rangle$ is given by

$$\begin{aligned}\langle\Psi_S^{\rm dist}(t)|\hat{O}|\Psi_S^{\rm dist}(t)\rangle &= \langle\Psi_S(0)|\hat{U}_H^\dagger(t)e^{i\hat{H}t}\hat{O}e^{-i\hat{H}t}\hat{U}_H(t)|\Psi_S(0)\rangle\\ &\approx \langle\Psi_S(0)|\left(1 + i\int_{-\infty}^{t} dt'\,\hat{H}_H^{\rm ext}(t') + \dots\right)\hat{O}_H(t)\\ &\quad\times\left(1 - i\int_{-\infty}^{t} dt'\,\hat{H}_H^{\rm ext}(t') + \dots\right)|\Psi_S(0)\rangle\\ &= \langle\Psi_H|\hat{O}_H(t)|\Psi_H\rangle - i\langle\Psi_H|\int_{-\infty}^{t} dt'\,\left[\hat{O}_H(t), \hat{H}_H^{\rm ext}(t')\right]|\Psi_H\rangle + \dots\ .\end{aligned} \tag{18.8}$$

We have identified the time-independent Heisenberg state with the time-dependent Schrödinger state at zero time in the usual manner, i.e., $|\Psi_H\rangle \equiv |\Psi_S(0)\rangle$. Thus the expectation value of $\hat{O}$ deviates from equilibrium by

$$\begin{aligned}\delta\langle\Psi_S(t)|\hat{O}|\Psi_S(t)\rangle &\equiv \langle\Psi_S^{\rm dist}(t)|\hat{O}(t)|\Psi_S^{\rm dist}(t)\rangle - \langle\Psi_S(t)|\hat{O}(t)|\Psi_S(t)\rangle\\ &= -i\int_{-\infty}^{t} dt'\,\langle\Psi_H|\left[\hat{O}_H(t), \hat{H}_H^{\rm ext}(t')\right]|\Psi_H\rangle.\end{aligned} \tag{18.9}$$

[1]Note that after the replacements $H \to H_0$, $H_H^{\rm ext} \to H_I^{\rm int}$, Eq. (18.4) coincides with the equation for the time evolution operator in the interaction picture to appear in Section 18.7. In contrast to that section, however, the present interaction is a nonpermanent artifact to be set equal to zero at the end, and H is the complicated total Hamiltonian, not a simple free one. This is why we do not speak of an interaction picture here.

If the left-hand side is transformed into the Heisenberg picture, it becomes

$$\delta\langle\Psi_S(t)|\hat{O}|\Psi_S(t)\rangle = \delta\langle\Psi_H|\hat{O}_H(t)|\Psi_H\rangle = \langle\Psi_H|\delta\hat{O}_H(t)|\Psi_H\rangle,$$

so that Eq. (18.9) takes the form

$$\langle\Psi_H|\delta\hat{O}_H(t)|\Psi_H\rangle = -i\int_{-\infty}^{t} dt'\,\langle\Psi_H|\left[\hat{O}_H(t),\hat{H}_H^{\rm ext}(t')\right]|\Psi_H\rangle. \qquad (18.10)$$

It is useful to use the retarded Green function of the operators $\hat{O}_H(t)$ and $\hat{H}_H(t')$ in the state $|\Psi_H\rangle$ [compare (3.40)]:

$$G^R_{OH}(t,t') \equiv \Theta(t-t')\langle\Psi_H|\left[\hat{O}_H(t),\hat{H}_H(t')\right]|\Psi_H\rangle. \qquad (18.11)$$

Then the deviation from equilibrium is given by the integral

$$\langle\Psi_H|\delta\hat{O}_H(t)|\Psi_H\rangle = -i\int_{-\infty}^{\infty} dt'\,G^R_{OH}(t,t'). \qquad (18.12)$$

Suppose now that the observable $\hat{O}_H(t)$ is capable of undergoing oscillations. Then an external disturbance coupled to $\hat{O}_H(t)$ will in general excite these oscillations. The simplest coupling is a linear one, with an interaction energy

$$\hat{H}^{\rm ext}(t) = -\hat{O}_H(t)\delta j(t), \qquad (18.13)$$

where $j(t)$ is some external source. Inserting (18.13) into (18.12) yields the linear-response formula

$$\langle\Psi_H|\delta\hat{O}_H(t)|\Psi_H\rangle = i\int_{-\infty}^{\infty} dt'\,G^R_{OO}(t,t')\delta j(t'), \qquad (18.14)$$

where G^R_{OO} is the retarded Green function of two operators $\hat{O}$:

$$G^R_{OO}(t,t') = \Theta(t-t')\langle\Psi_H|\left[\hat{O}_H(t),\hat{O}_H(t')\right]|\Psi_H\rangle. \qquad (18.15)$$

At frequencies where the Fourier transform of $G_{OO}(t,t')$ is singular, the slightest disturbance causes a large response. This is the well-known resonance phenomenon found in any oscillating system. Whenever the external frequency ω hits an eigenfrequency, the Fourier transform of the Green function diverges. Usually, the eigenfrequencies of a complicated N-body system are determined by calculating (18.15) and by finding the singularities in ω.

It is easy to generalize this description to a thermal ensemble at a nonzero temperature. The principal modification consists in the replacement of the ground state expectation by the thermal average

$$\langle\hat{O}\rangle_T \equiv \frac{{\rm Tr}\,(e^{-\hat{H}/T}\hat{O})}{{\rm Tr}\,(e^{-\hat{H}/T})}.$$

Using the free energy

$$F = -T \log \mathrm{Tr}\,(e^{-\hat{H}/T}),$$

this can also be written as

$$\langle \hat{O} \rangle_T = e^{F/T} \mathrm{Tr}\,(e^{-\hat{H}/T} \hat{O}). \tag{18.16}$$

In a grand-canonical ensemble, $\hat{H}$ must be replaced by $\hat{H} - \mu\hat{N}$ and F by its grand-canonical version F_G (see Section 1.17). At finite temperatures, the linear-response formula (18.14) becomes

$$\delta \langle \hat{O}(t) \rangle_T = i \int_{-\infty}^{\infty} dt'\, G^R_{OO}(t,t')\delta j(t'), \tag{18.17}$$

where $G^R_{OO}(t,t')$ is the *retarded Green function at nonzero temperature* defined by [recall (1.306)]

$$G^R_{OO}(t,t') \equiv G^R_{OO}(t-t') \equiv \Theta(t-t')\, e^{F/T} \mathrm{Tr}\, \left\{ e^{-\hat{H}/T} \left[\hat{O}_H(t), \hat{O}_H(t') \right] \right\}. \tag{18.18}$$

In a realistic physical system, there are usually many observables, say $\hat{O}^i_H(t)$ for $i = 1, 2, \ldots, l$, which perform coupled oscillations. Then the relevant retarded Green function is some $l \times l$ matrix

$$G^R_{ij}(t,t') \equiv G^R_{ij}(t-t') \equiv \Theta(t-t')\, e^{F/T} \mathrm{Tr}\, \left\{ e^{-\hat{H}/T} \left[\hat{O}^i_H(t), \hat{O}^j_H(t') \right] \right\}. \tag{18.19}$$

After a Fourier transformation and diagonalization, the singularities of this matrix render the important physical information on the resonance properties of the system.

The retarded Green function at $T \neq 0$ occupies an intermediate place between the real-time Green function of field theories at $T = 0$, and the imaginary-time Green function used before to describe thermal equilibria at $T \neq 0$ (see Subsection 3.8.2). The Green function (18.19) depends both on the real time and on the temperature via an imaginary time.

18.2 Spectral Representations of Green Functions for $T \neq 0$

The retarded Green functions are related to the imaginary-time Green functions of equilibrium physics by an analytic continuation. For two arbitrary operators $\hat{O}^1_H$, $\hat{O}^2_H$, the latter is defined by the thermal average

$$G_{12}(\tau, 0) \equiv G_{12}(\tau) \equiv e^{F/T} \mathrm{Tr}\, \left[e^{-\hat{H}/T} \hat{T}_\tau \hat{O}^1_H(\tau) \hat{O}^2_H(0) \right], \tag{18.20}$$

where $\hat{O}_H(\tau)$ is the *imaginary-time Heisenberg operator*

$$\hat{O}_H(\tau) \equiv e^{\hat{H}\tau} \hat{O} e^{-\hat{H}\tau}. \tag{18.21}$$

To see the relation between $G_{12}(\tau)$ and the retarded Green function $G^R_{12}(t)$, we take a complete set of states $|n\rangle$, insert them between the operators $\hat{O}^1$, $\hat{O}^2$, and expand $G_{12}(\tau)$ for $\tau \geq 0$ into the spectral representation

$$G_{12}(\tau) = e^{F/T} \sum_{n,n'} e^{-E_n/T} e^{(E_n - E_{n'})\tau} \langle n|\hat{O}^1|n'\rangle\langle n'|\hat{O}^2|n\rangle. \tag{18.22}$$

Since $G_{12}(\tau)$ is periodic under $\tau \to \tau + 1/T$, its Fourier representation contains only the discrete Matsubara frequencies $\omega_m = 2\pi m T$:

$$\begin{aligned} G_{12}(\omega_m) &= \int_0^{1/T} d\tau\, e^{i\omega_m \tau} G_{12}(\tau) \\ &= e^{F/T} \sum_{n,n'} e^{-E_n/T} \left(1 - e^{(E_n - E_{n'})/T}\right) \langle n|\hat{O}^1|n'\rangle\langle n'|\hat{O}^2|n\rangle \\ &\qquad\qquad\times \frac{-1}{i\omega_m - E_{n'} + E_n}. \end{aligned} \tag{18.23}$$

The retarded Green function satisfies no periodic (or antiperiodic) boundary condition. It possesses Fourier components with *all* real frequencies ω:

$$\begin{aligned} G^R_{12}(\omega) &= \int_{-\infty}^{\infty} dt\, e^{i\omega t}\, \Theta(t) e^{F/T} \mathrm{Tr}\left\{ e^{-\hat{H}/T} \left[\hat{O}^1_H(t), \hat{O}^2_H(0)\right]_{\mp} \right\} \\ &= e^{F/T} \int_0^{\infty} dt\, e^{i\omega t} \sum_{n,n'} \Big[\quad e^{-E_n/T} e^{i(E_n - E_{n'})t} \langle n|\hat{O}^1|n'\rangle\langle n'|\hat{O}^2|n\rangle \\ &\qquad\qquad \mp e^{-E_n/T} e^{-i(E_n - E_{n'})t} \langle n|\hat{O}^2|n'\rangle\langle n'|\hat{O}^1|n\rangle \Big]. \end{aligned} \tag{18.24}$$

In the second sum we exchange n and n' and perform the integral, after having attached to ω an infinitesimal positive-imaginary part $i\eta$ to ensure convergence [recall the discussion after Eq. (3.84)]. The result is

$$\begin{aligned} G^R_{12}(\omega) &= e^{F/T} \sum_{n,n'} e^{-E_n/T} \left[1 - e^{(E_n - E_{n'})/T}\right] \langle n|\hat{O}^1|n'\rangle\langle n'|\hat{O}^2|n\rangle \\ &\qquad\qquad \times \frac{i}{\omega - E_{n'} + E_n + i\eta}. \end{aligned} \tag{18.25}$$

By comparing this with (18.23) we see that the thermal Green functions are obtained from the retarded ones by replacing [1]

$$\frac{i}{\omega - E_{n'} + E_n + i\eta} \to \frac{-1}{i\omega_m - E_{n'} + E_n}. \tag{18.26}$$

A similar procedure holds for fermion operators $\hat{O}^i$ (which are not observable). There are only two changes with respect to the boson case. First, in the Fourier expansion of the imaginary-time Green functions, the bosonic Matsubara frequencies ω_m in (18.23) become fermionic. Second, in the definition of the retarded Green functions (18.19), the commutator is replaced by an anticommutator, i.e., the retarded Green function of fermion operators $\hat{O}_H^i$ is defined by

$$G_{ij}^R(t,t') \equiv G_{ij}^R(t-t') \equiv \Theta(t-t')e^{F/T}\mathrm{Tr}\left\{e^{-\hat{H}/T}\left[\hat{O}_H^i(t),\hat{O}_H^j(t')\right]_+\right\}. \quad (18.27)$$

These changes produce an opposite sign in front of the $e^{(E_n-E_{n'})/T}$-term in both of the formulas (18.23) and (18.25). Apart from that, the relation between the two Green functions is again given by the replacement rule (18.26).

At this point it is customary to introduce the *spectral function*

$$\begin{aligned}\rho_{12}(\omega') &= \left(1\mp e^{-\omega'/T}\right)e^{F/T} \\ &\quad \times \textstyle\sum_{n,n'} e^{-E_n/T}2\pi\delta(\omega-E_{n'}+E_n)\langle n|\hat{O}^1|n'\rangle\langle n'|\hat{O}^2|n\rangle,\end{aligned} \quad (18.28)$$

where the upper and the lower sign hold for bosons and fermions, respectively. Under an interchange of the two operators it behaves like

$$\rho_{12}(\omega') = \mp\rho_{12}(-\omega'). \quad (18.29)$$

Using this spectral function, we may rewrite the Fourier-transformed retarded and thermal Green functions as the following spectral integrals:

$$G_{12}^R(\omega) = \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\,\rho_{12}(\omega')\frac{i}{\omega-\omega'+i\eta}, \quad (18.30)$$

$$G_{12}(\omega_m) = \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\,\rho_{12}(\omega')\frac{-1}{i\omega_m-\omega'}. \quad (18.31)$$

These equations show how the imaginary-time Green functions arise from the retarded Green functions by a simple analytic continuation in the complex frequency plane to the discrete Matsubara frequencies, $\omega \to i\omega_m$. The inverse problem of reconstructing the retarded Green functions in the entire upper half-plane of ω from the imaginary-time Green functions defined only at the Matsubara frequencies ω_m is not solvable in general but only if other information is available [2]. For instance, the sum rules for canonical fields to be derived later in Eq. (18.66) with the ensuing asymptotic condition (18.67) are sufficient to make the continuation unique [3].

Going back to the time variables t and τ, the Green functions are

$$G_{12}^R(t) = \Theta(t)\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\,\rho_{12}(\omega')e^{-i\omega' t}, \quad (18.32)$$

$$G_{12}(\tau) = \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\,\rho_{12}(\omega')T\sum_{\omega_m}e^{-i\omega_m\tau}\frac{-1}{i\omega_m-\omega'}\,. \quad (18.33)$$

The sum over even or odd Matsubara frequencies on the right-hand side of $G_{12}(\tau)$ was evaluated in Section 3.3 for bosons and fermions as

$$\begin{aligned}T\sum_n e^{-i\omega_m\tau}\frac{-1}{i\omega_m-\omega} &= G_{\omega,e}^p(\tau) = e^{-\omega(\tau-1/2T)}\frac{1}{2\sin(\omega/2T)} \\ &= e^{-\omega\tau}(1+n_\omega)\end{aligned} \quad (18.34)$$

and

$$
\begin{aligned}
T\sum_n e^{-i\omega_m\tau}\frac{-1}{i\omega_m-\omega} &= G^a_{\omega,e}(\tau)=e^{-\omega(\tau-1/2T)}\frac{1}{2\cos(\omega/2T)} \\
&= e^{-\omega\tau}(1-n_\omega), \qquad (18.35)
\end{aligned}
$$

with the Bose and Fermi distribution functions [see (3.93), (7.542), (7.544)]

$$
n_\omega=\frac{1}{e^{\omega/T}\mp 1}, \qquad (18.36)
$$

respectively.

18.3 Other Important Green Functions

In studying the dynamics of systems at finite temperature, several other Green functions are useful whose spectral functions we shall now derive.

In complete analogy with the retarded Green functions for bosonic and fermionic operators, we may introduce their counterparts, the so-called *advanced Green functions* (compare page 38)

$$
G^A_{12}(t,t')\equiv G^A_{12}(t-t')=-\Theta(t'-t)e^{F/T}\mathrm{Tr}\left\{e^{-\hat H/T}\left[\hat O^1_H(t),\hat O^2_H(t')\right]_\mp\right\}. \qquad (18.37)
$$

Their Fourier transforms have the spectral representation

$$
G^A_{12}(\omega)=\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\,\rho_{12}(\omega')\frac{i}{\omega-\omega'-i\eta}, \qquad (18.38)
$$

differing from the retarded case (18.30) only by the sign of the $i\eta$-term. This makes the Fourier transforms vanish for $t>0$, so that the time-dependent Green function has the spectral representation [compare (18.32)]

$$
G^A_{12}(t)=-\Theta(-t)\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\rho_{12}(\omega)e^{-i\omega t}. \qquad (18.39)
$$

By subtracting retarded and advanced Green functions, we obtain the thermal expectation value of commutator or anticommutator:

$$
C_{12}(t,t')=e^{F/T}\mathrm{Tr}\left\{e^{-\hat H/T}\left[\hat O^1_H(t),\hat O^2_H(t')\right]_\mp\right\}=G^R_{12}(t,t')-G^A_{12}(t,t'). \qquad (18.40)
$$

Note the simple relations:

$$
\begin{aligned}
G^R_{12}(t,t') &= \Theta(t-t')C_{12}(t,t'), \qquad (18.41)\\
G^A_{12}(t,t') &= -\Theta(t'-t)C_{12}(t,t'). \qquad (18.42)
\end{aligned}
$$

When inserting the spectral representations (18.30) and (18.39) of $G^R_{12}(t)$ and $G^A_{12}(t)$ into (18.40), and using the identity (1.328),

$$\frac{i}{\omega-\omega'+i\eta}-\frac{i}{\omega-\omega'-i\eta} = 2\frac{\eta}{(\omega-\omega')^2+\eta^2}=2\pi\delta(\omega-\omega'), \tag{18.43}$$

we obtain the spectral integral representation for the commutator function:[2]

$$C_{12}(t)=\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\rho_{12}(\omega)e^{-i\omega t}. \tag{18.44}$$

Thus a knowledge of the commutator function $C_{12}(t)$ determines directly the spectral function $\rho_{12}(\omega)$ by its Fourier components

$$C_{12}(\omega)=\rho_{12}(\omega). \tag{18.45}$$

An important role in studying the dynamics of a system in a thermal environment is played by the time-ordered Green functions. They are defined by

$$G_{12}(t,t')\equiv G_{12}(t-t')=e^{F/T}\mathrm{Tr}\left[e^{-\hat H/T}\;\hat T\hat O^1_H(t)\hat O^2_H(t')\right]. \tag{18.46}$$

Inserting intermediate states as in (18.23) we find the spectral representation

$$\begin{aligned}
G_{12}(\omega) &= \int_{-\infty}^{\infty}dt\,e^{i\omega t}\;\Theta(t)\;\; e^{F/T}\mathrm{Tr}\left\{e^{-\hat H/T}\hat O^1_H(t)\hat O^2_H(0)\right\}\\
&+ \int_{-\infty}^{\infty}dt\,e^{i\omega t}\;\Theta(-t)e^{F/T}\mathrm{Tr}\left\{e^{-\hat H/T}\hat O^2_H(t)\hat O^1_H(0)\right\}\\
&= e^{F/T}\int_{0}^{\infty}dt\,e^{i\omega t}\sum_{n,n'}e^{-E_n/T}e^{i(E_n-E_{n'})t}\;\;\langle n|\hat O^1|n'\rangle\langle n'|\hat O^2|n\rangle\\
&\pm\; e^{F/T}\int_{-\infty}^{0}dt\,e^{i\omega t}\sum_{n,n'}e^{-E_n/T}e^{-i(E_n-E_{n'})t}\langle n|\hat O^2|n'\rangle\langle n'|\hat O^1|n\rangle\;.
\end{aligned} \tag{18.47}$$

Interchanging again n and n', this can be written in terms of the spectral function (18.28) as

$$G_{12}(\omega)=\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\rho_{12}(\omega')\left[\frac{1}{1\mp e^{-\omega'/T}}\frac{i}{\omega-\omega'+i\eta}+\frac{1}{1\mp e^{\omega'/T}}\frac{i}{\omega-\omega'-i\eta}\right]. \tag{18.48}$$

Let us also write down the spectral decomposition of a further operator expression complementary to $C_{12}(t)$ of (18.40), in which boson or fermion fields appear with the "wrong" commutator:

$$A_{12}(t-t')\equiv e^{F/T}\mathrm{Tr}\left\{e^{-\hat H/T}\left[\hat O^1_H(t),\hat O^2_H(t')\right]_\pm\right\}. \tag{18.49}$$

[2]Due to the relation (18.41), the same representation is found by dropping the factor $\Theta(t)$ in (18.32).

This function characterizes the size of fluctuations of the operators O^1_H and O^2_H. Inserting intermediate states, we find

$$\begin{aligned} A_{12}(\omega) &= \int_{-\infty}^{\infty} dt\, e^{i\omega t} e^{F/T} \mathrm{Tr}\left\{ e^{-\hat{H}/T} \left[\hat{O}^1_H(t), \hat{O}^2_H(0)\right]_{\pm} \right\} \\ &= e^{F/T} \int_{-\infty}^{\infty} dt\, e^{i\omega t} \sum_{n,n'} \Big[\ e^{-E_n/T} e^{i(E_n - E_{n'})t} \langle n|\hat{O}^1|n'\rangle\langle n'|\hat{O}^2|n\rangle \\ &\qquad\qquad \pm e^{-E_n/T} e^{-i(E_n - E_{n'})t} \langle n|\hat{O}^2|n'\rangle\langle n'|\hat{O}^1|n\rangle \Big]. \end{aligned} \tag{18.50}$$

In the second sum we exchange n and n' and perform the integral, which runs now over the entire time interval and gives therefore a δ-function:

$$\begin{aligned} A_{12}(\omega) &= e^{F/T} \sum_{n,n'} e^{-E_n/T} \left[1 \pm e^{(E_n - E_{n'})/T}\right] \langle n|\hat{O}^1|n'\rangle\langle n'|\hat{O}^2|n\rangle \\ &\qquad \times 2\pi\delta(\omega - E_{n'} + E_n). \end{aligned} \tag{18.51}$$

In terms of the spectral function (18.28), this has the simple form

$$A_{12}(\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \tanh^{\mp 1} \frac{\omega'}{2T} \rho_{12}(\omega')\, 2\pi\delta(\omega - \omega') = \tanh^{\mp 1} \frac{\omega}{2T} \rho_{12}(\omega). \tag{18.52}$$

Thus the expectation value (18.49) of the "wrong" commutator has the time dependence

$$A_{12}(t, t') \equiv A_{12}(t - t') = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \rho_{12}(\omega) \tanh^{\mp 1} \frac{\omega}{2T} e^{-i\omega(t - t')}. \tag{18.53}$$

There exists another way of writing the spectral representation of the various Green functions. For retarded and advanced Green functions G^R_{12}, G^A_{12}, we decompose in the spectral representations (18.30) and (18.38) according to the rule (1.329):

$$\frac{i}{\omega - \omega' \pm i\eta} = i\left[\frac{\mathcal{P}}{\omega - \omega'} \mp i\pi\delta(\omega - \omega')\right], \tag{18.54}$$

where $\mathcal{P}$ indicates principal value integration across the singularity, and write

$$G^{R,A}_{12}(\omega) = i \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \rho_{12}(\omega') \left[\frac{\mathcal{P}}{\omega - \omega'} \mp i\pi\delta(\omega - \omega')\right]. \tag{18.55}$$

Inserting (18.54) into (18.48) we find the alternative representation of the time-ordered Green function

$$G_{12}(\omega) = i \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \rho_{12}(\omega') \left[\frac{\mathcal{P}}{\omega - \omega'} - i\pi \tanh^{\mp 1} \frac{\omega}{2T} \delta(\omega - \omega')\right]. \tag{18.56}$$

The term proportional to $\delta(\omega - \omega')$ in the spectral representation is commonly referred to as the *absorptive* or *dissipative part* of the Green function. The first term proportional to the principal value is called the *dispersive* or *fluctuation part*.

The relevance of the spectral function $\rho_{12}(\omega')$ in determining both the *fluctuation part* as well as the *dissipative part* of the time-ordered Green function is the content of the important *fluctuation-dissipation theorem.* In more detail, this may be restated as follows: The common spectral function $\rho_{12}(\omega')$ of the commutator function in (18.44), the retarded Green function in (18.30), and the *fluctuation part* of the time-ordered Green function in (18.56) determines, after being multiplied by a factor $\tanh^{\mp 1}(\omega'/2T)$, the *dissipative part* of the time-ordered Green function in Eq. (18.56).

The three Green functions $-iG_{12}(\omega)$, $-iG^R_{12}(\omega)$, and $-iG^A_{12}(\omega)$ have the same real parts. By comparing Eqs. (18.30) and (18.31) we found that retarded and advanced Green functions are simply related to the imaginary-time Green function via an analytic continuation. The spectral decomposition (18.56) shows this is not true for the time-ordered Green function, due to the extra factor $\tanh^{\mp 1}(\omega/2T)$ in the absorptive term.

Another representation of the time-ordered Green is useful. It is obtained by expressing $\tan^{\mp 1}$ in terms of the Bose and Fermi distribution functions (18.36) as $\tan^{\mp 1} = 1 \pm 2n_\omega$. Then we can decompose

$$G_{12}(\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi}\, \rho_{12}(\omega') \left[\frac{i}{\omega - \omega' + i\eta} \pm 2\pi n_\omega\, \delta(\omega - \omega') \right]. \tag{18.57}$$

18.4 Hermitian Adjoint Operators

If the two operators $\hat{O}^1_H(t)$, $\hat{O}^2_H(t)$ are Hermitian adjoint to each other,

$$\hat{O}^2_H(t) = [\hat{O}^1_H(t)]^\dagger, \tag{18.58}$$

the spectral function (18.28) can be rewritten as

$$\begin{aligned} \rho_{12}(\omega') &= (1 \mp e^{-\omega'/T}) e^{F/T} \\ &\quad \times \sum_{n,n'} e^{-E_n/T} 2\pi\delta(\omega' - E_{n'} + E_n) |\langle n|\hat{O}^1_H(t)|n'\rangle\|^2. \end{aligned} \tag{18.59}$$

This shows that

$$\begin{aligned} \rho_{12}(\omega')\omega' &\geq 0 \qquad \text{for bosons,} \\ \rho_{12}(\omega') &\geq 0 \qquad \text{for fermions.} \end{aligned} \tag{18.60}$$

This property permits us to derive several useful inequalities between various diagonal Green functions in Appendix 18A.

Under the condition (18.58), the expectation values of anticommutators and commutators satisfy the time-reversal relations

$$G^A_{12}(t,t') = \mp G^R_{21}(t',t)^*, \tag{18.61}$$

$$A_{12}(t,t') = \pm A_{21}(t',t)^*, \tag{18.62}$$

$$C_{12}(t,t') = \mp C_{21}(t',t)^*. \tag{18.63}$$

$$G_{12}(t,t') = \pm G_{21}(t',t)^*. \tag{18.64}$$

Examples are the corresponding functions for creation and annihilation operators which will be treated in detail below. More generally, this properties hold for any interacting nonrelativistic particle fields $\hat{O}^1_H(t) = \hat{\psi}_{\mathbf{p}}(t)$, $\hat{O}^2_H(t) = \hat{\psi}^\dagger_{\mathbf{p}}(t)$ of a specific momentum $\mathbf{p}$.

Such operators satisfy, in addition, the canonical equal-time commutation rules at each momentum

$$\left[\hat{\psi}_{\mathbf{p}}(t), \hat{\psi}^\dagger_{\mathbf{p}}(t)\right] = 1 \tag{18.65}$$

(see Sections 7.6, 7.9). Using (18.40), (18.44) we derive from this *spectral function sum rule*:

$$\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \rho_{12}(\omega') = 1. \tag{18.66}$$

For a canonical free field with $\rho_{12}(\omega') = 2\pi\delta(\omega'-\omega)$, this sum rule is of course trivially fulfilled. In general, the sum rule ensures the large-ω behavior of imaginary-time, retarded, and advanced Green functions of canonically conjugate field operators to be the same as for a free particle, i.e.,

$$G_{12}(\omega_m) \xrightarrow[\omega_m\to\infty]{} \frac{i}{\omega_m}, \quad G^{A,R}_{12}(\omega) \xrightarrow[\omega\to\infty]{} \frac{1}{\omega}. \tag{18.67}$$

18.5 Harmonic Oscillator Green Functions for $T \neq 0$

As an example, consider a single harmonic oscillator of frequency Ω or, equivalently, a free particle at a point in the second-quantized field formalism (see Chapter 7). We shall start with the second representation.

18.5.1 Creation Annihilation Operators

The operators $\hat{O}^1_H(t)$ and $\hat{O}^2_H(t)$ are the creation and annihilation operators in the Heisenberg picture

$$\hat{a}^\dagger_H(t) = \hat{a}^\dagger e^{i\Omega t}, \quad \hat{a}_H(t) = \hat{a} e^{-i\Omega t}. \tag{18.68}$$

The eigenstates of the Hamiltonian operator

$$\hat{H} = \frac{1}{2}\left(\hat{p}^2 + \Omega^2 \hat{x}^2\right) = \frac{\omega}{2}\left(\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger\right) = \omega\left(\hat{a}^\dagger\hat{a} \pm \frac{1}{2}\right) \tag{18.69}$$

are

$$|n\rangle = \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n|0\rangle, \tag{18.70}$$

with the eigenvalues $E_n = (n \pm 1/2)\Omega$ for $n = 0, 1, 2, 3, \ldots$ or $n = 0, 1$, if $\hat{a}^\dagger$ and $\hat{a}$ commute or anticommute, respectively [compare Eq. (7.564)]. In the second-quantized field interpretation the energies are $E_n = n\Omega$ and the final Green functions are the same. The spectral function $\rho_{12}(\omega')$ is trivial to calculate. The Schrödinger operator $\hat{O}^2 = \hat{a}^\dagger$ can connect the state $|n\rangle$ only to $\langle n+1|$, with the matrix element $\sqrt{n+1}$. The operator $\hat{O}^1 = \hat{a}$ does the opposite. Hence we have

$$\rho_{12}(\omega') = 2\pi\delta(\omega' - \Omega)(1 \mp e^{-\Omega/T})e^{F/T} \sum_{n=0}^{\infty,0} e^{-(n\pm 1/2)\Omega/T}(n+1). \tag{18.71}$$

Now we make use of the explicit partition functions of the oscillator whose paths satisfy periodic and antiperiodic boundary conditions:

$$Z_\Omega \equiv e^{-F/T} = \sum_{n=0}^{\infty,1} e^{-(n\pm 1/2)\Omega/T} = \left\{ \begin{array}{c} [2\sinh(\Omega/2T)]^{-1} \\ 2\cosh(\Omega/2T) \end{array} \quad \text{for} \quad \begin{array}{c} \text{bosons} \\ \text{fermions} \end{array} \right\}. \tag{18.72}$$

These allow us to calculate the sums in (18.71) as follows

$$\sum_{n=0}^{\infty} e^{-(n+1/2)\Omega/T}(n+1) = \left(-T\frac{\partial}{\partial\Omega} + \frac{1}{2}\right) e^{-F/T} = \left(1 \mp e^{-\Omega/T}\right)^{-1} e^{-F/T},$$
$$\sum_{n=0}^{0} e^{-(n-1/2)\Omega/T}(n+1) = e^{\Omega/2T} = \left(1 + e^{-\Omega/T}\right)^{-1} e^{-F/T}. \tag{18.73}$$

The spectral function $\rho_{12}(\omega')$ of the a single oscillator quantum of frequency Ω is therefore given by

$$\rho_{12}(\omega') = 2\pi\delta(\omega' - \Omega). \tag{18.74}$$

With it, the retarded and imaginary-time Green functions become

$$G^R_\Omega(t,t') = \Theta(t-t')e^{-\Omega(t-t')}, \tag{18.75}$$

$$G_\Omega(\tau,\tau') = -T \sum_{m=-\infty}^{\infty} e^{-i\omega_m(\tau-\tau')} \frac{1}{i\Omega_m - \Omega} \tag{18.76}$$

$$= e^{-\Omega(\tau-\tau')} \left\{ \begin{array}{c} 1 \pm n_\Omega \\ \pm n_\Omega \end{array} \right. \quad \text{for} \quad \tau \begin{array}{c} \geq \\ < \end{array} \tau', \tag{18.77}$$

with the average particle number n_Ω of (18.36). The commutation function, for instance, is by (18.44) and (18.74):

$$C_{12}(t,t') = e^{-i\Omega(t-t')}, \tag{18.78}$$

and the correlation function of the "wrong commutator" is from (18.53) and (18.74):

$$A_\Omega(t,t') = \tanh^{\mp 1}\frac{\Omega}{2T} e^{-i\Omega(t-t')}. \tag{18.79}$$

Of course, these harmonic-oscillator expressions could have been obtained directly by starting from the defining operator equations. For example, the commutator function

$$C_\Omega(t,t') = e^{F/T}\text{Tr}\left\{e^{-\hat{H}/T}[\hat{a}_H(t), \hat{a}^\dagger_H(t')]_\mp\right\} \tag{18.80}$$

turn into (18.78) by using the commutation rule at different times

$$[\hat{a}_H(t), \hat{a}_H^\dagger(t')] = e^{-i\Omega(t-t')}, \tag{18.81}$$

which follows from (18.68). Since the right-hand side is a c-number, the thermodynamic average is trivial:

$$e^{F/T}\mathrm{Tr}\,(e^{-\hat{H}/T}) = 1. \tag{18.82}$$

After this, the relations (18.41), (18.42) determine the retarded and advanced Green functions

$$G_\Omega^R(t-t') = \Theta(t-t')e^{-i\Omega(t-t')}, \quad G_\Omega^A(t-t') = -\Theta(t'-t)e^{-i\Omega(t-t')}. \tag{18.83}$$

For the Green function at imaginary times

$$G_\Omega(\tau,\tau') \equiv e^{F/T}\mathrm{Tr}\left[e^{-\hat{H}/T}\hat{T}_\tau \hat{a}_H(\tau)\hat{a}_H^\dagger(\tau')\right], \tag{18.84}$$

the expression (18.77) is found using [see (18.85)]

$$\begin{aligned} \hat{a}_H^\dagger(\tau) &\equiv e^{\hat{H}\tau}\hat{a}^\dagger e^{-\hat{H}\tau} = \hat{a}^\dagger e^{\Omega\tau}, \\ \hat{a}_H(\tau) &\equiv e^{\hat{H}\tau}\hat{a}e^{-\hat{H}\tau} = \hat{a}e^{-\Omega\tau}, \end{aligned} \tag{18.85}$$

and the summation formula (18.73).

The "wrong" commutator function (18.79) can, of course, be immediately derived from the definition

$$A_{12}(t-t') \equiv e^{F/T}\mathrm{Tr}\left\{e^{-\hat{H}/T}\left[\hat{a}_H(t), \hat{a}_H^\dagger(t')\right]_\pm\right\} \tag{18.86}$$

and (18.68), by inserting intermediate states.

For the temporal behavior of the time-ordered Green function we find from (18.48)

$$G_\Omega(\omega) = \left(1 \mp e^{-\Omega/T}\right)^{-1} G_\Omega^R(\omega) + \left(1 \mp e^{\Omega/T}\right)^{-1} G_\Omega^A(\omega), \tag{18.87}$$

and from this by a Fourier transformation

$$\begin{aligned} G_\Omega(t,t') &= \left(1 \mp e^{-\Omega/T}\right)^{-1}\Theta(t-t')e^{-i\Omega(t-t')} - \left(1 \mp e^{\Omega/T}\right)^{-1}\Theta(t'-t)e^{-i\Omega(t-t')} \\ &= \left[\Theta(t-t') \pm (e^{\Omega/T} \mp 1)^{-1}\right]e^{-i\Omega(t-t')} = \left[\Theta(t-t') \pm n_\Omega\right]e^{-i\Omega(t-t')}. \end{aligned} \tag{18.88}$$

The same result is easily obtained by directly evaluating the defining equation using (18.68) and inserting intermediate states:

$$\begin{aligned} G_\Omega(t,t') &\equiv G_\Omega(t-t') = e^{F/T}\mathrm{Tr}\left[e^{-\hat{H}/T}\;\hat{T}\hat{a}_H(t)\hat{a}_H^\dagger(t')\right] \\ &= \Theta(t-t')\langle\hat{a}\,\hat{a}^\dagger\rangle e^{-i\Omega(t-t')} \pm \Theta(t'-t)\langle\hat{a}^\dagger\,\hat{a}\rangle e^{-i\Omega(t-t')} \\ &= \Theta(t-t')(1 \pm n_\Omega)e^{-i\Omega(t-t')} \pm \Theta(t'-t)n_\Omega e^{-i\Omega(t-t')}, \end{aligned} \tag{18.89}$$

which is the same as (18.88). For the correlation function with a and $a^\dagger$ interchanged,

$$\bar{G}_\Omega(t,t') \equiv G_\Omega(t-t') = e^{F/T}\text{Tr}\left[e^{-\hat{H}/T}\,\hat{T}\hat{a}_H^\dagger(t)\hat{a}_H(t')\right], \tag{18.90}$$

we find in this way

$$\begin{aligned}\bar{G}_\Omega(t,t') &= \Theta(t-t')\langle\hat{a}^\dagger\,\hat{a}\rangle e^{-i\Omega(t-t')} \pm \Theta(t'-t)\langle\hat{a}\,\hat{a}^\dagger\rangle e^{-i\Omega(t-t')} \\ &= \Theta(t-t')n_\Omega e^{-i\Omega(t-t')} \pm \Theta(t'-t)(1 \pm n_\Omega)e^{-i\Omega(t-t')},\end{aligned} \tag{18.91}$$

in agreement with (18.64).

18.5.2 Real Field Operators

From the above expressions it is easy to construct the corresponding Green functions for the position operators of the harmonic oscillator $\hat{x}(t)$. It will be useful to keep the discussion more general by admitting oscillators which are not necessarily mass points in space but can be field variables. Thus we shall use, instead of $\hat{x}(t)$, the symbol $\varphi(t)$, and call this a field variable. As in Eq. (7.295) we decompose the field as

$$\hat{x}(t) = \sqrt{\frac{\hbar}{2M\Omega}}\left[\hat{a}e^{-i\Omega t} + \hat{a}^\dagger e^{i\Omega t}\right]. \tag{18.92}$$

In this section we use physical units. The commutator function (18.40) is directly

$$C(t,t') \equiv \langle[\hat{\varphi}(t),\hat{\varphi}(t')]_\mp\rangle_\rho = -\frac{\hbar}{2M\Omega}2i\sin\Omega(t-t'), \tag{18.93}$$

implying a spectral function [recall (18.44)]

$$\rho(\omega') = \frac{1}{2M\Omega}\,2\pi\,[\delta(\omega'-\Omega) - \delta(\Omega'+\Omega)]. \tag{18.94}$$

The real operator $\hat{\varphi}(t)$ behaves like the difference of a particle of frequency Ω and $-\Omega$, with an overall factor $1/2M\Omega$. It is then easy to find the retarded and advanced Green functions of the operators $\hat{\varphi}(t)$ and $\hat{\varphi}(t')$:

$$G^R(t,t') = \frac{\hbar}{2M\Omega}\left[G_\Omega^R(t,t') - G_{-\Omega}^R(t,t')\right] = -\frac{\hbar}{2M\Omega}\Theta(t-t')\,2i\sin\Omega(t-t'), \tag{18.95}$$

$$G^A(t,t') = \frac{\hbar}{2M\Omega}\left[G_\Omega^A(t,t') - G_{-\Omega}^A(t,t')\right] = \frac{\hbar}{2M\Omega}\Theta(t-t')\,2i\sin\Omega(t'-t). \tag{18.96}$$

From the spectral representation (18.53), we obtain for the "wrong commutator"

$$A(t,t') = \langle[\hat{\varphi}(t),\hat{\varphi}(t')]_\mp\rangle = \frac{\hbar}{2M\Omega}\coth^{\pm 1}\frac{\Omega}{2k_BT}2\cos\Omega(t-t'). \tag{18.97}$$

The relation with (18.93) is again a manifestation of the fluctuation-dissipation theorem (18.53).

The average of these two functions yields the time-dependent correlation function at finite temperature containing only the product of the operators

$$G^P(t,t') \equiv \langle \hat\varphi(t)\hat\varphi(t')\rangle = \frac{\hbar}{2M\Omega}\left[(1\pm 2n_\Omega)\cos\Omega(t-t') - i\sin\Omega(t-t')\right], \quad (18.98)$$

with the average particle number n_Ω of (18.36). In the limit of zero temperature where $n_\Omega \equiv 0$, this reduces to

$$G^P(t,t') = \langle \hat\varphi(t)\hat\varphi(t')\rangle = \frac{\hbar}{2M\Omega}e^{-i\Omega(t-t')}. \quad (18.99)$$

The time-ordered Green function is obtained from this by the obvious relation

$$G(t,t') = \Theta(t-t')G^P(t,t') \pm \Theta(t'-t)G^P(t',t) = \frac{1}{2}\left[A(t,t') + \epsilon(t-t')C(t,t')\right], \quad (18.100)$$

where $\epsilon(t-t')$ is the step function of Eq. (1.316). Explicitly, the time-ordered Green function is

$$G(t,t') \equiv \langle \hat T\hat\varphi(t)\hat\varphi(t')\rangle = \frac{\hbar}{2M\Omega}\left[(1\pm 2n_\Omega)\cos\Omega|t-t'| - i\sin\Omega|t-t'|\right], \quad (18.101)$$

which reduces for $T\to 0$ to

$$G(t,t') = \langle \hat T\hat\varphi(t)\hat\varphi(t')\rangle = \frac{\hbar}{2M\Omega}e^{-i\Omega|t-t'|}. \quad (18.102)$$

Thus, as a mnemonic rule, a finite temperature is introduced into a zero-temperature Green function by simply multiplying the real part of the exponential function by a factor $1\pm 2n_\Omega$. This is another way of stating the *fluctuation-dissipation theorem*.

There is another way of writing the time-ordered Green function (18.101) in the bosonic case:

$$G(t,t') \equiv \langle \hat T\hat\varphi(t)\hat\varphi(t')\rangle = \frac{\hbar}{2M\Omega}\frac{\cosh\left[\frac{\Omega}{2}\left(\hbar\beta - i|t-t'|\right)\right]}{\sinh\frac{\hbar\Omega\beta}{2}}. \quad (18.103)$$

For $t-t'>0$, this coincides precisely with the periodic Green function $G_{\rm e}^{\rm p}(\tau,\tau') = G_{\rm e}^{\rm p}(\tau-\tau')$ at imaginary-times $\tau>\tau'$ [see (3.251)], if τ and τ' are continued analytically to it and it', respectively. Decomposing (18.101) into real and imaginary parts we see by comparison with (18.100) that anticommutator and commutator functions are the doubled real and imaginary parts of the time-ordered Green function:

$$A(t,t') = 2\,{\rm Re}\,G(t,t'), \qquad C(t,t') = 2i\,{\rm Im}\,G(t,t'). \quad (18.104)$$

In the fermionic case, the hyperbolic functions cosh and sinh in numerator and denominator are simply interchanged, and the result coincides with the analytically continued antiperiodic imaginary-time Green function (3.266).

The time-reversal properties (18.61)–(18.64) of the Green functions become for real fields $\hat{\varphi}(t)$:

$$
\begin{aligned}
G^A(t,t') &= \mp G^R(t',t), && (18.105)\\
A(t,t') &= \pm A(t',t), && (18.106)\\
C(t,t') &= \mp C(t',t), && (18.107)\\
G(t,t') &= \pm G(t',t). && (18.108)
\end{aligned}
$$

18.6 Nonequilibrium Green Functions

Up to this point we have assumed the system to be in intimate contact with a heat reservoir which ensures a constant temperature throughout the volume. The disturbance in (18.3) was taken to be small, so that only a small fraction of the particles could be excited. If the disturbance grows larger, large clouds of excitations can be formed in a local region. Such a system leaves thermal equilibrium, and the response is necessarily nonlinear. The system must be studied in its full quantum-mechanical time evolution. In order to describe such a process theoretically, we shall assume an initial equilibrium characterized by some density operator [compare (2.367)]

$$\hat{\rho} = \sum_n \rho_n |n\rangle\langle n|, \tag{18.109}$$

with eigenvalues

$$\rho_n = e^{-E_n/T}. \tag{18.110}$$

The disturbance sets in at some time t_0. If the initial state is out of equilibrium, the formalism to be described remains applicable, with only a few adaptations, if the initial state at t_0 is still characterized by a density operator of type (18.109), but has probabilities ρ_n different from (18.110). Of course, in the limit of very small deviations from thermal equilibrium, the formalism to be described reduces to the previously treated linear-response theory.

We first develop a perturbation theory for the time evolution of operators in a nonequilibrium situation. This serves to set up a path integral formalism for the description of the dynamical behavior of a single particle in contact with a thermal reservoir. This description can, in principle, be extended to ensembles of many particles by considering a similar path integral for a fluctuating field. After the discussion in Chapter 7, the necessary second quantization is straightforward and requires no detailed presentation.

The perturbation theory for nonequilibrium quantum-statistical mechanics to be developed now is known under the name of *closed-time path Green function formalism* (CTPGF). This formalism was developed by Schwinger [4] and Keldysh [5], and has been applied successfully to many nonequilibrium problems in statistical physics, in particular to superconductivity and plasma physics.

The fundamental problem of nonequilibrium statistical mechanics is finding the time evolution of thermodynamic averages of products of Heisenberg operators $\hat{\varphi}_H(t)$. For interesting applications it is useful to keep the formulation general and deal with relativistic *fields* of operators $\hat{\varphi}_H(\mathbf{x}, t)$. As in Section 7.6, an extra spatial argument $\mathbf{x}$ allows for a different time-dependent operator $\hat{\varphi}(t)$ at each point $\mathbf{x}$ in space. In order to prepare ourselves for the most interesting study of electromagnetic fields, we consider the simplest relativistically invariant classical action describing an observable field in D dimensions which has the form

$$\mathcal{A}_0 = \int dt d^D x \, \mathcal{L}_0(\mathbf{x}, t) \equiv \frac{1}{2} \int dt d^D x \left\{ [\dot{\varphi}(\mathbf{x}, t)]^2 - [\boldsymbol{\nabla}\varphi(\mathbf{x}, t)]^2 - m^2 \varphi^2(\mathbf{x}, t) \right\}. \tag{18.111}$$

As in Section 7.6, we go over to a countable set of infinite points $\mathbf{x}$ assuming that space is a fine lattice of spacing ϵ, with the continuum limit $\epsilon \to 0$ taken at the end. The associated Euler-Lagrange equation extremizing the action is the *Klein-Gordon equation*

$$\ddot{\varphi}(\mathbf{x}, t) + (-\partial_{\mathbf{x}}^2 + m^2)\varphi(\mathbf{x}, t) = 0. \tag{18.112}$$

This is solved by plane waves

$$f_{\mathbf{p}}(\mathbf{x}, t) = \frac{1}{\sqrt{2\omega_{\mathbf{p}} V}} e^{-i\omega_{\mathbf{p}} t + i\mathbf{p}\mathbf{x}}, \qquad \bar{f}_{\mathbf{p}}(\mathbf{x}, t) = \frac{1}{\sqrt{\omega_{\mathbf{p}} V}} e^{i\omega_{\mathbf{p}} t + i\mathbf{p}\mathbf{x}} \tag{18.113}$$

of positive and negative energy. As in Section 7.6, we imagine the system to be confined to a finite cubic volume V. Then the momenta $\mathbf{p}$ are discrete. The solutions (18.113) behave like an infinite set of harmonic oscillator solution, one for each momentum vector $\mathbf{p}$, with the $\mathbf{p}$-dependent frequencies

$$\omega_{\mathbf{p}} \equiv \sqrt{\mathbf{p}^2 + m^2}. \tag{18.114}$$

The general solution of (18.112) may be expanded as

$$\varphi(\mathbf{x}, t) = \sum_{\mathbf{p}} \frac{1}{2\omega_{\mathbf{p}} V} \left(a_{\mathbf{p}} e^{-i\omega_{\mathbf{p}} + i\mathbf{p}\mathbf{x}} + a_{\mathbf{p}}^* e^{i\omega_{\mathbf{p}} t + i\mathbf{p}\mathbf{x}} \right). \tag{18.115}$$

The canonical momenta of the field variables $\varphi(\mathbf{x}, t)$ are the field velocities

$$\pi(\mathbf{x}, t) \equiv p_{\mathbf{x}}(t) \equiv \dot{\varphi}(\mathbf{x}, t). \tag{18.116}$$

The fields are quantized by the canonical commutation rules

$$[\hat{\pi}(\mathbf{x}, t), \varphi(\mathbf{x}, t)] = -i\delta_{\mathbf{x}\mathbf{x}'}. \tag{18.117}$$

The quantum field is now expanded as in (18.115), but in terms of operators $\hat{a}_{\mathbf{p}}$ and their Hermitian adjoint operators $\hat{a}_{\mathbf{p}}^\dagger$. These satisfy the usual canonical commutation rules of creation and annihilation operators of Eq. (7.294):

$$[\hat{a}_{\mathbf{p}}(t), \hat{a}_{\mathbf{p}'}^\dagger(t)] = \delta_{\mathbf{p}\mathbf{p}'}, \qquad [\hat{a}_{\mathbf{p}}^\dagger(t), \hat{a}_{\mathbf{p}'}^\dagger(t)] = 0, \qquad [\hat{a}_{\mathbf{p}}(t), \hat{a}_{\mathbf{p}'}(t)] = 0. \tag{18.118}$$

The simplest nonequilibrium quantities to be studied are the thermal averages of one or two such field operators. More generally, we may investigate the averages of one or two fields with respect to an arbitrary initial density operator $\hat{\rho}$, the so-called *ρ-averages*:

$$\begin{aligned} \langle \hat{\varphi}_H(x) \rangle_\rho &= \text{Tr}\,[(\hat{\rho}\; \hat{\varphi}_H(x)]\,, \\ \langle \hat{\varphi}_H(x)\hat{\varphi}_H(y) \rangle_\rho &= \text{Tr}\,[\hat{\rho}\; \hat{\varphi}_H(x)\hat{\varphi}_H(y)]\,. \end{aligned} \tag{18.119}$$

For brevity, we have gone over to a four-vector notation and use spacetime coordinates $x \equiv (\mathbf{x}, t)$ to write $\hat{\varphi}_H(\mathbf{x}, t)$ as $\hat{\varphi}_H(x)$.

In general, the fields $\varphi(\mathbf{x}, t)$ will interact with each other and with further fields, adding to (18.111) some interaction $\mathcal{A}^{\text{int}}$. The behavior of an interacting field system can then be studied in perturbation theory. This is done by techniques related to those in Section 1.7. First we identify a time-independent part of the Hamiltonian for which we can solve the Schrödinger equation exactly. This is called the free part of the Hamiltonian $\hat{H}_0$. For the field $\varphi(\mathbf{x}, t)$ at hand this follows from the action (18.111) via the usual Legendre transformation (1.13). Its operator version is

$$\hat{H}_0 = \int d^D x\, \hat{\mathcal{H}}_0(\mathbf{x}, t) \equiv \frac{1}{2} \int d^D x \left\{ [\dot{\hat{\varphi}}(\mathbf{x}, t)]^2 + [\boldsymbol{\nabla} \hat{\varphi}(\mathbf{x}, t)]^2 + m^2 \hat{\varphi}^2(\mathbf{x}, t) \right\}. \tag{18.120}$$

The interaction $\mathcal{A}^{\text{int}}$ gives rise to an interaction Hamiltonian $\hat{H}^{\text{int}}(t)$. Then we introduce the field operators in Dirac's *interaction picture* $\hat{\varphi}(x)$. These are related to the Heisenberg operators via the free Hamiltonian $\hat{H}_0$, by

$$\hat{\varphi}(x) \equiv e^{i\hat{H}_0(t-t_0)} \hat{\varphi}_H(x, t_0) e^{-i\hat{H}_0(t-t_0)}. \tag{18.121}$$

The operators in the two pictures are equal to each other at a time t_0 at which the density operator $\hat{\rho}$ is known. We also introduce the interaction picture for the interaction Hamiltonian[3]

$$\hat{H}_I^{\text{int}}(t) \equiv e^{i\hat{H}t} \hat{H}^{\text{int}}(t) e^{-i\hat{H}t}. \tag{18.122}$$

This operator is used to set up the time evolution operator in the interaction picture

$$\hat{U}(t, t_0) \equiv \hat{T} \exp\left[i \int_{t_0}^{t} dt'\, \hat{H}_I^{\text{int}}(t') \right]. \tag{18.123}$$

It allows us to express the time dependence of the field operators $\hat{\varphi}(x)$ as follows:

$$\hat{\varphi}_H(x) = \hat{U}(t_0, t) \hat{\varphi}(x) \hat{U}(t, t_0). \tag{18.124}$$

[3]For consistency, the field operator $\hat{\varphi}(x)$ should carry the same subscript I which is, however, omitted to shorten the notation.

The ρ-averages of the Heisenberg fields in the interaction representation are therefore

$$\langle\hat\varphi_H(x)\rangle_\rho = \mathrm{Tr}\left[\hat\rho\,\hat U(t_0,t)\hat\varphi(x)\hat U(t,t_0)\right], \tag{18.125}$$

$$\langle\hat\varphi_H(x)\hat\varphi_H(x')\rangle_\rho = \begin{cases}\mathrm{Tr}\left[\hat\rho\,\hat U(t_0,t)\hat\varphi(x)\hat U(t,t')\hat\varphi(x')\hat U(t',t_0)\right], & t>t',\\ \mathrm{Tr}\left[\hat\rho\,\hat U(t_0,t')\hat\varphi(x')\hat U(t',t)\hat\varphi(x)\hat U(t,t_0)\right], & t'>t.\end{cases} \tag{18.126}$$

Now, suppose that the interaction has been active for a very long time, i.e., we let $t_0\to-\infty$. In this limit, (18.125) can be rewritten in terms of the scattering operator $\hat S\equiv\hat U(\infty,-\infty)$ of the system.[4] Using the time-ordering operator $\hat T$ of Eq. (1.241), we may write

$$\langle\hat\varphi_H(x)\rangle_\rho = \mathrm{Tr}\left[\hat\rho\,\hat S^\dagger\hat T\hat S\hat\varphi(x)\right], \tag{18.127}$$

$$\langle\hat\varphi_H(x)\hat\varphi_H(y)\rangle_\rho = \mathrm{Tr}\left[\hat\rho\,\hat S^\dagger\hat T\hat S\hat\varphi(x)\hat\varphi(y)\right]. \tag{18.128}$$

These expressions are indeed the same as those in (18.125) and (18.125); for instance

$$\begin{aligned}\hat S^\dagger\hat T\left(\hat S\hat\varphi(x)\right) &= \hat U(-\infty,t)\hat U(t,\infty)\hat T\left(\hat U(\infty,t)\hat\varphi(x)\hat U(t,-\infty)\right)\\ &= \hat U(-\infty,t)\hat\varphi(x)\hat U(t,-\infty).\end{aligned} \tag{18.129}$$

For further development it is useful to realize that the operators in the expectations (18.127) and (18.128) can be reinterpreted time-ordered products of a new type, ordered along a *closed-time contour* which extends from $t=-\infty$ to $t=\infty$ *and back*. This contour is imagined to encircle the time axis in the complex t-plane as shown in Figure 18.1. The contour runs from $t=-\infty$ to $t=\infty$ above the real

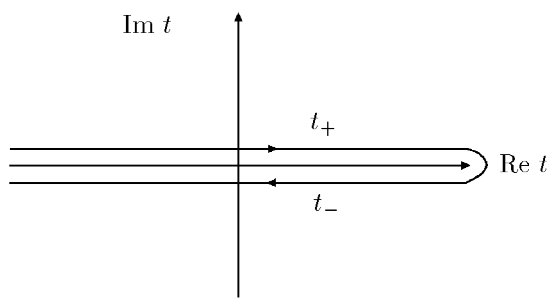

Figure 18.1 Closed-time contour in forward–backward path integrals.

time axis and returns below it. Accordingly, we distinguish t values from the upper branch and the lower branch by writing them as t_+ and t_-, respectively. Similarly we define $x(t_+)\equiv x_+$ and $x(t_-)\equiv x_-$. When viewed as a function of the closed-time contour, the operator

$$\hat S^\dagger\hat T\left(\hat S\hat\varphi(x)\right) \tag{18.130}$$

[4] The matrix elements of $\hat S$ between momentum eigenstates form the so-called S-matrix.

can be rewritten as

$$\hat{T}_{\mathrm{P}}\left(\hat{S}^{\dagger}\hat{S}\hat{\varphi}(x_{+})\right), \tag{18.131}$$

where $\hat{T}_{\mathrm{P}}$ performs a time ordering along the closed-time contour. The coordinate x lies on the positive branch of the contour, where it is denoted by x_{+}. The operator $\hat{T}_{\mathrm{P}}$ is called *path-ordering operator*.

We can then write down immediately a generating functional for an arbitrary product of field operators ordered along the closed-time path:

$$\hat{T}_{\mathrm{P}}\left\{\hat{S}^{\dagger}\hat{S}\exp\left[i\int dx\, j(x_{+})\hat{\varphi}(x_{+})\right]\right\}, \tag{18.132}$$

where dx is short for $d^3x dt$. Functional differentiation with respect to $j(x_{+})$ produces $\hat{\varphi}(x_{+})\equiv\hat{\varphi}(x)$. For symmetry reasons it is also useful to introduce the source $j(x_{-})$ coupled to the field on the lower time branch $\hat{\varphi}(x_{-})$. Thus we shall work with the symmetric generating functional

$$Z[j_{\mathrm{P}}]=\mathrm{Tr}\left(\hat{\rho}\;\hat{T}_{\mathrm{P}}\hat{S}^{\dagger}\hat{S}\exp\left\{i\left[\int dx\, j(x_{+})\hat{\varphi}(x_{+})+\int dx\, j(x_{-})\hat{\varphi}(x_{-})\right]\right\}\right).$$

It can be written as

$$Z[j_{\mathrm{P}}]=\mathrm{Tr}\left\{\hat{\rho}\;\hat{T}_{\mathrm{P}}\hat{S}^{\dagger}\hat{S}\exp\left[i\int_{\mathrm{P}} dx\, j_{\mathrm{P}}(x)\hat{\varphi}_{\mathrm{P}}(x)\right]\right\}, \tag{18.133}$$

with the subscript p distinguishing the time branches.

The path-ordering symbol serves to write down a useful formal expression for the interaction representation of the operator $\hat{S}^{\dagger}\hat{S}$:[5]

$$\hat{S}^{\dagger}\hat{S}=\hat{T}_{\mathrm{P}}\exp\left[-i\int_{\mathrm{P}} dt\, \hat{H}_I^{\mathrm{int}}(t)\right]. \tag{18.134}$$

In terms of this, $Z[j_{\mathrm{P}}]$ takes the suggestive form

$$Z[j_{\mathrm{P}}]=\mathrm{Tr}\left\{\hat{\rho}\;\hat{T}_{\mathrm{P}}\exp\left[-i\int_{\mathrm{P}} dt\hat{H}_I^{\mathrm{int}}(t)+i\int_{\mathrm{P}} dx\, j_{\mathrm{P}}(x)\hat{\varphi}_{\mathrm{P}}(x)\right]\right\}. \tag{18.135}$$

To calculate the integrals along the closed-time contour p, it is advantageous to traverse the lower time branch in the same direction as the upper from $t=-\infty$ to ∞ (since we are used to integrating in this direction), and rewrite the closed-contour integral in the source term,

$$\int_{\mathrm{P}} dx\, j_{\mathrm{P}}(x)\hat{\varphi}_{\mathrm{P}}(x)=\int d^3x\left[\int_{-\infty}^{\infty} dt\, j(\mathbf{x},t_{+})\hat{\varphi}(x_{+})+\int_{\infty}^{-\infty} dt\, j(\mathbf{x},t_{-})\hat{\varphi}(x_{-})\right], \tag{18.136}$$

[5] Note that the left-hand side is equal to 1 due to $\hat{S}$ being unitary. However, this identity cannot be inserted into the path-ordered expressions (18.131)–(18.133), since the current terms require a factorization of $\hat{S}$ or $\hat{S}^{\dagger}$ at specific times and an insertion of field operators between the factors.

as

$$\int_{\mathrm{P}} dx\, j_{\mathrm{P}}(x)\hat{\varphi}_{\mathrm{P}}(x) = \int d^3x \int_{-\infty}^{\infty} dt\, [j(\mathbf{x}, t_+)\hat{\varphi}(x_+) - j(\mathbf{x}, t_-)\hat{\varphi}(x_-)]\,. \tag{18.137}$$

Obviously, the functional derivative with respect to $-j(\mathbf{x}, t_-)$ produces a factor $\hat{\varphi}(x_-)$. Correspondingly, we shall imagine the two fields $\hat{\varphi}(x_+)$, $\hat{\varphi}(x_-)$ as two components of a vector

$$\hat{\vec{\varphi}}(x) = \begin{pmatrix} \hat{\varphi}(x_+) \\ \hat{\varphi}(x_-) \end{pmatrix}, \tag{18.138}$$

with the associated current

$$\vec{\jmath}\,(x) = \begin{pmatrix} j(x_+) \\ -j(x_-) \end{pmatrix}. \tag{18.139}$$

In this vector notation, the source term reads

$$\int dx\, \vec{\jmath}(x)\hat{\vec{\varphi}}(x), \tag{18.140}$$

and all closed-time path formulas go directly over into vector or matrix formulas whose integrals run only once along the positive time axis, for example

$$\int_{\mathrm{P}} dx\, j_{\mathrm{P}}(x)G_{\mathrm{P}}(x, x')j_{\mathrm{P}}(x') = \int dx\, \vec{\jmath}(x)G(x, x')\vec{\jmath}(x'), \tag{18.141}$$

where $G(x, x')$ on the right-hand side denotes the 2×2 matrix

$$G(x, y) = \begin{pmatrix} G_{++}(x, y) & G_{+-}(x, y) \\ G_{-+}(x, y) & G_{--}(x, y) \end{pmatrix} \equiv \begin{pmatrix} G(x_+, y_+) & G(x_+, y_-) \\ G(x_-, y_+) & G(x_-, y_-) \end{pmatrix}. \tag{18.142}$$

Since all formulas for j_{P} and $\hat{\varphi}_{\mathrm{P}}$ hold also for $\vec{\jmath}$ and $\hat{\vec{\varphi}}$, we shall identify the closed-time path objects with the corresponding vectors and matrices.

Differentiating the generating functional with respect to j_{P} produces all Green functions of the theory. Forming two derivatives gives the two-point Green function

$$G_{\mathrm{P}}(x, y) = \frac{\delta}{i\delta j_{\mathrm{P}}(x)} \frac{\delta}{i\delta j_{\mathrm{P}}(y)} Z[j_{\mathrm{P}}]\Big|_{j_{\mathrm{P}}=0} = \mathrm{Tr}\left[\hat{\rho}\; \hat{T}_{\mathrm{P}}\hat{S}^\dagger\hat{S}\; \hat{\varphi}_{\mathrm{P}}(x)\hat{\varphi}_{\mathrm{P}}(y)\right], \tag{18.143}$$

which we decompose according to the branches of the closed-time contour in the same way as the matrix (18.142):

$$G_{\mathrm{P}}(x, y) = \begin{pmatrix} G_{++}(x, y) & G_{+-}(x, y) \\ G_{-+}(x, y) & G_{--}(x, y) \end{pmatrix}. \tag{18.144}$$

The four matrix elements collect precisely the four physically relevant time-dependent Green functions discussed in the last section for the case of $\hat{\rho}$ being an equilibrium density operator. Here they may be out of thermal equilibrium, formed with an arbitrary ρ-average rather than the thermal average at a given temperature. Going back from the interaction picture to the Heisenberg picture, the matrix $G_{\rm P}(x,y)$ is the expectation

$$G_{\rm P}(x,y) = \langle \hat{T}_{\rm P}\hat{\varphi}_H(x_{\rm P})\hat{\varphi}_H(y_{\rm P})\rangle_\rho, \tag{18.145}$$

where $x_{\rm P}$ can be x_+ or x_-. Considering the different components we observe that the path order is trivial as soon as x and y lie on different branches of the time axis. Since y_+ lies always before x_-, the path-ordering operator can be omitted so that

$$G_{-+}(x,y) = \langle \hat{\varphi}_H(x)\hat{\varphi}_H(y)\rangle_\rho. \tag{18.146}$$

In the opposite configuration, the path order is opposite. When reestablishing the original order, a negative sign arises for fermion fields. Hence,

$$G_{+-}(x,y) = \langle \hat{\varphi}_H(y)\hat{\varphi}_H(x)\rangle_\rho = \pm\langle \hat{\varphi}_H(x)\hat{\varphi}_H(y)\rangle_\rho. \tag{18.147}$$

In either case, a distinction of the upper and lower time branches is superfluous after an explicit path ordering.

If both x and y lie on the upper branch, the path order coincides with the usual time order so that $G_{++}(x,y)$ is equal to the expectation

$$G_{++}(x,y) = \langle \hat{T}\hat{\varphi}_H(x)\hat{\varphi}_H(y)\rangle_\rho \equiv G(x,y), \tag{18.148}$$

i.e., the ρ-average of the usual time-ordered Green function. Similarly, if x and y both lie on the lower branch, the path order coincides with the usual anti-time order and

$$G_{--}(x,y) = \langle \hat{\bar{T}}\hat{\varphi}_H(x)\hat{\varphi}_H(y)\rangle_\rho \equiv \bar{G}(x,y). \tag{18.149}$$

From these relations it is easy to see that only three of the four matrix elements of $G_{\rm P}(x,y)$ are linearly independent, since there exists the relation

$$G_{++} + G_{--} = G_{+-} + G_{-+}. \tag{18.150}$$

This can be verified by writing out explicitly the time order and antiorder on the left-hand side. In the linear-response theory of Sections 18.1 and 18.2, the most convenient independent Green functions are the retarded and the advanced ones, together with the expectation of the anticommutator (the commutator for fermions). By analogy, we also define here, in the nonequilibrium case,

$$G^R(x,y) \;=\; \Theta(x-y)\langle[\hat{\varphi}_H(x),\hat{\varphi}_H(y)]_\mp\rangle_\rho, \tag{18.151}$$

$$G^A(x,y) \;=\; -\Theta(y-x)\langle[\hat{\varphi}_H(x),\hat{\varphi}_H(y)]_\mp\rangle_\rho, \tag{18.152}$$

$$A(x,y) \;=\; \langle[\hat{\varphi}_H(x),\hat{\varphi}_H(y)]_\pm\rangle_\rho. \tag{18.153}$$

As in (18.53), the last expression coincides with the absorptive or dissipative part of the Green function. The expectation of the commutator (the anticommutator for fermions),

$$C(x,y) = \langle [\hat{\varphi}_H(x), \hat{\varphi}_H(y)]_{\mp} \rangle_\rho, \tag{18.154}$$

is not an independent quantity. It is related to the others by

$$C(x,y) = G^R(x,y) - G^A(x,y). \tag{18.155}$$

A comparison of the Fourier decomposition of the field (18.115) with (18.92) shows that the Green functions are simple plane-wave superpositions of harmonic oscillator of all momenta $\mathbf{p}$ and frequency $\Omega = \omega_{\mathbf{p}}$. The normalization factor $\hbar/M$ becomes $1/V$. For instance

$$G^R(x,x') = \sum_{\mathbf{p}} \frac{M}{\hbar V} e^{i\mathbf{p}(\mathbf{x}-\mathbf{x}')} G^R(t,t')|_{\Omega=\omega_{\mathbf{p}}}. \tag{18.156}$$

In the continuum limit, where the sum over momenta goes over into an integral with the rule (7.571), this becomes, from (18.95),

$$G^R(x,x') = -\Theta(x-x') \int \frac{d^D p}{2\omega_{\mathbf{p}}(2\pi)^D} e^{i\mathbf{k}(\mathbf{x}-\mathbf{x}')}\, 2i \sin \omega_{\mathbf{p}}(t-t'). \tag{18.157}$$

Similarly we find from (18.102)

$$A(x,x') = \int \frac{d^D p}{2\omega_{\mathbf{p}}(2\pi)^D} e^{i\mathbf{k}(\mathbf{x}-\mathbf{x}')}\, 2 \cos \omega_{\mathbf{p}}(t-t'). \tag{18.158}$$

These and the other Green functions satisfy identities analogous to those formed from the position operator $\hat{\varphi}(t)$ of a simple harmonic oscillator in (18.105)–(18.108):

$$G^A(x,x') = \mp G^R(x',x), \tag{18.159}$$
$$A(x,x') = \pm A(x',x), \tag{18.160}$$
$$C(x,x') = \mp C(x',x). \tag{18.161}$$
$$G(x,x') = \pm G(x',x)^*. \tag{18.162}$$

It is now easy to express the matrix elements of the 2×2 Green function $G_{\mathrm{P}}(x,y)$ in (18.144) in terms of the three independent quantities (18.153). Since

$$\begin{aligned} G^R &= G_{-+} - G_{--} = G_{++} - G_{+-}, \\ G^A &= G_{+-} - G_{--} = G_{++} - G_{-+}, \\ A &= G_{-+} + G_{+-} = G_{++} + G_{--}, \\ C &= G_{-+} - G_{+-} = G^R - G^A, \end{aligned} \tag{18.163}$$

we find

$$\begin{aligned} G_{-+} &= \frac{1}{2}(A+C) = \tfrac{1}{2}(A+G^R-G^A), \\ G_{+-} &= \frac{1}{2}(A-C) = \tfrac{1}{2}(A-G^R+G^A), \end{aligned} \tag{18.164}$$

and

$$\begin{aligned} G_{++} &= G^R + G_{+-} = \tfrac{1}{2}(A+G^R+G^A), \\ G_{--} &= G_{+-} + G_{-+} - G_{++} \\ &= A - G_{++} = \tfrac{1}{2}(A-G^R-G^A). \end{aligned} \tag{18.165}$$

The matrix $G_{\rm P}(x,y)$ can therefore be written as follows:

$$G_{\rm P} = \frac{1}{2}\begin{pmatrix} A+G^R+G^A & A-G^R+G^A \\ A+G^R-G^A & A-G^R-G^A \end{pmatrix}. \tag{18.166}$$

For actual calculations it is somewhat more convenient to use a transformation introduced by Keldysh [5]. It arises from the similarity transformation

$$\tilde{G} = QG_{\rm P}Q^{-1}, \quad \text{with} \quad Q = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} = (Q^T)^{-1}, \tag{18.167}$$

producing the simpler triangular Green function matrix

$$\begin{aligned} \tilde{G}(x,y) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \frac{1}{2}\begin{pmatrix} A+G^R+G^A & A-G^R+G^A \\ A+G^R-G^A & A-G^R-G^A \end{pmatrix} \\ \times \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} = \begin{pmatrix} 0 & G^A \\ G^R & A \end{pmatrix}. \end{aligned} \tag{18.168}$$

Due to the calculational advantages it is worth re-expressing all quantities in the new basis. The linear source term, for example, becomes

$$\begin{aligned} \textstyle\int_{\rm P} dx\, j_{\rm P}(x)\hat{\varphi}_{\rm P}(x) &= \textstyle\int dx\, (j(x_+), -j(x_-)) \begin{pmatrix} \hat{\varphi}(x_+) \\ \hat{\varphi}(x_-) \end{pmatrix} \\ &= \textstyle\int dx\, \tilde{\jmath}(x)\tilde{\hat{\varphi}}(x), \end{aligned} \tag{18.169}$$

with the source vectors

$$\tilde{\hat{\varphi}}(x) \equiv Q\begin{pmatrix} \hat{\varphi}(x_+) \\ \hat{\varphi}(x_-) \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} \hat{\varphi}(x_+) - \hat{\varphi}(x_-) \\ \hat{\varphi}(x_+) + \hat{\varphi}(x_-) \end{pmatrix}, \tag{18.170}$$

and the field vectors

$$\tilde{\jmath}(x) \equiv \begin{pmatrix} j_1(x) \\ j_2(x) \end{pmatrix} = Q\begin{pmatrix} j(x_+) \\ -j(x_-) \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} j(x_+) + j(x_-) \\ j(x_+) - j(x_-) \end{pmatrix}. \tag{18.171}$$

The quadratic source term

$$\begin{aligned}&\int dx\,dx'\,j_{\rm P}(x)G_{\rm P}(x,x')j_{\rm P}(x') \\ &\quad=\int dx\,dx'\,(j(x_+),-j(x_-))\left(\begin{array}{cc}G_{++} & G_{+-}\\ G_{-+} & G_{--}\end{array}\right)(x,x')\left(\begin{array}{c}j(x'_+)\\ -j(x'_-)\end{array}\right)\end{aligned} \tag{18.172}$$

becomes

$$\int dx\,dx'\,\tilde{\jmath}^T(x)\tilde{G}(x,x')\tilde{\jmath}(x'). \tag{18.173}$$

The product[6] of two Green functions $\tilde{G}^{(1)}$ and $\tilde{G}^{(2)}$ has the same triangular form as each factor. The three nonzero entries are composed as follows:

$$\begin{aligned}\tilde{G}^{12} &= \tilde{G}^{(1)}\tilde{G}^{(2)}=QG_{\rm P}^{(1)}Q^{-1}QG_{\rm P}^{(2)}Q^{-1}\\ &= \left(\begin{array}{cc}0 & G_1^AG_2^A\\ G_1^RG_2^R & G_1^RA_2+A_1G_2^A\end{array}\right).\end{aligned} \tag{18.174}$$

More details on these Green functions can be found in the literature [6].

18.7 Perturbation Theory for Nonequilibrium Green Functions

The interaction picture can be used to develop a perturbation expansion for nonequilibrium Green functions. For this we go back to the generating functional (18.135) and assume that the interaction depends only on the field operators. Usually it will be a local interaction, i.e., a spacetime integral over an interaction density:

$$\exp\left[-i\int_{\rm P}dt\,\hat{H}_I^{\rm int}(t)\right]=\exp\left[i\int_{\rm P}dt\,\int d^3x\,L^{\rm int}(\hat{\varphi}_{\rm P}({\bf x},t))\right]. \tag{18.175}$$

The subsequent formal development applies also to the case of a more general nonlocal interaction

$$\exp\left\{i\mathcal{A}_{\rm P}^{\rm int}[\hat{\varphi}_{\rm P}]\right\}. \tag{18.176}$$

To account for the interaction, we use the fact used in Section 3.18, that within the expectation (18.135) the field $\hat{\varphi}_{\rm P}$ can be written as a differential operator $\delta/i\delta j_{\rm P}(x)$ applied to the source term. In this form, the interaction term can be moved outside the thermal expectation. The result is the generating functional in the interaction picture

$$Z[j_{\rm P}]=\exp\left\{i\mathcal{A}_{\rm P}^{\rm int}\left[\delta/i\delta j_{\rm P}\right]\right\}Z_0[j_{\rm P}], \tag{18.177}$$

[6] The product is meant in the functional sense, i.e., $(G^{(1)}G^{(2)})(x,y)=\int dz\,G^{(1)}(x,z)G^{(2)}(z,y)$.

where

$$Z_0[j_{\rm P}] = {\rm Tr}\left\{\hat\rho\,\hat T_{\rm P}\exp\left[i\int_{\rm P} dx\,\hat\varphi_{\rm P}(x)\,j_{\rm P}(x)\right]\right\} \tag{18.178}$$

is the free partition function.

To apply this formula, we have to find $Z_0[j_{\rm P}]$ explicitly. By expanding the exponential in powers of $i\mathcal{A}_{\rm P}^{\rm int}[\delta/i\delta j_{\rm P}]$ and performing the functional derivatives $\delta/i\delta j_{\rm P}$, we obtain the desired perturbation expansion for $Z[j_{\rm P}]$.

For a general density operator $\hat\rho$, the free partition function $Z_0[j_{\rm P}]$ cannot be written down in closed form. Here we give $Z_0[j_{\rm P}]$ explicitly only for a harmonic system in thermal equilibrium, where the ρ-averages $\langle\ldots\rangle_\rho$ are the thermal averages $\langle\ldots\rangle_T$ calculated in Sections 18.1 and 18.2. Since the fluctuation terms in the field $\varphi(t)$ are quadratic, $Z_0[j_{\rm P}]$ must have an exponent quadratic in the sources $j_{\rm P}$. To satisfy (18.143), the functional is necessarily given by

$$Z_0[j_{\rm P}] = \exp\left[-\frac{1}{2}\int dxdy\,j_{\rm P}(x)G_{\rm P}(x,y)j_{\rm P}(y)\right]. \tag{18.179}$$

Inserting the 4×4-matrix (18.166), this becomes

$$\begin{aligned}
Z_0[j_+,j_-] &= \exp\left[-\frac{1}{2}\int dx\int dx'\,(j_+,-j_-)Q^{-1}\begin{pmatrix} 0 & G^A \\ G^R & A\end{pmatrix} Q\begin{pmatrix} j_+ \\ -j_-\end{pmatrix}\right]\\
&= \exp\Big\{-\frac{1}{4}\int dx\int dx'\Big[(j_+ + j_-)(x)G^A(x,x')(j_+ - j_-)(x')\\
&\qquad\qquad + (j_+ - j_-)(x)G^R(x,x')(j_+ + j_-)(x')\\
&\qquad\qquad + (j_+ - j_-)(x)A(x,x')(j_+ - j_-)(x')\Big]\Big\},
\end{aligned} \tag{18.180}$$

where

$$j_+(x)\equiv j(x_+),\quad j_-(x)\equiv j(x_-). \tag{18.181}$$

The advanced Green functions are different from zero only for $t<t'$. Using relation (18.159), the second term is seen to be the same as the first. For the real field at hand, these terms are purely imaginary [see (18.156)]. The anticommutation function $A(x,x')$ is symmetric by (18.160). We therefore rewrite (18.180) as

$$\begin{aligned}
Z_0[j_+,j_-] &= \exp\Big\{-\frac{1}{2}\int dx\int dx'\,\Theta(x'-x)\\
&\times\Big[(j_+ - j_-)(x)G^R(x,x')(j_+ + j_-)(x') + (j_+ - j_-)(x)A(x,x')(j_+ - j_-)(x')\Big]\Big\}.
\end{aligned} \tag{18.182}$$

For any given spectral function, the exponent can easily be written down explicitly using the spectral representations (18.44) and (18.53).

As an important example consider the simple case of a single harmonic oscillator of frequency Ω. Then the field $\hat\varphi(x)$ depends only on the time t, and the commutator and "wrong" commutator functions are given by (18.93) and (18.102). Reintroducing all factors $\hbar$ and k_B, we have

$$Z_0[j_+,j_-] = \exp\Big\{ -\frac{1}{2\hbar^2}\int dt \int dt' \Theta(t-t') \times\Big[(j_+-j_-)(t)C(t,t')(j_++j_-)(t') + (j_+-j_-)(t)A(t,t')(j_+-j_-)(t')\Big]\Big\} \tag{18.183}$$

or, more explicitly,

$$\begin{aligned} Z_0[j_+,j_-] = \exp\Big\{ &-\frac{1}{2M\Omega\hbar}\int dt \int dt'\, \Theta(t'-t) \\ &\times\Big[-(j_+-j_-)(t) \quad i\sin\Omega(t-t') \quad (j_++j_-)(t') \\ &+ (j_+-j_-)(t)\ \coth\frac{\hbar\Omega}{2k_BT}\cos\Omega(t-t')\ (j_+-j_-)(t')\Big]\Big\}. \end{aligned} \tag{18.184}$$

We have taken advantage of the presence of the Heaviside function to express the retarded Green function for $t>t'$ as a commutator function $C(t,t')$ [recall (18.151), (18.154)]. Together with the anticommutator function $A(t,t')$, we obtain for $t>t'$

$$G(t,t') = \frac{1}{2}\left[A(t,t')+C(t,t')\right] = \frac{\hbar}{2M\Omega}\frac{\cosh\dfrac{\Omega}{2}\left[\hbar\beta - i(t-t')\right]}{\sinh\dfrac{\hbar\Omega\beta}{2}}, \tag{18.185}$$

which coincides with the time-ordered Green function (18.101) for $t>t'$, and thus with the analytically continued periodic imaginary-time Green function (3.251). The exponent in this generating functional is thus quite similar to the equilibrium source term (3.221).

The generating functional (18.180) can, of course, be derived without the previous operator discussion completely in terms of path integrals for the harmonic oscillator in thermal equilibrium. Using the notation $\hat{X}(t)$ for a purely time-dependent oscillator field $\hat{\varphi}(x)$, we can take the generating functional directly from Eq. (3.168):

$$\begin{aligned} (X_bt_b|X_at_a)^j_\Omega &= \int \mathcal{D}X(t)\exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b}dt\left[\frac{M}{2}(\dot{X}^2-\Omega^2X^2)+jX\right]\right\} \\ &= e^{(i/\hbar)\mathcal{A}_{\mathrm{cl},j}}F_{\Omega,j}(t_b,t_a). \end{aligned} \tag{18.186}$$

with a total classical action

$$\begin{aligned} \mathcal{A}_{\mathrm{cl},j} &= \frac{1}{2}\frac{M\Omega}{\sin\Omega(t_b-t_a)}\Big[(X_b^2+X_a^2)\cos\Omega(t_b-t_a)-2X_bX_a\Big] \\ &+ \frac{1}{\sin\Omega(t_b-t_a)}\int_{t_a}^{t_b}dt[X_a\sin\Omega(t_b-t)+X_b\sin\Omega(t-t_a)]j(t), \end{aligned} \tag{18.187}$$

and the fluctuation factor (3.170), and express (18.187) as in (3.171) in terms of the two independent solutions $D_a(t)$ and $D_b(t)$ of the homogenous differential equations (3.48) introduced in Eqs. (2.228) and (2.229):

$$\mathcal{A}_{\mathrm{cl},j} = \frac{M}{2D_a(t_b)}\Big[X_b^2\dot{D}_a(t_b)-X_a^2\dot{D}_b(t_a)-2X_bX_a\Big]$$

$$+ \quad \frac{1}{D_a(t_b)} \int_{t_a}^{t_b} dt\, [X_b D_a(t) + X_a D_b(t)] j(t). \tag{18.188}$$

The fluctuation factor is taken as in (3.172). Then we calculate the thermal average of the forward–backward path integral of the oscillator $X(t)$ via the Gaussian integral

$$Z_0[j_+, j_-] = \int dX_b\, dX_a\ (X_b\, \hbar\beta | X_a 0)_\Omega\ (X_b t_b | X_a t_a)_\Omega^{j+}\ (X_b t_b | X_a t_a)_\Omega^{j-*}. \tag{18.189}$$

Here $(X_b\, \hbar\beta | X_a 0)_\Omega$ is the imaginary-time amplitude (2.411):

$$(X_b \hbar\beta | X_a 0) = \frac{1}{\sqrt{2\pi\hbar/M}} \sqrt{\frac{\Omega}{\sinh \hbar\beta}} \times \exp\left\{ -\frac{1}{2\hbar} \frac{M\Omega}{\sinh \hbar\beta\Omega} [(X_b^2 + X_a^2) \cosh \hbar\beta\Omega - 2X_b X_a] \right\}. \tag{18.190}$$

We have preferred deriving $Z_0[j_+, j_-]$ in the operator language since this illuminates better the physical meaning of the different terms in the result (18.185).

18.8 Path Integral Coupled to Thermal Reservoir

After these preparations, we can embark on a study of a simple but typical problem of nonequilibrium thermodynamics. We would like to understand the quantum-mechanical behavior of a particle coupled to a thermal reservoir of temperature T and moving in an arbitrary potential $V(x)$ [7]. Without the reservoir, the probability of going from x_a, t_a to x_b, t_b would be given by[7]

$$|(x_b t_b | x_a t_a)|^2 = \left| \int \mathcal{D}x(t)\ \exp\left\{ \frac{i}{\hbar} \int dt\ \left[\frac{M}{2} \dot{x}^2 - V(x) \right] \right\} \right|^2. \tag{18.191}$$

This may be written as a path integral over two independent orbits, to be called $x_+(t)$ and $x_-(t)$:

$$(x_b t_b | x_a t_a)(x_b t_b | x_a t_a)^* = \int \mathcal{D}x_+(t)\, \mathcal{D}x_-(t) \times \exp\left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} dt\ \left[\frac{M}{2} (\dot{x}_+^2 - \dot{x}_-^2) - (V(x_+) - V(x_-)) \right] \right\}. \tag{18.192}$$

In accordance with the development in Section 18.7, the two orbits are reinterpreted as two branches of a single closed-time orbit $x_\mathrm{P}(t)$. The time coordinate t_P of the path runs from t_a to t_b slightly above the real time axis and returns slightly below it, just as in Fig. 18.1. The probability distribution (18.191) can then be written as a path integral over the closed-time contour encircling the interval (t_a, t_b):

$$|(x_b t_b | x_a t_a)|^2 = \int \mathcal{D}x_\mathrm{P}\ \exp\left\{ \frac{i}{\hbar} \int_\mathrm{P} dt\ \left[\frac{M}{2} \dot{x}_\mathrm{P}^2 - V(x_\mathrm{P}) \right] \right\}. \tag{18.193}$$

[7] In the sequel, we display the constants $\hbar$ and k_B explicitly.

We now introduce a coupling to a thermal reservoir for which we use, as in the equilibrium discussion in Section 3.13, a bath of independent harmonic oscillators $\hat{\varphi}_i(t)$ of masses M_i and frequencies Ω_i in thermal equilibrium at temperature T. For simplicity, the coupling is assumed to be linear in $\hat{\varphi}_i(t)$ and the position of the particle $x(t)$. The bath contributes to (18.193) a factor involving the thermal expectation of the linear interaction

$$|(x_b t_b|x_a t_a)|^2 = \int \mathcal{D}x_{\rm P} \exp\left\{\frac{i}{\hbar}\int_{\rm P} dt\, \left[\frac{M}{2}\dot{x}_{\rm P}^2 - V(x_{\rm P})\right]\right\} \times {\rm Tr}\left\{\hat{\rho}\,\hat{T}_{\rm P}\exp\left[\frac{i}{\hbar}\sum_i c_i \int_{\rm P} dt\,\hat{\varphi}_{\rm P}^i(t)\,x_{\rm P}(t)\right]\right\}. \qquad (18.194)$$

Here, $\hat{\varphi}_{\rm P}^i(t)$ for $i = 1, 2, 3, \ldots$ are the position operators of the auxiliary harmonic oscillators. Since the oscillators are independent, the trace of the exponentials factorizes into a product of single-oscillator expressions

$${\rm Tr}\left\{\hat{\rho}\,\hat{T}_{\rm P}\exp\left[\frac{i}{\hbar}\sum_i c_i\int_{\rm P} dt\,\hat{\varphi}_{\rm P}^i(t)x_{\rm P}(t)\right]\right\} = \prod_i {\rm Tr}\left\{\hat{\rho}\,\hat{T}_{\rm P}\exp\left[\frac{i}{\hbar}c_i\int_{\rm P} dt\,\hat{\varphi}_{\rm P}^i(t)x_{\rm P}(t)\right]\right\}. \qquad (18.195)$$

The density operator $\hat{\rho}$ has the eigenvalues (18.110).

Each factor on the right-hand side is of the form (18.178) with $\hat{\varphi}(t) = c_i\hat{\varphi}_{\rm P}^i(t)/\hbar$ and $j_{+,-} = x_{+,-}(t)$, so that (18.195) leads to the partition function (18.183), which reads here

$$Z_0^{\rm b}[x_+, x_-] = \exp\left\{-\frac{1}{2\hbar^2}\int dt\int dt'\,\Theta(t-t') \times\Big[(x_+ - x_-)(t)C_{\rm b}(t,t')(x_+ + x_-)(t') + (x_+ - x_-)(t)A_{\rm b}(t,t')(x_+ - x_-)(t')\Big]\right\}, \qquad (18.196)$$

where $C_{\rm b}(t,t')$ and $A_{\rm b}(t,t')$ collect the commutator and anticommutator functions of the bath. They are sums of correlation functions (18.93) and (18.102) of the individual oscillators of mass M_i and frequency Ω_i, each contributing with a weight c_i^2. Thus we may write

$$C_{\rm b}(t,t') = \sum_i c_i^2\,\langle[\hat{\varphi}_i(t), \hat{\varphi}_i(t')]\rangle_T = -\hbar\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\rho_{\rm b}(\omega')i\sin\omega'(t-t'), \qquad (18.197)$$

$$A_{\rm b}(t,t') = \sum_i c_i^2\,\langle\{\hat{\varphi}_i(t), \hat{\varphi}_i(t')\}\rangle_T = \hbar\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\rho_{\rm b}(\omega')\coth\frac{\hbar\omega'}{2k_BT}\cos\omega'(t-t'), \qquad (18.198)$$

where the ensemble averages at a fixed temperature T are now denoted by a subscript T, and

$$\rho_{\rm b}(\omega') \equiv 2\pi\sum_i\frac{c_i^2}{2M_i\Omega_i}[\delta(\omega'-\Omega_i) - \delta(\omega'+\Omega_i)] \qquad (18.199)$$

is the spectral function of the bath. It is the antisymmetric continuation of the spectral function (3.408) to negative ω'. Since the spectral function of the bath $\rho_{\rm b}(\omega')$

of (18.199) is odd in ω', we can replace both trigonometric functions $-i\sin\omega'(t-t')$ and $\cos\omega'(t-t')$ in (18.199) by the exponentials $e^{-i\omega'(t-t')}$.

The expression in the exponent of (18.196) may be considered as an effective action in the path integral, caused by the thermal bath. We shall therefore write

$$Z_0[x_+,x_-]=\exp\left\{\frac{i}{\hbar}\mathcal{A}^{\rm FV}[x_+,x_-]\right\}=\exp\left\{\frac{i}{\hbar}\left(\mathcal{A}_D^{\rm FV}[x_+,x_-]+\mathcal{A}_F^{\rm FV}[x_+,x_-]\right)\right\},\quad(18.200)$$

where the effective action $\mathcal{A}^{\rm FV}[x_+,x_-]$ consists of a dissipative part $\mathcal{A}_D^{\rm FV}[x_+,x_-]$ and a fluctuation part $\mathcal{A}_F^{\rm FV}[x_+,x_-]$. The expression $Z_0[x_+,x_-]$ is the famous *influence functional* first introduced by Feynman and Vernon.

Inserting (18.200) into (18.194) and displaying explicitly the two branches of the path $x_P(t)$ with the proper limits of time integrations, we obtain from (18.194) the probability for the particle to move from x_at_a to $x_b\,t_b$ as the path integral

$$\begin{aligned}|(x_bt_b|x_at_a)|^2 &= \int\mathcal{D}x_+(t)\int\mathcal{D}x_-(t)\times\\ &\times\exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b}dt\,\left[\frac{M}{2}(\dot x_+^2-\dot x_-^2)-(V(x_+)-V(x_-))\right]+\frac{i}{\hbar}\mathcal{A}^{\rm FV}[x_+,x_-]\right\}.\end{aligned}\quad(18.201)$$

For a better understanding of the influence functional, we introduce an auxiliary retarded function

$$\gamma(t-t')\equiv\Theta(t-t')\frac{1}{M}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{\sigma_{\rm b}(\omega)}{\omega}e^{-i\omega(t-t')}.\quad(18.202)$$

Then we can write

$$\Theta(t-t')C_{\rm b}(t,t')=i\hbar M\dot\gamma(t-t')+i\hbar M\Delta\omega^2\delta(t-t'),\quad(18.203)$$

where the quantity

$$\Delta\omega^2\equiv-\frac{1}{M}\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{\sigma_{\rm b}(\omega')}{\omega'}=-\frac{1}{M}\sum_i\frac{c_i^2}{M_i\Omega_i^2}\quad(18.204)$$

was introduced before in Eq. (3.420). Inserting the first term of the decomposition (18.203) into (18.196), the dissipative part of the influence functional can be integrated by parts in t' and becomes

$$\begin{aligned}\mathcal{A}_D^{\rm FV}[x_+,x_-] &= -\frac{M}{2}\int_{t_a}^{t_b}dt\int_{t_a}^{t_b}dt'\,(x_+-x_-)(t)\gamma(t-t')(\dot x_++\dot x_-)(t')\\ &\quad+\frac{M}{2}\int_{t_a}^{t_b}dt(x_+-x_-)(t)\gamma(t-t_b)(x_++x_-)(t_a).\end{aligned}\quad(18.205)$$

The δ-function in (18.203) contributes to $\mathcal{A}_D^{\rm FV}[x_+,x_-]$ a term analogous to (3.421)

$$\Delta\mathcal{A}_{\rm loc}[x_+,x_-]=\frac{M}{2}\int_{t_a}^{t_b}dt\Delta\omega^2(x_+^2-x_-^2)(t),\quad(18.206)$$

which may simply be absorbed into the potential terms of the path integral (18.201), renormalizing them to

$$-\frac{i}{\hbar}\int_{t_a}^{t_b} dt\, \left[V_{\rm ren}(x_+) - V_{\rm ren}(x_-)\right]. \tag{18.207}$$

This renormalization is completely analogous to that in the imaginary-time formula (3.423).

The odd bath function $\rho_{\rm b}(\omega')$ can be expanded in a power series with only odd powers of ω'. The lowest approximation

$$\rho_{\rm b}(\omega') \approx 2M\gamma\omega', \tag{18.208}$$

describes Ohmic dissipation with some friction constant γ [recall (3.427)]. For frequencies much larger than the atomic relaxation rates, the friction goes to zero. This behavior is modeled by the Drude form (3.428) of the spectral function

$$\rho_{\rm b}(\omega') \approx 2M\gamma\omega' \frac{\omega_D^2}{\omega_D^2 + \omega'^2}. \tag{18.209}$$

Inserting this into Eq. (18.202), we obtain the Drude form of the function $\gamma(t)$:

$$\gamma_D^R(t) \equiv \Theta(t)\, \gamma\omega_D e^{-\omega_D t}. \tag{18.210}$$

The superscript emphasizes the retarded nature. This can also be written as a Fourier integral

$$\gamma_D^R(t) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \gamma_D^R(\omega') e^{-i\omega' t}, \tag{18.211}$$

with the Fourier components

$$\gamma_D^R(\omega') = \gamma \frac{i\omega_D}{\omega' + i\omega_D}. \tag{18.212}$$

The position of the pole in the lower half-plane ensures the retarded nature of the friction term by producing the Heaviside function in (18.210) [recall (1.312)].

The imaginary-time expansion coefficients γ_m of Eq. (3.431) are related to these by

$$\gamma_m = \gamma(\omega')\big|_{\omega'=i|\omega_m|}, \tag{18.213}$$

by close analogy with the relation between the retarded and imaginary-time Green functions (18.30) and (18.31).

In the Ohmic limit (18.208), the dissipative part of the influence functional simplifies. Then $\gamma_D^R(t)$ becomes narrowly peaked at positive t, and may be approximated by a right-sided *retarded* δ-function as

$$\gamma_D^R(t) \to \gamma\, \delta^R(t), \tag{18.214}$$

whose superscript R indicates the retarded asymmetry of the δ-function. With this, (18.205) becomes a local action

$$\mathcal{A}_D^{\rm FV}[x_+, x_-] = -\frac{M}{2}\gamma \int_{t_a}^{t_b} dt (x_+ - x_-)(\dot{x}_+ + \dot{x}_-)^R - \frac{M}{2}\gamma(x_+^2 - x_-^2)(t_a). \tag{18.215}$$

The right-sided nature of the function $\delta^R(t)$ causes an infinitesimal *negative* shift in the time argument of the velocities $(\dot{x}_+ + \dot{x}_-)(t)$ with respect to the factor $(x_+ - x_-)(t)$, indicated by the superscript R. It expresses the *causality* of the friction forces and will be seen to be crucial in producing a probability conserving time evolution of the probability distribution.

The second term changes only the curvature of the effective potential at the initial time, and can be ignored.

It is useful to incorporate the slope information (18.208) also into the bath correlation function $A_{\rm b}(t, t')$ in (18.198), and factorize it as

$$A_{\rm b}(t, t') = 2M\gamma k_B T K(t, t'), \tag{18.216}$$

where

$$K(t, t') = K(t - t') \equiv \frac{1}{2M\gamma k_B T} \sum_i c_i^2 \langle \{\hat{\varphi}_i(t), \hat{\varphi}_i(t')\} \rangle_T. \tag{18.217}$$

The prefactor in (18.216) is conveniently abbreviated by the constant

$$w \equiv 2M\gamma k_B T, \tag{18.218}$$

which is related to the so-called *diffusion constant*

$$D \equiv k_B T / M\gamma \tag{18.219}$$

by

$$w = 2\gamma^2 M^2 D. \tag{18.220}$$

The Fourier decomposition of (18.217) is

$$K(t, t') = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} K(\omega') e^{-i\omega'(t-t')}, \tag{18.221}$$

with

$$K(\omega') \equiv \frac{1}{2M\gamma} \frac{\rho_{\rm b}(\omega')}{\omega'} \frac{\hbar\omega'}{2k_B T} \coth \frac{\hbar\omega'}{2k_B T}. \tag{18.222}$$

In the limit of a purely Ohmic dissipation this simplifies to

$$K(\omega') \to K^{\rm Ohm}(\omega') \equiv \frac{\hbar\omega'}{2k_B T} \coth \frac{\hbar\omega'}{2k_B T}. \tag{18.223}$$

The function $K(\omega')$ has the normalization $K(0)=1$, giving $K(t-t')$ a unit temporal area:

$$\int_{-\infty}^{\infty} dt\, K(t-t') = 1. \tag{18.224}$$

In the classical limit $\hbar \to 0$, the Drude spectral function (18.209) leads to

$$K_D^{\rm cl}(\omega') = \frac{\omega_D^2}{\omega'^2 + \omega_D^2}, \tag{18.225}$$

with the Fourier transform

$$K_D^{\rm cl}(t-t') = \frac{1}{2\omega_D} e^{-\omega_D(t-t')}. \tag{18.226}$$

In the limit of Ohmic dissipation, this becomes a δ-function. Thus $K(t-t')$ may be viewed as a δ-function broadened by quantum fluctuations and relaxation effects.

With the function $K(t,t')$, the fluctuation part of the influence functional in (18.196), (18.200), (18.201) becomes

$$\mathcal{A}_F^{\rm FV}[x_+,x_-] = i\frac{w}{2\hbar}\int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt'\,(x_+ - x_-)(t)\, K(t,t')\,(x_+ - x_-)(t'). \tag{18.227}$$

Here we have used the symmetry of the function $K(t,t')$ to remove the Heaviside function $\Theta(t-t')$ from the integrand, and to extend the range of t'-integration to the entire interval (t_a,t_b).

In the Ohmic limit, the probability of the particle to move from $x_a t_a$ to $x_b t_b$ is given by the path integral

$$\begin{aligned}
|(x_bt_b|x_at_a)|^2 =& \int \mathcal{D}x_+(t) \int \mathcal{D}x_-(t) \\
&\times \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b} dt\left[\frac{M}{2}(\dot x_+^2 - \dot x_-^2) - (V(x_+) - V(x_-))\right]\right\} \\
&\times \exp\left\{-i\int_{t_a}^{t_b} dt\,\frac{M\gamma}{2\hbar}(x_+ - x_-)(t)(\dot x_+ + \dot x_-)^R(t)\right. \\
&\left. \qquad - \frac{w}{2\hbar^2}\int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt'\,(x_+ - x_-)(t)\, K^{\rm Ohm}(t,t')\,(x_+ - x_-)(t')\right\}.
\end{aligned} \tag{18.228}$$

This is the *closed-time path integral* of a particle in contact with a thermal reservoir.

The paths $x_+(t), x_-(t)$ may also be associated with a forward and a backward movement of the particle in time. For this reason, (18.228) is also called a *forward–backward path integral*. The hyphen is pronounced as *minus*, to emphasize the opposite signs in the partial actions.

It is now convenient to change integration variables and go over to average and relative coordinates of the two paths x_+, x_-:

$$\begin{aligned} x &\equiv (x_+ + x_-)/2, \\ y &\equiv x_+ - x_- . \end{aligned} \tag{18.229}$$

Then (18.228) becomes

$$\begin{aligned} |(x_bt_b|x_at_a)|^2 &= \int \mathcal{D}x(t) \int \mathcal{D}y(t) \\ &\times \exp\left\{ -\frac{i}{\hbar}\int_{t_a}^{t_b} dt \left[M\left(-\dot{y}\dot{x} + \gamma y \dot{x}^R\right) + V\left(x+\frac{y}{2}\right) - V\left(x-\frac{y}{2}\right)\right]\right. \\ &\left. \quad - \frac{w}{2\hbar^2}\int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt'\, y(t) K^{\rm Ohm}(t,t') y(t') \right\}. \end{aligned} \quad (18.230)$$

18.9 Fokker-Planck Equation

At high temperatures, the Fourier transform of the Kernel $K(t,t')$ in Eq. (18.223) tends to unity such that $K(t,t')$ becomes a δ-function, so that the path integral (18.230) for the probability distribution of a particle coupled to a thermal bath simplifies to

$$\begin{aligned} P(x_bt_b|x_at_a) \equiv |(x_bt_b|x_at_a)|^2 &= \int \mathcal{D}x(t) \int \mathcal{D}y(t) \\ \times \exp&\left\{ -\frac{i}{\hbar}\int_{t_a}^{t_b} dt\, y[M\ddot{x} + M\gamma\dot{x}^R + V'(x)] - \frac{w}{2\hbar^2}\int_{t_a}^{t_b} dt\, y^2 \right\}. \end{aligned} \quad (18.231)$$

The superscript R records the infinitesimal backward shift of the time argument as in Eq. (18.215). The y-variable can be integrated out, and we obtain

$$P(x_bt_b|x_at_a) = \mathcal{N}\int \mathcal{D}x(t)\, \exp\left\{ -\frac{1}{2w}\int_{t_a}^{t_b} dt\, [M\ddot{x} + M\gamma\dot{x}^R + V'(x)]^2 \right\}. \quad (18.232)$$

The proportionality constant $\mathcal{N}$ can be fixed by the normalization integral

$$\int dx_b\, P(x_bt_b|x_at_a) = 1. \quad (18.233)$$

Since the particle is initially concentrated around x_a, the normalization may also be fixed by the initial condition

$$\lim_{t_b \to t_a} P(x_bt_b|x_at_a) = \delta(x_b - x_a). \quad (18.234)$$

The right-hand side of (18.232) looks like a Euclidean path integral associated with the Lagrangian [8]

$$L_{\rm e} = \frac{1}{2w}[M\ddot{x} + M\gamma\dot{x} + V'(x)]^2. \quad (18.235)$$

The result will, however, be different, due to time-ordering of the $\dot{x}^R$-term.

Apart from this, the Lagrangian is not of the conventional type since it involves a second time derivative. The action principle $\delta\mathcal{A} = 0$ now yields the Euler-Lagrange equation

$$\frac{\partial L}{\partial x} - \frac{d}{dt}\frac{\partial L}{\partial \dot{x}} + \frac{d^2}{dt^2}\frac{\partial L}{\partial \ddot{x}} = 0. \quad (18.236)$$

This equation can also be derived via the usual Lagrange formalism by considering x and $\dot{x}$ as independent generalized coordinates x, v.

18.9.1 Canonical Path Integral for Probability Distribution

In Section 2.1 we have constructed path integrals for time evolution amplitudes to solve the Schrödinger equation. By analogy, we expect the path integral (18.232) for the probability distribution to satisfy a differential equation of the Schrödinger type. This equation is known as a *Fokker-Planck equation*. As in Section 2.1, the relation is established by rewriting the path integral in canonical form. Treating $v = \dot{x}$ as an independent dynamical variable, the canonical momenta of x and v are [9]

$$\begin{aligned} p &= i\frac{\partial L}{\partial \dot{x}} = i\frac{M\gamma}{w}[M\ddot{x} + M\gamma\dot{x} + V'(x)] = i\frac{M\gamma}{w}[M\dot{v} + M\gamma v + V'(x)], \\ p_v &= i\frac{\partial L}{\partial \ddot{x}} = \frac{1}{\gamma}p. \end{aligned} \tag{18.237}$$

The Hamiltonian is given by the Legendre transform

$$H(p, p_v, x, v) = L_{\rm e}(\dot{x}, \ddot{x}) - \sum_{i=1}^{2} \frac{\partial L_{\rm e}}{\partial \dot{x}_i}\dot{x}_i = L_{\rm e}(v, \dot{v}) + ipv + ip_v\dot{v}, \tag{18.238}$$

where $\dot{v}$ has to be eliminated in favor of p_v using (18.237). This leads to

$$H(p, p_v, x, v) = \frac{w}{2M^2}p_v^2 - ip_v\left[\gamma v + \frac{1}{M}V'(x)\right] + ipv. \tag{18.239}$$

The canonical path integral representation for the probability distribution reads therefore

$$\begin{aligned} P(x_bt_b|x_at_a) = \int \mathcal{D}x \int \frac{\mathcal{D}p}{2\pi} \int \mathcal{D}v \int \frac{\mathcal{D}p_v}{2\pi} \\ \times \exp\left\{\int_{t_a}^{t_b} dt\ [i(p\dot{x} + p_v\dot{v}) - H(p, p_v, x, v)]\right\}. \end{aligned} \tag{18.240}$$

It is easy to verify that the path integral over p enforces $v \equiv \dot{x}$, after which the path integral over p_v leads back to the initial expression (18.232). We may keep the auxiliary variable $v(t)$ as an independent fluctuating quantity in all formulas and decompose the probability distribution $P(x_bt_b|x_at_a)$ with respect to the content of v as an integral

$$P(x_bt_b|x_at_a) = \int_{-\infty}^{\infty} dv_b \int_{-\infty}^{\infty} dv_a\, P(x_bv_bt_b|x_av_at_a). \tag{18.241}$$

The more detailed probability distribution on the right-hand side has the path integral representation

$$\begin{aligned} P(x_bv_bt_b|x_av_at_a) = |(x_bv_bt_b|x_av_at_a)|^2 = \int \mathcal{D}x \int \frac{\mathcal{D}p}{2\pi} \int \mathcal{D}v \int \frac{\mathcal{D}p_v}{2\pi} \\ \times \exp\left\{\int_{t_a}^{t_b} dt\,[i(p\dot{x} + p_v\dot{v}) - H(p, p_v, x, v)]\right\}, \end{aligned} \tag{18.242}$$

where the endpoints of v are now kept fixed at $v_b = v(t_b)$, $v_a = v(t_a)$.

We now use the relation between a canonical path integral and the Schrödinger equation discussed in Section 2.1 to conclude that the probability distribution (18.242) satisfies the Schrödinger-like differential equation [10]:

$$H(\hat{p}, \hat{p}_v, x, v)P(x\, v\, t_b|x_a v_a t_a) = -\partial_t P(x\, v\, t|x_a v_a t_a). \tag{18.243}$$

It is called the *Klein-Kramers equation* for the motion of an inert point particle with dissipation. It is a special case of a two-variable *Fokker-Planck equation* whose general version deals with N variables $\mathbf{x}x_1, \ldots, x_N$ collected in a vector $\mathbf{x}$, and has the form

$$\partial_t P(\mathbf{x}\, t|\mathbf{x}_a v_a t_a) = \left[-\partial_i D_i(\mathbf{x}) + \partial_i \partial_j D^{(2)}_{ij}(\mathbf{x})\right] P(\mathbf{x}\, t|\mathbf{x}_a v_a t_a). \tag{18.244}$$

The above equation (18.243) is a special case of this for $N = 2$;

$$\partial_t P(\mathbf{x}\, t|t_a \mathbf{x}_a) = \left(-\kappa_{ij}\partial_i x_j + D_{ij}\partial_i\partial_j\right) P(\mathbf{x}\, t|t_a \mathbf{x}_a). \tag{18.245}$$

with the *diffusion matrix*

$$\mathbf{D} = \begin{pmatrix} 0 & 0 \\ 0 & w/2M^2 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & \gamma k_B T/M \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & \gamma^2 D \end{pmatrix}, \tag{18.246}$$

and

$$\boldsymbol{\kappa} = \begin{pmatrix} 0 & -1 \\ V'(x)/M & \gamma \end{pmatrix}. \tag{18.247}$$

It must be realized that when going over from the classical Hamiltonian (18.239) to the Hamiltonian operator in the differential equation (18.243), there is an operator ordering problem. Such a problem was encountered in Section 10.5 and discussed further at the end of Section 11.3. In this respect the analogy with the simple path integrals in Section 2.1 is not perfect. When writing down Eq. (18.243) we do not know in which order the momentum operator $\hat{p}_v$ must stand with respect to v. If we were dealing with an ordinary functional integral in (18.232) we would know the order. It would be found as in the case of the electromagnetic interaction in Eq. (11.89) to have the symmetric order $-(\hat{p}_v v + v\hat{p}_v)/2$.

On physical grounds, it is easy to guess the correct order. The differential equation (18.243) has to conserve the total probability

$$\int dx\, dv P(x\, v\, t_b|x_a v_a t_a) = 1 \tag{18.248}$$

for all times t. This is guaranteed if all momentum operators stand to the left of all coordinates in the Hamiltonian operator. Indeed, integrating the Fokker-Planck equation (18.243) over x and v, only a left-hand position of the momentum operators leads to a vanishing integral, and thus to a time independent total probability. We suspect that this order must be derivable from the retarded nature of the velocity in the term $y\dot{x}^R$ in (18.231). This will be shown in the next section.

18.9.2 Solving the Operator Ordering Problem

The ordering problem in the Hamiltonian operator associated with (18.239) does not involve the potential $V(x)$. We may therefore study this problem most simply by considering the classical free Hamiltonian

$$\tilde{H}_0(p, p_v, x, v) = \frac{w}{2M^2} p_v^2 - i\gamma p_v v + ipv, \tag{18.249}$$

associated with the Lagrangian path integral

$$P_0(x_b t_b | x_a t_a) = \mathcal{N} \int \mathcal{D}x(t) \, \exp\left\{-\frac{1}{2w} \int_{t_a}^{t_b} dt \, [M\ddot{x} + M\gamma \dot{x}^R]^2\right\}, \tag{18.250}$$

if we ignore the operator ordering problem. We may further concentrate our attention upon the probability distribution with $x_b = x_a = 0$, and assume $t_b - t_a$ to be very large. Then the frequencies of all Fourier decompositions are continuous.

In spite of the restrictions to large $t_b - t_a$, the result to be derived will be valid for any time interval. The reason is that operator order is a property of extremely short time intervals, so that it does not matter, how long the time interval is on which we solve the problem.

Forgetting for a moment the retarded nature of the velocity $\dot{x}$, the Gaussian path integral can immediately be done and yields

$$\begin{aligned} P_0(0\, t_b | 0\, t_a) &\propto \text{Det}^{-1}(-\partial_t^2 - \gamma \partial_t) \\ &\propto \exp\left[-(t_b - t_a) \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \log(\omega'^2 - i\gamma\omega')\right], \end{aligned} \tag{18.251}$$

where γ is *positive*. The integral on the right-hand side diverges. This is a consequence of the fact that we have not used Feynman's time slicing procedure for defining the path integral. As for an ordinary harmonic oscillator discussed in detail in Sections 2.3 and 2.14), this would lead to a finite integral in which ω' is replaced by $\tilde{\omega}' \equiv (2 - 2\cos a\omega')/a^2$:

$$\frac{1}{2} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \log[\tilde{\omega}'^4 + \gamma^2 \tilde{\omega}'^2] = \frac{1}{2} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \log \tilde{\omega}'^2 + \frac{1}{2} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \log[\tilde{\omega}'^2 + \gamma^2] = 0 + \frac{\gamma}{2}. \tag{18.252}$$

For a derivation see Section 2.14, in particular the first term in Eq. (2.485). The same result can equally well be obtained without time slicing by regularizing the divergent integral in (18.251) analytically, as shown in (2.504). Recall the discussion in Section 10.6 where analytic regularization was seen to be the only method that allows to define path integrals without time slicing in such a way that they are invariant under coordinate transformations [11]. It is therefore suggestive to apply the same procedure also to the present path integrals with dissipation and to use the dimensionally regularized formula (2.541):

$$\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \log(\omega' \pm i\gamma) = \frac{\gamma}{2}, \quad \gamma > 0. \tag{18.253}$$

Applying this to the functional determinant in (18.251) yields

$$\begin{aligned}\mathrm{Det}(-\partial_t^2-\gamma\partial_t) &= \mathrm{Det}(i\partial_t)\mathrm{Det}(i\partial_t+i\gamma)=\exp\left[\mathrm{Tr}\,\log(i\partial_t)+\mathrm{Tr}\,\log(i\partial_t+i\gamma)\right]\\ &= \exp\left[(t_b-t_a)\frac{\gamma}{2}\right], \qquad (18.254)\end{aligned}$$

and thus

$$P_0(0\,t_b|0\,t_a) \;\propto\; \exp\left[-(t_b-t_a)\frac{\gamma}{2}\right]. \qquad (18.255)$$

This corresponds to an energy $\gamma/2$, and an ordering $-i\gamma(\hat p_v v+v\hat p_v)/2$ in the Hamiltonian operator.

We now take the retardation of the time argument of $\dot x^R$ into account. Specifically, we replace the term $\gamma y\dot x^R$ in (18.230) by the Drude form on the left-hand side (18.214) before going to the limit $\omega_D\to\infty$:

$$\gamma y\dot x^R(t)\to\int dt'\,y(t)\,\gamma_D^R(t-t')\,x(t'), \qquad (18.256)$$

containing now explicitly the retarded Drude function (18.210) of the friction. Then the frequency integral in (18.251) becomes

$$\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\log\left(\omega'^2-\gamma\frac{\omega'\omega_D}{\omega'+i\omega_D}\right)=\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\left[-\log(\omega'+i\omega_D)+\log\left(\omega'^2+i\omega'\omega_D-\gamma\omega_D\right)\right], \qquad (18.257)$$

where we have omitted a vanishing integral over $\log\omega'$ on account of (18.253). We now decompose

$$\log\left(\omega'^2+i\omega'\omega_D-\gamma\omega_D\right)=\log(\omega'+i\omega_1)+\log(\omega'+i\omega_2), \qquad (18.258)$$

with

$$\omega_{1,2}=\frac{\omega_D}{2}\left(1\pm\sqrt{1-\frac{4\gamma}{\omega_D}}\right), \qquad (18.259)$$

and use formula (2.541) to find

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\left[-\log(\omega'+i\omega_D)+\log\left(\omega'^2+i\omega'\omega_D-\gamma\omega_D\right)\right]=-\frac{\omega_D}{2}+\frac{\omega_1}{2}+\frac{\omega_2}{2}=0. \qquad (18.260)$$

The vanishing frequency integral implies that the retarded functional determinant is trivial:

$$\mathrm{Det}(-\partial_t^2-\gamma\partial_t^R)=\exp\left[\mathrm{Tr}\,\log(-\partial_t^2-\gamma\partial_t^R)\right]=1, \qquad (18.261)$$

instead of (18.254) obtained from the frequency integral without the Drude modification. With the determinant (18.261), the probability becomes a constant

$$P_0(0\,t_b|0\,t_a)=\mathrm{const.} \qquad (18.262)$$

This shows that the retarded nature of the friction force has *subtracted* an energy $\gamma/2$ from the energy in (18.255). Since the ordinary path integral corresponds to a Hamiltonian operator with a symmetrized term $-i(\hat{p}_v v + v\,\hat{p}_v)/2$, the subtraction of $\gamma/2$ changes this term to $-i\gamma\hat{p}_v v$.

Note that the opposite case of an *advanced* velocity term $\dot{x}^A$ in (18.250) would be approximated by a Drude function $\gamma_D^A(t)$ which looks just like $\gamma_D^R(t)$ in (18.212), but with *negative* ω_D. The right-hand side of (18.260) would then become 2γ rather than zero. The corresponding formula for the functional determinant is

$$\mathrm{Det}(-\partial_t^2 - \gamma\partial_t^A) = \exp\left[\mathrm{Tr}\,\log(-\partial_t^2 - \gamma\partial_t^A)\right] = \exp\left[(t_b - t_a)\gamma\right], \qquad (18.263)$$

where $\gamma\partial_t^A$ stands for the advanced version of the functional matrix (18.256) in which ω_D is replaced by $-\omega_D$. Thus we would find

$$P_0(0\,t_b|0\,t_a) \quad \propto \quad \exp\left[-(t_b - t_a)\gamma\right], \qquad (18.264)$$

with an *additional* energy $\gamma/2$ with respect to the ordinary formula (18.255). This corresponds to the opposite (unphysical) operator order $-i\gamma v\hat{p}_v$ in $\hat{H}_0$, which would violate the probability conservation of time evolution twice as much as the symmetric order.

The above formulas for the functional determinants can easily be extended to the slightly more general case where $V(x)$ is the potential of a harmonic oscillator $V(x) = M\omega_0^2 x^2/2$. Then the path integral (18.232) for the probability distribution becomes

$$P_0(x_b t_b|x_a t_a) = \mathcal{N}\int \mathcal{D}x(t)\,\exp\left\{-\frac{1}{2w}\int_{t_a}^{t_b} dt\,[M\ddot{x} + M\gamma\dot{x}^R + \omega_0^2 x]^2\right\}, \quad (18.265)$$

which we evaluate at $x_b = x_a = 0$, where it is given by the properly retarded expression

$$\begin{aligned} P_0(0\,t_b|0\,t_a) \quad &\propto \quad \mathrm{Det}^{-1}(-\partial_t^2 - \gamma\partial_t + \omega_0^2) \\ &\propto \quad \exp\left[-(t_b - t_a)\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\log(\omega'^2 - i\gamma\omega' - \omega_0^2)\right]. \end{aligned} \qquad (18.266)$$

The logarithm can be decomposed into a sum $\log(\omega' + i\omega_1) + \log(\omega' + i\omega_2)$ with

$$\omega_{1,2} = \frac{\gamma}{2}\left(1 \pm \sqrt{1 - \frac{4\omega_0^2}{\gamma^2}}\right). \qquad (18.267)$$

We now apply the analytically regularized formula (2.541) to obtain

$$\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\left[\log(\omega' + i\omega_1) + \log(\omega' + i\omega_2)\right] = \frac{\omega_1}{2} + \frac{\omega_2}{2} = \gamma. \qquad (18.268)$$

Both under- and overdamped motion yield the same result. This is one of the situations where our remarks after Eqs. (2.544) and (2.543) concerning the cancellation of oscillatory parts apply. For the functional determinant (18.266), the result is

$$\mathrm{Det}(-\partial_t^2 - \gamma\partial_t - \omega_0^2) = \exp\left[\mathrm{Tr}\,\log(-\partial_t^2 - \gamma\partial_t - \omega_0^2)\right] = \exp\left[(t_b - t_a)\frac{\gamma}{2}\right]. \ (18.269)$$

Note that the result is independent of ω_0. This can simply be understood by forming the derivative of the logarithm of the functional determinant in (18.254) with respect to ω_0^2. Since $\log \mathrm{Det} M = \mathrm{Tr} \log M$, this yields the trace of the associated Green function:

$$\frac{\partial}{\partial \omega_0^2} \mathrm{Tr} \log(-\partial_t^2 - \gamma\partial_t - \omega_0^2) = -\int dt\, (-\partial_t^2 - \gamma\partial_t - \omega_0^2)^{-1}(t,t). \tag{18.270}$$

In Fourier space, the right-hand side turns into the frequency integral

$$-\int \frac{d\omega'}{2\pi} \frac{1}{(\omega' + i\omega_1)(\omega' + i\omega_1)}. \tag{18.271}$$

Since the two poles lie below the contour of integration, we may close it in the upper half-plane and obtain zero. Closing it in the lower half plane would initially lead to two nonzero contributions from the residues of the two poles which, however, cancel each other.

The Green function (18.270) is causal, in contrast to the oscillator Green function in Section 3.3 whose left-hand pole lies in the upper half-plane (recall Fig. 3.3). Thus it carries a Heaviside function as a prefactor [recall Eq. (1.305) and the discussion of causality there]. The vanishing of the integral (18.270) may be interpreted as being caused by the Heaviside function (1.304).

The γ-dependence of (18.269) can be calculated likewise:

$$\frac{\partial}{\partial \gamma} \log \mathrm{Det} \partial_t(-\partial_t^2 - \gamma\partial_t - \omega_0^2) = -\int dt\, [\partial_t(-\partial_t^2 - \gamma\partial_t - \omega_0^2)^{-1}](t,t). \tag{18.272}$$

We perform the trace in frequency space:

$$i\int \frac{d\omega'}{2\pi} \frac{\omega'}{(\omega' + i\omega_1)(\omega' + i\omega_1)}. \tag{18.273}$$

If we now close the contour of integration with an infinite semicircle in the upper half plane to obtain a vanishing integral from the residue theorem, we must subtract the integral over the semicircle $i \int d\omega'/2\pi\omega'$ and obtain $1/2$, in agreement with (18.269).

Formula (18.269) can be generalized further to time-dependent coefficients

$$\mathrm{Det}\left[-\partial_t^2 - \gamma(t)\partial_t - \Omega^2(t)\right] = \exp\left\{\mathrm{Tr} \log\left[-\partial_t^2 - \gamma(t)\partial_t - \Omega^2(t)\right]\right\} = \exp\left[\int_{t_a}^{t_b} dt \frac{\gamma(t)}{2}\right]. \tag{18.274}$$

This follows from the factorization

$$\mathrm{Det}\left[-\partial_t^2 - \gamma(t)\partial_t - \Omega^2(t)\right] = \mathrm{Det}[\partial_t + \Omega_1(t)]\, \mathrm{Det}[\partial_t + \Omega_2(t)]\,, \tag{18.275}$$

with

$$\Omega_1(t) + \Omega_2(t) = \gamma(t), \qquad \partial_t\Omega_2(t) + \Omega_1(t)\Omega_2(t) = \Omega^2(t), \tag{18.276}$$

and applying formula (3.134).

The probability obtained from the general path integral (18.232) without retardation of the velocity term is therefore

$$P_0(0\,t_b|0\,t_a) \;\;\propto\;\; \exp\left[-(t_b-t_a)\frac{\gamma}{2}\right], \tag{18.277}$$

as in (18.255).

Let us now introduce retardation of the velocity term by using the ω'-dependent Drude expression (18.212) for the friction coefficient. First we consider again the harmonic path integral (18.265), for which (18.266) becomes

$$P_0(0\,t_b|0\,t_a) \propto \exp\left\{-(t_b-t_a)\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\log\left[\omega'^2 - i\gamma_D^R(\omega')\omega' - \omega_0^2\right]\right\}. \tag{18.278}$$

Rewriting the logarithm as $-\log(\omega' + i\omega_D) + \Sigma_{k=1}^3 \log(\omega' + i\omega_k)$ with

$$\omega_{1,2} = \frac{\gamma}{2}\left(1 \pm \sqrt{1-\frac{4\omega_0^2}{\gamma^2}}\right), \qquad \omega_3 = \omega_D - \gamma \tag{18.279}$$

[recall Eq. (3.454) in the equilibrium discussion of Section 3.15], we use again formula (2.541) to find

$$\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\left[-\log(\omega'+i\omega_D) + \sum_{k=1}^{3}\log(\omega'+i\omega_k)\right] = -\omega_D + \sum_{k=1}^{3}\frac{\omega_k}{2} = 0. \tag{18.280}$$

Thus γ and ω_0 disappear from the functional determinant, and we remain with

$$P_0(0\,t_b|0\,t_a) \;\;=\;\; \text{const}\,. \tag{18.281}$$

This implies a unit functional determinant [12]

$$\text{Det}(\partial_t^2 + i\gamma\partial_t^R + \omega_0^2) = 1, \tag{18.282}$$

in contrast to the unretarded determinant (18.269). The γ-independence of this can also be seen heuristically as in (18.270) by forming the derivative with respect to γ:

$$\frac{\partial}{\partial\gamma}\text{Det}(-\partial_t^2 - \gamma\partial_t^R - \omega_0^2) = -\int dt\,[\partial_t^R(\partial_t^2 - \gamma\partial_t - \omega_0^2)^{-1}(t,t). \tag{18.283}$$

Since the retarded derivative carries a Heaviside factor $\Theta(t-t')$ of (1.304), we find zero for $t = t'$.

The result 1/2 of the unretarded derivative in (18.272) can similarly be understood as a consequence of the average Heaviside function (1.313) at $t = t'$.

An advanced time derivative in the determinant (18.282) would, of course, have produced the result

$$\text{Det}(\partial_t^2 + i\gamma\partial_t^A + \omega_0^2) = \gamma. \tag{18.284}$$

By analogy with (18.275), the general retarded determinant is also independent of $\gamma(t)$ and $\Omega(t)$.

$$\mathrm{Det}\left[-\partial_t^2 - \gamma(t)\partial_t^R - \Omega^2(t)\right] = 1. \tag{18.285}$$

In the advanced case, we would find similarly

$$\mathrm{Det}\left[-\partial_t^2 - \gamma(t)\partial_t^A - \Omega^2(t)\right] = \exp\left[\int dt\,\gamma(t)\right]. \tag{18.286}$$

By comparing the functional determinants (18.269) and (18.282) we see that the retardation prescription can be avoided by a trivial additive change of the Lagrangian (18.235) to

$$L_\mathrm{e}(x,\dot{x}) = \frac{1}{2w}\left[\ddot{x} + M\gamma\dot{x} + V'(x)\right]^2 - \frac{\gamma}{2}. \tag{18.287}$$

From this, the path integral can be calculated with the usual time slicing, and the result can be deduced directly from Ref. [8].

The Hamiltonian associated with this Lagangian is only slightly modified with respect to the naive form (18.249):

$$H_0(p,p_v,x,v) = \frac{w}{2M^2}p_v^2 - i\gamma p_v v + ipv - \frac{\gamma}{2}. \tag{18.288}$$

The extra $\gamma/2$ ensures that the operator version of the Hamiltonian (18.239) has $\hat{p}_v$ to the left of v.

18.9.3 Strong Damping

For $\gamma \gg V''(x)/M$, the dynamics is dominated by dissipation, and the Lagrangian (18.235) takes a more conventional form in which only x and $\dot{x}$ appear:

$$L_\mathrm{e}(x,\dot{x}) = \frac{1}{2w}\left[M\gamma\dot{x}^R + V'(x)\right]^2 = \frac{1}{4D}\left[\dot{x}^R + \frac{1}{M\gamma}V'(x)\right]^2, \tag{18.289}$$

where $\dot{x}^R$ lies slightly *earlier* $V'(x(t))$. The probability distribution

$$P(x_b t_b|x_a t_a) = \mathcal{N}\int \mathcal{D}x\,\exp\left[-\int_{t_a}^{t_b} dt\,L_\mathrm{e}(x,\dot{x}^R)\right] \tag{18.290}$$

looks like an ordinary Euclidean path integral for the density matrix of a particle of mass $M = 1/2D$. As such it obeys a differential equation of the Schrödinger type. Forgetting for a moment the subtleties of the retardation, we introduce an auxiliary momentum integration and go over to the canonical representation of (18.290):

$$P(x_b t_b|x_a t_a) = \int \mathcal{D}x \int \frac{\mathcal{D}p}{2\pi}\,\exp\left\{\int_{t_a}^{t_b} dt\,\left[ip\dot{x} - 2D\frac{p^2}{2} + ip\frac{1}{M\gamma}V'(x)\right]\right\}. \tag{18.291}$$

This probability distribution satisfies therefore the Schrödinger type of equation

$$H(\hat{p}_b, x_b)P(x_bt_b|x_at_a) = -\partial_{t_b}P(x_bt_b|x_at_a), \tag{18.292}$$

with the Hamiltonian operator

$$H(\hat{p}, x) \equiv 2D\frac{\hat{p}^2}{2} - i\hat{p}\frac{1}{M\gamma}V'(x) = -D\,\partial_x\left[\partial_x + \frac{1}{DM\gamma}V'(x)\right]. \tag{18.293}$$

In order to conserve probability, the momentum operator has to stand to the left of the potential term. Only then does the integral over x_b of Eq. (18.292) vanish. Equation (18.292) is the overdamped Klein-Kramers equation, also called the *Smoluchowski equation*. It is a special case of ordinary Fokker-Planck equation.

Without the retardation on $\dot{x}$ in (18.290), the path integral would give a symmetrized operator $-i[\hat{p}V'(x) + V'(x)\hat{p}]/2$ in $\hat{H}$. This follows from the fact that the coupling $(1/2DM\gamma)\dot{x}V'(x)$ looks precisely like the coupling of a particle to a magnetic field with a "vector potential" $A(x) = (1/2DM\gamma)V'(x)$ [see (10.171)].

Realizing this it is not difficult to account quite explicitly for the effect of retardation of the velocity in the path integral (18.289) Let us assume, for a moment, that w is very small. Then the path integral (18.290) without the retardation,

$$P_0(x_bt_b|x_at_a) = \mathcal{N}\int\mathcal{D}x\,\exp\left\{-\frac{1}{2w}\int_{t_a}^{t_b}dt\,\left[M\gamma\dot{x} + V'(x)\right]^2\right\}, \tag{18.294}$$

can be performed in the Gaussian approximation resulting for $x_b = x_a = 0$ in the inverse functional determinant

$$P_0(0\,t_b|0\,t_a) \;=\; \mathrm{Det}^{-1}\left[\partial_t + V''(x)/M\gamma\right], \tag{18.295}$$

whose value is according to formula (3.134)

$$\mathrm{Det}\left[\partial_t + V''(x)/M\gamma\right] = \exp\left[\int dt\,V''(x)/2M\gamma\right]. \tag{18.296}$$

The retarded version of this determinant is trivial:

$$\mathrm{Det}\left[\partial_t^R + V''(x)/M\gamma\right] = 1, \tag{18.297}$$

as we learned from Eq. (18.285. The advanced version would be [compare (18.286)]

$$\mathrm{Det}\left[\partial_t^A + V''(x)/M\gamma\right] = \exp\left[\int dt\,V''(x)/M\gamma\right]. \tag{18.298}$$

Although the determinants (18.296), (18.297), and (18.298) were discussed here only for a large time interval $t_b - t_a$, the formulas remain true for all time intervals, due to the trivial first-order nature of the differential operator. In a short time interval, however, the second derivative is approximately time-independent. For this reason the difference between ordinary and retarded path integrals (18.290) is given by the difference between the functional determinants (18.296) and (18.297) not only if w is very small but for all w. Thus we can avoid the retardation of the velocity as in Eq. (18.287) by adding to the Lagrangian (18.289) a term containing the second derivative of the potential:

$$L_{\rm e}(x,\dot{x}) = \frac{1}{4D}\left[\dot{x} + \frac{1}{M\gamma}V'(x)\right]^2 - \frac{1}{2M\gamma}V''(x). \tag{18.299}$$

From this, the path integral can be calculated with the same slicing as for the gauge-invariant coupling in Section 10.5:

$$P_0(x_bt_b|x_at_a) = \mathcal{N}\int \mathcal{D}x(t)\exp\left[-\int_{t_a}^{t_b} dt\left\{\frac{1}{4D}\left[\dot{x}+\frac{V'(x)}{M\gamma}\right]^2 - \frac{V''(x)}{2M\gamma}\right\}\right]. \tag{18.300}$$

As an example consider a harmonic potential $V(x) = M\omega_0^2x^2/2$, where the Lagrangian (18.299) becomes

$$L_{\rm e}(x,\dot{x}) = \frac{1}{4D}\left(\dot{x}+\kappa x\right)^2 - \frac{\kappa}{2}, \tag{18.301}$$

with the abbreviation $\kappa \equiv \omega_0^2/\gamma$. The equation of motion reads

$$-\ddot{x} + \kappa^2 x = 0, \tag{18.302}$$

and its solution connecting x_a, t_a with x_b, t_b is

$$x(t) = \frac{1}{e^{2\kappa t_a} - e^{2\kappa t_b}}\left[e^{\kappa(t+t_a)}x_a - e^{\kappa(-t+t_a+2\kappa t_b)}x_a - e^{\kappa(t+t_b)}x_b + e^{\kappa(-t+2\,t_a+t_b)}x_b\right]. \tag{18.303}$$

This has the total Euclidean action

$$\mathcal{A}_{\rm e} = \frac{\kappa(e^{\kappa t_b}\,x_b - e^{\kappa t_a}\,x_a)^2}{2\,D\,\left(e^{2\kappa t_b} - e^{2\kappa t_a}\right)} - \frac{\kappa}{2}. \tag{18.304}$$

The fluctuation determinant is from Eq. (2.171), after an appropriate substitution of variables,

$$F_\kappa(t_b - t_a) = \frac{1}{\sqrt{2\pi\sinh\kappa(t_b - t_a)}}. \tag{18.305}$$

The probability distribution is then given by

$$P(x_bt_b|x_at_a) = F_\kappa(t_b - t_a)e^{-\mathcal{A}_{\rm e}} = \frac{1}{\sqrt{2\pi\sigma^2(t_b-t_a)}}\exp\left\{-\frac{[x_b - \bar{x}(t_b-t_a)]^2}{2\sigma^2(t_b-t_a)}\right\}, \tag{18.306}$$

where $\bar{x}(t)$, $\sigma^2(t)$ are the averages

$$\bar{x}(t) \equiv \langle x(t)\rangle = x_a e^{-\kappa t}, \quad \sigma^2(t) \equiv \langle [x(t)-\bar{x}(t)]^2\rangle = \frac{D}{\kappa}\left(1 - e^{-2\kappa t}\right), \tag{18.307}$$

obtained from the integrals[8]

$$\bar{x}(t_b - t_a) \equiv \langle x(t_b - t_a)\rangle \equiv \int_{-\infty}^{\infty} x_b P(x_b t_b | x_a t_a), \tag{18.308}$$

$$\langle [x(t_b - t_a) - \bar{x}(t_b - t_a)]^2\rangle \equiv \int_{-\infty}^{\infty} [x_b - \bar{x}(t_b - t_a)]^2 P(x_b t_b | x_a t_a). \tag{18.309}$$

The canonical momentum associated with the Lagrangian (18.301) is $p = (\dot{x} + \kappa x)/2D$ so that the Hamiltonian operator becomes, via the Euclidean Legendre transformation (2.340), and with the operator ordering fixed as discussed after Eq. (18.247):

$$\hat{H}(p, x) = D\hat{p}^2 + i\kappa\hat{p}x, \qquad p \equiv -i\partial_x. \tag{18.310}$$

This is the same operator as in Eq. (18.293), and the Fokker-Planck equation (18.292) reads, for the harmonic potential:

$$\left(-D\partial_{x_b}^2 + \kappa\partial_{x_b} x_b\right) P(x_b t_b | x_a t_a) = -\partial_{t_b} P(x_b t_b | x_a t_a). \tag{18.311}$$

For $t_b \to t_a$, the probability distribution (18.306) starts out as a δ-function around the initial position x_a. In the limit of large $t_b - t_a$, it converges against the limiting distribution

$$\lim_{t_b \to \infty} P(x_b t_b | x_a t_a) = \sqrt{\frac{\kappa}{2\pi D}} \exp\left\{-\kappa \frac{x_b^2}{2D}\right\}. \tag{18.312}$$

Replacing κ again by $\omega_0^2/\gamma = V''(0)/M\gamma$, and D from (18.219), this becomes

$$\lim_{t_b \to \infty} P(x_b t_b | x_a t_a) = \sqrt{\frac{V''(0)}{2\pi k_B T}} \exp\left\{-\frac{1}{k_B T} V(x_b)\right\}. \tag{18.313}$$

Thus, the limiting distribution of (18.290) depends only on x_b. It is given by the Boltzmann factor associated with the potential $V(x)$, in which the particle moves. This result can be generalized to a large class of potentials.

An interesting related result can be derived by introducing an external source term $j_b\, x(t_b)$ into the Lagrangian (18.299). By repeated functional differentiation with respect to j_b we find that the expectation values

$$\langle x^n \rangle = \lim_{t_b \to \infty} \langle x^n(t_b)\rangle = \lim_{t_b \to \infty} \frac{\int \mathcal{D}x\, x^n(t_b) e^{-\int_{t_a}^{t_b} dt\, L_{\rm e}(x, \dot{x}^R)}}{\int \mathcal{D}x\, e^{-\int_{t_a}^{t_b} dt\, L_{\rm e}(x, \dot{x}^R)}} \tag{18.314}$$

have the large-time limit

$$\lim_{t_b \to \infty} \langle x^n(t_b)\rangle = \langle x^n \rangle = \frac{\int dx\, x^n e^{-V(x)/k_B T}}{\int dx\, e^{-V(x)/k_B T}}. \tag{18.315}$$

The generalization of this relation to quantum field theory forms the basis of *stochastic quantization* in Section 18.12.

[8]An alternative method for calculating such expectation values will be presented in Section 18.15.

18.10 Langevin Equations

Consider the forward–backward path integral (18.230) for high γT. Then the second exponent limits the fluctuations of y to satisfy $|y| \ll |x|$, and $K(t,t')$ will be assumed to take the Drude form (18.226), which becomes a δ-function for $\omega_D \to \infty$. Then we can expand

$$V\left(x+\frac{y}{2}\right) - V\left(x-\frac{y}{2}\right) \sim yV'(x) + \frac{y^3}{24}V'''(x) + \dots\ , \tag{18.316}$$

keeping only the first term. We further introduce an auxiliary quantity $\eta(t)$ by

$$\eta(t) \equiv M\ddot{x}(t) + M\gamma\dot{x}^R(t) + V'(x(t)). \tag{18.317}$$

With this, the exponential function in (18.230) becomes after a partial integration of the first term using the endpoint properties $y(t_b) = y(t_a) = 0$:

$$\exp\left\{-\frac{i}{\hbar}\int_{t_a}^{t_b} dt\, y\eta - \frac{w}{2\hbar^2}\int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt'\, y(t)K(t,t')y(t')\right\}. \tag{18.318}$$

The variable y can obviously be integrated out and we find a probability distribution

$$P[\eta] \propto \exp\left\{-\frac{1}{2w}\int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt'\, \eta(t)K^{-1}(t,t')\eta(t')\right\}, \tag{18.319}$$

where the fluctuation width w was given in (18.218), and $K^{-1}(t,t')$ denotes the inverse functional matrix of $K(t,t')$.

The defining equation (18.317) for $\eta(t)$ may be viewed as a *stochastic differential equation* to be solved for arbitrary initial positions $x(t_a) = x_a$ and velocities $\dot{x}(t_a) = v_a$. The differential equation is driven by a Gaussian random *noise* variable $\eta(t)$ with a correlation function

$$\langle \eta(t)\rangle_\eta = 0, \qquad \langle \eta(t)\eta(t')\rangle_\eta = w\, K(t-t'), \tag{18.320}$$

where the expectation value of an arbitrary functional of $F[x]$ is defined by the path integral

$$\langle F[x]\rangle_\eta \equiv \mathcal{N}\int_{x(t_a)=x_a} \mathcal{D}x\, P[\eta]F[x]. \tag{18.321}$$

The normalization factor $\mathcal{N}$ is fixed by the condition $\mathcal{N}\int \mathcal{D}\eta\, P[\eta] = 1$, so that $\langle\, 1\,\rangle_\eta = 1$. In the sequel, this factor will always be absorbed in the measure $\mathcal{D}\eta$.

For each noise function $\eta(t)$, the solution of the differential equation yields a path $x_\eta(x_a, x_b, t_a)$ with a final position $x_b = x_\eta(x_a, x_b, t_b)$ and velocity $v_b = \dot{x}_\eta(x_a, x_b, t_b)$, all being functionals of $\eta(t)$. From this we can calculate the distribution $P(x_b v_b t_b | x_a v_a t_a)$ of the final x_b and v_b by summing over all paths resulting from the noise functions $\eta(t)$ with the probability distribution (18.319). The result is of course the same as the distribution (18.242) obtained previously from the canonical path integral.

It is useful to exhibit clearly the dependence on initial and final velocities by separating the stochastic differential equation (18.317) into two first-order equations

$$M\dot{v}(t) + M\gamma v^R(t) + V'(x(t)) = \eta(t), \tag{18.322}$$
$$\dot{x}(t) = v(t), \tag{18.323}$$

to be solved for initial values $x(t_a) = x_a$ and $\dot{x}(t_a) = v_a$. For a given noise function $\eta(t)$, the final positions and velocities have the probability distribution

$$P_\eta(x_b v_b t_b | x_a v_a t_a) = \delta(x_\eta(t) - x_b)\delta(\dot{x}_\eta(t) - v_b). \tag{18.324}$$

Given these distributions for all possible noise functions $\eta(t)$, we find the final probability distribution $P(x_b v_b t_b | x_a v_a t_a)$ from the path integral over all $\eta(t)$ calculated with the noise distribution (18.319). We shall write this in the form

$$P(x_b v_b t_b | x_a v_a t_a) = \langle P_\eta(x_b v_b t_b | x_a v_a t_a)\rangle_\eta. \tag{18.325}$$

Let us change of integration variable from $x(t)$ to $\eta(t)$. This produces a Jacobian

$$J[x] \equiv \mathrm{Det}[\delta\eta(t)/\delta x(t')] = \det\left[M\partial_t^2 + M\gamma\partial_t^R + V''(x(t))\right]. \tag{18.326}$$

In Eq. (18.285) we have seen that due to the retardation of ∂_t^R, this Jacobian is unity. Hence we can rewrite the expectation value (18.321) as a functional integral

$$\langle F[x]\rangle_\eta \equiv \int \mathcal{D}\eta\, P[\eta]\, F[x]\Big|_{x(t_a)=x_a}. \tag{18.327}$$

From the probability distribution $P(x_b v_b t_b | x_a v_a t_a)$ we find the pure position probability $P(x_b t_b | x_a t_a)$ by integrating over all initial and final velocities as in Eq. (18.241). Thus we have shown that a solution of the forward–backward path integral at high temperature (18.232) can be obtained from a solution of the stochastic differential equations (18.317), or more specifically, from the pair of stochastic differential equations (18.322) and (18.323).

The stochastic differential equation (18.317) together with the correlation function (18.320) is called *semiclassical Langevin equation*. The fluctuation width w in (18.320) was given in (18.218). The attribute *semiclassical* emphasizes the truncation of the expansion (18.316) after the first term, which can be justified only for nearly harmonic potentials. For a discussion of the range of applicability of the truncation see the literature [14]. The untruncated path integral is equivalent to an operator form of the Langevin equation, the so-called *quantum Langevin equation* [15]. This equivalence will be discussed further in Subsection 18.19.

The physical interpretation of Eq. (18.320) goes as follows. For $T \to 0$ and $\hbar \to 0$ at $\hbar/T = \text{const}$, the random variable $\eta(t)$ does not fluctuate at all and (18.317) reduces to the classical equation of motion of a particle in a potential $V(x)$, with an additional friction term proportional to γ. For T and $\hbar$ both finite, the particle is shaken around its classical path by thermal and quantum fluctuations. At high temperatures (at fixed $\hbar$), $K(\omega')$ reduces to

$$\lim_{T\to\infty} K(\omega') \equiv 1. \tag{18.328}$$

Then $\eta(t)$ is an instantaneous random variable with zero average and a nonzero pair correlation function:

$$\langle \eta(t)\rangle_\eta = 0, \qquad \langle \eta(t)\eta(t')\rangle_\eta = w\,\delta(t-t'), \tag{18.329}$$

All higher correlation functions vanish. A random variable with these characteristics is referred to as *white noise*. The stochastic differential equation (18.317) with the white noise (18.329) reduces to the *classical Langevin equation with inertia* [16].

In the opposite limit of small temperatures, $K(\omega')$ diverges like

$$K(\omega') \xrightarrow[T\to 0]{} \frac{\hbar|\omega'|}{2k_BT}, \tag{18.330}$$

so that $w\,K(\omega')$ has the finite limit

$$\lim_{T\to 0} wK(\omega') = M\gamma\hbar|\omega'|. \tag{18.331}$$

To find the Fourier transformation of this, we use the Fourier decomposition of the Heaviside function (1.306)

$$\Theta(\omega') = \frac{1}{2\pi}\int_{-\infty}^{\infty} dt\, e^{-i\omega' t}\frac{i}{t+i\eta} \tag{18.332}$$

to form the antisymmetric combination

$$\begin{aligned}\Theta(\omega') - \Theta(-\omega') &= \frac{1}{2\pi}\int_{-\infty}^{\infty} dt\, e^{-i\omega' t}\left(\frac{i}{t+i\eta}+\frac{i}{t-i\eta}\right)\\ &\equiv \frac{i}{\pi}\int_{-\infty}^{\infty} dt\, e^{-i\omega' t}\frac{\mathcal{P}}{t}.\end{aligned} \tag{18.333}$$

A multiplication by ω' yields

$$\begin{aligned}|\omega'| = \omega'[\Theta(\omega') - \Theta(-\omega')] &= -\frac{1}{\pi}\int_{-\infty}^{\infty} dt\, \partial_t e^{-i\omega' t}\frac{\mathcal{P}}{t} = \frac{1}{\pi}\int_{-\infty}^{\infty} dt\, e^{-i\omega' t}\partial_t\frac{\mathcal{P}}{t}\\ &= -\frac{1}{\pi}\int_{-\infty}^{\infty} dt\, e^{-i\omega' t}\frac{\mathcal{P}}{t^2}.\end{aligned} \tag{18.334}$$

By comparison with (18.331) we see that the pure quantum limit of $K(t-t')$ can be written as

$$wK(t-t') \underset{T=0}{=} -\frac{M\gamma\hbar}{\pi}\frac{\mathcal{P}}{(t-t')^2}. \tag{18.335}$$

Hence the quantum-mechanical motion in contact with a thermal reservoir looks just like a classical motion, but disturbed by a random source with temporally long-range correlations

$$\langle \eta(t)\eta(t')\rangle_\eta = -\frac{M\gamma\hbar}{\pi}\frac{\mathcal{P}}{(t-t')^2}. \tag{18.336}$$

The temporal range is found from the temporal average

$$\langle(\Delta t)^2\rangle_t \equiv \int_{-\infty}^{\infty} d\Delta t\,(\Delta t)^2 K(\Delta t) = -\frac{\partial^2}{\partial\omega'^2}K(\omega')\Big|_{\omega'=0} = -\frac{1}{6}\left(\frac{\hbar}{k_BT}\right)^2. \tag{18.337}$$

Apart from the negative sign (which would be positive for Euclidean times), the random variable acquires more and more memory as the temperature decreases and the system moves deeper into the quantum regime. Note that no extra normalization factor is required to form the temporal average (18.337), due to the unit normalization of $K(t-t')$ in (18.224).

In the overdamped limit, the classical Langevin equation with inertia (18.317) reduced to the *overdamped Langevin equation*:

$$\dot{x}(t) = -V'(x(t))/M\gamma + \eta(t)/M\gamma. \tag{18.338}$$

At high temperature, the noise variable $\eta(t)$ has the correlation functions (18.329). Then the stochastic differential equation (18.338) is said to describe a *Wiener process*.The first term on the right-hand side $r_x(x(t)) \equiv -V'(x(t))/M\gamma$ is called the *drift* of the process.

The probability distribution of $x(t)$ resulting from this process is calculated as in Eqs. (18.325), (18.321) from the path integral

$$P(x_bt_a|x_at_a) = \int \mathcal{D}\eta\, P[\eta]\,\delta(x_\eta(t)-x_b), \tag{18.339}$$

and $\mathcal{D}\eta$ is normalized so that $\int\mathcal{D}\eta\,P[\eta]=1$.

A path integral representation closely related to this is obtained by using the identity

$$\int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}x\,\delta[\dot{x}-\eta] = \delta(x_\eta(t_b)-x_b), \tag{18.340}$$

which can easily be proved by time-slicing the Fourier representation of the δ-functional

$$\delta[\dot{x}-\eta] = \int \mathcal{D}p\, e^{i\int dt\, p\,(\dot{x}-\eta)} \tag{18.341}$$

and performing all the momentum integrals. This brings the path integral (18.339) to the form

$$P(x_bt_b|x_at_a) = \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}x \int \mathcal{D}\eta\, P[\eta]\,\delta[\dot{x}-\eta]. \tag{18.342}$$

For a harmonic potential $V(x) = M\omega_0^2 x^2/2$, where the overdamped Langevin equation reads

$$\dot{x}(t) = -\omega_0^2\, x(t)/M\gamma + \eta(t)/M\gamma = -\kappa\, x(t)/M\gamma + \bar{\eta}(t), \tag{18.343}$$

where the noise variable $\bar{\eta}(t) \equiv \eta(t)/M\gamma$ has the correlation functions

$$\langle \bar{\eta}(t) \rangle = 0, \quad \langle \bar{\eta}(t)\bar{\eta}(t') \rangle_\eta = \frac{w}{M^2\gamma^2}\delta(t-t') = 2D\delta(t-t'), \tag{18.344}$$

the calculation of the stochastic path integral yields, of course, once more the probability (18.306).

18.11 Path Integral Solution of Klein-Kramers Equation

For a free particle at finite temperature, there exists another way of representing the solution (18.440). Consider the original path integral for the probability in Eq. (18.240) with the Hamiltonian (18.288). Let us introduce the thermal velocity $v_T \equiv \sqrt{k_B T/M}$ and write the action as [compare (2.340)]

$$\mathcal{A}_{\rm e} = \int_{t_a}^{t_b} dt \left[-i(p\dot{x} + p_v \dot{v}) + H(p, p_v, v, x) \right], \tag{18.345}$$

with

$$H(p, p_v, v, x) = \gamma v_T^2 \left(p_v - i\frac{v}{2v_T^2} \right)^2 + \frac{\gamma}{4v_T^2}\left(v + 2i\frac{v_T^2}{\gamma}p \right)^2 + \frac{v_T^2}{\gamma}p^2 + \frac{\gamma}{2}\,. \tag{18.346}$$

In the path integral (18.240), we may integrate out $x(t)$, which converts the path integral over $p(t)$ into an ordinary integral, so that we obtain the integral representation

$$P(x_b v_b t_b | x_a v_a t_a) = \int \frac{dp}{2\pi}\, P(v_b t_b | v_a p_a)_p e^{ip(x_b - x_a) - v_T^2 p^2 (t_b - t_a)/\gamma}, \tag{18.347}$$

where

$$P_p(v_b t_b | v_a t_a) = \int \mathcal{D}v \int \frac{\mathcal{D}p_v}{2\pi} \exp\left\{ \int_{t_a}^{t_b} dt\ \left[ip_v \dot{v} - H_p(p_v, v) \right] \right\}, \tag{18.348}$$

with the p-dependent Hamiltonian governing p_v and v:

$$H_p(p_v, v) \equiv \gamma v_T^2 \left(p_v - i\frac{v}{2v_T^2} \right)^2 + \frac{\gamma}{4v_T^2}\left(v + 2i\frac{v_T^2}{\gamma}p \right)^2 - \frac{\gamma}{2}. \tag{18.349}$$

In the associated Hamiltonian operator, the shift of p_v by $-iv/2v_T^2$ can be removed by a similarity transformation to

$$\tilde{H}_p(p_v, v) \equiv e^{v^2/4v_T^2} \hat{H}_p e^{-v^2/4v_T^2} = \gamma v_T^2 p_v^2 + \frac{\gamma}{4v_T^2}\left(v + 2i\frac{v_T^2}{\gamma}p \right)^2 - \frac{\gamma}{2}. \tag{18.350}$$

Thus we can rewrite $P_p(v_bt_b|v_at_a)$ as

$$P_p(v_bt_b|v_at_a) = e^{-v_b^2/4v_T^2}\tilde{P}_p(v_bt_b|v_at_a)e^{v_a^2/4v_T^2} \tag{18.351}$$

where $\tilde{P}_p(v_bt_b|v_at_a)$ is the probability associated with the Hamiltonian $\tilde{H}_p(p_v, v)$. This describes a harmonic oscillator with frequency γ around the p-dependent center at $v_p = -2iv_T^2 p/\gamma$. If we denote the mass of this oscillator by $m = 1/2\gamma v_T^2$, we can immediately write down the wave eigenfunctions as $\psi_n(v - v_p)$ with $\psi(x)$ of Eq. (2.302). The energies are $n\gamma$. Thus we may express the probability distribution of x and v as a spectral representation

$$P(x_bv_bt_b|x_av_at_a) = e^{-(v_b^2-v_a^2)/4v_T^2}\int\frac{dp}{2\pi}\sum_{n=0}^{\infty}\psi_n(v_b - v_p)\psi_n(v_a - v_p)e^{-n\gamma(t_b-t_a)} \times e^{ip(x_b-x_a)-v_T^2p^2(t_b-t_a)/\gamma}, \tag{18.352}$$

where

$$\psi_n(v) = \frac{1}{(2^n n!\sqrt{\pi})^{1/2}(\sqrt{2}v_T)^{1/2}}e^{-v^2/4v_T^2}H_n(v/\sqrt{2}v_T). \tag{18.353}$$

In the limit of strong damping, only $n = 0$ contributes to the sum, and we find

$$P(x_bv_bt_b|x_av_at_a) = \frac{e^{-(v_b^2-v_a^2)/4v_T^2}}{\sqrt{2\pi}v_T}\int\frac{dp}{2\pi}e^{-[(v_b-v_p)^2+(v_a-v_p)^2]/4v_T^2}e^{ip(x_b-x_a)-v_T^2p^2(t_b-t_a)/\gamma}.$$

Integrating this over v_b leads to

$$P(x_bt_b|x_av_at_a) = \int\frac{dp}{2\pi}\,e^{ip(x_b-x_a-v_a/\gamma)-v_T^2p^2(t_b-t_a)/\gamma} = \frac{1}{\sqrt{4\pi v_T^2/\gamma}}e^{-\frac{\gamma(x_b-x_a-v_a/\gamma)^2}{4v_T^2(t_b-t_a)}}, \tag{18.354}$$

where we have neglected terms of order γ^{-2} in the exponent. A compact expression for the general solution will be derived in (18.440) by stochastic calculus.

18.12 Stochastic Quantization

In Eq. (18.314) we observed that the expectation value of powers of a classical variable x in a potential $V(x)$ can be recovered as a result of a path integral associated with the Lagrangian (18.299). From Eq. (18.339) we know that the path integral (18.314) can be replaced by the stochastic path integral:

$$\langle x^n\rangle = \lim_{s\to\infty}\langle x^n(s)\rangle = \lim_{s\to\infty}\int\mathcal{D}\eta\, x_\eta^n(s)P[\eta]\,, \tag{18.355}$$

where

$$P[\eta] \equiv \int\mathcal{D}\eta e^{-(1/4k_BT)\int_{s_a}^s ds'\eta^2(s')}, \tag{18.356}$$

To simplify the equations, we have replaced the physical time by a rescaled parameter $s = t/M\gamma$.

Equivalently we may say that we obtain the expectation values (18.355) by solving the stochastic differential equation of the Wiener process

$$x'(s) = -V'(x) + \eta(s), \tag{18.357}$$

where $\eta(s)$ is a white noise with the pair correlation functions

$$\langle \eta(s) \rangle_T = 0, \qquad \langle \eta(s)\eta(s') \rangle_T = 2k_BT\,\delta(s - s'), \tag{18.358}$$

and going to the large-s limit of the expectation values $\langle x^n(s) \rangle$.

This can easily be generalized to Euclidean quantum mechanics. Suppose we want to calculate the correlation functions (3.298)

$$\langle x(\tau_1)x(\tau_2)\cdots x(\tau_n) \rangle \equiv Z^{-1} \int \mathcal{D}x\, x(\tau_1)x(\tau_2)\cdots x(\tau_n) \exp\left(-\frac{1}{\hbar}\mathcal{A}_{\rm e}\right). \tag{18.359}$$

We introduce an additional auxiliary time variable s and set up a stochastic differential equation

$$\partial_s x(\tau; s) = -\frac{\delta \mathcal{A}_{\rm e}}{\delta x(\tau; s)} + \eta(\tau; s), \tag{18.360}$$

where $\eta(\tau; s)$ has correlation functions

$$\langle \eta(\tau; s) \rangle = 0, \quad \langle \eta(\tau; s)\eta(\tau'; s') \rangle = 2\hbar\delta(\tau - \tau')\delta(s - s'). \tag{18.361}$$

The role of the thermal fluctuation width $2k_BT$ in (18.358) is now played by $2\hbar$. The correlation functions (18.359) can now be calculated from the auxiliary correlation functions of $x(\tau, s)$ in the large-s limit:

$$\langle x(\tau_1)x(\tau_2)\cdots x(\tau_n) \rangle = \lim_{s\to\infty} \langle x(\tau_1, s)x(\tau_2, s)\cdots x(\tau_n, s) \rangle. \tag{18.362}$$

Due to the extra time variable of stochastic variable $x(\tau; s)$ with respect to (18.357), the probability distribution associated with the stochastic differential equation (18.379) is a functional $P[x_b(\tau), s_b; x_a(\tau), s_a]$ given by the functional generalization of the path integral (18.300):

$$\begin{aligned} P[x_b(\tau_b), s; x_a(\tau), s_a] &= \mathcal{N} \int \mathcal{D}x(\tau; s) \\ &\times\ e^{-\int_{s_a}^{s_b} ds \left\{ \frac{1}{4\hbar} \int_{-\infty}^{\infty} d\tau \left[\partial_s x(\tau;s) + \frac{\delta}{\delta x(\tau;s)}\mathcal{A}_{\rm e}\right] - \frac{1}{2\hbar}\frac{\delta^2}{\delta x(\tau;s)^2}\mathcal{A}_{\rm e} \right\}}. \end{aligned} \tag{18.363}$$

This satisfies the functional generalization of the Fokker-Planck equation (18.292):

$$H[\hat{p}(\tau), x(\tau)]P(x(\tau)s|x_a(\tau); s_a) = -\partial_s P(x(\tau)s|x_a(\tau); s_a), \tag{18.364}$$

with the Hamiltonian

$$H[\hat{p}(\tau), x(\tau)] = \int_{-\infty}^{\infty} d\tau \left[\hbar \hat{p}^2(\tau) - i\hat{p}(\tau)\frac{\delta}{\delta x(\tau)}\mathcal{A}_{\rm e}\right], \tag{18.365}$$

where $\hat{p}(\tau) \equiv \delta/\delta x(\tau)$. We have dropped the subscript b of the final state, for brevity. Explicitly, the Fokker-Planck equation (18.364) reads

$$-\int_{-\infty}^{\infty} d\tau \frac{\hbar\delta}{\delta x(\tau)}\left[\frac{\hbar\delta}{\delta x(\tau)} + \frac{\delta \mathcal{A}_{\rm e}}{\delta x(\tau)}\right] P[x(\tau), s; x_a(\tau), s_a] = -\hbar\partial_s P[x(\tau), s; x_a(\tau), s_a]. \tag{18.366}$$

For $s \to \infty$, the distribution becomes independent of the initial path $x_a(\tau)$, and has the limit [compare (18.314)]

$$\lim_{s\to\infty} P[x(\tau), s; x_a(\tau), s_a] = \frac{e^{-\mathcal{A}_{\rm e}[x]/\hbar}}{\int \mathcal{D}x(\tau)\, e^{-\mathcal{A}_{\rm e}[x]/\hbar}}, \tag{18.367}$$

and the correlation functions (18.378) are given by the usual path integral, apart from the normalization which is here such that $\langle 1 \rangle = 1$.

As an example, consider a harmonic oscillator where Eq. (18.360) reads

$$\partial_s x(\tau; s) = -M(-\partial_\tau^2 + \omega^2)x(\tau; s) + \eta(\tau; s). \tag{18.368}$$

This is solved by

$$x(\tau; s) = \int_0^s ds'\, e^{-M(-\partial_\tau^2+\omega^2)(s'-s)}\eta(\tau; s'). \tag{18.369}$$

The correlation function reads, therefore,

$$\langle x(\tau_1; s_1)x(\tau_2; s_2)\rangle = \int_0^{s_1} ds_1' \int_0^{s_2} ds_2'\, e^{M(-\partial_\tau^2+\omega^2)(s_1'+s_2'-s_1-s_2)}\langle \eta(\tau_1; s_1')\eta(\tau_2; s_2')\rangle. \tag{18.370}$$

Inserting (18.361), this becomes

$$\langle x(\tau_1; s_1)x(\tau_2; s_2)\rangle = \hbar \int_0^{\infty} ds \left[e^{-M(-\partial_\tau^2+\omega^2)(s+|s_1-s_2|)} - e^{-M(-\partial_\tau^2+\omega^2)(s+s_1+s_2)}\right], \tag{18.371}$$

or

$$\langle x(\tau_1; s_1)x(\tau_2; s_2)\rangle = \frac{\hbar}{M}\frac{1}{-\partial_\tau^2+\omega^2}\left[e^{-M(-\partial_\tau^2+\omega^2)|s_1-s_2|} - e^{-M(-\partial_\tau^2+\omega^2)(s_1+s_2)}\right]. \tag{18.372}$$

For Dirichlet boundary conditions ($x_b = x_a = 0$) where operator $(-\partial_\tau^2 + \omega^2)$ has the sinusoidal eigenfunctions of the form (3.63) with eigenfrequencies (3.64), this has the spectral representation

$$\begin{aligned}\langle x(\tau_1; s_1)x(\tau_2; s_2)\rangle &= \frac{\hbar}{M}\frac{2}{t_b - t_a}\sum_{n=1}^{\infty}\frac{1}{\nu_n^2+\omega^2}\sin\nu_n(\tau_1-\tau_a)\sin\nu_n(\tau_2-\tau_a)\\ &\times \left[e^{-M(\nu_n^2+\omega^2)|s_1-s_2|} - e^{-M(-\nu_n^2+\omega^2)(s_1+s_2)}\right].\end{aligned} \tag{18.373}$$

For large s_1, s_2, the second term can be omitted. If, in addition, $s_1 = s_2$, we obtain the imaginary-time correlation function [compare (3.69), (3.304), and (3.36)]:

$$\lim_{s_1=s_2\to\infty}\langle x(\tau_1;s)x(\tau_2;s)\rangle = \langle x(\tau_1)x(\tau_2)\rangle = \frac{\hbar}{M}\frac{1}{-\partial_\tau^2+\omega^2}(\tau_1,\tau_2)$$
$$= \frac{\hbar}{M}\frac{\sinh\omega(\tau_b-\tau_>)\,\sinh\omega(\tau_<-\tau_a)}{\omega\sinh\omega(\tau_b-\tau_a)}. \tag{18.374}$$

We can use these results to calculate the time evolution amplitude according to an imaginary-time version of Eq. (3.318):

$$(\mathbf{x}_b\tau_b|\mathbf{x}_a\tau_a) = C(\mathbf{x}_b,\mathbf{x}_a)e^{-A_{\rm e}(\mathbf{x}_b,\mathbf{x}_a;\tau_b-\tau_a)/\hbar}e^{-\int_{\tau_a}^{\tau_b}\frac{M}{2}d\tau_b'\langle L_{\rm e,fl}(\mathbf{x}_b,\dot{\mathbf{x}}_b)\rangle/\hbar}, \tag{18.375}$$

where $A_{\rm e}(\mathbf{x}_b,\mathbf{x}_a;\tau_b-\tau_a)$ is the Euclidean version of the classical action (4.87). If the Lagrangian has the standard form, then

$$\langle L_{\rm e,fl}(\mathbf{x}_b,\dot{\mathbf{x}}_b)\rangle = \frac{M}{2}\langle\delta\dot{\mathbf{x}}_b^2\rangle, \tag{18.376}$$

and we obtain the imaginary-time evolution amplitude in an expression like (3.318). The constant of integration is determined by solving the differential equation (3.319), and a similar equation for $\mathbf{x}_a$. From this we find as before that $C(\mathbf{x}_b,\mathbf{x}_a)$ is independent of $\mathbf{x}_b$ and $\mathbf{x}_a$.

For the harmonic oscillator with Dirichlet boundary conditions we calculate from this

$$\frac{M}{2}\langle\delta\dot{\mathbf{x}}_b^2\rangle = \frac{\hbar\omega}{2}D\coth\omega(\tau_b-\tau_a). \tag{18.377}$$

Integrating this over τ_b yields $\hbar(D/2)\log[2\sinh\omega(\tau_b-\tau_a)]$, so that the second exponential in (18.375) reduces to the correct fluctuation factor in the D-dimensional imaginary-time amplitude [compare (2.411)].

The formalism can easily be carried over to real-time quantum mechanics. We replace $t\to -i\tau$ and $\mathcal{A}_{\rm e}\to -i\mathcal{A}$, and find that the real-time correlation functions are obtained from the large-s limit

$$\langle x(t_1)x(t_2)\cdots x(\tau_n)\rangle = \lim_{s\to\infty}\langle x(t_1,s)x(t_2,s)\cdots x(t_n,s)\rangle, \tag{18.378}$$

where $x(t;s)$ satisfies the stochastic differential equation

$$\hbar\partial_s x(t;s) = i\frac{\delta\mathcal{A}}{\partial x(t;s)} + \eta(t;s), \tag{18.379}$$

where the noise $\eta(t;s)$ has the same correlation functions as in (18.361), if we replace τ by t. This procedure of calculating quantum-mechanical correlation functions is called *stochastic quantization* [17].

18.13 Stochastic Calculus

The relation between Langevin and Fokker-Planck equations is a major subject of the so-called *stochastic calculus*. Given a Langevin equation, the time order of the potential $V(x)$ with respect to $\dot{x}$ and $\ddot{x}$ is a matter of choice. Different choices form the basis of the *Itō* or the *Stratonovich calculus*. The retarded position which appears naturally in the derivation from the forward–backward path integral favors the use of the Itō calculus. A midpoint ordering as in the gauge-invariant path integrals in Section 10.5 corresponds to the Stratonovich calculus.

18.13.1 Kubo's stochastic Liouville equation

It is worthwhile to trace how the retarded operator order of the friction term enters the framework of stochastic calculus. Thus we assume that the stochastic differential equations (18.322) and (18.323) have been solved for a specific noise function $\eta(t)$ such that we know the probability distribution $P_\eta(x\,v\,t|x_av_at_a)$ in (18.324). Now we observe that the time dependence of this distribution is governed by a simple differential equation known as *Kubo's stochastic Liouville equation* [18], which is derived as follows [19]. A time derivative of (18.324) yields

$$\partial_t P_\eta(x\,v\,t|x_av_at_a) = \dot{x}_\eta(t)\delta'(x_\eta(t)-x)\delta(\dot{x}_\eta(t)-v) + \ddot{x}_\eta(t)\delta(x_\eta(t)-x)\delta'(\dot{x}_\eta(t)-v). \tag{18.380}$$

The derivatives of the δ-functions are initially with respect to the arguments $x_\eta(t)$ and $\dot{x}_\eta(t)$. These can, however, be expressed in terms of derivatives with respect to $-x$ and $-v$. However, since $\ddot{x}_\eta(t)$ depends on $\dot{x}_\eta(t)$ we have to be careful where to put the derivative $-\partial_v$. The general formula for such an operation may be expressed as follows: Given an arbitrary dynamical variable $z(t)$ which may be any local function (local in the temporal sense) of $x(t)$ and $\dot{x}(t)$, and whose derivative is some function of $z(t)$, i.e., $\dot{z}(t) = F(z(t))$, then

$$\frac{d}{dt}\delta(z(t)-z) = \dot{z}(t)\frac{\partial}{\partial z(t)}\delta(z(t)-z) = -\frac{\partial}{\partial z}[\dot{z}(t)\delta(z(t)-z)] = -\frac{\partial}{\partial z}[F(z)\delta(z(t)-z)]. \tag{18.381}$$

To prove this formula, we multiply each expression by an arbitrary smooth test function $g(z)$ and integrate over z. Each integral yields indeed the same result $\dot{g}(z(t)) = \dot{z}(t)g'(z(t)) = F(z)g'(z(t))$. Applying the identity (18.381) to (18.380), we obtain an equation for $P_\eta(x\,v\,t|x_av_at_a)$:

$$\partial_t P_\eta(x\,v\,t|x_av_at_a) \;=\; -[\partial_x\dot{x}_\eta(t) + \partial_v\ddot{x}_\eta(t)]P_\eta(x\,v\,t|x_av_at_a). \tag{18.382}$$

We now express $\ddot{x}_\eta(t)$ with the help of the Langevin equation (18.317) in terms of the friction force $-M\gamma\dot{x}_\eta(t)$, the force $-V'(x_\eta(t))$, and the noise $\eta(t)$. In the presence of the δ-function $\delta(\dot{x}_\eta(t)-v)$, the velocity $\dot{x}_\eta(t)$ can everywhere be replaced by v, and Eq. (18.382) becomes

$$\partial_t P_\eta(x\,v\,t|x_av_at_a) = -\left\{v\partial_x + \frac{1}{M}\left[\eta(t)+f(x,v)\right]\right\}P_\eta(x\,v\,t|x_av_at_a), \tag{18.383}$$

where

$$f(x,v) \equiv -M\gamma v - V'(x) \tag{18.384}$$

is the sum of potential and friction forces. This is Kubo's stochastic Liouville equation which, together with the correlation function (18.218) of the noise variable and the prescription (18.325) of forming expectation values, determines the temporal behavior of the probability distribution $P(x\,v\,t|x_a v_a t_a)$.

18.13.2 From Kubo's to Fokker-Planck Equations

Let us calculate the expectation value of $P_\eta(x\,v\,t|x_a v_a t_a)$ with respect to noise fluctuations and show that $P(x\,v\,t|x_a v_a t_a)$ of Eq. (18.325) satisfies the Fokker-Planck equation with inertia (18.243). First we observe that in a Gaussian expectation value (18.321), the multiplication of a functional $F[\eta]$ by η produces the same result as the functional differentiation with respect to η with a subsequent functional multiplication by the correlation function $\langle \eta(t)\eta(t')\rangle$:

$$\langle \eta(t)F[\eta]\rangle_\eta = \int dt' \langle \eta(t)\eta(t')\rangle_\eta \left\langle \frac{\delta\eta(t)}{\delta\eta(t')}F[\eta]\right\rangle_\eta . \tag{18.385}$$

This follows from the fact that $\eta(t)$ can be obtained from a functional derivative of the Gaussian distribution in (18.321) as:

$$\eta(t)e^{-\frac{1}{2w}\int dtdt'\eta(t)K^{-1}(t,t')\eta(t')} = -w\int dt' K(t,t')\frac{\delta}{\delta\eta(t')}e^{-\frac{1}{2w}\int dtdt'\eta(t)K^{-1}(t,t')\eta(t')}. \tag{18.386}$$

Inside the functional integral (18.321) over $\eta(t)$, an integration by parts moves the functional derivative $-\delta/\delta\eta(t')$ in front of $F[\eta]$ with a sign change. The surface terms can be discarded since the integrand decrease exponentially fast for large noises $\eta(t)$. Thus we obtain indeed the useful formula (18.385).

With the goal of a Gaussian average (18.321) in mind, we can therefore replace Eq. (18.383) by

$$\partial_t P_\eta(x\,v\,t|x_a v_a t_a) = -\left\{v\partial_x + \frac{1}{M}\partial_v\left[w\int dt' K(t,t')\frac{\delta}{\delta\eta(t')} + f(x,v)\right]\right\}P_\eta(x\,v\,t|x_a v_a t_a). \tag{18.387}$$

After this, we observe that

$$\frac{\delta}{\delta\eta(t')}\delta(x_\eta(t)-x)\delta(\dot{x}_\eta(t)-v) = -\left[\frac{\delta x_\eta(t)}{\delta\eta(t')}\partial_x + \frac{\delta\dot{x}_\eta(t)}{\delta\eta(t')}\partial_v\right]\delta(x_\eta(t)-x)\delta(\dot{x}_\eta(t)-v). \tag{18.388}$$

From the stochastic differential equation (18.317) we deduce the following behavior of the functional derivatives:

$$\frac{\delta \ddot{x}_\eta(t)}{\delta\eta(t')} = \frac{1}{M}\delta(t-t') - \gamma\Theta(t-t') \ + \ \text{smooth function of } t-t', \quad (18.389)$$

$$\frac{\delta \dot{x}_\eta(t)}{\delta\eta(t')} = \frac{1}{M}\Theta(t-t') + \mathcal{O}(t-t'), \quad (18.390)$$

$$\frac{\delta x_\eta(t)}{\delta\eta(t')} = \mathcal{O}((t-t')^2). \quad (18.391)$$

Inserting (18.380) with (18.390) and (18.391) into (18.387), the functional derivatives (18.390) and (18.391) are multiplied by $K(t,t')$ and integrated over t'.

Consider now the regime of large temperatures. There the function $K(t,t')$ is narrowly peaked around $t=t'$, forming almost a δ-function [recall the unit normalization (18.328)]. We shall emphasize this by writing $K(t,t') \equiv \delta_\epsilon(t-t')$, with the subscript indicating the width ϵ of $K(t,t')$ which goes to zero like $\hbar/k_BT$ for large T [recall (18.337)]. In this limit, the contribution of the derivative (18.391) vanishes, whereas (18.390) contributes to (18.387) a term

$$\int dt' K(t,t')\frac{\delta}{\delta\eta(t')}\delta(x_\eta(t)-x)\delta(\dot{x}_\eta(t)-v) \quad (18.392)$$
$$= -\int dt'\delta_\epsilon(t-t')\frac{\delta\dot{x}_\eta(t)}{\delta\eta(t')}\partial_v\delta(x_\eta(t)-x)\delta(\dot{x}_\eta(t)-v) = -\frac{1}{2M}\partial_v\delta(x_\eta(t)-x)\delta(\dot{x}_\eta(t)-v).$$

The factor 1/2 on the right-hand side arises from the fact that the would-be δ-function $\delta_\epsilon(t-t')$ is symmetric in $t-t'$, so that its convolution with the Heaviside function $\Theta(t-t')$ is nonzero only over half the peak. Taking the noise average (18.325), we obtain from (18.387) the Fokker-Planck equation with inertia (18.243):

$$\partial_t P(x\,v\,t|x_a v_a t_a) = \left\{-v\partial_x + \frac{1}{M}\partial_v\left[\frac{w}{2M}\partial_v - f(x,v)\right]\right\} P(x\,v\,t|x_a v_a t_a). \quad (18.393)$$

Note that the differential operators have precisely the same order as in Eq. (18.239) as a consequence of formula, here (18.381).

In the overdamped limit, the derivation of the Fokker-Planck equation becomes simple. Then we have to consider only the pure x-space distribution

$$P_\eta(x\,t|x_a t_a) = \int dv\, P_\eta(x\,v\,t|x_a v_a t_a) = \delta(x_\eta(t)-x), \quad (18.394)$$

whose time derivative is given by

$$\partial_t P_\eta(x\,t|x_a v_a t_a) = -\partial_x\dot{x}_\eta(t)P_\eta(x\,t|x_a v_a t_a)$$
$$= -\frac{1}{M\gamma}\partial_x[\eta(t)-V'(x)]P_\eta(x\,t|x_a v_a t_a). \quad (18.395)$$

After treating the noise term $\eta(t)$ according to the rule (18.385),

$$\eta(t) \to w\int dt'\delta_\epsilon(t-t')\frac{\delta}{\delta\eta(t')}, \quad (18.396)$$

we use

$$\frac{\delta}{\delta\eta(t')}\delta(x_\eta(t)-x) = -\frac{\delta x_\eta(t)}{\delta\eta(t')}\delta(x_\eta(t)-x) \tag{18.397}$$

and

$$\begin{aligned}\frac{\delta\dot{x}_\eta(t)}{\delta\eta(t')} &= \frac{1}{M\gamma}\delta(t-t') + \text{ smooth function of } t-t', \\ \frac{\delta x_\eta(t)}{\delta\eta(t')} &= \frac{1}{M\gamma}\Theta(t-t') + \mathcal{O}(t-t'),\end{aligned} \tag{18.398}$$

to find the overdamped Fokker-Planck equation (18.292):

$$\partial_t P(x\,t|x_a t_a) = \left[D\partial^2 + \frac{1}{M\gamma}V'(x)\right]P(x\,t|x_a t_a). \tag{18.399}$$

The distributions $P(x\,t|x_a t_a)$ and $P(x\,v\,t|x_a v_a t_a)$ develop from initial δ-function distributions $P(x\,t_a|x_a t_a) = \delta(x-x_a)$ and $P(x\,v\,t_a|x_a t_a) = \delta(x-x_a)\delta(v-x_a)$.

Let us multiply these δ-functions with arbitrary initial probabilities $P(x,t_a)$ and $P(x\,v,t_a)$ and integrate over x and v. Then we obtain the stochastic path integrals

$$P(x\,,t) = \int \mathcal{D}\eta\, e^{-(1/2w)\int dtdt'\,\eta(t)K^{-1}(t,t')\eta(t')}P(x_{a\eta}(t),t_a), \tag{18.400}$$

$$P(x\,v,t) = \int \mathcal{D}\eta\, e^{-(1/2w)\int dtdt'\,\eta(t)K^{-1}(t,t')\eta(t')}P(x_{a\eta}(t),v_{a\eta},t), \tag{18.401}$$

where $x_{a\eta}$ and $v_{a\eta}$ are initial positions and velocities of paths which arrive at the final x and v following the equation of motion with a fixed noise $\eta(t)$:

$$x_{a\eta}(t) = x - \int_{t_a}^t dt'\,\dot{x}(t'), \qquad v_{a\eta}(t) = x - \int_{t_a}^t dt'\,\dot{v}(t'). \tag{18.402}$$

At high temperatures, the overdamped equation can be written with (18.338) as

$$P(x\,,t) = \int \mathcal{D}\eta\, e^{-(1/2w)\int dt\,\eta^2(t)}P\left(x - \frac{1}{M\gamma}\int_{t_a}^t dt'\,\left[\eta(t') - V'(x(t'))\right],t\right). \tag{18.403}$$

The time evolution equation (18.399) follows from this by calculating for a short time increment ϵ:

$$\begin{aligned}P(x\,,t+\epsilon) = \int \mathcal{D}\eta\, e^{-(1/2w)\int dt\,\eta^2(t)}\Bigg\{&-\frac{\epsilon}{M\gamma}\int_t^{t+\epsilon} dt'\left[\eta(t') - V'(x(t'))\right]\partial_x \\ &+\frac{1}{2M^2\gamma^2}\int_t^{t+\epsilon} dt'\int_t^{t+\epsilon} dt''\left[\eta(t') - V'(x(t'))\right]\left[\eta(t'') - V'(x(t''))\right]\partial_x^2 + \dots\Bigg\} \\ &\times P\left(x - \frac{1}{M\gamma}\int_{t_a}^t dt'\,\left[\eta(t') - V'(x(t'))\right],t\right).\end{aligned} \tag{18.404}$$

We now use the correlation functions (18.329), ignore all powers higher than linear in ϵ, and find in the limit $\epsilon \to 0$ directly the equation (18.399).

18.13.3 Itō's Lemma

An important tool for dealing with stochastic variables is suplied by *Itō's lemma*. Let $x(t)$ be a stochastic variable following a Wiener process with a drift $r_x(x(t),t)$ which is supposed to be a smooth function of $x(t)$ and t [compare (18.338)], i.e., $\dot{x}(t)$ fluctuates harmonically with a white noise around its average $\langle\dot{x}(t)\rangle = r_x(x(t),t)$ according to a stochastic differential equation

$$\dot{x}(t) = \langle\dot{x}(t)\rangle + \eta(t) = r_x + \eta(t). \tag{18.405}$$

We shall omit the smooth dependence of r_x on its arguments since this will be irrelevant for the subsequent arguments. The white noise has zero average $\langle\eta(t)\rangle = 0$, and its only nonzero correlation function is

$$\langle\eta(t)\eta(t')\rangle \; = \sigma^2\delta(t-t'). \tag{18.406}$$

The value of $x(t)$ at a slightly later time $t+\epsilon$ is $x(t+\epsilon) = x(t) + \Delta x(t)$, where

$$\Delta x(t) \equiv \int_t^{t+\epsilon} dt'\,\dot{x}(t') = \epsilon r_x + \int_t^{t+\epsilon} dt'\,\eta(t'). \tag{18.407}$$

Consider now an arbitrary function $f(x(t))$. Its value at the time $t+\epsilon$ has the Taylor expansion

$$\begin{aligned} f(x(t+\epsilon)) \;=\; & f(x(t)) + f'(x(t))\Delta x(t) \\ & + \frac{1}{2} f''(x(t))[\Delta x(t)]^2 + \frac{1}{3!} f^{(3)}[\Delta x(t)]^3 + \ldots\,. \end{aligned} \tag{18.408}$$

The linear term in $\Delta x(t)$ on the right-hand side of (18.408) has the average

$$\langle\Delta x(t)\rangle \;=\; \int_t^{t+\epsilon} dt'\,\langle\dot{x}(t') + \eta(t')\rangle = \int_t^{t+\epsilon} dt'\,\langle\dot{x}(t')\rangle \approx \epsilon r_x, \tag{18.409}$$

where we have omitted the arguments $x(t)$ and t of $r_x(x(t),t)$, since the variation of $r_x(x(t),t)$ in the small interval $(t,t+\epsilon)$ can be neglected to lowest order in ϵ.

The average of the quadratic term $\langle[\Delta x(t)]^2\rangle$ is

$$\begin{aligned} \langle[\Delta x(t)]^2\rangle \;&=\; \int_t^{t+\epsilon} dt_1 \int_t^{t+\epsilon} dt_2\, \langle[\langle\dot{x}(t_1)\rangle + \eta(t_1)]\,[\langle\dot{x}(t_2)\rangle + \eta(t_2)]\rangle \\ &\approx\; \epsilon^2 r_x^2 + \langle\eta(t_1)\eta(t_2)\rangle. \end{aligned}$$

The second term is of the order ϵ due to the δ-function in the correlation function (18.406). Thus we find

$$\langle[\Delta x(t)]^2\rangle = \epsilon\sigma^2 + \mathcal{O}(\epsilon^2). \tag{18.410}$$

The average of the cubic term $\langle[\Delta x(t)]^3\rangle$ is given by the integral

$$\begin{aligned} &\int_t^{t+\epsilon} dt_1 \int_t^{t+\epsilon} dt_2 \int_t^{t+\epsilon} dt_3\, \langle[\langle\dot{x}(t_1)\rangle + \eta(t_1)]\,[\langle\dot{x}(t_2)\rangle + \eta(t_2)]\,[\langle\dot{x}(t_3)\rangle + \eta(t_2)]\rangle \\ &= \int_t^{t+\epsilon} dt_1 \int_t^{t+\epsilon} dt_2 \int_t^{t+\epsilon} dt_3 \Big[\langle\dot{x}(t_1)\rangle\langle\dot{x}(t_2)\rangle\langle\dot{x}(t_3)\rangle + \langle\dot{x}(t_1)\rangle\langle\eta(t_2)\eta(t_3)\rangle \\ &\qquad\qquad + \langle\dot{x}(t_2)\rangle\langle\eta(t_1)\eta(t_3)\rangle + \langle\dot{x}(t_3)\rangle\langle\eta(t_1)\eta(t_2)\rangle\Big] \\ &= \epsilon^3 r_x^3 + 3\epsilon^2 r_x\sigma^2 = \mathcal{O}(\epsilon^2). \end{aligned} \tag{18.411}$$

The averages of the higher powers $[\Delta x(t)]^n$ are obviously at least of order $\epsilon^{n/2}$. Thus we find in the limit $\epsilon \to 0$ the simple formula

$$\langle \dot{f}(x(t))\rangle = \langle f'(x(t))\rangle\langle \dot{x}(t)\rangle + \frac{\sigma^2}{2}\langle f''(x(t))\rangle. \tag{18.412}$$

Note that in a time-sliced formulation, $f(x(t))\dot{x}(t)$ has the form $f(x_n)(x_{n+1}-x_n)/\epsilon$, with independently fluctuating x_n and x_{n+1}, so that we may treat x_n and $(x_{n+1} - x_n)/\epsilon$ as independent fluctuating variables. In the continuum limit $x(t)$ and $\dot{x}(t)$ become independent.

The important point noted by Itō is now that this result is not only true for the averages but also for the derivative $\dot{f}(x(t))$ itself, i.e., $f(x(t))$ obeys the stochastic differential equation

$$\dot{f}(x(t)) = f'(x(t))\,\dot{x}(t) + \frac{\sigma^2}{2} f''(x(t)), \tag{18.413}$$

which is known as Itō's lemma.

In order to prove this we must show that the omitted fluctuations in the higher powers $[\Delta x(t)]^n$ for $n \geq 2$ are of higher order in ϵ than the leading fluctuation of $\Delta x(t)$ which is of order ϵ. Indeed, let us denote the fluctuating part of $[\Delta x(t)]^n$ by $z_n(t)$. For $n = 1, 2$, these are

$$z_1(t) = \int_t^{t+\epsilon} dt\,\eta(t), \qquad z_2(t) \equiv [z_{2,1}(t) + z_{2,2}(t)]\,, \tag{18.414}$$

where the two parts of $z_2(t)$ are

$$z_{2,1}(t) = 2\int_t^{t+\epsilon} dt_1\,\langle \dot{x}(t_1)\rangle\, z_1(t) \approx 2\epsilon r_x\, z_1(t), \quad z_{2,2}(t) = [z_1(t)]^2. \tag{18.415}$$

The fluctuations of $z_{2,1}(t)$ are smaller than the leading ones of $z_1(t)$ by a factor ϵ. They can therefore be ignored in the limit $\epsilon \to 0$.

The size of the fluctuations $z_{2,2}(t)$ are estimated by calculating its variance $\langle [z_{2,2}(t)]^2\rangle - \langle z_{2,2}(t)\rangle^2$. The first of the two expectation values is

$$\left\langle [z_{2,2}(t)]^2 \right\rangle = \int_t^{t+\epsilon} dt_1 \int_t^{t+\epsilon} dt_2 \int_t^{t+\epsilon} dt_3 \int_t^{t+\epsilon} dt_4\, \langle \eta(t_1)\eta(t_2)\eta(t_3)\eta(t_4)\rangle. \tag{18.416}$$

According to Wick's rule (3.305) for harmonic fluctuations, the expectation value on the right-hand sid is equal to the sum of three pair contractions

$$\langle \eta(t_1)\eta(t_2)\rangle\langle \eta(t_3)\eta(t_4)\rangle + \langle \eta(t_1)\eta(t_3)\rangle\langle \eta(t_2)\eta(t_4)\rangle\langle \eta(t_1)\eta(t_4)\rangle\langle \eta(t_2)\eta(t_3)\rangle. \tag{18.417}$$

Inserting (18.406) and performing the integrals yields

$$\left\langle [z_{2,2}(t)]^2 \right\rangle = 3\epsilon^2\sigma^4. \tag{18.418}$$

The second term in the variance of $z_{2,2}(t)$ is

$$\langle z_{2,2}(t)\rangle^2 = \langle z_1^2(t)\rangle^2 = \left[\int_t^{t+\epsilon} dt_1 \int_t^{t+\epsilon} dt_2 \, \langle \eta(t_1)\eta(t_2)\rangle\right]^2 = \epsilon^2\sigma^4. \tag{18.419}$$

Hence we obtain for the variance of $z_{2,2}(t)$:

$$\langle [z_{2,2}(t)]^2\rangle - \langle z_{2,2}(t)\rangle^2 = 2\sigma^4\epsilon^2. \tag{18.420}$$

This must be compared with the variance of the leading fluctuations $z_1(t)$ in (18.413):

$$\langle [z_1(t)]^2\rangle - \langle z_1(t)\rangle^2 = \int_t^{t+\epsilon} dt_1 \int_t^{t+\epsilon} dt_2 \, \langle \eta(t_1)\eta(t_2)\rangle = \epsilon\sigma^2, \tag{18.421}$$

which implies that $z_1(t)$ is of the order of $\sigma\sqrt{\epsilon}$. Thus the fluctuating part of $[\Delta x(t)]^2$ is by a factor $\sqrt{\epsilon}$ smaller than that of $\Delta x(t)$, so that it can be ignored in the continuum limit $\epsilon \to 0$.

Thus we have proved that not only the expectation value $\langle [\Delta x(t)]^2\rangle$ becomes equal to $\epsilon\sigma^2$ as stated in Eq. (18.410), but also the fluctuating quantity $[\Delta x(t)]^2$ itself:

$$[\Delta x(t)]^2 = \epsilon\sigma^2 + \mathcal{O}(\epsilon^2). \tag{18.422}$$

In a similar way we can derive the estimates $[\Delta x(t)]^n = \mathcal{O}((\sigma\sqrt{\epsilon})^n)$ for all higher fluctuations $z_n(t)$ in the Taylor expansion (18.408). These can all be neglected compared to $z_1(t)$, thus proving Itō's lemma (18.413).

For an exponential function, Itō's lemma yields

$$\frac{d}{dt}e^{Px} = \left(P\dot{x} + \frac{\sigma^2 P^2}{2}\right) e^{Px}. \tag{18.423}$$

This can be integrated to

$$e^{Px} = e^{\int_0^t dt' \, P\dot{x}} \, e^{P^2\sigma^2 t/2}. \tag{18.424}$$

The expectation value of this can also be formulated as a rule for calculating the expectation value of an exponential of an integral over a Gaussian noise variable with zero average:

$$\left\langle e^{P\int_0^t dt' \, \eta(t')} \right\rangle = e^{P^2 \int_0^t dt' \int_0^t dt'' \langle \eta(t')\eta(t'')\rangle} = e^{P^2\sigma^2 t/2}. \tag{18.425}$$

This rule can also be derived directly from Wick's rule (3.310). The right-hand side corresponds to the *Debye-Waller factor* introduced in solid-state physics to describe the reduction of the intensities of Bragg peaks by thermal fluctuations of the atomic positions [see Eq. (3.311)].

There is a simple mnemonic way of formalizing this derivation of Eq. (18.413) in a sloppy differential notation. We expand

$$f(x(t+dt)) = f(x(t)+\dot{x}dt) = f(x(t)) + f'(x(t))\dot{x}(t)dt + \frac{1}{2}f''(x(t))\dot{x}^2(t)dt^2 + \dots\ , \tag{18.426}$$

and insert in the higher-order expansion terms $\dot{x} = \langle\dot{x}\rangle + \eta(t)$ where $\langle\eta(t)\rangle = 0$ and the expectation

$$\langle\eta^2(t)\rangle\, dt = \sigma^2, \tag{18.427}$$

which expresses infinitesimally the correct equation

$$\int_t^{t+\epsilon} dt'\, \langle\eta(t')\eta(t)\rangle = \int_t^{t+\epsilon} dt'\, \sigma^2\, \delta(t'-t) = \sigma^2. \tag{18.428}$$

The variable $\dot{x}^2(t)dt^2$ has an expectation value $\sigma^2 dt$ and a variance $\langle[\dot{x}^2(t)dt^2]^2 - \langle\dot{x}^2(t)dt\rangle^2\rangle = 2\sigma^2 dt^2$, so that $\dot{x}^2(t)dt^2$ in (18.426) can be replaced as follows:

$$\dot{x}^2(t)dt^2 \to \sigma^2 dt/2. \tag{18.429}$$

A corresponding estimate holds for all higher powers:

$$z_n \approx \mathcal{O}((\sigma\sqrt{\epsilon})^n). \tag{18.430}$$

or

$$\dot{x}^n(t)dt^n \approx \mathcal{O}((\sigma\sqrt{dt})^n). \tag{18.431}$$

These can all be omitted in the expansion (18.426), thus leading back to Itō's rule (18.412).

It must be realized that Itō's lemma is valid only in the limit $\epsilon \to 0$. For a discrete time axis with small but finite time intervals $\Delta t = \epsilon$, the fluctuations of $z_n(t)$ cannot strictly be ignored but are only suppressed by a small factor $\sigma\sqrt{\Delta T}$. The discrete version of Itō's lemma expands the fluctuating difference $\Delta f(x(t_n)) \equiv f(x(t_{n+1})) - f(x(t_n))$ as follows:

$$\frac{\Delta f(x(t_n))}{\Delta t} = f'(x(t_n))\frac{\Delta x(t_n)}{\Delta t} + \frac{\sigma^2}{2}f''(x(t_n)) + \mathcal{O}(\sigma\sqrt{\Delta t}). \tag{18.432}$$

18.14 Solving the Langevin Equation

In Eq. (18.306) we have found the probability distribution for the motion of a particle with large dissipation by solving the path integral (18.300) for the harmonic oscillator potential $V(x) = \omega_0^2 x^2/2$. For completeness, let us calculated the same result within stochastic calculus. The stochastic differential equation associated with the Lagrangian (18.301) is

$$\dot{x}(t) = -\kappa x(t) + \bar{\eta}(t), \tag{18.433}$$

where

$$\langle \bar{\eta}(t) \rangle_\eta, \quad \langle \bar{\eta}(t)\bar{\eta}(t') \rangle_\eta = 2D\delta(t-t'). \tag{18.434}$$

This equation is solved by

$$x(t) = x_0 e^{-\kappa t} + \int_0^t dt_1\, e^{-\kappa(t-t_1)}\bar{\eta}(t_1), \tag{18.435}$$

so that we obtain $\langle x(t) \rangle_\eta = x_0 e^{-\gamma t}$ and

$$\begin{aligned} \langle x(t)x(t') \rangle_\eta &= x_0^2 e^{-\kappa(t+t')} + 2D \int_0^t dt_1\, e^{-\kappa(t-t_1)} \int_0^{t'} dt_2\, e^{-(t'-t_2)}\delta(t_1-t_2) \\ &= x_0^2 e^{-\kappa(t+t')} + \kappa^{-1} D \left(e^{-\kappa|t-t'|} - e^{-\kappa(t+t')} \right), \end{aligned} \tag{18.436}$$

and the mean-square deviation

$$\langle [x(t) - \langle x(t) \rangle]^2 \rangle_\eta = \kappa^{-1} D \left(1 - e^{-2\kappa t} \right). \tag{18.437}$$

From these expectation values we recover immediately the previous distribution function (18.306).

This result can easily be generalized to a D-component Langevin equation

$$\dot{\mathbf{x}}(t) = -\boldsymbol{\kappa}\, \mathbf{x}(t) + \bar{\boldsymbol{\eta}}(t), \tag{18.438}$$

where $\boldsymbol{\kappa}$ is a matrix, and $\bar{\boldsymbol{\eta}}(t)$ a noise vector. Its correlation functions may be expressed in terms of a diffusion matrix $\mathbf{D}$ as

$$\langle \bar{\boldsymbol{\eta}}(t) \rangle = 0, \quad \langle \bar{\boldsymbol{\eta}}(t) \bar{\boldsymbol{\eta}}^T(t') \rangle_{\boldsymbol{\eta}} = 2\mathbf{D}\delta(t-t'), \tag{18.439}$$

to be compared with the one-dimensional expressions (18.329).

Then the probability (18.306) becomes

$$\begin{aligned} P(\mathbf{x}_b t_b | \mathbf{x}_a t_a) &= \frac{1}{\sqrt{2\pi}^D} \frac{1}{\sqrt{\det\left[\sigma^2(t_b-t_a)\right]}^D} \\ &\times \exp\left\{ -\frac{1}{2} [x_b - \bar{x}(t_b - t_a)]^i [\sigma^2_{ij}(t_b - t_a)]^{-1} [x_b - \bar{x}(t_b - t_a)]^j \right\}, \end{aligned} \tag{18.440}$$

where

$$\bar{\mathbf{x}}(t) = e^{-\boldsymbol{\kappa} t}\, \mathbf{x}_a\,, \tag{18.441}$$

and

$$\sigma^2_{ij}(t) \equiv \langle [x(t) - \bar{x}(t)]^i [x(t) - \bar{x}(t)]^j \rangle_{\boldsymbol{\eta}}\,. \tag{18.442}$$

The probability (18.440) solves the Fokker-Planck equation (18.245)

$$\partial_t P(\mathbf{x}\, t | t_a \mathbf{x}_a) = \left(-\kappa_{ij} \partial_i x_j + D_{ij} \partial_i \partial_j \right) P(\mathbf{x}\, t | t_a \mathbf{x}_a). \tag{18.443}$$

The D-component result (18.440) allows us to solve the Langevin equation with inertia in Eq. (18.317). We simply rewrite the equivalent pair of equations (18.322) and (18.323) in the matrix form (18.438) with $x_1 = x$ and $x_2 = v$, and identify

$$\boldsymbol{\kappa} = \begin{pmatrix} 0 & -1 \\ \omega_0^2 & \gamma \end{pmatrix}, \qquad \bar{\boldsymbol{\eta}}(t) = \frac{1}{M}\begin{pmatrix} 0 \\ \eta(t) \end{pmatrix}, \tag{18.444}$$

so that the diffusion matrix takes the form (18.246).

The eigenvalues of the nonhermitian matrix $\boldsymbol{\kappa}$ in (18.441) are $\kappa_{1,2} = \frac{1}{2}(\gamma \pm \sqrt{\gamma^2 - 4\omega_0^2})$. The associated eigenvectors $\mathbf{u}^{(1,2)}$ satisfying $\boldsymbol{\kappa}\mathbf{u}^{(1,2)} = \kappa_{1,2}\mathbf{u}^{(1,2)}$ are $(-1, \kappa_1)$ and $(1, -\kappa_2)$, respectively, while those to the left satisfying $\mathbf{v}^{(1,2)}\boldsymbol{\kappa} = \kappa_{(1,2)}\mathbf{v}^{(1,2)}$ are $(\kappa_2, 1)/(\kappa_1 - \kappa_2)$ and $(\kappa_1, 1)/(\kappa_1 - \kappa_2)$, respectively. The two sets of eigenvectors are mutually orthonormal and complete: $\mathbf{u}^{(i)} \cdot \mathbf{v}^{(j)} = \delta^{ij}$, $\sum_k v_i^{(k)} u_j^{(k)} = \delta_{ij}$. The matrix $\boldsymbol{\kappa}$ has then the spectral representation $\kappa_{ij} = \sum_k \kappa_k u_i^{(k)} v_j^{(k)}$, and an exponential $(e^{-\boldsymbol{\kappa}t})_{ij} = \sum_k e^{-\kappa_k t} u_i^{(k)} v_j^{(k)}$. which reads explicitly

$$e^{-\boldsymbol{\kappa}t} = \frac{1}{\kappa_1 - \kappa_2}\begin{pmatrix} \kappa_1 e^{-\kappa_2 t} - \kappa_2 e^{-\kappa_1 t} & e^{-\kappa_2 t} - e^{-\kappa_1 t} \\ \omega_0^2(e^{-\kappa_1 t} - e^{-\kappa_2 t}) & \kappa_1 e^{-\kappa_1 t} - \kappa_2 e^{-\kappa_2 t} \end{pmatrix}. \tag{18.445}$$

The inverse matrix $[\sigma_{ij}^2(t_b - t_a)]^{-1}$ is given by

$$[\sigma_{ij}^2(t)]^{-1} = \left[\det \sigma_{ij}^2(t)\right]^{-1}\begin{pmatrix} \sigma_{vv}^2(t) & -\sigma_{xv}^2(t) \\ -\sigma_{xv}^2(t) & \sigma_{xx}^2(t) \end{pmatrix} \tag{18.446}$$

where the matrix elements $\sigma_{ij}^2(t_b - t_a)$ are calculated from the expectation values (18.442). This is done by expressing the solution of (18.438) as in (18.435) in the form

$$\mathbf{x}(t) = e^{-\boldsymbol{\kappa}t}\,\mathbf{x}_a + \int_{t_a}^{t} dt\,\bar{\boldsymbol{\eta}}(t), \tag{18.447}$$

and using the correlation functions (18.439) to find

$$\begin{aligned}
\sigma_{xx}^2(t) &= \frac{\gamma^2 D}{(\kappa_1 - \kappa_2)^2}\left[\frac{1}{\kappa_1}\left(1 - e^{-2\kappa_1 t}\right) + \frac{1}{\kappa_2}\left(1 - e^{-2\kappa_2 t}\right) - \frac{4}{\kappa_1 + \kappa_2}\left(1 - e^{-\kappa_1 + \kappa_2)t}\right)\right], \\
\sigma_{xv}^2(t) &= \frac{\gamma^2 D}{(\kappa_1 - \kappa_2)^2}\left(e^{-\kappa_1 t} - e^{-\kappa_2 t}\right)^2, \qquad\qquad (18.448) \\
\sigma_{vv}^2(t) &= \frac{\gamma^2 D}{(\kappa_1 - \kappa_2)^2}\left[\kappa_1\left(1 - e^{-2\kappa_1 t}\right) + \kappa_2\left(1 - e^{-2\kappa_2 t}\right) - \frac{4}{\kappa_1^{-1} + \kappa_2^{-1}}\left(1 - e^{-\kappa_1 + \kappa_2)t}\right)\right].
\end{aligned}$$

After a long time, these converge to

$$\sigma_{xx}^2(t) \to \frac{\gamma D}{\kappa_1 \kappa_2} = \frac{\gamma D}{\omega_0^2}, \qquad \sigma_{xv}^2(t) \to 0, \qquad \sigma_{vv}^2(t) \to \gamma D, \tag{18.449}$$

so that the determinant $\det \sigma_{ij}^2(t)$ becomes $\gamma^2 D^2/\omega_0^2$, and the distribution (18.440) turns into the Boltzmann distribution

$$\lim_{t_b \to \infty} P(x_b v_b t_b | x_a v_a t_a) = \frac{\omega_0}{2\pi\gamma D} e^{-(v_b^2 + \omega_0^2 x_b^2)/2\gamma D} = \frac{M\omega_0}{2\pi k_B T} e^{-M(v_b^2 + \omega_0^2 x_b^2)/2k_B T}. \tag{18.450}$$

The velocity shows the well-known *Maxwell distribution*:

$$P(v_b) = \frac{1}{\sqrt{2\pi\gamma D}} e^{-v_b^2/2\gamma D} = \frac{1}{\sqrt{2\pi k_B T/M}} e^{-Mv_b^2/2k_BT} = \frac{1}{\sqrt{2\pi} v_T} e^{-v_b^2/2v_T^2}, \quad (18.451)$$

which exhibits an average thermal velocity

$$v_T \equiv \sqrt{k_B T/M}. \quad (18.452)$$

If we integrate the two-dimensional result $P(x_b v_b t_b|x_a v_a t_a)$ over all final velocities, we obtain

$$P(x_b t_b|x_a v_a t_a) = \int dv_b \, P(x_b v_b t_b|x_a v_a t_a) = \frac{1}{\sqrt{2\pi\sigma_{xx}^2(t_b - t_a)}} \exp\left\{-\frac{1}{2}\frac{[x_b - \bar{x}(t_b - t_a)]^2}{\sigma_{xx}^2(t_b - t_a)}\right\}. \quad (18.453)$$

Note that this depends on v_a via $\bar{x}(t_b - t_a) = x_a + \gamma^{-1}(1 - e^{-\gamma(t_b - t_a)})v_a$.

In the absence of an external potential, i.e. for $\omega_0 = 0$, the eigenvalues $\kappa_{1,2}$ are γ and 0, respectively, and the matrix $e^{-\boldsymbol{\kappa} t}$ reduces to

$$e^{-\boldsymbol{\kappa} t} = \begin{pmatrix} 1 & \gamma^{-1}(1 - e^{-\gamma t}) \\ 0 & e^{-\gamma t} \end{pmatrix}. \quad (18.454)$$

The matrix elements $\sigma_{ij}^2(t)$ are simply[9]

$$\sigma_{xx}^2(t) = \gamma^{-1} D(2\gamma t - 3 + 4e^{-\gamma t} - e^{-2\gamma t}), \;\; \sigma_{xv}^2(t) = D(1 - e^{-\gamma t})^2, \;\; \sigma_{vv}^2(t) = \gamma D(1 - e^{-2\gamma t}), \quad (18.455)$$

whose determinant is

$$\det \sigma_{ij}^2(t) = D^2 \left[2\gamma t(1 - e^{-2\gamma t}) + (1 - e^{-\gamma t})^2(-4 - 2e^{-\gamma t} + e^{-3\gamma t})\right]. \quad (18.456)$$

In the large-time limit, these become

$$\sigma_{xx}^2(t) \to 2Dt, \;\; \sigma_{xv}^2(t) \to D, \;\; \sigma_{vv}^2(t) \to \gamma D, \quad \det \sigma_{ij}^2(t) \to 2\gamma t D^2. \quad (18.457)$$

The last result can, of course, be derived by integrating the pair of Langevin equations with inertia (18.322) and (18.323) for zero potential $V(x)$ successively. First the equation for $v(t)$ which reads $v(t) = v_0 e^{-\gamma t} + \int_0^t dt_1 \, e^{-\gamma(t - t_1)} \eta(t_1)/M$, and yields $\langle v(t)v(t')\rangle_\eta = v_0^2 e^{-\gamma(t+t')} + \gamma D\left(e^{-\gamma|t-t'|} - e^{-\gamma(t+t')}\right)$, using the white noise correlation functions (18.329). The equations for $x(t)$ are obtained from these by integration over t.

[9]See Section 18.15 for an alternative method of calculating the expectation values (18.442).

18.15 Heisenberg Picture for Probability Evolution

It is possible to develop a Heisenberg operator description of the time dependence of thermal expectations. This goes by complete analogy with the development in Section 2.23 for the quantum-mechanical time evolution amplitude. Consider the thermal expectations of x and x^2 for a particle which sits at the initial time $t = t_a$ at x_a. They are given by the integrals

$$\langle x \rangle \equiv \int_{-\infty}^{\infty} dx_b \, x_b P(x_b t_b | x_a t_a), \tag{18.458}$$

$$\langle x^2 \rangle \equiv \int_{-\infty}^{\infty} dx_b \, x_b^2 P(x_b t_b | x_a t_a). \tag{18.459}$$

For simplicity, let us first look at the case of a dominant friction term. As in quantum mechanics, it is useful to introduce a bra-ket notation, but for the *probabilities* rather than the amplitudes,

$$\langle x_b t_b | x_a t_a \rangle \equiv |(x_b t_b | x_a t_a)|^2. \tag{18.460}$$

The fact that this probability satisfies the Fokker-Planck equation implies that we can write it as

$$\langle x_b t_b | x_a t_a \rangle = e^{-(t_b - t_a) H(\hat{p}_b, x_b)} \delta(x_b - x_a). \tag{18.461}$$

Thus we may introduce time-independent basis vectors $|x_a\rangle$ satisfying

$$\langle x_b | x_a \rangle = \delta(x_b - x_a). \tag{18.462}$$

On this basis, the operators $\hat{p}$, $\hat{x}$ are defined in the usual way. They satisfy

$$\langle x_b | \hat{x} = x_b \langle x_b |, \qquad \langle x_b | \hat{p} = -i \frac{\partial}{\partial x_b} \langle x_b |. \tag{18.463}$$

Then we may rewrite (18.461) in bra-ket notation as

$$\langle x_b t_b | x_a t_a \rangle = \langle x_b | e^{-H(\hat{p}, \hat{x})(t_b - t_a)} | x_a \rangle. \tag{18.464}$$

The expectation value of any function $f(x)$ is calculated as follows

$$\begin{aligned} \langle f(x) \rangle &= \int_{-\infty}^{\infty} dx_b \, f(x_b) \langle x_b | e^{-(t_b - t_a) H(\hat{p}, \hat{x})} | x_a \rangle \\ &= \int_{-\infty}^{\infty} dx_b \, \langle x_b | f(\hat{x}) e^{-(t_b - t_a) H(\hat{p}, \hat{x})} | x_a \rangle \\ &= \int_{-\infty}^{\infty} dx_b \int_{-\infty}^{\infty} dx \, \langle x_b | e^{-(t_b - t_a) H(\hat{p}, \hat{x})} | x \rangle \langle x | f(\hat{x}(t_b - t_a)) | x_a \rangle. \end{aligned} \tag{18.465}$$

In the last term we have introduced the time-dependent Heisenberg type of operator

$$\hat{x}(t) \equiv e^{tH(\hat{p}, \hat{x})} \hat{x} e^{-tH(\hat{p}, \hat{x})}. \tag{18.466}$$

The probability $P(x_b t_b | x_a t_a)$ satisfies the normalization condition

$$\begin{aligned} \int_{-\infty}^{\infty} dx_b \, P(x_b t_b | x_a t_a) &= \int_{-\infty}^{\infty} dx_b \, \langle x_b t_b | x_a t_a \rangle \\ &= \int_{-\infty}^{\infty} dx_b \, \langle x_b | e^{-(t_b - t_a) H(\hat{p}, \hat{x})} | x_a \rangle = 1. \end{aligned} \tag{18.467}$$

Appliying this to the last line of (18.465), we arrive at the simple formula

$$\langle f(x) \rangle = \int_{-\infty}^{\infty} dx_b \, \langle x_b | f(\hat{x}(t_b - t_a)) | x_a \rangle. \tag{18.468}$$

For the Brownian motion of a point particle where

$$L_{\rm e} = \frac{\dot{x}^2}{4D}, \qquad H = Dp^2, \tag{18.469}$$

the Heisenberg operators are

$$\hat{p}(t) = \hat{p}, \qquad \hat{x}(t) = e^{\hat{H}t}\hat{x}e^{-\hat{H}t} = \hat{x} - i2D\hat{p}t, \tag{18.470}$$

and

$$\begin{aligned} \hat{x}^2(t) &= \hat{x}^2 - i2D\cdot(\hat{p}\hat{x} + \hat{x}\hat{p})t - 4D^2\hat{p}^2t^2, \\ &= \hat{x}^2 + 2Dt - i2D\cdot 2\hat{x}\hat{p} - 4D^2\hat{p}^2 t. \end{aligned} \tag{18.471}$$

It is easy to calculate the following matrix elements:

$$\begin{aligned} \int_{-\infty}^{\infty} dx_b\, \langle x_b|\hat{x}|x_a\rangle &= x_a, \\ \int_{-\infty}^{\infty} dx_b\, \langle x_b|\hat{p}|x_a\rangle &= -i\int_{-\infty}^{\infty} dx_b\, \frac{\partial}{\partial x_b}\delta(x_b - x_a) = 0, \\ \int_{-\infty}^{\infty} dx_b\, \langle x_b|\hat{x}^2|x_a\rangle &= \int_{-\infty}^{\infty} dx_b\, {x_b}^2\delta(x_b - x_a) = {x_a}^2, \\ \int_{-\infty}^{\infty} dx_b\, \langle x_b|\hat{p}^2|x_a\rangle &= -\int_{-\infty}^{\infty} dx_b\, \frac{\partial^2}{\partial {x_b}^2}\delta(x_b - x_a) = 0, \\ \int_{-\infty}^{\infty} dx_b\, \langle x_b|\hat{p}\hat{x}|x_a\rangle &= -i\int_{-\infty}^{\infty} dx_b\, \frac{\partial}{\partial x_b}\delta(x_b - x_a)x_a = 0. \end{aligned} \tag{18.472}$$

The vanishing integrals reflect the translational invariance of the integrated bra state $\int_{-\infty}^{\infty} dx_b\, \langle x_b|$, which is therefore annihilated by a translational operator $\hat{p}_b$ on its right:

$$\int_{-\infty}^{\infty} dx_b\, \langle x_b|\hat{p} = 0. \tag{18.473}$$

With the help of Eqs. (18.472), we obtain

$$\langle x\rangle = x_a, \qquad \langle x^2\rangle = {x_a}^2 + 2D(t_b - t_a), \tag{18.474}$$

and

$$\langle (x - x_a)^2\rangle = 2D(t_b - t_a). \tag{18.475}$$

Clearly, a similar formalism can be developed for the general case with the Lagrangian containing $\ddot{x}$-terms. All we have to do is define time-dependent Heisenberg operators for both sets of canonical coordinates x, p, v, p_v. For instance, consider the case of a free particle, where $V(x) = 0$ and the Hamiltonian (18.239) reduces to

$$H = \frac{w}{2M^2}p_v^2 - i\gamma p_v v + ipv. \tag{18.476}$$

If we want to calculate expectations $\langle f(x, v)\rangle$ for a particle initially at x_a with an initial velocity $\dot{x}_a = v_a$, we now have to evaluate integrals of the form

$$\begin{aligned} \langle f(x,v)\rangle &= \int_{-\infty}^{\infty} dx_b \int_{-\infty}^{\infty} dv_b\, f(x_b, v_b)P(x_b v_b t_b|x_a v_a t_a) \\ &= \int_{-\infty}^{\infty} dx_b \int_{-\infty}^{\infty} dv_b\, \langle x_b v_b|f(\hat{x}(t_b - t_a), \hat{v}(t_b - t_a))|x_a v_a\rangle. \end{aligned} \tag{18.477}$$

Here we introduce basis vectors $|xv\rangle$ which diagonalize the operators $\hat{x}$, $\hat{v}$. The momentum operators satisfy

$$\langle xv|\hat{p} = -\frac{\partial}{\partial x}\langle xv|, \qquad \langle xv|\hat{p}_v = -\frac{\partial}{\partial v}\langle xv|. \tag{18.478}$$

Then we can write

$$\langle x^2\rangle = \int_{-\infty}^{\infty} dx_b \int_{-\infty}^{\infty} dv_b\, \langle x_b v_b|\hat{x}^2(t_b - t_a)|x_a v_a\rangle, \tag{18.479}$$

where $\hat{x}(t)$ is the Heisenberg operator defined by

$$\hat{x}(t) = e^{tH(\hat{p},\hat{p}_v,\hat{x},\hat{v})}\hat{x}e^{-tH(\hat{p},\hat{p}_v,\hat{x},\hat{v})}. \tag{18.480}$$

The Heisenberg equations of motions are

$$\begin{aligned}
\dot{\hat{p}}(t) &= [\hat{H}, \hat{p}(t)] = 0,\\
\dot{\hat{p}}_v(t) &= [\hat{H}, \hat{p}_v(t)] = \gamma\hat{p}_v(t) - \hat{p}(t),\\
\dot{\hat{x}}(t) &= [\hat{H}, \hat{x}(t)] = \hat{v}(t),\\
\dot{\hat{v}}(t) &= [\hat{H}, \hat{v}(t)] = -i\frac{w}{M^2}\hat{p}_v(t) - \gamma\hat{v}(t).
\end{aligned} \tag{18.481}$$

According to the first equation, $\hat{p}(t)$ is a constant operator:

$$\hat{p}(t) \equiv \hat{p} = \text{const.}$$

The second equation is solved by

$$\hat{p}_v(t) = \hat{p}_v e^{\gamma t} - \frac{1}{\gamma}\hat{p}(e^{\gamma t} - 1), \tag{18.482}$$

where $\hat{p}_v$ is the initial value of $\hat{p}_v(t)$ at $t = 0$. With this, the fourth equation in (18.481) can be integrated to give

$$\begin{aligned}
\hat{v}(t) &= \hat{v}e^{-\gamma t} - i\frac{w}{M^2}\int_0^t dt'\, e^{-\gamma(t-t')}\hat{p}_v(t')\\
&= \hat{v}e^{-\gamma t} - i\frac{w}{\gamma M^2}\left[\hat{p}_v \sinh\gamma t - \frac{1}{\gamma}\hat{p}(\cosh\gamma t - 1)\right].
\end{aligned} \tag{18.483}$$

Inserting this into the third equation in (18.481) we obtain immediately

$$\hat{x}(t) = \hat{x} + \hat{v}\frac{1}{\gamma}(1 - e^{-\gamma t}) - i\frac{w}{\gamma M^2}\left[p_v \cosh\gamma t - \frac{1}{\gamma}p(\sinh\gamma t - \gamma t)\right]. \tag{18.484}$$

Using now the relations extending (18.473):

$$\int_{-\infty}^{\infty} dx_b \int_{-\infty}^{\infty} dx_{2b}\, \langle x_b x_{2b}| \left\{ \begin{array}{c} \hat{p} \\ \hat{p}_v \end{array} \right\} = 0 \tag{18.485}$$

to express the translational invariance of the integrated bra state, we find directly

$$\langle x\rangle = x_a + \dot{x}_a\frac{1}{\gamma}\left(1 - e^{-\gamma(t_b - t_a)}\right), \qquad \langle v\rangle = v_a e^{-\gamma(t_b - t_a)}, \tag{18.486}$$

in agreement with (18.441) and (18.454). The expectations values of the quadratic cumulants $\left\langle(x - \langle x\rangle)^2\right\rangle$, $\left\langle(x - \langle x\rangle)(v - \langle v\rangle)\right\rangle$, $\left\langle(v - \langle v\rangle)^2\right\rangle$ are found to be the same as in (18.457).

18.16 Supersymmetry

An interesting new symmetry can be derived from the functional determinant (18.296) which causes the extra last term in the exponent of the path integral (18.300). Let us rewriting this implicitly as

$$P_0(x_bt_b|x_at_a) \propto \int \mathcal{D}x(t)\,\mathrm{Det}\left[\partial_t + \frac{V''(x)}{M\gamma}\right] \exp\left\{-\int_{t_a}^{t_b} dt\,\frac{1}{4D}\left[\dot{x} + \frac{V'(x)}{M\gamma}\right]^2\right\}. \tag{18.487}$$

In this expression, the time ordering of the velocity $\dot{x}$ with respect to $V'(x)/M\gamma$ is arbitrary. It may be quantum-mechanical (Stratonovich-like), but equally well retarded (Itō-like), or advanced, as long as the same ordering is used in both the Lagrangian and the determinant.

The new symmetry arises if one generates the determinant with the help of an auxiliary fermion field $c(t)$ from a path integral over $c(t)$:

$$\det\left[\partial_t + V''(x(t))/M\gamma\right] \propto \int \mathcal{D}c\mathcal{D}\bar{c}\, e^{-\int dt\bar{c}(t)\left[M\gamma\partial_t + V''(x(t))\right]c(t)}. \tag{18.488}$$

In quantum field theory, such auxiliary fermionic fields are referred to as *ghost fields*. With these we can rewrite the path integral (18.290) for the probability distribution as an ordinary path integral

$$P(x_bt_b|x_at_a) = \int \mathcal{D}x \int \mathcal{D}c\mathcal{D}\bar{c}\, \exp\left\{-\mathcal{A}_{\rm PS}[x,c,\bar{c}]\right\}, \tag{18.489}$$

where $\mathcal{A}_{\rm PS}$ is the Euclidean action

$$\mathcal{A}_{\rm PS} = \frac{1}{2DM^2\gamma^2}\int_{t_a}^{t_b} dt\left\{\frac{1}{2}\left[M\gamma\dot{x} + V'(x)\right]^2 + \bar{c}(t)\left[M\gamma\partial_t + V''(x(t))\right]c(t)\right\}, \tag{18.490}$$

first written down by Parisi and Sourlas [20] and by McKane [21]. This action has a particular property. If we denote the expression in the first brackets by

$$U_x \equiv M\gamma\partial_t x + V'(x), \tag{18.491}$$

the operator between the Grassmann variables in (18.490) is simply the functional derivative of U_x:

$$U_{xy} \equiv \frac{\delta U_x}{\delta y} = M\gamma\partial_t + V''(x). \tag{18.492}$$

Thus we may write

$$\mathcal{A}_{\rm PS} = \frac{1}{2D}\int_{t_a}^{t_b} dt\left[\frac{1}{2}U_x^2 + \bar{c}(t)\,U_{xy}\,c(t)\right], \tag{18.493}$$

where $U_{xy}c(t)$ is the usual short notation for the functional matrix multiplication $\int dt' U_{xy}(t,t')c(t')$. The relation between the two terms makes this action *supersymmetric*. It is invariant under transformations which mix the Fermi and Bose degrees of freedom. Denoting by ε and $\bar{\varepsilon}$ a small anticommuting Grassmann variable and its conjugate (see Section 7.10), the action is invariant under the field transformations

$$\delta x(t) = \bar{\varepsilon}c(t) + \bar{c}(t)\varepsilon, \tag{18.494}$$

$$\delta\bar{c}(t) = -\bar{\varepsilon}U_x, \tag{18.495}$$

$$\delta c(t) = U_x\varepsilon. \tag{18.496}$$

The invariance follows immediately after observing that

$$\delta U_x = \bar{\varepsilon}U_{xy}c(t) + \bar{c}(t)U_{xy}\varepsilon. \tag{18.497}$$

Formally, a similar construction is also possible for a particle with inertia in the path integral (18.232), which is an ordinary path integral involving the Lagrangian (18.287). Here we can write

$$P(x_bt_b|x_at_a) = \mathcal{N}\int \mathcal{D}x\, J[x] \exp\left\{-\frac{1}{2w}\int_{t_a}^{t_b} dt\,[M\ddot{x}+M\gamma\dot{x}+V'(x)]^2\right\}, \tag{18.498}$$

where $J[x]$ abbreviates the determinant

$$J[x] = \det\,[M\partial_t^2 + M\gamma\partial_t + V''(x(t))], \tag{18.499}$$

which is known from formula (18.274). The path integral (18.498) is valid for *any* ordering of the velocity term, as long as it is the same in the exponent and the functional determinant.

We may now express the functional determinant as a path integral over fermionic ghost fields

$$J[x] = \det\,[M\partial_t^2 + M\gamma\partial_t + V''(x(t))] \propto \int \mathcal{D}c\mathcal{D}\bar{c}\, e^{-\int dt\,\bar{c}(t)\left[M\partial_t^2+M\gamma\partial_t+V''(x(t))\right]c(t)}, \tag{18.500}$$

and rewrite the probability distribution $P(x_bt_b|x_at_a)$ as an ordinary path integral

$$P(x_bt_b|x_at_a) \propto \int \mathcal{D}x \int \mathcal{D}c\mathcal{D}\bar{c}\exp\{-\mathcal{A}^{\rm KS}[x,ˌ\bar{c}]\}, \tag{18.501}$$

where $\mathcal{A}[x,ˌ\bar{c}]$ is the Euclidean action

$$\mathcal{A}^{\rm KS}[x,ˌ\bar{c}] \equiv \int_{t_a}^{t_b} dt\left\{\frac{1}{2w}[M\ddot{x}+M\gamma\dot{x}+V'(x)]^2 + \bar{c}(t)\left[M\partial_t^2+M\gamma\partial_t+V''(x(t))\right]c(t)\right\}. \tag{18.502}$$

This formal expression contains subtleties arising from the boundary conditions when calculating the Jacobian (18.500) from the functional integral on the right-hand side. It is necessary to factorize the second-order operator in the functional determinant and express the determinant of each first-order factor as a functional integral over Grassmann variables as in (18.488). At the end, the action is again supersymmetric, but there are twice as many auxiliary Fermi fields [22].

As a check of this formula, we may let the coupling to the thermal reservoir go to zero, $\gamma \to 0$. Then the first factor in (18.501),

$$\exp\left(-\int_{t_a}^{t_b} dt\left\{\frac{1}{2w}[M\ddot{x}+M\gamma\dot{x}+V'(x)]^2\right\}\right)$$

becomes proportional to a δ-functional $\delta[M\ddot{x}+V'(x)]$. The argument is simply the functional derivative of the original action of the quantum system in (18.191), so that we obtain in the limit $\delta[\delta\mathcal{A}/\delta x]$. The functional matrix between the Grassmann fields in (18.501), on the other hand, reduces to $\delta^2\mathcal{A}/\delta x(t)\delta x(t')$, and we arrive at the path integral

$$P(x_bt_b|x_at_a) \underset{\gamma\to 0}{\propto} \int \mathcal{D}x\,\delta[\delta\mathcal{A}/\delta x] \times \int \mathcal{D}c\mathcal{D}\bar{c}\exp\left\{-\int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt'\,\bar{c}(t)\delta^2\mathcal{A}/\partial x(t)\partial x(t')c(t')\right\}. \tag{18.503}$$

Performing the integral over the Grassmann variables yields

$$P(x_bt_b|x_at_a) \underset{\gamma\to 0}{\propto} \int \mathcal{D}x\,\delta[\delta\mathcal{A}/\delta x]\,{\rm Det}\left[\delta^2\mathcal{A}/\partial x(t)\partial x(t')\right]. \tag{18.504}$$

The δ-functional selects from all paths only those which obey the Euler-Lagrange equations of motion. With the help of the functional identity

$$\delta[M\ddot{x}+V'(x)] = \delta[x-x_{\rm cl}] \times {\rm Det}^{-1}[M\ddot{x}+V''(x)], \tag{18.505}$$

which generalizes identity $\delta(f(x)) = \delta(x)/f'(x)$ if $f(0) = 0$, the above path integral becomes simply

$$P(x_bt_b|x_at_a) \underset{\gamma\to 0}{\propto} \int \mathcal{D}x\, \delta[x - x_{\rm cl}], \tag{18.506}$$

which is the correct probability distribution of classical physics. Note the important difference with respect to the classical amplitude in Eq. (4.96), where the concentration of the path integral on the classical path is enforced by a strongly oscillating complex expression requiring the semiclassical fluctuation factor in Eq. (4.97) for proper normalization. In the probability (18.506) this is achieved by a real δ-functional.

Note that by a Fourier decomposition of the δ-functional (18.503) we obtain the alternative path integral representation of classical physics

$$P(x_bt_b|x_at_a) \underset{\gamma\to 0}{\propto} \int \mathcal{D}x\mathcal{D}\lambda\mathcal{D}c\mathcal{D}\bar{c}\, e^{-\int_{t_a}^{t_b} dt \delta\mathcal{A}/\delta x(t)\lambda(t) - \int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt' \bar{c}(t)\delta^2\mathcal{A}/\delta x(t)\delta x(t')c(t')}. \tag{18.507}$$

This is supersymmetric under the transformations

$$\delta x = \bar{\varepsilon}c\,, \quad \delta c = 0\,, \quad \delta\bar{c} = -\bar{\varepsilon}\lambda\,, \quad \delta\lambda = 0\,, \tag{18.508}$$

as observed by Gozzi [23].

There exists a compact way of rewriting the action using *superfields*. We define a three-dimensional *superspace* consisting of time and two auxiliary Grassmann variables θ and $\bar{\theta}$. Then we define a superfield

$$X(t) \equiv x(t) + i\bar{\theta}c(t) - i\bar{\theta}c(t) - \bar{\theta}\lambda(t). \tag{18.509}$$

We now consider the superaction

$$\mathcal{A}^{\rm super} \equiv \int d\bar{\theta}d\theta\mathcal{A}[X] \quad \equiv \quad \int d\bar{\theta}d\theta\mathcal{A}[x + i\bar{\theta}c - i\theta\bar{c} - \bar{\theta}\theta\lambda] \tag{18.510}$$

and expand the action into a functional Taylor series:

$$\int d\bar{\theta}d\theta \left\{ \mathcal{A}[x] + \frac{\delta\mathcal{A}}{\delta x}(i\bar{\theta}c - i\theta\bar{c} - \bar{\theta}\theta\lambda) + \frac{1}{2}(i\bar{\theta}c - i\theta\bar{c} - \bar{\theta}\theta\lambda)\frac{\partial^2\mathcal{A}}{\delta x\delta x}(i\bar{\theta}c - i\theta\bar{c}c - \bar{\theta}\theta\lambda) \right\}.$$

Due to the nilpotency (7.375) of the Grassmann variables, the expansion stops after the second term. Recalling now the integration rules (7.378) and (7.379), this becomes

$$\frac{\delta\mathcal{A}}{\delta x}\lambda + \frac{1}{2}\bar{c}\frac{\partial^2\mathcal{A}}{\delta x\delta x}c,$$

which is precisely the short-hand functional notation for the negative exponent in the path integral (18.507).

18.17 Stochastic Quantum Liouville Equation

At lower temperatures, where quantum fluctuations become important, the forward–backward path integral (18.230) does not allow us to derive a Schrödinger-like differential equation for the probability distribution $P(x\,v\,t|x_av_at_t)$. To see the obstacle, we go over to the canonical representation of (18.230):

$$|(x_bt_b|x_at_a)|^2 = \int \mathcal{D}x\,\mathcal{D}y \int \frac{\mathcal{D}p}{2\pi}\,\frac{\mathcal{D}p_y}{2\pi}\,\exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b} dt\,\left[p\dot{x} + p_y\dot{y} - H_T\right]\right\}, \tag{18.511}$$

where

$$H_T = \frac{1}{M} p_y p_x + \gamma p_y y + V(x + y/2) - V(x - y/2) - i\frac{w}{2\hbar} y \hat{K}^{\rm Ohm} y \tag{18.512}$$

plays the role of a temperature-dependent quasi-Hamiltonian for an Ohmic system associated with the Lagrangian of the forward–backward path integral (18.230). The notation $\hat{K}^{\rm Ohm} y(t)$ abbreviates the product of the functional matrix $K^{\rm Ohm}(t, t')$ with the functional vector $y(t')$ defined by $\hat{K}^{\rm Ohm} y(t) \equiv \int dt' K^{\rm Ohm}(t, t') y(t')$. Hence is H_T a nonlocal object (in the temporal sense), and this is the reason for calling it quasi-Hamiltonian.

It is useful to omit y-integrations at the endpoints in the path integral (18.511), and set up a path integral representation for the product of amplitudes

$$U(x_b y_b t_b | x_a y_a t_a) \equiv (x_b + y_b/2\ t_b | x_a + y_a/2\ t_a)(x_b - y_b/2\ t_b | x_a - y_a/2\ t_a)^*. \tag{18.513}$$

Given some initial density matrix $\rho(x_+, x_-; t) = \rho(x + y/2, x - y/2; t)$ at time $t = t_a$, which may actually be in equilibrium and time-independent, as in Eq. (2.367), the functional matrix $U(x_b y_b t_b | x_a y_a t_a)$ allows us to calculate $\rho(x_+, x_-; t)$ at any time by the time evolution equation

$$\rho(x + y/2, x - y/2; t) = \int dx_a\, dy_a\, U(x\, y\, t | x_a y_a t_a)\, \rho(x_a + y_a/2, x_a - y_a/2; t_a). \tag{18.514}$$

Recall that the Fourier transform of $\rho(x + y/2, x - y/2; t)$ with respect to y is the Wigner function (1.224).

When considering the change of $U(x\, y\, t | x_a y_a t_a)$ over a small time interval ϵ, the momentum variables p and p_y have the same effect as differential operators $-i\partial_{x_b}$ and $-i\partial_{y_b}$, respectively. The last term in H_T, however, is nonlocal in time, thus preventing a derivation of a Schrödinger-like differential equation.

The locality problem can be removed by introducing a noise variable $\eta(t)$ with the correlation function determined by (18.321):

$$\langle \eta(t) \eta(t') \rangle_T = \frac{w}{2} [K^{\rm Ohm}]^{-1}(t, t'). \tag{18.515}$$

Then we can define a temporally local η-dependent Hamiltonian operator

$$\hat{H}_\eta \equiv \frac{1}{M} (\hat{p}_x + \gamma y)\, \hat{p}_y + V(x + y/2) - V(x - y/2) - y\eta, \tag{18.516}$$

which governs the evolution of η-dependent versions of the amplitude products (18.513) via the *stochastic Schrödinger equation*

$$i\hbar \partial_t U_\eta(x\, y\, t | x_a y_a t_a) = \hat{H}_\eta\, U_\eta(x\, y\, t | x_a y_a t_a). \tag{18.517}$$

The same equation is obeyed by the noise-dependent density matrix $\rho_\eta(x, y; t)$.

Averaging these equation over η with the distribution (18.321) yields for $y_a = y_b = 0$ the same probability distribution as the forward–backward path integral (18.230):

$$|(x_b t_b | x_a t_a)|^2 = U(x_b\, 0\, t_b | x_a\, 0\, t_a) \equiv \langle U(x_b\, 0\, t_b | x_a\, y_a\, t_a) \rangle_\eta. \tag{18.518}$$

At high temperatures, the noise averaged stochastic Schrödinger equation (18.517) takes the form

$$i\hbar \partial_t U(x\, y\, t | x_a\, y_a\, t_a) = \hat{\bar{H}}_T U(x\, y\, t | x_a\, y_a\, t_a), \tag{18.519}$$

where $\hat{\bar{H}}$ is now a local (in the temporal sense)

$$\hat{\bar{H}}_T \equiv \frac{1}{M} \hat{p}_y \hat{p}_x + \gamma y \hat{p}_y + V(x + y/2) - V(x - y/2) - i\frac{w}{2\hbar} y^2, \tag{18.520}$$

arising from the Hamiltonian (18.512) in the high-temperature limit $K^{\rm Ohm} \to 1$ [recall (18.223)]. In terms of the separate path positions $x_\pm = x \pm y/2$ where $p_x = \partial_+ + \partial_-$ and $p_y = (\partial_+ - \partial_-)/2$, this takes the more familiar form [24]

$$\hat{\bar{H}}_T \equiv \frac{1}{2M}\left(\hat{p}_+^2 - \hat{p}_-^2\right) + V(x_+) - V(x_-) + \frac{\gamma}{2}(x_+ - x_-)(\hat{p}_+ - \hat{p}_-) - i\frac{w}{2\hbar}(x_+ - x_-)^2. \tag{18.521}$$

The last term is often written as $-i\hbar\Lambda(x_+ - x_-)^2$, where Λ is the so-called *decoherence rate per square distance*

$$\Lambda \equiv \frac{w}{2\hbar^2} = \frac{M\gamma k_B T}{\hbar^2}. \tag{18.522}$$

It is composed of the damping rate γ and the squared thermal length (2.353):

$$\Lambda = \frac{2\pi\gamma}{l_{\rm e}^2(\hbar\beta)}, \tag{18.523}$$

and controls the decay of interference peaks [25].

Note that the order of the operators in the mixed term of the form $y\hat{p}_y$ in Eq. (18.520) is opposite to the mixed term $-i\hat{p}_v v$ in the differential operator (18.239) of the Fokker-Planck equation. This order is necessary to guarantee the conservation of probability. Indeed, multiplying the time evolution equation (18.519) by $\delta(y)$, and integrating both sides over x and y, the left-hand side vanishes.

The correctness of this order can be verified by calculating the fluctuation determinant of the path integral for the product of amplitudes (18.513) in the Lagrangian form, which looks just like (18.230), except that the difference between forward and backward trajectories $y(t) = x_+(t) - x_-(t)$ is nonzero at the endpoints. For the fluctuation which vanish at the endpoints, this is irrelevant. As explained before, the order is a short-time issue, and we can take $t_b - t_a \to \infty$. Moreover, since the order is independent of the potential, we may consider only the free case $V(x \pm y/2) \equiv 0$. The relevant fluctuation determinant was calculated in formula (18.254). In the Hamiltonian operator (18.520), this implies an additional energy $-i\gamma/2$ with respect to the symmetrically ordered term $\gamma\{y, \hat{p}_y\}/2$, which brings it to $\gamma y\hat{p}_y$, and thus the order in (18.521).

18.18 Master Equation for Time Evolution

In the high-temperature limit, the Hamiltonian (18.521) becomes local. Then the evolution equation (18.514) for the density matrix $\rho(x_{+a}, x_{-a}; t_a)$ can be converted into an operator equation

$$i\hbar\partial_t\rho(x_+, x_-; t_a) = \hat{\bar{H}}_T\rho(x_+, x_-; t_a), \tag{18.524}$$

where $\hat{\bar{H}}_T$ is the operator version of the temperature-dependent Hamiltonian (18.521). Such an equation does not exist at low temperatures, due to the nonlocality of the last term in (18.512). Then one cannot avoid solving the stochastic Schrödinger equation (18.517) with the subsequent averaging (18.518). For moderately high temperatures, however, a Hamiltonian formalism can still be set up, although it requires solving a recursion relation. For this purpose we write down the quasi-Hamiltonian in D dimensions

$$\begin{aligned}\hat{\bar{H}}_T \equiv\; & \frac{1}{2M}\left(\hat{\mathbf{p}}_+^2 - \hat{\mathbf{p}}_-^2\right) + V(\mathbf{x}_+) - V(\mathbf{x}_-) + \frac{M\gamma}{2}(\hat{\mathbf{x}}_+ - \hat{\mathbf{x}}_-)(\hat{\dot{\mathbf{x}}}_+ + \hat{\dot{\mathbf{x}}}_-)^R \\ & - i\frac{w}{2\hbar}(\hat{\mathbf{x}}_+ - \hat{\mathbf{x}}_-)\hat{K}^{\rm Ohm}(\hat{\mathbf{x}}_+ - \hat{\mathbf{x}}_-),\end{aligned} \tag{18.525}$$

where the Fourier transform of $K^{\rm Ohm}(t, t')$ is expanded in powers of ω' [recall (18.223)]

$$K^{\rm Ohm}(\omega') = 1 + \frac{1}{3}\left(\frac{\hbar\omega'}{2k_BT}\right)^2 + \dots\, . \tag{18.526}$$

Each power of ω'^2 stands for the operator $-\overleftarrow{\partial}_t\partial_t$. In this way we find for the last term the locally looking high-temperature expansion

$$-i(\hat{\mathbf{x}}_+-\hat{\mathbf{x}}_-)\hat{K}^{\rm Ohm}(\hat{\mathbf{x}}_+-\hat{\mathbf{x}}_-)=-i(\hat{\mathbf{x}}_+-\hat{\mathbf{x}}_-)^2+i\frac{w\hbar}{24(k_BT)^2}(\hat{\dot{\mathbf{x}}}_+-\hat{\dot{\mathbf{x}}}_-)^2+\dots\,. \tag{18.527}$$

The expression is not really local, since the operator $\hat{\dot{\mathbf{x}}}$ is defined implicitly as an abbreviations for the commutator

$$\hat{\dot{\mathbf{x}}}\equiv\frac{i}{\hbar}[\hat{\bar{H}}_T,\hat{\mathbf{x}}]. \tag{18.528}$$

If the expansion (18.527) is carried further, higher derivatives of $\mathbf{x}$ arise, which are all defined recursively:

$$\hat{\ddot{\mathbf{x}}}\equiv\frac{i}{\hbar}[\hat{\bar{H}}_T,\hat{\dot{\mathbf{x}}}],\quad \hat{\dddot{\mathbf{x}}}\equiv\frac{i}{\hbar}[\hat{\bar{H}}_T,\hat{\ddot{\mathbf{x}}}],\quad\dots\,. \tag{18.529}$$

Thus Eq. (18.525) with the expansion (18.527) is a recursive equation for the Hamiltonian operator $\hat{\bar{H}}_T$. For small γ (and thus $w=2M\gamma k_BT$), the recursion can be solved iteratively, in the first step by inserting $\hat{\dot{\mathbf{x}}}\approx\hat{\mathbf{p}}/M$ into Eq. (18.530).

It is useful to re-express (18.524) in the Dirac operator form where the density matrix has a bra–ket representation $\hat{\rho}(t)=\sum_{mn}\rho_{mn}(t)|m\rangle\langle n|$. Denoting $\hat{\mathbf{p}}^2/2M+\hat{V}$ in (18.525) by $\hat{H}$, we obtain with the expansion (18.527) the local *master equation*:

$$\begin{aligned} i\hbar\partial_t\hat{\rho}=\hat{\bar{H}}_T\,\hat{\rho} \quad &\equiv \quad [\hat{H},\hat{\rho}]+\frac{M\gamma}{2}\left(\hat{\mathbf{x}}\hat{\dot{\mathbf{x}}}\hat{\rho}-\hat{\rho}\hat{\dot{\mathbf{x}}}\hat{\mathbf{x}}+\hat{\mathbf{x}}\,\hat{\rho}\,\hat{\dot{\mathbf{x}}}-\hat{\dot{\mathbf{x}}}\,\hat{\rho}\,\hat{\mathbf{x}}\right)\\ &- \quad \frac{iw}{2\hbar}[\hat{\mathbf{x}},[\hat{\mathbf{x}},\hat{\rho}]]-\frac{iw\hbar^2}{24(k_BT)^2}[\hat{\dot{\mathbf{x}}},[\hat{\dot{\mathbf{x}}},\hat{\rho}]]+\dots\,. \end{aligned} \tag{18.530}$$

The validity of the above iterative procedure is most easily proved in the time-sliced path integral. The final slice of infinitesimal width ϵ reads

$$\begin{aligned} &U(\mathbf{x}_{+b},\mathbf{x}_{-b},t_b|\mathbf{x}_{+a},\mathbf{x}_{-a},t_b-\epsilon)\\ &\qquad=\int\frac{d\mathbf{p}_+(t_b)}{(2\pi)^3}\int\frac{d\mathbf{p}_-(t_b)}{(2\pi)^3}e^{\frac{i}{\hbar}\left\{\mathbf{p}_+(t_b)[\mathbf{x}_+(t_b)-\mathbf{x}_+(t_b-\epsilon)]-\mathbf{p}_-\dot{\mathbf{x}}_--\bar{H}_T(t_b)\right\}}. \end{aligned} \tag{18.531}$$

Consider now a term of the generic form $\dot{F}_+(\mathbf{x}_+(t))F_-(\mathbf{x}_-(t))$ in $\bar{H}_T(t)$. When differentiating $U(\mathbf{x}_{+b},\mathbf{x}_{-b},t_b|\mathbf{x}_{+a},\mathbf{x}_{-a},t_b-\epsilon)$ with respect to the final time t_b, the integrand receives a factor $-\bar{H}_T(t_b)$. At t_b, the term $\dot{F}_+(\mathbf{x}_+(t))F_-(\mathbf{x}_-(t))$ in $\bar{H}_T(t)$ has the explicit form $\epsilon^{-1}\left[F_+(\mathbf{x}_+(t_b))-F_+(\mathbf{x}_+(t_b-\epsilon))\right]F_-(\mathbf{x}_-(t_b))$. It can be taken out of the integral, yielding

$$\epsilon^{-1}\left[F_+(\mathbf{x}_+(t_b))U-UF_+(\mathbf{x}_+(t_b-\epsilon))\right]F_-(\mathbf{x}_-(t_b)). \tag{18.532}$$

In operator language, the amplitude U is associated with $\hat{U}\approx 1-i\epsilon\hat{\bar{H}}_T/\hbar$, such the term $\dot{F}_+(\mathbf{x}_+(t))F_-(\mathbf{x}_-(t))$ in $\hat{\bar{H}}_T$ yields a Schrödinger operator

$$\frac{i}{\hbar}\left[\hat{\bar{H}}_T,\hat{F}_+(\mathbf{x}_+)\right]F_-(\mathbf{x}_-) \tag{18.533}$$

in the time evolution equation (18.530).

For functions of the second derivative $\ddot{\mathbf{x}}$ we have to split off the last two time slices in (18.531) and convert the two intermediate integrals over $\mathbf{x}$ into operator expressions, which obviously leads to the repeated commutator of $\hat{\bar{H}}_T$ with $\hat{\mathbf{x}}$, and so on.

The operator order in the terms in the parentheses of Eq. (18.530) is fixed by the retardation of $\dot{\mathbf{x}}_\pm$ with respect to $\mathbf{x}_\pm$ in (18.521). This implies that the associated operator $\hat{\dot{\mathbf{x}}}(t)$ has a time argument which lies slightly *before* that of $\hat{\mathbf{x}}_\pm$, thus acting upon $\hat\rho$ before $\hat{\mathbf{x}}$. This puts $\hat{\dot{\mathbf{x}}}(t)$ to the right of $\hat{\mathbf{x}}$, i.e., next to $\hat\rho$. On the right-hand side of $\hat\rho$, the time runs in the opposite direction such that $\hat{\dot{\mathbf{x}}}$ must lie to the left of $\hat{\mathbf{x}}$, again next to $\hat\rho$. In this way we obtain an operator order which ensures that Eq. (18.530) conserves the total probability.

This property and the positivity of $\hat\rho$ are actually guaranteed by the observation, that the master equation (18.530) can be written in the *Lindblad form* [26]

$$\partial_t\hat\rho \quad = \quad -\frac{i}{\hbar}[\hat H,\hat\rho]-\sum_{n=1}^{2}\left(\frac{1}{2}\hat L_n\hat L_n^\dagger\hat\rho+\frac{1}{2}\hat\rho\hat L_n\hat L_n^\dagger-\hat L_n^\dagger\hat\rho\hat L_n\right), \tag{18.534}$$

with the two Lindblad operators [27]

$$\hat L_1\equiv\frac{\sqrt{w}}{2\hbar}\hat{\mathbf{x}}, \qquad \hat L_2\equiv\frac{\sqrt{3w}}{2\hbar}\left(\hat{\mathbf{x}}-i\frac{\hbar}{3k_BT}\hat{\dot{\mathbf{x}}}\right). \tag{18.535}$$

Note that the operator order in Eq. (18.530) prevents the term $\hat{\mathbf{x}}\hat{\dot{\mathbf{x}}}\hat\rho$ from being a pure divergence. If we rewrite it as a sum of a commutator and an anticommutator, $[\hat{\mathbf{x}},\hat{\dot{\mathbf{x}}}]/2+\{\hat{\mathbf{x}},\hat{\dot{\mathbf{x}}}\}/2$, then the latter term is a pure divergence, and we can think of the first two γ-terms in (18.530) as being due to an additional anti-Hermitian term in the Hamiltonian operator $\hat H$, the *dissipation operator*

$$\hat H_\gamma=\gamma M\frac{1}{4}[\hat{\mathbf{x}},\hat{\dot{\mathbf{x}}}]. \tag{18.536}$$

18.19 Relation to Quantum Langevin Equation

The stochastic Liouville equation (18.517) can also be derived from an operator version of the Langevin equation (18.317), the so-called *Quantum Langevin equation*

$$M\ddot{\hat x}(t)+M\gamma\dot{\hat x}(t)+V'(\hat x(t))=\hat\eta(t), \tag{18.537}$$

where $\hat\eta(t)$ is an operator noise variable with the commutation rule

$$[\hat\eta_t,\hat\eta_{t'}]=w\frac{i\hbar}{k_BT}\partial_t\delta(t-t'), \tag{18.538}$$

and the correlation function [28]

$$\frac{1}{2}\langle[\hat\eta_t,\hat\eta_{t'}]_+\rangle_{\hat\eta} \quad = \quad w\,K(t,t'). \tag{18.539}$$

The commutator (18.538) and the correlation function (18.539) are related to each other as required by the fluctuation-dissipation theorem: By omitting the factor $\coth(\hbar\omega/2k_BT)$ in Eq. (18.223), the Fourier integral (18.221) for $K(t,t')$ reduces to $(\hbar/2k_BT)\partial_t\delta(t-t')$. A comparison with the general spectral representation (18.53) shows that the expectation value (18.539) has the spectral function

$$\rho_{\rm b}(\omega')=2M\gamma\hbar\omega'. \tag{18.540}$$

By inserting this into the spectral representation (18.53) we obtain the right-hand side of the commutator equation (18.538).

A noise variable with the properties (18.538) and (18.539) can be constructed explicitly by superimposing quantized oscillator velocities of frequencies ω as follows:

$$\hat\eta(t)=-i\sqrt{\frac{M\hbar\gamma}{\pi}}\int_0^\infty d\Omega'\sqrt{\Omega'}[a_{\Omega'}e^{-i\omega't}-a_{\omega'}^\dagger e^{i\omega't}]. \tag{18.541}$$

It is worth pointing out that there exists a direct derivation of the quantum Langevin equation (18.537), whose noise operator $\hat\eta(t)$ satisfies the commutator and fluctuation properties (18.538) and (18.539), from Kubo's stochastic Liouville equation, and thus from the forward–backward path integral (18.230) [29].

18.20 Electromagnetic Dissipation and Decoherence

There exists a thermal bath of particular importance: atoms are usually observed at a finite temperature where they interact with a grand-canonical ensemble of photons in thermal equilibrium. This interaction will broaden the natural line width of atomic levels even if all major mechanisms for the broadening are removed. To study this situation, let us set up a forward–backward path integral description for a bath of photons, and derive from it a master equation for the density matrix which describes electromagnetic dissipation and decoherence. As an application, we shall calculate the Wigner-Weisskopf formula for the natural line width of an atomic state at zero temperature, find the finite-temperature effects, and calculate the Lamb shift between atomic s- and p-wave states of principal quantum number $n=2$ with the term notation $2S_{1/2}$ and $2P_{1/2}$. The master equation may eventually have applications to dilute interstellar gases or to few-particle systems in cavities.

18.20.1 Forward–Backward Path Integral

With the application to atomic physics in mind, we shall consider a three-dimensional quantum system described by a time-dependent quantum-mechanical density matrix $\rho(\mathbf{x}_+,\mathbf{x}_-;t)$. In contrast to Eq. (18.514), we use here the forward and backward variables as arguments, and write the time evolution equation as

$$\rho(\mathbf{x}_{+b},\mathbf{x}_{-a};t_b)=\int d\mathbf{x}_{+a}\,d\mathbf{x}_{-a}\,U(\mathbf{x}_{+b},\mathbf{x}_{-b},t_b|\mathbf{x}_{+a},\mathbf{x}_{-a},t_a)\rho(\mathbf{x}_{+a},\mathbf{x}_{-a};t_a). \tag{18.542}$$

In an external electromagnetic vector potential $\mathbf{A}(\mathbf{x},t)$, the time-evolution kernel is determined by a forward–backward path integral of the type (18.192), in which the forward and backward paths start at different initial and final points $\mathbf{x}_{+a},\mathbf{x}_{-a}$ and $\mathbf{x}_{+b},\mathbf{x}_{-b}$, respectively:

$$U(\mathbf{x}_{+b},\mathbf{x}_{-b},t_b|\mathbf{x}_{+a},\mathbf{x}_{-a},t_a)\equiv(\mathbf{x}_{+b},t_b|\mathbf{x}_{+a},t_a)(\mathbf{x}_{-b},t_b|\mathbf{x}_{-a},t_a)^*=\int\mathcal{D}\mathbf{x}_+\mathcal{D}\mathbf{x}_-$$
$$\times\exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b}\left[\frac{M}{2}\left(\mathbf{x}_+^2-\mathbf{x}_-^2\right)-V(\mathbf{x}_+)+V(\mathbf{x}_-)-\frac{e}{c}\dot{\mathbf{x}}_+\mathbf{A}(\mathbf{x}_+,t)+\frac{e}{c}\dot{\mathbf{x}}_-\mathbf{A}(\mathbf{x}_-,t)\right]\right\}. \tag{18.543}$$

The vector potential $\mathbf{A}(\mathbf{x},t)$ is a superposition of oscillators $\mathbf{X}_\mathbf{k}(t)$ of frequency $\Omega_\mathbf{k}=c|\mathbf{k}|$ in a volume V:

$$\mathbf{A}(\mathbf{x},t)=\sum_\mathbf{k}c_\mathbf{k}(\mathbf{x})\mathbf{X}_\mathbf{k}(t),\qquad c_\mathbf{k}=\frac{e^{i\mathbf{k}\mathbf{x}}}{\sqrt{2\Omega_\mathbf{k}V}},\qquad \sum_\mathbf{k}=\int\frac{d^3kV}{(2\pi)^3}. \tag{18.544}$$

At a finite temperature T, these oscillators are assumed to be in equilibrium, where we shall write their time-ordered correlation functions as

$$G^{ij}_{\mathbf{k}\mathbf{k}'}(t,t')=\langle\hat{T}\hat{X}^i_\mathbf{k}(t),\hat{X}^j_{-\mathbf{k}'}(t')\rangle=\delta^{ij\,\mathrm{tr}}_{\mathbf{k}\mathbf{k}'}G_{\Omega_\mathbf{k}}(t,t')\equiv\delta_{\mathbf{k}\mathbf{k}'}P^{\perp\,ij}_\mathbf{k}G_{\Omega_\mathbf{k}}(t,t'). \tag{18.545}$$

The transverse projection matrix is the result of the sum over the transverse polarization vectors of the photons:

$$P^{\perp\,ij}_\mathbf{k}=\sum_{h=\pm}\epsilon^i(\mathbf{k},h)\epsilon^{j\,*}(\mathbf{k},h)=(\delta^{ij}-k^ik^j/\mathbf{k}^2). \tag{18.546}$$

The function $G_{\Omega_\mathbf{k}}(t,t')$ on the right-hand side of (18.545) is the Green function (18.185) of a single oscillator of frequency $\Omega_\mathbf{k}$. It is decomposed into real and imaginary parts, defining $A_{\Omega_\mathbf{k}}(t,t')$ and $C_{\Omega_\mathbf{k}}(t,t')$ as in (18.185), which are commutator and anticommutator functions of the oscillator at temperature T: $C_{\Omega_\mathbf{k}}(t,t')\equiv\langle[\hat{X}(t),\hat{X}(t')]\rangle_T$ and $A_{\Omega_\mathbf{k}}(t,t')\equiv\langle[\hat{X}(t),\hat{X}(t')]\rangle_T$, respectively.

The thermal average of the evolution kernel (18.543) is then given by the forward–backward path integral

$$U(\mathbf{x}_{+b},\mathbf{x}_{-b},t_b|\mathbf{x}_{+a},\mathbf{x}_{-a},t_a) = \int \mathcal{D}\mathbf{x}_+(t) \int \mathcal{D}\mathbf{x}_-(t) \times \exp\left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} dt \left[\frac{M}{2}(\dot{\mathbf{x}}_+^2 - \dot{\mathbf{x}}_-^2) - (V(\mathbf{x}_+) - V(\mathbf{x}_-)) \right] + \frac{i}{\hbar}\mathcal{A}^{\rm FV}[\mathbf{x}_+,\mathbf{x}_-] \right\}, \tag{18.547}$$

where $\exp\{i\mathcal{A}^{\rm FV}[\mathbf{x}_+,\mathbf{x}_-]/\hbar\}$ is the Feynman-Vernon influence functional defined in Eq. (18.200). The influence action $\mathcal{A}^{\rm FV}[\mathbf{x}_+,\mathbf{x}_-]$ is the sum of a dissipative and a fluctuating part $\mathcal{A}_D^{\rm FV}[\mathbf{x}_+,\mathbf{x}_-]$ and $\mathcal{A}_F^{\rm FV}[\mathbf{x}_+,\mathbf{x}_-]$, whose explicit forms are now

$$\begin{aligned}\mathcal{A}_D^{\rm FV}[\mathbf{x}_+,\mathbf{x}_-] = \frac{ie^2}{2\hbar c^2} \int dt \int dt'\, \Theta(t-t') \\ \times \Big[\dot{\mathbf{x}}_+(t)\mathbf{C}_{\rm b}(\mathbf{x}_+\,t,\mathbf{x}'_+\,t')\dot{\mathbf{x}}_+(t') - \dot{\mathbf{x}}_+(t)\mathbf{C}_{\rm b}(\mathbf{x}_+\,t,\mathbf{x}'_-\,t')\dot{\mathbf{x}}_-(t') \\ - \dot{\mathbf{x}}_-(t)\mathbf{C}_{\rm b}(\mathbf{x}_-\,t,\mathbf{x}'_+\,t')\dot{\mathbf{x}}_+(t') + \dot{\mathbf{x}}_-(t)\mathbf{C}_{\rm b}(\mathbf{x}_-\,t,\mathbf{x}'_-\,t')\dot{\mathbf{x}}_-(t')\Big],\end{aligned} \tag{18.548}$$

and

$$\begin{aligned}\mathbf{A}_F^{\rm FV}[\mathbf{x}_+,\mathbf{x}_-] = \frac{ie^2}{2\hbar c^2} \int dt \int dt'\, \Theta(t-t') \\ \times \Big[\dot{\mathbf{x}}_+(t)\mathbf{A}_{\rm b}(\mathbf{x}_+\,t,\mathbf{x}'_+\,t')\dot{\mathbf{x}}_+(t') + \dot{\mathbf{x}}_+(t)\mathbf{A}_{\rm b}(\mathbf{x}_+\,t,\mathbf{x}'_-\,t')\dot{\mathbf{x}}_-(t') \\ + \dot{\mathbf{x}}_-(t)\mathbf{A}_{\rm b}(\mathbf{x}_-\,t,\mathbf{x}'_+\,t')\dot{\mathbf{x}}_+(t') + \dot{\mathbf{x}}_-(t)\mathbf{A}_{\rm b}(\mathbf{x}_-\,t,\mathbf{x}'_-\,t')\dot{\mathbf{x}}_-(t')\Big],\end{aligned} \tag{18.549}$$

with $\mathbf{C}_{\rm b}(\mathbf{x}_-\,t,\mathbf{x}'_-\,t')$ and $\mathbf{A}_{\rm b}(\mathbf{x}_-\,t,\mathbf{x}'_-\,t')$ collecting the 3×3 commutator and anticommutator functions of the bath of photons. They are sums of correlation functions over the bath of the oscillators of frequency $\Omega_{\mathbf{k}}$, each contributing with a weight $c_{\mathbf{k}}(\mathbf{x})c_{-\mathbf{k}}(\mathbf{x}') = e^{i\mathbf{k}(\mathbf{x}-\mathbf{x}')}/2\Omega_{\mathbf{k}}V$. Thus we may write, generalizing (18.197) and (18.198),

$$\begin{aligned}C_{\rm b}^{ij}(\mathbf{x}\,t,\mathbf{x}'\,t') &= \sum_{\mathbf{k}} c_{-\mathbf{k}}(\mathbf{x})c_{\mathbf{k}}(\mathbf{x}') \left\langle [\hat{X}^i_{-\mathbf{k}}(t),\hat{X}^j_{\mathbf{k}}(t')] \right\rangle_T \\ &= -i\hbar \int \frac{d\omega' d^3k}{(2\pi)^4} \rho_{\mathbf{k}}(\omega') P_{\mathbf{k}}^{\perp\,ij} e^{i\mathbf{k}(\mathbf{x}-\mathbf{x}')} \sin\omega'(t-t'),\end{aligned} \tag{18.550}$$

$$\begin{aligned}A_{\rm b}^{ij}(\mathbf{x}\,t,\mathbf{x}'\,t') &= \sum_{\mathbf{k}} c_{-\mathbf{k}}(\mathbf{x})c_{\mathbf{k}}(\mathbf{x}') \left\langle \left\{ \hat{X}^i_{-\mathbf{k}}(t),\hat{X}^j_{\mathbf{k}}(t') \right\} \right\rangle_T \\ &= \hbar \int \frac{d\omega' d^3k}{(2\pi)^4} \rho_{\mathbf{k}}(\omega') P_{\mathbf{k}}^{\perp\,ij} \coth\frac{\hbar\omega'}{2k_BT}\; e^{i\mathbf{k}(\mathbf{x}-\mathbf{x}')} \cos\omega'(t-t'),\end{aligned} \tag{18.551}$$

where $\rho_{\mathbf{k}}(\omega')$ is the spectral density contributed by the oscillator of momentum $\mathbf{k}$:

$$\rho_{\mathbf{k}}(\omega') \equiv \frac{2\pi}{2\Omega_{\mathbf{k}}}[\delta(\omega'-\Omega_{\mathbf{k}}) - \delta(\omega'+\Omega_{\mathbf{k}})]. \tag{18.552}$$

At zero temperature, we recognize in (18.550) and (18.551) twice the imaginary and real parts of the Feynman propagator of a massless particle for $t > t'$, which in four-vector notation with $k = (\omega/c,\mathbf{k})$ and $x = (ct,\mathbf{x})$ reads

$$\begin{aligned}G(x,x') &= \frac{1}{2}[A(x,x') + C(x,x')] = \int \frac{d^4k}{(2\pi)^4} e^{ik(x-x')} \frac{i\hbar}{k^2 + i\eta} \\ &= \int \frac{d\omega\, d^3k}{(2\pi)^4} \frac{ic\hbar}{\omega^2 - \Omega_{\mathbf{k}}^2 + i\eta} e^{-i[\omega(t-t') - \mathbf{k}(\mathbf{x}-\mathbf{x}')]},\end{aligned} \tag{18.553}$$

where η is an infinitesimally small number > 0.

We shall now focus attention upon systems which are so small that the effects of retardation can be neglected. Then we can ignore the $\mathbf{x}$-dependence in (18.551) and (18.552) and find

$$C_{\rm b}^{ij}(\mathbf{x}\,t,\mathbf{x}'\,t') \approx C_{\rm b}^{ij}(t,t') = i\frac{\hbar}{2\pi c}\frac{2}{3}\delta^{ij}\partial_t\delta(t-t'). \tag{18.554}$$

Inserting this into (18.548) and integrating by parts, we obtain two contributions. The first is a diverging term

$$\Delta\mathcal{A}_{\rm loc}[\mathbf{x}_+,\mathbf{x}_-] = \frac{\Delta M}{2}\int_{t_a}^{t_b} dt\,(\dot{\mathbf{x}}_+^2 - \dot{\mathbf{x}}_-^2)(t), \tag{18.555}$$

where

$$\Delta M \equiv -\frac{e^2}{c^2}\int\frac{d\omega' d^3k}{(2\pi)^4}\frac{\sigma_{\mathbf{k}}(\omega')}{\omega'}\delta_{\mathbf{kk}}^{ij\,\rm tr} = -\frac{e^2}{3\pi^2c^3}\int_0^\infty dk \tag{18.556}$$

diverges linearly. This simply renormalizes the kinetic terms in the path integral (18.547), renormalizing them to

$$\frac{i}{\hbar}\int_{t_a}^{t_b} dt\,\frac{M_{\rm ren}}{2}\left(\dot{\mathbf{x}}_+^2 - \dot{\mathbf{x}}_-^2\right). \tag{18.557}$$

By identifying M with $M_{\rm ren}$ this renormalization may be ignored.

The second term has the form [compare (18.205)]

$$\mathcal{A}_D^{\rm FV}[\mathbf{x}_+,\mathbf{x}_-] \;=\; -\gamma\frac{M}{2}\int_{t_a}^{t_b} dt\,(\dot{\mathbf{x}}_+ - \dot{\mathbf{x}}_-)(t)(\ddot{\mathbf{x}}_+ + \ddot{\mathbf{x}}_-)^R(t), \tag{18.558}$$

with the friction constant of the photon bath encountered before in Eq. (3.444):

$$\gamma \equiv \frac{e^2}{6\pi c^3 M} = \frac{2}{3}\frac{\alpha}{\omega_M}, \tag{18.559}$$

where $\alpha \equiv e^2/\hbar c \approx 1/137$ is the fine-structure constant (1.505) and $\omega_M \equiv Mc^2/\hbar$ the Compton frequency associated with the mass M. Note once more that in contrast to the usual friction constant γ in Section 3.13, this has the dimension 1/frequency.

As discussed in Section 18.8, the retardation enforced by the Heaviside function in the exponent of (18.548) removes the left-hand half of the δ-function [see (18.214)]. It ensures the *causality* of the dissipation forces, which has been shown in Section 18.9.2 to be crucial for producing a probability conserving time evolution of the probability distribution [13]. The superscript R in (18.558) shifts the acceleration $(\ddot{\mathbf{x}}_+ + \ddot{\mathbf{x}}_-)(t)$ slightly towards an earlier time with respect to the velocity factor $(\dot{\mathbf{x}}_+ - \dot{\mathbf{x}}_-)(t)$.

We now turn to the anticommutator function. Inserting (18.552) and the friction constant γ from (18.559), it becomes

$$\frac{e^2}{c^2}A_{\rm b}(\mathbf{x}\,t,\mathbf{x}'\,t') \approx 2\gamma k_BTK^{\rm Ohm}(t,t'), \tag{18.560}$$

as in Eq. (18.216), with the same function $K^{\rm Ohm}(t,t')$ as in Eq. (18.223), whose high-temperature expansion starts out as in Eq. (18.526).

In terms of the function $K^{\rm Ohm}(t,t')$, the fluctuation part of the influence functional in (18.549), (18.548), (18.547) becomes [compare (18.227)]

$$\mathcal{A}_F^{\rm FV}[\mathbf{x}_+,\mathbf{x}_-] = i\frac{w}{2\hbar}\int_{t_a}^{t_b} dt\int_{t_a}^{t_b} dt'\,(\dot{\mathbf{x}}_+ - \dot{\mathbf{x}}_-)(t)\,K^{\rm Ohm}(t,t')\,(\dot{\mathbf{x}}_+ - \dot{\mathbf{x}}_-)(t'). \tag{18.561}$$

Here we have used the symmetry of the function $K^{\rm Ohm}(t,t')$ to remove the Heaviside function $\Theta(t-t')$ from the integrand, extending the range of t'-integration to the entire interval (t_a,t_b). We also have introduced the constant

$$w \equiv 2Mk_BT\gamma, \tag{18.562}$$

for brevity.

In the high-temperature limit, the time evolution amplitude for the density matrix is given by the path integral

$$\begin{aligned} U(\mathbf{x}_{+b},\mathbf{x}_{-b},t_b|\mathbf{x}_{+a},\mathbf{x}_{-a},t_a) &= \int \mathcal{D}\mathbf{x}_+(t)\int \mathcal{D}\mathbf{x}_-(t) \\ &\times \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b} dt\,\left[\frac{M}{2}(\dot{\mathbf{x}}_+^2-\dot{\mathbf{x}}_-^2)-(V(\mathbf{x}_+)-V(\mathbf{x}_-))\right]\right\} \\ &\times \exp\left\{-\frac{i}{2\hbar}M\gamma\int_{t_a}^{t_b} dt\;(\dot{\mathbf{x}}_+-\dot{\mathbf{x}}_-)(\ddot{\mathbf{x}}_++\ddot{\mathbf{x}}_-)^R-\frac{w}{2\hbar^2}\int_{t_a}^{t_b} dt\,(\dot{\mathbf{x}}_+-\dot{\mathbf{x}}_-)^2\right\}, \end{aligned} \tag{18.563}$$

where the last term is now local since $K^{\rm Ohm}(t,t')\to\delta(t-t')$. In this limit (as in the classical limit $\hbar\to 0$), this term squeezes the forward and backward paths together. The density matrix (18.563) becomes diagonal. The γ-term, however, remains and describes classical radiation damping.

At moderately high temperature, we should include also the first correction term in (18.526) which adds to the exponent an additional term

$$-\frac{w}{24(k_BT)^2}\int_{t_a}^{t_b} dt\,(\ddot{\mathbf{x}}_+-\ddot{\mathbf{x}}_-)^2. \tag{18.564}$$

The extended expression is the desired *closed-time path integral* of a particle in contact with a thermal reservoir.

18.20.2 Master Equation for Time Evolution in Photon Bath

It is possible to derive a master equation for the evolution of the density matrix $\rho(\mathbf{x}_{+a},\mathbf{x}_{-a};t_a)$ analogous to Eq. (18.530) for a quantum particle in a photon bath. Since the dissipative and fluctuating parts of the influence functional in Eq. (18.555) and (18.561) coincide with the corresponding terms in (18.230), except for an extra dot on top of the coordinates, the associated temperature-dependent Hamiltonian operator is directly obtained from (18.525) with the expansion (18.527) by adding the extra dots: In the high-temperature limit we obtain

$$\hat{\mathcal{H}} \equiv \frac{1}{2M}\left(\hat{\mathbf{p}}_+^2-\hat{\mathbf{p}}_-^2\right)+V(\mathbf{x}_+)-V(\mathbf{x}_-)+\frac{M\gamma}{2}\,(\hat{\dot{\mathbf{x}}}_+-\hat{\dot{\mathbf{x}}}_-)(\hat{\dot{\mathbf{x}}}_++\hat{\dot{\mathbf{x}}}_-)^R-i\frac{w}{2\hbar}(\hat{\dot{\mathbf{x}}}_+-\hat{\dot{\mathbf{x}}}_-)^2, \tag{18.565}$$

extended at moderately high temperatures by the Hamiltonian corresponding to (18.564):

$$\Delta\hat{\bar{H}}_T \equiv i\frac{w\hbar}{24(k_BT)^2}(\hat{\dot{\mathbf{x}}}_+-\hat{\dot{\mathbf{x}}}_-)^2. \tag{18.566}$$

The master equation corresponding to the Ohmic equation (18.530) reads now

$$\begin{aligned} i\hbar\partial_t\hat{\rho} = \hat{\bar{H}}_T\,\hat{\rho} \;\;&\equiv\;\; [\hat{H},\hat{\rho}]+\frac{M\gamma}{2}\left(\hat{\dot{\mathbf{x}}}\hat{\ddot{\mathbf{x}}}\hat{\rho}-\hat{\rho}\hat{\ddot{\mathbf{x}}}\hat{\dot{\mathbf{x}}}+\hat{\dot{\mathbf{x}}}\,\hat{\rho}\,\hat{\ddot{\mathbf{x}}}-\hat{\ddot{\mathbf{x}}}\,\hat{\rho}\,\hat{\dot{\mathbf{x}}}\right) \\ &-\;\; \frac{iw}{2\hbar}[\hat{\dot{\mathbf{x}}},[\hat{\dot{\mathbf{x}}},\hat{\rho}]]-\frac{iw\hbar^2}{24(k_BT)^2}[\hat{\ddot{\mathbf{x}}},[\hat{\ddot{\mathbf{x}}},\hat{\rho}]]. \end{aligned} \tag{18.567}$$

The conservation of total probability and the positivity of $\hat{\rho}$ are ensured by the observation, that Eq. (18.567) can be written in the *Lindblad form*

$$\partial_t\hat{\rho} \;=\; -\frac{i}{\hbar}[\hat{H},\hat{\rho}]-\sum_{n=1}^{2}\left(\frac{1}{2}\hat{L}_n\hat{L}_n^\dagger\hat{\rho}+\frac{1}{2}\hat{\rho}\hat{L}_n\hat{L}_n^\dagger-\hat{L}_n^\dagger\hat{\rho}\hat{L}_n\right), \tag{18.568}$$

with the two Lindblad operators

$$\hat{L}_1 \equiv \frac{\sqrt{w}}{2\hbar}\hat{\mathbf{x}}, \qquad \hat{L}_2 \equiv \frac{\sqrt{3w}}{2\hbar}\left(\hat{\dot{\mathbf{x}}} - i\frac{\hbar}{3k_BT}\hat{\ddot{\mathbf{x}}}\right). \tag{18.569}$$

As noted in the discussion of Eq. (18.530), the operator order in (18.567) prevents the term $\hat{\dot{\mathbf{x}}}\hat{\ddot{\mathbf{x}}}\hat{\rho}$ from being a pure divergence. By rewriting it as a sum of a commutator and an anticommutator, $[\hat{\dot{\mathbf{x}}}, \hat{\ddot{\mathbf{x}}}]/2 + \{\hat{\dot{\mathbf{x}}}, \hat{\ddot{\mathbf{x}}}\}/2$, the latter term is a pure divergence, and we can think of the first two γ-terms in (18.567) as being due to an additional anti-Hermitian *dissipation operator*

$$\hat{H}_\gamma = \gamma M \frac{1}{4}[\hat{\dot{\mathbf{x}}}, \hat{\ddot{\mathbf{x}}}]. \tag{18.570}$$

For a free particle with $V(\mathbf{x}) \equiv 0$ and $[\hat{H}, \hat{\mathbf{p}}] = 0$, one has $\hat{\dot{\mathbf{x}}}_\pm = \hat{\mathbf{p}}_\pm/M$ to all orders in γ, such that the time evolution equation (18.567) becomes

$$i\hbar\partial_t\hat{\rho} \;\; = \;\; [\hat{H}, \hat{\rho}] - \frac{iw}{2M^2\hbar}[\hat{\mathbf{p}}, [\hat{\mathbf{p}}, \hat{\rho}]]. \tag{18.571}$$

In the momentum representation of the density matrix $\hat{\rho} = \sum_{\mathbf{pp}'} \rho_{\mathbf{pp}'}|\mathbf{p}\rangle\langle\mathbf{p}'|$, the last term simplifies to $-i\Gamma \equiv -iw(\mathbf{p}-\mathbf{p}')^{\mathbf{2}}/2M^2\hbar^2$ multiplying $\hat{\rho}$, which shows that a free particle does not dissipate energy by radiation, and that the off-diagonal matrix elements decay with the rate Γ.

For small e^2, the implicit equation Eq. (18.565) with the expansion term (18.566) can be solved approximately in a single iteration step, inserting $\hat{\dot{\mathbf{x}}} \approx \hat{\mathbf{p}}/M$ and $\hat{\ddot{\mathbf{x}}} \approx -\boldsymbol{\nabla}V/M$.

18.20.3 Line Width

Let us apply the master equation (18.567) to atoms, where $V(\mathbf{x})$ is the Coulomb potential, assuming it to be initially in an eigenstate $|i\rangle$ of H, with a density matrix $\hat{\rho}(0) = |i\rangle\langle i|$. Since atoms decay rather slowly, we may treat the γ-term in (18.567) perturbatively. It leads to a time derivative of the density matrix

$$\begin{aligned} \partial_t\langle i|\hat{\rho}(t)|i\rangle &= -\frac{\gamma}{\hbar M}\langle i|[\hat{H}, \hat{\mathbf{p}}]\,\hat{\mathbf{p}}\,\hat{\rho}(0)|i\rangle = \frac{\gamma}{M}\sum_{f\neq i}\omega_{if}\langle i|\mathbf{p}|f\rangle\langle f|\mathbf{p}|i\rangle \\ &= -M\gamma\sum_f \omega_{if}^3\,|\mathbf{x}_{fi}|^2, \end{aligned} \tag{18.572}$$

where $\hbar\omega_{if} \equiv E_i - E_f$, and $\mathbf{x}_{fi} \equiv \langle f|\mathbf{x}|i\rangle$ are the matrix elements of the dipole operator.

An extra width comes from the last two terms in (18.567):

$$\begin{aligned} \partial_t\langle i|\hat{\rho}(t)|i\rangle &= -\frac{w}{M^2\hbar^2}\langle i|\mathbf{p}^2|i\rangle - \frac{w}{12M^2(k_BT)^2}\langle i|\dot{\mathbf{p}}^2|i\rangle \\ &= -w\sum_n \omega_{if}^2\left[1 + \frac{\hbar^2\omega_{if}^2}{12(k_BT)^2}\right]|\mathbf{x}_{fi}|^2. \end{aligned} \tag{18.573}$$

This time dependence is caused by spontaneous emission and induced emission and absorption. To identify the different contributions, we rewrite the spectral decompositions (18.550) and (18.551) in the $\mathbf{x}$-independent approximation as

$$\begin{aligned} &C_b(t,t') + A_b(t,t') \\ &= \frac{4\pi}{3}\hbar\int\frac{d\omega' d^3k}{(2\pi)^4}\frac{\pi}{2M\Omega_{\mathbf{k}}}\left\{1 + \coth\frac{\hbar\omega'}{2k_BT}\right\}\left[\delta(\omega'-\Omega_{\mathbf{k}}) - \delta(\omega'+\Omega_{\mathbf{k}})\right]e^{-i\omega'(t-t')}, \end{aligned} \tag{18.574}$$

or

$$\begin{aligned} &C_b(t,t') + A_b(t,t') \\ &= \frac{4\pi}{3}\hbar\int\frac{d\omega' d^3k}{(2\pi)^4}\frac{\pi}{2M\Omega_{\mathbf{k}}}\left\{2\delta(\omega'-\Omega_{\mathbf{k}}) + \frac{2}{e^{\hbar\Omega_{\mathbf{k}}/k_BT}-1}\left[\delta(\omega'-\Omega_{\mathbf{k}}) + \delta(\omega'+\Omega_{\mathbf{k}})\right]\right\}e^{-i\omega'(t-t')}. \end{aligned} \tag{18.575}$$

Following Einstein's intuitive interpretation, the first term in curly brackets is due to spontaneous emission, the other two terms accompanied by the Bose occupation function account for induced emission and absorption. For high and intermediate temperatures, (18.575) has the expansion

$$\frac{4\pi}{3}\hbar\int\frac{d\omega' d^3k}{(2\pi)^4}\frac{\pi}{2M\Omega_{\mathbf{k}}}\left\{2\delta(\omega'-\Omega_{\mathbf{k}})\right.$$
$$\left.+\left(\frac{2k_BT}{\hbar\Omega_{\mathbf{k}}}-1+\frac{1}{6}\frac{\hbar\Omega_{\mathbf{k}}}{k_BT}\right)[\delta(\omega'-\Omega_{\mathbf{k}})+\delta(\omega'+\Omega_{\mathbf{k}})]\right\}e^{-i\omega'(t-t')}. \tag{18.576}$$

The first term in curly brackets corresponds to the spontaneous emission. It contributes to the rate of change $\partial_t\langle i|\hat\rho(t)|i\rangle$ a term $-2M\gamma\sum_{f<i}\omega_{if}^3\,|\mathbf{x}_{fi}|^2$. This differs from the right-hand side of Eq. (18.572) in two important respects. First, the sum is restricted to the lower states $f<i$ with $\omega_{if}>0$, since the δ-function allows only for decays. Second, there is an extra factor 2. Indeed, by comparing (18.574) with (18.576) we see that the spontaneous emission receives equal contributions from the 1 and the $\coth(\hbar\omega'/2k_BT)$ in the curly brackets of (18.574), i.e., from dissipation and fluctuation terms $C_{\rm b}(t,t')$ and $A_{\rm b}(t,t')$.

Thus our master equation yields for the natural line width of atomic levels the equation

$$\Gamma=2M\gamma\sum_{f<i}\omega_{if}^3\,|\mathbf{x}_{fi}|^2, \tag{18.577}$$

in agreement with the historic *Wigner-Weisskopf formula*.

In terms of Γ, the rate (18.572) can therefore be written as

$$\partial_t\langle i|\hat\rho(t)|i\rangle \;=\; -\Gamma+M\gamma\sum_{f<i}\omega_{if}^3\,|\mathbf{x}_{fi}|^2+M\gamma\sum_{f>i}|\omega_{if}|^3\,|\mathbf{x}_{fi}|^2. \tag{18.578}$$

The second and third terms do not contribute to the total rate of change of $\langle i|\hat\rho(t)|i\rangle$ since they are canceled by the induced emission and absorption terms associated with the -1 in the big parentheses of the fluctuation part of (18.576). The finite lifetime changes the time dependence of the state $|i,t\rangle$ from $|i,t\rangle=|i,0\rangle e^{-iEt}$ to $|i,0\rangle e^{-iEt-\Gamma t/2}$.

Note that due to the restriction to $f<i$ in (18.577), there is no operator local in time whose expectation value is Γ. Only the combination of spontaneous and induced emissions and absorptions in (18.578) can be obtained from a local operator, which is in fact the dissipation operator (18.570).

For all temperatures, the spontaneous and induced transitions together lead to the rate of change of $\langle i|\hat\rho(t)|i\rangle$:

$$\partial_t\langle i|\hat\rho(t)|i\rangle \;=\; -2M\gamma\left(\sum_{f<i}\omega_{if}^3+\sum_f\omega_{if}^3\frac{1}{e^{\hbar\omega_{if}/k_BT}-1}\right)|\mathbf{x}_{fi}|^2. \tag{18.579}$$

For a state with principal quantum number n the temperature effects become detectable only if T becomes larger than $-1/(n+1)^2+1/n^2\approx 2/n^3$ times the Rydberg temperature $T_{\rm Ry}=157886.601K$. Thus we have to go to $n\gtrsim 20$ to have observable effects at room temperature.

18.20.4 Lamb shift

For atoms, the Feynman influence functional (18.547) allows us to calculate the celebrated Lamb shift. Being interested in the time behavior of the pure-state density matrix $\rho=|i\rangle\langle i|$, we may calculate the effect of the actions (18.548) and (18.549) perturbatively. For this, consider the dissipative part of the influence action (18.548), and in it the first term involving $\mathbf{x}_+(t)$ and $\mathbf{x}_+(t')$, and integrate the external positions in the path integral (18.547) over the initial wave functions, forming

$$U_{ii,t_b;ii,t_a} = \int d\mathbf{x}_{+b}\, d\mathbf{x}_{-b} \int d\mathbf{x}_{+a}\, d\mathbf{x}_{-a} \langle i|\mathbf{x}_{+b}\rangle\langle i|\mathbf{x}_{-b}\rangle \times\; U(\mathbf{x}_{+b},\mathbf{x}_{-b},t_b|\mathbf{x}_{+a},\mathbf{x}_{-a},t_a)\langle \mathbf{x}_{+b}|i\rangle\langle \mathbf{x}_{-b}|i\rangle. \tag{18.580}$$

To lowest order in γ, the effect of the $\mathbf{C}_\mathrm{b}$-term in (18.548) can be evaluated in the local approximation (18.554) as follows. We take the linear approximation to the exponential $\exp[\int dtdt'\mathcal{O}(t,t')] \approx 1+\int dtdt'\mathcal{O}(t,t')$ and propagate the initial state with the help of the amplitude $U_{ii,t';ii,t_a}$ to the first time t', then with $U_{fi,t;fi,t'}$ to the later time t, and finally with $U_{ii,t_a;ii,t}$ to the final time t_b. The intermediate state between the times t and t' are arbitrary and must be summed. Details how to do such a perturbation expansion are given in Section 3.17. Thus we find

$$\Delta_C U_{ii,t_b;ii,t_a} = i\frac{e^2}{2\hbar^2c^2}\int_{t_a}^{t_b} dtdt' \sum_f \int d\mathbf{x}_+ \int d\mathbf{x}'_+\, U_{ii,t_a;ii,t}\langle i|\mathbf{x}_+\rangle\mathbf{x}_+\langle \mathbf{x}_+|f\rangle \times[\partial_t\partial_{t'}\mathbf{C}_\mathrm{b}(t,t')]U_{fi,t;fi,t'}\langle f|\mathbf{x}'_+\rangle\mathbf{x}'_+\langle \mathbf{x}'_+|i\rangle U_{ii,t';ii,t_a}. \tag{18.581}$$

Inserting $U_{ii,t_a;ii,t} = e^{-iE_i(t_a-t)/\hbar}$ etc., this becomes

$$\begin{aligned}\Delta_C U_{ii,t_b;ii,t_a} &= -\frac{e^2}{2\hbar^2c^2}\int_{t_a}^{t_b} dtdt'\,\langle i|\hat{\mathbf{x}}(t)\,[\partial_t\partial_{t'}\mathbf{C}_\mathrm{b}(t,t')]\,\hat{\mathbf{x}}(t')|i\rangle\\ &= -\frac{e^2}{2\hbar^2c^2}\sum_f\int_{t_a}^{t_b} dtdt'\, e^{i\omega_{if}(t-t')}\langle i|\hat{\mathbf{x}}|f\rangle\mathbf{C}_\mathrm{b}(t,t')\langle f|\hat{\mathbf{x}}|i\rangle.\end{aligned} \tag{18.582}$$

Expressing $C_\mathrm{b}^{ij}(t,t')$ of Eq. (18.554) in the form

$$C_\mathrm{b}^{ij}(t,t') = \frac{\hbar}{2\pi c}\frac{2}{3}\delta^{ij}\int\frac{d\omega}{2\pi}\,\omega\, e^{-i\omega(t-t')}, \tag{18.583}$$

the integration over t and t' yields

$$\Delta_C U_{ii,t_b;ii,t_a} = -i\frac{e^2}{4\pi\hbar c^3}\frac{2}{3}\int_{t_a}^{t_b} dt\int\frac{d\omega}{2\pi}\sum_f\frac{\omega}{\omega-\omega_{if}-i\eta}|\hat{\mathbf{x}}_{fi}|^2. \tag{18.584}$$

The same treatment is applied to the A_b in the action (18.549), where the first term involving $\mathbf{x}_+(t)$ and $\mathbf{x}_+(t')$ changes (18.585) to

$$\Delta U_{ii,t_b;ii,t_a} = -i\frac{e^2}{4\pi\hbar c^3}\frac{2}{3}\int_{t_a}^{t_b} dt\int\frac{d\omega}{2\pi}\sum_f\frac{\omega}{\omega-\omega_{if}+i\eta}\left(1+\coth\frac{\hbar\omega}{2k_BT}\right)|\hat{\mathbf{x}}_{fi}|^2. \tag{18.585}$$

The ω-integral is conveniently split into a zero-temperature part

$$I(\omega_{if},0) \equiv \int_0^\infty\frac{d\omega}{\pi}\sum_f\frac{\omega}{\omega-\omega_{if}+i\eta}, \tag{18.586}$$

and a finite-temperature correction

$$\Delta I_T(\omega_{if},T) \equiv 2\int_0^\infty\frac{d\omega}{\pi}\sum_f\frac{\omega}{\omega-\omega_{if}+i\eta}\frac{1}{e^{\hbar\omega/k_BT}-1}. \tag{18.587}$$

Decomposing $1/(\omega_{if}-\omega+i\eta) = \mathcal{P}/(\omega-\omega_{if}) - i\pi\delta(\omega_{if}-\omega)$, the imaginary part of the ω-integral yields half of the natural line width in (18.572). The other half comes from the part of the integral

(18.548) involving $\mathbf{x}_-(t)$ and $\mathbf{x}_-(t')$. The principal-value part of the zero-temperature integral diverges linearly, the divergence yielding again the mass renormalization (18.556). Subtracting this divergence from $I(\omega_{if},0)$, the remaining integral has the same form as $I(\omega_{if},0)$, but with ω in the numerator replaced by $\omega_{if}=0$. This integral diverges logarithmically like $(\omega_{if}/\pi)\log[(\Lambda-\omega_{if})/|\omega_{if}|]$, where Λ is Bethe's cutoff [30]. For $\Lambda\gg|\omega_{if}|$, the result (18.585) implies an energy shift of the atomic level $|i\rangle$:

$$\Delta E_i=\frac{e^2}{4\pi c^3}\frac{2}{3\pi}\sum_f \omega_{if}^3|\hat{\mathbf{x}}_{fi}|^2\log\frac{\Lambda}{|\omega_{if}|},\tag{18.588}$$

which is the *Lamb shift*.

Usually, the weakly varying logarithm is approximated by a weighted average $L=\log[\Lambda/\langle|\omega_{if}|\rangle]$ over energy levels and taken out of the integral. Then contribution of the term (18.585) can be attributed to an extra term

$$\hat{H}_{\rm LS}\approx -i\frac{L}{\pi}\gamma M\frac{1}{4}[\hat{\mathbf{x}},\hat{\ddot{\mathbf{x}}}]\tag{18.589}$$

in the Hamiltonian (18.567). In this form, the Lamb shift appears as a Hermitian logarithmically divergent correction to the operator (18.570) governing the spontaneous emission of photons.

To lowest order in γ, the commutator is for a Coulomb potential $V(\mathbf{x})=-e^2/r$ equal to

$$-\frac{i}{M^2}[\hat{\mathbf{p}},\hat{\dot{\mathbf{p}}}]=\frac{\hbar}{M^2}\boldsymbol{\nabla}^2V(\mathbf{x})=\frac{\hbar^2c\,\alpha}{M^2}\,4\pi\delta^{(3)}(\mathbf{x}),\tag{18.590}$$

leading to

$$\Delta E_i=\frac{4\alpha^2\hbar^3}{3M^2c}\langle i|\delta^{(3)}(\mathbf{x})|i\rangle.\tag{18.591}$$

For an atomic state of principal quantum number n with a wave function $\psi_n(\mathbf{x})$, this becomes

$$\Delta E_n=\frac{4\alpha\hbar^3}{3M^2c^2}\alpha L\,|\psi_n(\mathbf{0})|^2.\tag{18.592}$$

Only atomic s-states can contribute, since the wave functions of all other angular momenta vanish at the origin. Explicitly, the s-states of the hydrogen atom (13.219) have the value at the origin

$$\psi_n(\mathbf{0})=\frac{1}{\sqrt{n^3\pi}}\left(\frac{1}{a_H}\right)^{3/2},\tag{18.593}$$

where $a_H=\hbar/Mc\alpha$ is the Bohr radius (4.376). If the nuclear charge is Z, then $a_{\rm B}$, is diminished by this factor. Thus we obtain the energy shift

$$\Delta E_n=\frac{4\alpha^2\hbar^3}{3M^2c}\left(\frac{Mc\alpha}{\hbar}\right)^3\frac{L}{n^3\pi}.\tag{18.594}$$

For a hydrogen atom with $n=2$, this becomes

$$\Delta E_2=\frac{\alpha^3}{6\pi}\alpha^2Mc^2L.\tag{18.595}$$

The quantity $Mc^2\alpha^2$ is the unit energy of atomic physics determining the hydrogen spectrum to be $E_n=-Mc^2\alpha^2/2n^2$. Thus

$$M\alpha^2=4.36\times10^{-11}\text{erg}=27.21\text{eV}=2\,\text{Ry}=2\cdot3.288\times10^{15}\text{Hz}.\tag{18.596}$$

Inserting this together with $\alpha \approx 1/137.036$ into (18.595) yields[10]

$$\Delta E_2 \approx 135.6\text{MHz} \times L. \tag{18.597}$$

The constant L can be calculated approximately as

$$L \approx 9.3, \tag{18.598}$$

leading to the estimate

$$\Delta E_2 \approx 1261\text{MHz}. \tag{18.599}$$

The experimental Lamb shift

$$\Delta E_{\text{Lamb shift}} \approx 1057 \text{ MHz} \tag{18.600}$$

is indeed contained in this range. In this calculation, two effects have been ignored: the vacuum polarization of the photon and the form factor of the electron caused by radiative corrections. They reduce the frequency (18.599) by $(27.3+51)$MHz bringing the theoretical number closer to experiment. The vacuum polarization will be discussed in detail in Section 19.4.

At finite temperature, (18.588) changes to

$$\Delta E_i = \frac{e^2}{4\pi c^3}\frac{2}{3\pi}\sum_f \omega_{if}^3 |\hat{\mathbf{x}}_{fi}|^2 \left[\log\frac{\Lambda}{|\omega_{if}|} + \left(\frac{k_BT}{\hbar\omega_{ij}}\right)^2 J\left(\frac{\hbar\omega_{if}}{k_BT}\right)\right], \tag{18.601}$$

where $J(z)$ denotes the integral

$$J(z) \equiv z\int_0^\infty dz\, \frac{\mathcal{P}}{z'-z}\frac{z'}{e^{z'}-1}, \tag{18.602}$$

which has the low-temperature (large-z) expansion $J(z) = -\pi^2/6 - 2\zeta(3)/z + \dots$, and goes to zero for high temperature (small z) like $-z\log z$, as shown in Fig. 18.2.

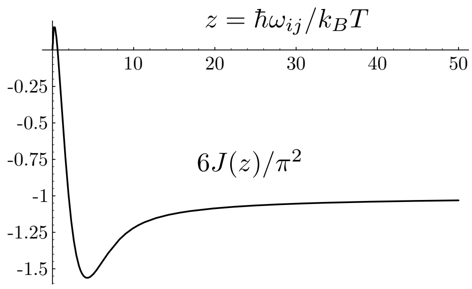

Figure 18.2 Behavior of function $6J(z)/\pi^2$ in finite-temperature Lamb shift.

The above equations may have applications to dilute interstellar gases or, after a reformulation in a finite volume, to few-particle systems contained in cavities. So far, a master equation has been set up only for a finite number of modes [31].

[10]The precise value of the Lamb constant $\alpha^4 M/6\pi$ is 135.641± 0.004 MHz.

18.20.5 Langevin Equations

For high γT, the last term in the forward–backward path integral (18.563) makes the size of the fluctuations in the difference between the paths $\mathbf{y}(t) \equiv \mathbf{x}_+(t) - \mathbf{x}_-(t)$ very small. It is then convenient to introduce the average of the two paths as $\mathbf{x}(t) \equiv [\mathbf{x}_+(t) + \mathbf{x}_-(t)]/2$, and expand

$$V\left(\mathbf{x}+\frac{\mathbf{y}}{2}\right) - V\left(\mathbf{x}-\frac{\mathbf{y}}{2}\right) \sim \mathbf{y}\cdot\boldsymbol{\nabla}V(\mathbf{x}) + \mathcal{O}(\mathbf{y}^3)\dots\ , \tag{18.603}$$

keeping only the first term. We further introduce an auxiliary quantity $\boldsymbol{\eta}(t)$ by

$$\dot{\boldsymbol{\eta}}(t) \equiv M\ddot{\mathbf{x}}(t) - M\gamma\dddot{\mathbf{x}}(t) + \boldsymbol{\nabla}V(\mathbf{x}(t)). \tag{18.604}$$

With this, the exponential function in (18.563) becomes

$$\exp\left[-\frac{i}{\hbar}\int_{t_a}^{t_b} dt\,\dot{\mathbf{y}}\boldsymbol{\eta} - \frac{w}{2\hbar^2}\int_{t_a}^{t_b} dt\,\dot{\mathbf{y}}^2(t)\right], \tag{18.605}$$

where w is the constant (18.562).

Consider now the diagonal part of the amplitude (18.603) with $\mathbf{x}_{+b} = \mathbf{x}_{-b} \equiv \mathbf{x}_b$ and $\mathbf{x}_{+a} = \mathbf{x}_{-a} \equiv \mathbf{x}_a$, implying that $\mathbf{y}_b = \mathbf{y}_a = 0$. It represents a probability distribution

$$P(\mathbf{x}_b\,t_b|\mathbf{x}_a\,t_a) \equiv |(\mathbf{x}_b, t_b|\mathbf{x}_a, t_a)|^2 \equiv U(\mathbf{x}_b, \mathbf{x}_b, t_b|\mathbf{x}_a, \mathbf{x}_a, t_a). \tag{18.606}$$

Now the variable $\mathbf{y}$ can simply be integrated out in (18.605), and we find the probability distribution

$$P[\boldsymbol{\eta}] \propto \exp\left[-\frac{1}{2w}\int_{t_a}^{t_b} dt\,\boldsymbol{\eta}^2(t)\right]. \tag{18.607}$$

The expectation value of an arbitrary functional of $F[x]$ can be calculated from the path integral

$$\langle F[\mathbf{x}]\rangle_\eta \equiv \mathcal{N}\int \mathcal{D}\mathbf{x}\,P[\boldsymbol{\eta}]F[\mathbf{x}], \tag{18.608}$$

where the normalization factor $\mathcal{N}$ is fixed by the condition $\langle\,1\,\rangle = 1$. By a change of integration variables from $x(t)$ to $\eta(t)$, the expectation value (18.608) can be rewritten as a functional integral

$$\langle F[\mathbf{x}]\rangle_\eta \equiv \mathcal{N}\int \mathcal{D}\boldsymbol{\eta}\,P[\boldsymbol{\eta}]\;F[\mathbf{x}]. \tag{18.609}$$

Note that the probability distribution (18.607) is $\hbar$-independent. Hence in the approximation (18.603) we obtain the classical Langevin equation. In principle, the integrand contains a factor $J^{-1}[x]$, where $J[x]$ is the functional Jacobian

$$J[\mathbf{x}] \equiv \mathrm{Det}[\delta\eta^i(t)/\delta x^j(t')] = \det\left[\left(M\partial_t^2 - M\gamma\partial_t^{3R}\right)\delta_{ij} + \nabla_i\nabla_j V(\mathbf{x}(t))\right]. \tag{18.610}$$

By the same procedure as in Section 18.9.2 it can be shown that the determinant is unity, due to the retardation of the friction term, thus justifying its omission in (18.609).

The path integral (18.609) may be interpreted as an expectation value with respect to the solutions of a *stochastic differential equation* (18.604) driven by a Gaussian random *noise* variable $\eta(t)$ with a correlation function

$$\langle\eta^i(t)\eta^j(t')\rangle_T = \delta^{ij}w\,\delta(t-t'). \tag{18.611}$$

Since the dissipation carries a third time derivative, the treatment of the initial conditions is nontrivial and will be discussed elsewhere. In most physical applications γ leads to slow decay rates. In this case the simplest procedure to solve (18.604) is to write the stochastic equation as

$$M\ddot{\mathbf{x}}(t) + \boldsymbol{\nabla}V(\mathbf{x}(t)) = \dot{\boldsymbol{\eta}}(t) + M\gamma\dddot{\mathbf{x}}(t), \tag{18.612}$$

and solve it iteratively, first without the γ-term, inserting the solution on the right-hand side, and such a procedure is equivalent to a perturbative expansion in γ in Eq. (18.563).

Note that the lowest iteration of Eq. (18.612) with $\boldsymbol{\eta} \equiv 0$ can be multiplied by $\dot{\mathbf{x}}$ and leads to the equation for the energy change of the particle

$$\frac{d}{dt}\left[\frac{M}{2}\dot{\mathbf{x}}^2 + V(\mathbf{x}) - M\gamma\dot{\mathbf{x}}\ddot{\mathbf{x}}\right] = -M\gamma\,\ddot{\mathbf{x}}^2. \tag{18.613}$$

The right-hand side is the classical electromagnetic power radiated by an accelerated particle. The extra term in the brackets is known as *Schott term* [32].

18.21 Fokker-Planck Equation in Spaces with Curvature and Torsion

According to the new equivalence principle found in Chapter 10, equations of motion can be transformed by a nonholonomic transformation $dx^i = e^i{}_\mu(q)dq^\mu$ into spaces with curvature and torsion, where they are applicable to the diffusion of atoms in crystals with defects [33]. If we denote $g_{\mu\nu}\dot{q}^\nu$ by v_μ, the Langevin equation (18.317) goes over into

$$\dot{v}_\mu = F_\mu(q,v) + e^i{}_\mu(q)\eta_i \tag{18.614}$$

where $F_\mu(q,v)$ is the sum of all forces after the nonholonomic transformation:

$$F_\mu(q,v) \equiv M\left[\Gamma_{\nu\lambda\mu}(q)v^\nu v^\lambda - \gamma v_\mu\right] - \partial_\mu V(q). \tag{18.615}$$

In addition to the transformed force (18.384), $F_\mu(q,v)$ contains the apparent forces resulting from the coordinate transformation. For a distribution

$$P_\eta(qvt|q_av_at_a) = \delta(q_\eta(t)-q)\delta(\dot{q}_\eta - v_\mu) \tag{18.616}$$

one obtains, instead of (18.383), the Kubo equation

$$\partial_t P_\eta(q\,v\,t|q_av_at_a) = \left\{-\partial_\mu g^{\mu\nu}(q)v_\nu - \frac{1}{M}\partial^v_\mu\left[e^i{}_\mu(q)\eta_i + F_\mu(q,v)\right]\right\}P_\eta(q\,v\,t|q_av_at_a), \tag{18.617}$$

and from this the generalization of the Fokker-Planck equation (18.393) to spaces with curvature and torsion:

$$\partial_t P(x\,v\,t|x_av_at_a) = \left\{-\partial_\mu g^{\mu\nu}v_\nu + \frac{1}{M}\partial^v_\mu\left[\frac{w}{2M}\partial^v_\mu - F_\mu(q,v)\right]\right\}P(x\,v\,t|x_av_at_a). \tag{18.618}$$

In the overdamped limit, the integrated probability distributions

$$P(q\,t|q_at_a) \equiv \int d^Dv P(q\,v\,t|q_av_at_a) \tag{18.619}$$

satisfies the equation [generalizing (18.399)]

$$\partial_t P(q\,t|q_at) \;=\; \left[D\partial_\mu e_i{}^\mu\partial_\nu e_i{}^\nu + \frac{1}{M\gamma}\partial_\nu g^{\mu\nu}V_\nu(q)\right]P(q\,t|q_at), \tag{18.620}$$

where $V_\nu(q) \equiv \partial_\nu V(q)$.

In the Fokker-Planck equations (18.617) and (18.620), the probability distributions $P(q\,v\,t|q_av_at_a)$ and $P(qt|q_at)$ have the unit normalizations

$$\int d^Dqd^Dv\,P(q\,v\,t|q_av_at_a) = 1, \qquad \int d^Dq\,P(q\,t|q_at_a) = 1, \tag{18.621}$$

as can be seen from the definitions (18.616) and (18.619). For distributions normalized with the invariant volume integral $\int d^D q\sqrt{g}$, to be denoted by $P^{\rm inv}(qt|q_a t_a) \equiv \sqrt{g}^{-1}P(qt|q_a t)$, we obtain from (18.620) the following invariant Fokker-Planck equation:

$$\partial_t P^{\rm inv}(q\,t|q_a t_a) = \left\{ \frac{D}{\sqrt{g}}\partial_\mu g^{\mu\nu}\sqrt{g}\left[\partial_\nu + 2S_\nu + \frac{1}{k_B T}V_\nu(x)\right]\right\} P^{\rm inv}(q\,t|q_a t_a). \tag{18.622}$$

The first term on the right-hand side contains the Laplace-Beltrami operator (11.13).

With the help of the covariant derivative D^*_μ defined in Eq. (11.96), which arises from D_μ by a partial integration, this equation can also be written as

$$\partial_t P^{\rm inv}(q\,t|q_a t_a) = \left[D\, g^{\mu\nu} D^*_\mu D^*_\nu + \frac{1}{M\gamma}\bar{D}_\mu V^\mu(x)\right] P^{\rm inv}(q\,t|q_a t_a), \tag{18.623}$$

where $\bar{D}_\mu$ is the covariant derivative (10.37) associated with the Christoffel symbol.

18.22 Stochastic Interpretation of Quantum-Mechanical Amplitudes

In the last section we have seen that the probability distribution $|(x_b,t_b|x_a,t_a)|^2$ is the result of a stochastic differential equation describing a classical path disturbed by a noise term $\eta(t)$ with the correlation function (18.320). It is interesting to observe that the quantum-mechanical amplitude $(x_b,t_b|x_a,t_a)$ possesses quite a similar stochastic interpretation, albeit with some imaginary factors i and an unsatisfactory aspect as we shall see. Recall the path integral representation of the time evolution amplitude in Eq. (2.712). It involves the action $A(x,t;x_a,t_a)$ from the initial point x_a to the actual particle position x. Recalling the definition of the fluctuation factor $F(x_b,x_a;t_b-t_a)$ in Eq. (4.97), we see that this factor is given by the path integral

$$F(x_b,x_a;t_b-t_a) = \int_{(x_a,t_a)\rightsquigarrow(x_b,t_b)} \mathcal{D}x \exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b} dt \frac{M}{2}\left(\dot{x}-v\right)^2\right], \tag{18.624}$$

where $v(x,t) = (1/M)\partial_x A(x,x_a;t_b-t_a)$ is the classical particle velocity. Up to a factor i and the absence of the retardation symbol, this path integral has the same form as the one for the probability (18.290) at large damping. As in (2.713) we introduce the momentum variable $p(t)$ and obtain the canonical path integral

$$F(x_b,x_a;t_b-t_a) = \int_{(x_a,t_a)\rightsquigarrow(x_b,t_b)} \mathcal{D}'x\frac{\mathcal{D}p}{2\pi\hbar} e^{(i/\hbar)\int_{t_a}^{t_b} dt\left\{p(t)[\dot{x}(t)-v(x(t),t)]-p^2(t)/2M\right\}}, \tag{18.625}$$

which looks similar to the stochastic path integral (18.290). The role of the diffusion constant $D = k_B T/M\gamma$ is now played by $\hbar/2$. By analogy with the path integral of a particle in a magnetic field in (2.654), the fluctuation factor satisfies a Schrödinger-like equation

$$\left(\frac{\hat{p}_b^2}{2M} + \frac{1}{2}\{\hat{p}_b, v_b\}\right) F(x_b,x_a;t_b-t_a) = i\hbar F(x_b,x_a;t_b-t_a). \tag{18.626}$$

This can easily be verified for the free particle, where $v_b = (x_b-x_a)/(t_b-t_a)$, and the fluctuation factor is from (2.130) $F(x_b,x_a;t_b-t_a) = \sqrt{2\pi i\hbar(t_b-t_a)}$. Note the symmetric operator order of the product $\hat{p}v$ in accordance with the time slicing in Section 10.5, and the ensuing operator order observed in Eq. (11.88). By reordering the Hamiltonian operator on the left-hand side of (18.626) to position $\hat{p}$ to the left of the velocity,

$$\hat{H} \to \frac{\hat{p}^2}{2M} + \hat{p}v + \frac{i}{2}\nabla v. \tag{18.627}$$

Without the last term, the path integral (18.625) would describe fluctuating paths obeying the stochastic differential equation analogous to the classical Langevin equation (18.338) [34]:

$$\dot{x}(t) - v(x(t), t) = p(t)/M. \tag{18.628}$$

The momentum variable $p(t)$ plays the role of the noise variable $\eta(t)$. Up to a factor i, this *quantum noise* has the same correlation functions as a white-noise variable:

$$\langle p(t)p(t')\rangle = -iM\hbar\delta(t-t'). \tag{18.629}$$

The "Fokker-Planck equation" associated with this "process" would be the ordinary Schrödinger equation for the amplitude $(x_b t_b|x_a t_a)$.

For a free particle, the ordering problem can be solved by noting that in the path integral (18.624), the constant v can be removed from the path integral leaving

$$F(x_b, x_a; t_b - t_a) = e^{-iA(x_b,x_a;t_b-t_a)/\hbar} \int_{(x_a,t_a)\rightsquigarrow(x_b,t_b)} \mathcal{D}x \exp\left(\frac{i}{\hbar}\int_{t_a}^{t_b} dt \frac{M}{2}\dot{x}^2\right), \tag{18.630}$$

the right-hand factor being the path integral for the amplitude $(x_b t_b|x_a t_a)$ itself. This is identical with the path integral for the probability distribution of Brownian motion, and quantum-mechanical fluctuations are determined by the process

$$\dot{x}(t) = p(t)/M, \tag{18.631}$$

with the quantum noise (18.629).

But also in the presence of a potential, it is possible to specify a process which properly represents quantum-mechanical fluctuations, although the situation is more involved [35]. To find it we rewrite the action in (18.624) as

$$\mathcal{A} = \int_{t_a}^{t_b} dt \frac{M}{2}(\dot{x}-v)^2 = \int_{t_a}^{t_b} dt \frac{M}{2}\left[(\dot{x}-s)^2 - \frac{i\hbar}{2}s'^2\right], \tag{18.632}$$

with some as yet unknown function $s(x)$. The associated Hamiltonian is now

$$\hat{H} \to \frac{\hat{p}^2}{2M} + \frac{1}{2}\{\hat{p}, s\} + i\hbar s'^2 = \frac{\hat{p}^2}{2M} + \hat{p}s, \tag{18.633}$$

with the proper operator order. In order for (18.632) to hold, the function $s(x)$ must satisfy the equations

$$v = s', \qquad -i\hbar s'^2 + s^2 = v^2. \tag{18.634}$$

Recalling Eqs. (4.12) and (4.5) we see that the equations in (18.634) can be satisfied with the help of the full eikonal $S(x)$:

$$s(x) = S(x)/M. \tag{18.635}$$

The process which describes the quantum-mechanical fluctuations is therefore

$$\dot{x}(t) - S(x)/M = p(t)/M. \tag{18.636}$$

The analogy is, however, not really satisfactory, since the full eikonal contains information on all fluctuations. Indeed, by the definition (4.4), it is given by the logarithm of the amplitude $(x\,t|x_a t_a)$, or any superposition $\psi(x,t) = \int dx_a\,(x\,t|x_a t_a)\psi(x_a t_a)$ of it:

$$S(x) = -i\hbar \log(x\,t|x_a t_a). \tag{18.637}$$

For the fluctuation factor this implies

$$s(x)-v(x)=\delta v(x)\equiv-\frac{i}{M}\hbar F(x\,t|x_at_a). \tag{18.638}$$

The path integral representation (18.624) for the fluctuation factor which has maximal analogy with the stochastic path integral (18.300) is therefore

$$F(x_bt_b,x_at_a)=\int_{(x_a,t_a)\rightsquigarrow(x_b,t_b)}\mathcal{D}x\exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b}dt\frac{M}{2}\left[\dot{x}^R-v+\frac{i}{M}\hbar\log F(x_bt_b,x_at_a)\right]^2\right\}. \tag{18.639}$$

Since we have to know $F(x_bt_b,x_at_a)$ to describe quantum-mechanical fluctuations as a process, this representation is of little practical use. The initial representation (18.624) which does not correspond to a proper process can, however, be used to solve quantum-mechanical problems.

18.23 Stochastic Equation for Schrödinger Wave Function

It is possible to write a stochastic type of path integral for the Schrödinger wave function $\psi(\mathbf{x},t)$ in D dimensions. By close analogy with Eq. (18.403), it reads

$$\psi(\mathbf{x}_b,t_b)=\int\mathcal{D}\mathbf{v}\,e^{(i/\hbar)\int_{t_a}^{t_b}dt\left[(M/2)\mathbf{v}^2(t)-V(\mathbf{x}_\mathbf{v}(t_b,t))\right]}\psi\left(\mathbf{x}_\mathbf{v}(t_b,t_a),t_a\right), \tag{18.640}$$

where

$$\mathbf{x}_\mathbf{v}(t_b,t)\equiv\mathbf{x}(t_b)-\int_t^{t_b}dt'\,\mathbf{v}(t') \tag{18.641}$$

is a functional of $\mathbf{v}(t')$ parameterizing all possible fluctuating paths arriving at the fixed final point $\mathbf{x}(t_b)$ after having started from an arbitrary initial point $\mathbf{x}(t)$. They are *Brownian bridges* between the two points. The variables $\mathbf{v}(t)$ are the independently fluctuating velocities of the particle. The natural appearance of the velocities in the measure of the stochastic path integral (18.640) is in agreement with our observation in Eq. (10.141) that the time-sliced measure should contain the coordinate *differences* $\Delta\mathbf{x}_n$ as the integration variables rather than the coordinates themselves, which was the starting point for the nonholonomic coordinate transformations to spaces with curvature and torsion.

We easily verify that (18.640) satisfies the Schrödinger equation by calculating the wave function at a slightly later time $t_b+\epsilon$, and expanding the right-hand side in powers of ϵ. Using the correlation functions

$$\langle v^i(t)\rangle=0,\qquad\langle v^i(t)v^j(t')\rangle=i\hbar\delta^{ij}\,\delta(t-t'), \tag{18.642}$$

we find, via a similar intermediate step as in (18.404), the desired result:

$$i\partial_t\psi(\mathbf{x},t)=\left[-\frac{\hbar^2}{2M}\partial_\mathbf{x}^2+V(\mathbf{x})\right]\psi(\mathbf{x},t). \tag{18.643}$$

One may also write down a corresponding path integral for the time evolution amplitude

$$(\mathbf{x}_bt_b|\mathbf{x}_at_a)=\int\mathcal{D}\mathbf{v}\,e^{(i/\hbar)\int_{t_a}^{t_b}dt\left[(M/2)\mathbf{v}^2(t)-V(\mathbf{x}_\mathbf{v}(t_b,t))\right]}\delta^{(D)}(\mathbf{x}_a-\mathbf{x}_b+\int_{t_a}^{t_b}dt\,\mathbf{v}(t)), \tag{18.644}$$

which returns the Schrödinger amplitude (18.640) after convolution with $\psi(\mathbf{x}_a,t_a)$ (and reduces to $\delta^{(D)}(\mathbf{x}_a-\mathbf{x}_b)$ for $t_b\to t_a$, as it should).

The addition of an interaction with a vector potential is nontrivial. The electromagnetic interaction in (10.168)

$$\mathcal{A}_{\rm em} = \int_{t_a}^{t} dt\, \mathbf{A}(\mathbf{x}(t)) \cdot \dot{\mathbf{x}} \tag{18.645}$$

cannot be simply inserted into the exponent of the path integral (18.640) since in the evaluation via the correlation functions (18.642) assumes the independence of the noise variables $\mathbf{v}(t)$. This, however, is not true in the interaction (18.645). Recall the discussion in Section 10.6 which showed that the time-sliced version of the interaction (18.645) must contain the midpoint ordering of the vector potential with respect to the intervals $\Delta\mathbf{x}$ to be compatible with the classical field equation. In Section 11.3 we have furthermore seen that this guaranteed gauge invariance. For the time-sliced short-time action, this implies that (18.645) has the form [see (10.179)]

$$\mathcal{A}^{\epsilon}_{\rm em} = \mathbf{A}(\bar{\mathbf{x}}) \cdot \Delta\mathbf{x}. \tag{18.646}$$

In this expression, a variation of $\Delta\mathbf{x}$ changes also $\bar{\mathbf{x}}$, implying that in the sum over all sliced actions, the $\Delta\mathbf{x}$ are not independent. This is only achieved by the re-expanded postpoint interaction [see 10.178]. In the continuum, we shall indicate the postpoint product as before in (18.231) by a retardation symbol R, and rewrite (18.645) as

$$\mathcal{A}_{\rm em} = \int_{t_a}^{t} dt \left[\mathbf{A}(\mathbf{x}(t))\dot{\mathbf{x}}^R(t) - i\epsilon\frac{\hbar}{2M}\boldsymbol{\nabla}\cdot\mathbf{A}(\mathbf{x}(t))\right]. \tag{18.647}$$

In the theory of stochastic differential equations, this postpoint expression is called an *Itō integral*. The ordinary midpoint integral (18.645) is referred to as *Stratonovich integral*.

The Itō integral can now be added to the action in (18.644) with $\dot{\mathbf{x}}(t)$ replaced by $\mathbf{v}(t)$, and we obtain

$$(\mathbf{x}_b t_b|\mathbf{x}_a t_a) = \int \mathcal{D}\mathbf{v}\, \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b} dt\, \left[\frac{M}{2}\mathbf{v}^2(t) + \mathbf{A}(\mathbf{x}_{\mathbf{v}}(t_b,t))\mathbf{v}^R(t) - V(\mathbf{x}_{\mathbf{v}}(t_b,t))\right]\right\}$$
$$\times \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b} dt\, \left[-i\epsilon\frac{\hbar}{2M}\boldsymbol{\nabla}\cdot\mathbf{A}(\mathbf{x}_{\mathbf{v}}(t_b,t))\right]\right\}\delta^{(D)}(\mathbf{x}_a - \mathbf{x}_b + \int_{t_a}^{t_b} dt\, \mathbf{v}(t)). \tag{18.648}$$

Expanding the functional integrand in powers of $\mathbf{v}(t)$ as in (18.403) and using the correlation functions (18.642) we obtain the Schrödinger equation

$$i\partial_t(\mathbf{x}\,t|\mathbf{x}_a t_a) = \left[-\frac{\hbar^2}{2M}\left[\boldsymbol{\nabla} - i\mathbf{A}(\mathbf{x})\right]^2 + V(\mathbf{x})\right](\mathbf{x}\,t|\mathbf{x}_a t_a). \tag{18.649}$$

The advantage of the Itō integral is that such a calculation becomes quite simple using the correlation functions (18.642). The integral itself, however, is awkward to handle since it cannot be modified by partial integration. This is only possible for the ordinary, Stratonovich integral.

18.24 Real Stochastic and Deterministic Equation for Schrödinger Wave Function

The noise variable in the previous stochastic differential equation had an imaginary correlation function (18.629). It is possible to set up a completely real stochastic differential equation and modify this into a simple deterministic model which possesses the quantum properties of a particle in an arbitrary potential. In particular, the model has a discrete energy spectrum with a definite ground state energy, in this respect going beyond an earlier model by 't Hooft [36], whose spectrum was unbounded from below.

Let $\mathbf{u}(\mathbf{x}) = \big(u^1(\mathbf{x}), u^2(\mathbf{x})\big)$ be a time-independent field in two dimensions to be called *mother field*. The reparametrization freedom of the spatial coordinates is fixed by choosing harmonic coordinates in which

$$\boldsymbol{\nabla}^2 u(\mathbf{x}) = 0, \tag{18.650}$$

where $\boldsymbol{\nabla}^2$ is the Laplace operator. Equivalently, the components $u^1(\mathbf{x})$ and $u^2(\mathbf{x})$ may be assumed to satisfy the Cauchy-Riemann equations

$$\partial_\mu u^\nu = \epsilon_\mu{}^\rho \epsilon^\nu{}_\sigma \partial_\rho u^\sigma, \quad (\mu, \nu, \ldots = 1, 2), \tag{18.651}$$

where $\epsilon_{\mu\nu}$ is the antisymmetric Levi-Civita pseudotensor. The metric is $\delta_{\mu\nu}$, so that indices can be sub- or superscripts.

18.24.1 Stochastic Differential Equation

Consider now a point particle in contact with a heat bath of "temperature" $\hbar$. Its classical orbit $\mathbf{x}(t)$ is assumed to follow a stochastic differential equation consisting of a fixed rotation and a random translation in the diagonal direction $\mathbf{n} \equiv (1, 1)$:

$$\dot{\mathbf{x}}(t) \;\; = \;\; \boldsymbol{\omega} \times \mathbf{x}(t) + \mathbf{n}\, \eta(t), \tag{18.652}$$

where $\boldsymbol{\omega}$ is the rotation vector of length ω pointing orthogonal to the plane, and $\eta(t)$ a white-noise variable with zero expectation and the correlation function

$$\langle \eta(t)\eta(t')\rangle = \hbar\, \delta(t - t'). \tag{18.653}$$

For a particle starting at $\mathbf{x}(0) = \mathbf{x}$, the position $\mathbf{x}(t)$ at a later time t is a function of $\mathbf{x}$ and a *functional* of the noise variable $\eta(t')$ for $0 < t' < t$:

$$\mathbf{x}(t) = \mathbf{X}_\eta(\mathbf{x}, t). \tag{18.654}$$

As earlier in Section 18.13, a subscript η is used to indicate the functional dependence on the noise variable ν.

We now use the orbits ending at all possible final points $\mathbf{x} = \mathbf{x}(t)$ to define a time-dependent field $\mathbf{u}(\mathbf{x}; t)$ which is equal to $\mathbf{u}(\mathbf{x})$ at $t = 0$, and evolves with time as follows:

$$\mathbf{u}(\mathbf{x}; t) = \mathbf{u}_t[\mathbf{x}; \eta] \equiv \mathbf{u}\left(\mathbf{X}_0[t, \mathbf{x}; \eta]\right), \tag{18.655}$$

where the notation $\mathbf{u}_t[\mathbf{x}; \eta]$ indicates the variables as in (18.654).

As a consequence of the dynamic equation (20A.1), the change of the field $\mathbf{u}(\mathbf{x}, t)$ in a small time interval from $t = 0$ to $t = \Delta t$ has the expansion

$$\begin{aligned}\Delta \mathbf{u}_\eta(\mathbf{x}, 0) \;\; = \;\; & \Delta t \,[\boldsymbol{\omega} \times \mathbf{x}] \cdot \boldsymbol{\nabla}\, \mathbf{u}_\eta(\mathbf{x}, 0) + \int_0^{\Delta t} dt'\, \eta(t') \; (\mathbf{n} \cdot \boldsymbol{\nabla})\, \mathbf{u}_\eta(\mathbf{x}, 0) \\ & + \frac{1}{2} \int_0^{\Delta t} dt' \int_0^{\Delta t} dt''\, \eta(t')\eta(t'')\, (\mathbf{n} \cdot \boldsymbol{\nabla})^2\, \mathbf{u}_\eta(\mathbf{x}, 0) + \ldots\; .\end{aligned} \tag{18.656}$$

The omitted terms are of order $\Delta t^{3/2}$.

18.24.2 Equation for Noise Average

We now perform the noise average of Eq. (20A.2), defining the average field

$$\mathbf{u}(\mathbf{x}, t) \equiv \langle \mathbf{u}_\eta(\mathbf{x}, t)\rangle. \tag{18.657}$$

Using the vanishing average of $\eta(t)$ and the correlation function (18.653), we obtain in the limit $\Delta t \to 0$ the time derivative

$$\partial_t \mathbf{u}(\mathbf{x}, t) = \hat{\mathcal{H}}\, \mathbf{u}(\mathbf{x}, t), \quad \text{at} \ \ t = 0, \tag{18.658}$$

with the time evolution operator

$$\hat{\mathcal{H}} \equiv \{[\boldsymbol{\omega} \times \mathbf{x}] \cdot \boldsymbol{\nabla}\} + \frac{\hbar}{2}(\mathbf{n} \cdot \boldsymbol{\nabla})^2. \tag{18.659}$$

The average over η has made the operator $\hat{\mathcal{H}}$ time-independent. For this reason, the average field $\mathbf{u}(\mathbf{x}, t)$ at an arbitrary time t is obtained by the operation

$$\mathbf{u}(\mathbf{x}, t) = \hat{\mathcal{U}}(t)\mathbf{u}(\mathbf{x}, 0), \tag{18.660}$$

where $\hat{\mathcal{U}}(t)$ is a simple exponential

$$\hat{\mathcal{U}}(t) \equiv e^{\hat{\mathcal{H}} t}, \tag{18.661}$$

as follows immediately from (18.658) and the trivial property $\hat{\mathcal{H}}\hat{\mathcal{U}}(t) = \hat{\mathcal{U}}(t)\hat{\mathcal{H}}$.

Note that the operator $\hat{\mathcal{H}}$ commutes with the Laplace operator $\boldsymbol{\nabla}^2$, thus ensuring that the harmonic property (18.650) of $\mathbf{u}(\mathbf{x})$ remains true for all times, i.e.,

$$\boldsymbol{\nabla}^2 \mathbf{u}(\mathbf{x}, t) \equiv 0. \tag{18.662}$$

18.24.3 Harmonic Oscillator

We now show that Eq. (18.658) describes the quantum mechanics of a harmonic oscillator. Let us restrict our attention to the line with arbitrary $x_1 \equiv x$ and $x_2 = 0$. Applying the Cauchy-Riemann equations (18.651), we can rewrite Eq. (18.658) in the pure x-form

$$\partial_t u^1(x, t) \;=\; \omega\, x\, \partial_x u^2(x, t) - \frac{\hbar}{2}\partial_x^2\, u^2(x, t), \tag{18.663}$$

$$\partial_t u^2(x, t) \;=\; -\omega\, x\, \partial_x u^1(x, t) + \frac{\hbar}{2}\partial_x^2\, u^1(x, t), \tag{18.664}$$

where we have omitted the second spatial coordinates $x_2 = 0$. Now we introduce a complex field

$$\psi(x, t) \equiv e^{-\omega x^2/2\hbar} \left[u^1 (x, t) + i u^2 (x, t)\right]. \tag{18.665}$$

This satisfies the differential equation

$$i\hbar \partial_t \psi(x, t) = \left(-\frac{\hbar^2}{2}\partial_x^2 + \frac{\omega^2}{2}x^2 - \frac{\hbar\omega}{2}\right) \psi(x, t), \tag{18.666}$$

which is the Schrödinger equation of a harmonic oscillator with the discrete energy spectrum $E_n = (n + 1/2)\hbar\omega,\ \ n = 0, 1, 2, \dots$.

18.24.4 General Potential

The method can easily be generalized to an arbitrary potential. We simply replace (18.652) by

$$\begin{aligned} \dot{x}^1(t) &= -\partial_2 S^1(\mathbf{x}(t)) + n^1\, \eta(t), \\ \dot{x}^2(t) &= -\partial_1 S^1(\mathbf{x}(t)) + n^2\, \eta(t), \end{aligned} \tag{18.667}$$

where $\mathbf{S}(\mathbf{x})$ shares with $\mathbf{u}(\mathbf{x})$ the harmonic property (18.650):

$$\boldsymbol{\nabla}^2 \mathbf{S}(\mathbf{x}) = 0, \tag{18.668}$$

i.e., the functions $S^\mu(\mathbf{x})$ with $\mu = 1,2$ fulfill Cauchy-Riemann equations like $u^\mu(\mathbf{x})$ in (18.651). Repeating the above steps we find, instead of the operator (18.659),

$$\hat{\mathcal{H}} \equiv -(\partial_2 S^1)\partial_1 - (\partial_1 S^1)\partial_2 + \frac{\hbar}{2}(\mathbf{n}\cdot\boldsymbol{\nabla})^2, \tag{18.669}$$

and Eqs. (18.663) and (18.664) become:

$$\partial_t u^1(x,t) = (\partial_x S^1)\partial_x u^2(x,t) - \frac{\hbar}{2}\partial_x^2\, u^2(x,t), \tag{18.670}$$

$$\partial_t u^2(x,t) = -(\partial_x S^1)\,\partial_x u^1(x,t) + \frac{\hbar}{2}\partial_x^2\, u^1(x,t). \tag{18.671}$$

This time evolution preserves the harmonic nature of $\mathbf{u}(\mathbf{x})$. Indeed, using the harmonic property $\boldsymbol{\nabla}^2\mathbf{S}(\mathbf{x}) = 0$ we can easily derive the following time dependence of the Cauchy-Riemann combinations in Eq. (18.651):

$$\partial_t(\partial_1 u^1 - \partial_2 u^2) = \hat{\mathcal{H}}(\partial_1 u^1 - \partial_2 u^2) - \partial_2\partial_1 S^1(\partial_1 u^1 - \partial_2 u^2) + \partial_2^2 S^1(\partial_2 u^1 + \partial_1 u^2),$$
$$\partial_t(\partial_2 u^1 + \partial_1 u^2) = \hat{\mathcal{H}}(\partial_2 u^1 + \partial_1 u^2) - \partial_2\partial_1 S^1(\partial_2 u^1 + \partial_1 u^2) - \partial_2^2 S^1(\partial_1 u^1 - \partial_2 u^2).$$

Thus $\partial_1 u^1 - \partial_2 u^2$ and $\partial_2 u^1 + \partial_1 u^2$ which are zero at any time remain zero at all times.

On account of Eqs. (18.671), the combination

$$\psi(x,t) \equiv e^{-S^1(x)/\hbar}\left[u^1(x,t) + iu^2(x,t)\right] \tag{18.672}$$

satisfies the Schrödinger equation

$$i\hbar\partial_t\psi(x,t) = \left[-\frac{\hbar^2}{2}\partial_x^2 + V(x)\right]\psi(x,t), \tag{18.673}$$

where the potential is related to $S^1(x)$ by the Riccati differential equation

$$V(x) = \frac{1}{2}[\partial_x S^1(x)]^2 - \frac{\hbar}{2}\partial_x^2 S^1(x). \tag{18.674}$$

The harmonic oscillator is recovered for the pair of functions

$$S^1(\mathbf{x}) + iS^2(\mathbf{x}) = \omega(x^1 + ix^2)^2/2. \tag{18.675}$$

18.24.5 Deterministic Equation

The noise $\eta(t)$ in the stochastic differential equation Eq. (18.667) can also be replaced by a source composed of deterministic classical oscillators $q_k(t)$, $k = 1,2,\ldots$ with the equations of motion

$$\dot{q}_k = p_k, \qquad \dot{p}_k = -\omega_k^2 q_k, \tag{18.676}$$

as

$$\eta(t) \equiv \sum_k \dot{q}_k(t). \tag{18.677}$$

The initial positions $q_k(0)$ and momenta $p_k(0)$ are assumed to be randomly distributed with a Boltzmann factor $e^{-\beta H_{\rm osc}/\hbar}$, such that

$$\langle q_k(0)q_k(0)\rangle = \hbar/\omega_k^2, \quad \langle p_k(0)p_k(0)\rangle = \hbar. \tag{18.678}$$

Using the equation of motion

$$\dot{q}_k(t) = \omega_k q_k(0)\sin\omega_k t + p_k(0)\sin\omega_k t, \tag{18.679}$$

we find the correlation function

$$\begin{aligned}\langle \dot{q}_k(t)\dot{q}_k(t')\rangle &= \omega_k^2 \cos\omega_k t \cos\omega_k t' \langle q_k(0)q_k(0)\rangle + \sin\omega_k t \sin\omega_k t \langle p_k(0)p_k(0)\rangle \\ &= \cos\omega_k(t-t').\end{aligned} \tag{18.680}$$

We may now assume that the oscillators $q_k(t)$ are the Fourier components of a massless field, for instance the gravitational field whose frequencies are $\omega_k = k$, and whose random initial conditions are caused by the big bang. If the sum over k is simply a momentum integral $\int_{-\infty}^{\infty} dk$, then (18.680) yields a white-noise correlation function (18.653) for $\eta(t)$.

Thus it is indeed possible to simulate the quantum-mechanical wave functions $\psi(x,t)$ and the energy spectrum of an arbitrary potential problem by deterministic equations with random initial conditions at the beginning of the universe.

It remains to solve the open problem of finding a classical origin of the second important ingredient of quantum theory: the theory of quantum measurement to be extracted from the wave function $\psi(x,t)$. Only then shall we understand how God throws dice [37].

Appendix 18A Inequalities for Diagonal Green Functions

Let us introduce several diagonal Green functions consisting of thermal averages of equal-time commutators and anticommutators of bosonic and fermionic field operators, elementary or composite. For brevity, we write

$$\langle \ldots \rangle_T = \mathrm{Tr}\left[\exp(-\hat{H}/T)\ldots\right] \Big/ \mathrm{Tr}\left[\exp(-\hat{H}/T)\right] = \langle \ldots \rangle_T \tag{18A.1}$$

and define the averages with obvious spectral representations

$$\begin{aligned} c &\equiv \langle[\hat{\psi},\hat{\psi}^\dagger]_\mp\rangle_T = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\rho_{12}(\omega), \\ a &\equiv \langle[\hat{\psi},\hat{\psi}^\dagger]_\pm\rangle_T = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\rho_{12}(\omega)\tanh^{\mp 1}\frac{\omega}{2T}.\end{aligned} \tag{18A.2}$$

We shall also introduce a quantity obtained by integrating the imaginary-time Green function over a period $\tau \in [0, 1/T)$. This gives for boson and fermion fields the nonnegative expression [see (18.23)]

$$\begin{aligned} g &\equiv G(\omega_m = 0) = \int_0^{1/T} d\tau\, \langle\hat{\psi}(\tau)\hat{\psi}^\dagger(0)\rangle_T \\ &= \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\rho_{12}(\omega)\frac{1}{\omega}\left\{\begin{array}{c} 1 \\ \tanh(\omega/2T)\end{array}\right\} \geq 0.\end{aligned} \tag{18A.3}$$

Note that for fermion fields, the spectral weight in this integral is accompanied by an extra factor $\tanh(\omega/2T)$. This is due to the fact that $\omega_m = 0$ is *no* fermionic Matsubara frequency, but a "wrong" bosonic one. In fact, the sum (18.23) for $G(\omega_m)$ contains a factor $1 - e^{(E_n - E_{n'})/T}$ for both bosons and fermions, while $\rho_{12}(\omega)$ in the spectral representation (18A.3) introduces, via (18.59), a factor $1 - e^{-\omega/T}$ for bosons and a factor $1 + e^{\omega/T}$ for fermions, thus explaining the relative factor $\tanh(\omega/2T)$ in (18A.3).

The integration over τ leads to the factor $1/\omega$ in (18A.3). This factor is also found by integrating the retarded Green function $G_{12}(t)$ and the commutator function $C_{12}(t)$ over all real times, resulting in the spectral representations

$$\begin{aligned} i\int_{-\infty}^{\infty} dt\,\Theta(t)\langle[\hat{\psi}(t),\hat{\psi}^\dagger(0)]_\mp\rangle_T &= \int\frac{d\omega}{2\pi}\,\rho_{12}(\omega)\frac{1}{\omega}, \\ i\int_{-\infty}^{\infty} dt\,\Theta(t)\langle[\hat{\psi}(t),\hat{\psi}^\dagger(0)]_\pm\rangle_T &= \int\frac{d\omega}{2\pi}\,\rho_{12}(\omega)\frac{1}{\omega}\tanh^{\mp 1}\frac{\omega}{2T}.\end{aligned} \tag{18A.4}$$

Another set of thermal expectation values involves products of field operators with time derivatives rather than integrals. Their spectral representations contain an extra factor ω. For example, the τ-derivative of the expectation value in (18A.3) leads to

$$-\langle\dot{\hat\psi}(0),\hat\psi^\dagger(0)\rangle_T=\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\rho_{12}(\omega)\omega(1\pm n_\omega). \tag{18A.5}$$

The real-time derivatives of the expectation values in (18A.4) have the spectral integrals

$$\begin{aligned} d &\equiv i\langle[\dot{\hat\psi}(0),\hat\psi^\dagger(0)]_\mp\rangle_T=\textstyle\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\rho_{12}(\omega)\omega,\\ e &\equiv i\langle[\dot{\hat\psi}(0),\hat\psi^\dagger(0)]_\pm\rangle_T=\textstyle\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\rho_{12}(\omega)\omega\tanh^{\mp1}\frac{\omega}{2T}. \end{aligned} \tag{18A.6}$$

The expectation values c, a, g, d, e satisfy several rigorous inequalities. To derive these, we observe that

$$\mu(\omega)=\frac{1}{g}\frac{1}{2\pi}\rho_{12}(\omega)\frac{1}{\omega}\left\{\begin{array}{c}1\\ \tanh(\omega/2T)\end{array}\right\} \tag{18A.7}$$

is a positive function. This follows directly from (18.59), according to which $\rho_{12}(\omega)$ at negative ω is negative for bosons and positive for fermions. Having divided out the total integral g defined in (18A.3), the integral over $\mu(\omega)$ is normalized to unity,

$$\int_{-\infty}^{\infty}d\omega\,\mu(\omega)=1, \tag{18A.8}$$

for both bosons and fermions. Using $\mu(\omega)$, we form the following ratios:

$$\frac{c}{g}=\int_{-\infty}^{\infty}d\omega\,\mu(\omega)\omega\left\{\begin{array}{c}1\\ \coth(\omega/2T)\end{array}\right\}, \tag{18A.9}$$

$$\frac{a}{g}=\int_{-\infty}^{\infty}d\omega\,\mu(\omega)\omega\left\{\begin{array}{c}\coth(\omega/2T)\\ 1\end{array}\right\}, \tag{18A.10}$$

$$\frac{d}{g}=\int_{-\infty}^{\infty}d\omega\,\mu(\omega)\omega^2\left\{\begin{array}{c}1\\ \coth(\omega/2T)\end{array}\right\}, \tag{18A.11}$$

$$\frac{e}{g}=\int_{-\infty}^{\infty}d\omega\,\mu(\omega)\omega^2\left\{\begin{array}{c}\coth(\omega/2T)\\ 1\end{array}\right\}. \tag{18A.12}$$

The inequalities to be derived are based on the Jensen-Peierls inequality for convex functions derived in Chapter [5]. Recall that a convex function $f(\omega)$ satisfies

$$f\left(\frac{\omega_1+\omega_2}{2}\right)\le\frac{f(\omega_1)+f(\omega_2)}{2}, \tag{18A.13}$$

which is generalized to

$$f\left(\sum_i\mu_i\omega_i\right)\le\sum_i\mu_i f(\omega_i), \tag{18A.14}$$

where μ_i is an arbitrary set of positive numbers with $\sum_i\mu_i=1$. In the continuum limit, this becomes

$$f\left(\int_{-\infty}^{\infty}d\omega\,\mu(\omega)\omega\right)\le\int_{-\infty}^{\infty}d\omega\,\mu(\omega)f(\omega). \tag{18A.15}$$

It is obvious that a similar Jensen-Peierls inequality holds also for concave functions with inequality sign in the opposite direction.

The Jensen-Peierls inequality (18A.15) is now applied to the function

$$f(\omega) = \omega \coth \frac{\omega}{2T}, \tag{18A.16}$$

which looks like a slightly distorted hyperbola coming in from infinity along the diagonal lines $|\omega|$ and crossing the f-axis at $\omega = 0$, $f(0) = 2T$. The second derivative of $f(\omega)$ is positive everywhere, ensuring the convexity. The function (18A.16) appears in the integrand of the boson part of Eq. (18A.10). The right-hand side of (18A.15) can therefore be written as a/g. The left-hand side is obviously equal to $(c/g)\coth(c/2Tg)$. Hence we arrive at the inequality

$$c \coth \frac{c}{2Tg} \leq a. \tag{18A.17}$$

In terms of the original field operators, this amounts to

$$\langle[\hat{\psi}, \hat{\psi}^\dagger]_+\rangle_T \geq \langle[\hat{\psi}, \hat{\psi}^\dagger]_-\rangle_T \coth \frac{\langle[\hat{\psi}, \hat{\psi}^\dagger]_-\rangle_T}{2T\int_0^{1/T} d\tau\, \langle\hat{\psi}(\tau)\hat{\psi}^\dagger(0)\rangle_T}. \tag{18A.18}$$

In the special case that $\hat{\psi}$ is a *canonical* interacting boson field of momentum $\mathbf{p}$, the commutator is simply $[\hat{\psi}, \hat{\psi}^\dagger]_- = 1$, and the inequality becomes

$$1 + 2\langle\hat{\psi}^\dagger_{\mathbf{p}}\hat{\psi}_{\mathbf{p}}\rangle_T \quad \geq \quad \coth(1/2Tg) = 1 + \frac{2}{e^{1/gT} - 1} = 1 + 2n_{g^{-1}}, \tag{18A.19}$$

i.e.,

$$\langle\hat{\psi}^\dagger_{\mathbf{p}}\hat{\psi}_{\mathbf{p}}\rangle_T \geq \frac{1}{e^{1/gT} - 1} \equiv n_{g^{-1}}, \tag{18A.20}$$

where $n_{g^{-1}}$ is the free-boson distribution function (18.36) for an energy g^{-1}.

This is quite an interesting relation. The quantity g is the Euclidean equilibrium Green function $G(\omega_m, \mathbf{p})$ at $\omega_m = 0$. For free particles in contact with a reservoir, it is given by

$$g^{-1} = G(0, \mathbf{p})^{-1} = \frac{\mathbf{p}^2}{2M} - \mu \equiv \xi(\mathbf{p}), \tag{18A.21}$$

i.e., it is equal to the particle energy measured with respect to the chemical potential μ. Moreover, we know that for free particles

$$\langle\hat{\psi}^\dagger_{\mathbf{p}}\hat{\psi}_{\mathbf{p}}\rangle_T = n_{\xi(\mathbf{p})}, \tag{18A.22}$$

so that the inequality (18A.20) becomes an equality. The content of the inequality (18A.20) may therefore be phrased as follows: For any interaction, the occupation of a state with momentum $\mathbf{p}$ is never *smaller* than for a free boson level of energy $g^{-1} = G(0, \mathbf{p})$.

Another inequality can be derived from the concave function

$$\bar{f}(y) = \sqrt{y} \coth \frac{\sqrt{y}}{2T}, \tag{18A.23}$$

using $y = \omega^2$ and the measure

$$\int_{-\infty}^{\infty} d\omega\, \mu(\omega) = \int_0^\infty \frac{dy}{\sqrt{y}}\, \mu(\sqrt{y}) = 1. \tag{18A.24}$$

As argued before, concave functions satisfy the inequality opposite to (18A.15), from which we derive the inequality

$$\bar{f}\left(\int_0^\infty \frac{dy}{\sqrt{y}}\,\mu(\sqrt{y})y\right) \geq \int_0^\infty \frac{dy}{\sqrt{y}}\,\mu(\sqrt{y})\bar{f}(y), \tag{18A.25}$$

which can be rewritten as

$$\bar{f}\left(\int_{-\infty}^\infty d\omega\,\mu(\omega)\omega^2\right) \geq \int_{-\infty}^\infty d\omega\,\mu(\omega)\bar{f}(\omega^2). \tag{18A.26}$$

Again, the right-hand side is a/g, but now it is bounded from above by

$$\frac{a}{g} \leq \sqrt{\frac{d}{g}}\coth\left(\frac{1}{2T}\sqrt{\frac{d}{g}}\right). \tag{18A.27}$$

The combined inequality

$$c\,\coth\frac{c}{2Tg} \leq a \leq \sqrt{dg}\coth\left(\frac{1}{2T}\sqrt{\frac{d}{g}}\right) \tag{18A.28}$$

may be used to derive further inequalities:

$$\begin{aligned} c^2 &\leq dg, \\ c\,\coth(d/2Tc) &\leq a, \\ g &\leq \coth(c/2Ta), \\ c &\leq d\tanh(c/2Ta), \\ c &\leq a\tanh(d/2Tc). \end{aligned} \tag{18A.29}$$

For fermion fields we see that an inequality like (18A.17) holds with c and a interchanged, i.e.,

$$a\coth\frac{a}{2Tg} \leq c, \tag{18A.30}$$

which leads to

$$\langle[\hat{\psi},\hat{\psi}^\dagger]_-\rangle_T \leq \langle[\hat{\psi},\hat{\psi}^\dagger]_+\rangle_T\tanh\frac{\langle[\hat{\psi},\hat{\psi}^\dagger]_+\rangle_T}{2T\int_0^{1/T}d\tau\,\langle\hat{\psi}(\tau)\hat{\psi}^\dagger(0)\rangle_T}. \tag{18A.31}$$

For canonical fermion fields with $[\hat{\psi},\hat{\psi}^\dagger]_+ = 1$, this becomes

$$1-2\langle\hat{\psi}^\dagger\hat{\psi}\rangle_T \quad\leq\quad \tanh(1/2gT) = 1-\frac{2}{e^{1/gT}+1}, \tag{18A.32}$$

i.e., the fermionic counterpart of (18A.20):

$$\langle\hat{\psi}^\dagger_{\mathbf{p}}\hat{\psi}_{\mathbf{p}}\rangle_T \leq \frac{1}{e^{1/gT}+1} = n_{g^{-1}}, \tag{18A.33}$$

where $n_{g^{-1}}$ is the free-fermion distribution function (18.36) at an energy g^{-1}. As in the Bose case, free particles fulfill

$$\langle\hat{\psi}^\dagger_{\mathbf{p}}\hat{\psi}_{\mathbf{p}}\rangle_T = n_{\xi(\mathbf{p})}, \tag{18A.34}$$

with $g^{-1} = \xi(\mathbf{p})$, so that the inequality (18A.33) becomes an equality. The inequality implies that an interacting Fermi level is never occupied *more* than a free fermion level of energy $g^{-1} = G(0,\mathbf{p})^{-1}$.

Also the second inequality in (18A.29) can be taken over to fermions which amounts to (18A.30), but with a and d replaced by c and e.

Appendix 18B General Generating Functional

For a field operator $a(t)$ of frequency Ω and its Hermitian conjugate $a^\dagger(t)$, the retarded and advanced Green functions and the expectation values of commutators and anticommutators were derived in Eqs. (18.68)–(18.77):

$$\begin{aligned} G^R_\Omega(t,t') &= \Theta(t-t')e^{-i\Omega(t-t')}, \\ G^A_\Omega(t,t') &= -\Theta(t'-t)e^{-i\Omega(t-t')}, \\ C_\Omega(t,t') &= e^{-i\Omega(t-t')}, \\ A_\Omega(t,t') &= \left(\tanh\frac{\Omega}{2T}\right)^{\mp 1} e^{-i\Omega(t-t')}. \end{aligned} \tag{18B.1}$$

Introducing complex sources $\eta(t)$ and $\eta^\dagger(t)$ associated with these operators, the generating functional for these functions is

$$Z_0[\eta_{\rm P},\eta^\dagger_{\rm P}] = \mathrm{Tr}\left\{\hat\rho\,\hat T_{\rm P}\exp\left[-i\int_{t_a}^{t_b} dt(\hat a^\dagger\eta+\eta^\dagger\hat a)\right]\right\}. \tag{18B.2}$$

The complex sources are distinguished according to the closed-time contour branches by a subscript P. The generating functional can then be written down immediately as

$$Z_0[\eta_{\rm P},\eta^\dagger_{\rm P}] = \exp\left\{-\int dt\int dt'\eta^\dagger_{\rm P}(t)G_{\rm P}(t,t')\eta_{\rm P}(t')\right\}, \tag{18B.3}$$

generalizing (18.179), where the matrix

$$G_{\rm p} = \frac{1}{2}\begin{pmatrix} A_\Omega + G^R_\Omega + G^A_\Omega & A_\Omega - G^R_\Omega + G^A_\Omega \\ A_\Omega + G^R_\Omega - G^A_\Omega & A_\Omega - G^R_\Omega - G^A_\Omega \end{pmatrix} \tag{18B.4}$$

contains the following operator expectations on the two time branches:

$$\begin{aligned} G_{\rm p}(t,t') &= \begin{pmatrix} \langle\hat T_{\rm P}\hat a_H(t_+)\hat a^\dagger_H(t'_+)\rangle_T & \langle\hat T_{\rm P}\hat a_H(t_+)\hat a^\dagger_H(t'_-)\rangle_T \\ \langle\hat T_{\rm P}\hat a_H(t_-)\hat a^\dagger_H(t'_+)\rangle_T & \langle\hat T_{\rm P}\hat a_H(t_-)\hat a^\dagger_H(t'_-)\rangle_T \end{pmatrix} \\ &= \begin{pmatrix} \langle\hat T\hat a_H(t_+)\hat a^\dagger_H(t'_+)\rangle_T & \pm\langle\hat a^\dagger_H(t'_-)\hat a_H(t_+)\rangle_T \\ \langle\hat a_H(t_-)\hat a^\dagger_H(t'_+)\rangle_T & \langle\hat{\bar T}\hat a_H(t_-)\hat a^\dagger_H(t'_-)\rangle_T \end{pmatrix}. \end{aligned} \tag{18B.5}$$

Note that $\hat a_H(t_+),\hat a^\dagger_H(t_+)$ and $\hat a_H(t_-),\hat a^\dagger_H(t_-)$ obey the Heisenberg equations of motion with the Hamiltonians

$$\begin{aligned} \hat H_+ &\equiv \frac{\Omega}{2}\left[\hat a^\dagger_H(t_+)\hat a_H(t_+) \pm \hat a_H(t_+)\hat a^\dagger_H(t_+)\right], \\ \hat H_- &\equiv -\frac{\Omega}{2}\left[\hat a^\dagger_H(t_-)\hat a_H(t_-) \pm \hat a_H(t_-)\hat a^\dagger_H(t_-)\right]. \end{aligned} \tag{18B.6}$$

In the second-quantized field interpretation, they read

$$\begin{aligned} \hat H_+ &\equiv \frac{\Omega}{2}\hat a^\dagger_H(t_+)\hat a_H(t_+), \\ \hat H_- &\equiv -\frac{\Omega}{2}\hat a^\dagger_H(t_-)\hat a_H(t_-). \end{aligned}$$

The explicit time dependence of the matrix elements of $G_{\rm P}(t,t')$ in Eq. (18B.5) is

$$G_{\rm P}(t,t') = e^{-i\Omega(t-t')}\begin{pmatrix} \Theta(t-t')\pm n_\Omega & \pm n_\Omega \\ 1\pm n_\Omega & \Theta(t'-t)\pm n_\Omega \end{pmatrix}, \tag{18B.7}$$

with $n_\Omega = (e^{\Omega/T} \pm 1)^{-1}$.

This Green function can, incidentally, be decomposed as

$$G^0_{\rm P}(t,t') + G^N_{\rm P}(t,t'), \tag{18B.8}$$

where $G^0_{\rm P}(t,t')$ is the Green function at zero temperature, i.e., the expression (18B.7) for $n_\Omega \equiv 0$. The matrix $G^N(t,t')$ contains the expectations of the *normal products*:

$$\begin{aligned} G^N_{\rm P}(t,t') &\equiv \left(\begin{array}{cc} \langle \hat N \hat a_H(t_+)\hat a^\dagger_H(t'_+)\rangle_T & \langle \hat N \hat a_H(t_+)\hat a^\dagger_H(t'_-)\rangle_T \\ \langle \hat N \hat a_H(t_-)\hat a^\dagger_H(t'_+)\rangle_T & \langle \hat N \hat a_H(t_-)\hat a^\dagger_H(t'_-)\rangle_T \end{array}\right) \\ &\equiv \pm \left(\begin{array}{cc} \langle \hat a^\dagger_H(t'_+)\hat a_H(t_+)\rangle_T & \langle \hat a^\dagger_H(t'_-)\hat a_H(t_+)\rangle_T \\ \langle \hat a^\dagger_H(t'_+)\hat a_H(t_-)\rangle_T & \langle \hat a^\dagger_H(t'_-)\hat a_H(t_-)\rangle_T \end{array}\right). \end{aligned} \tag{18B.9}$$

For an arbitrary product of operators, the normal product $\hat N(\dots)$ is defined by reordering the operators so that all annihilation operators come to act first upon the state on the right-hand side. At the end, the product receives the phase factor $(-)^F$, where F is the number of fermion permutations to arrive at the normal order. A similar decomposition exists at the operator level *before* taking expectation values. For any pair of operators $\hat A(t), \hat B(t')$ which are linear combinations of creation and annihilation operators, the time-ordered product can be decomposed as

$$\hat T \hat A(t)\hat B(t') = \langle \hat T \hat A(t)\hat B(t')\rangle_0 + \hat N \hat A(t)\hat B(t'), \tag{18B.10}$$

where $\langle \dots\rangle_0 \equiv {\rm Tr}\,(|0\rangle\langle 0|\dots)$ denotes the zero-temperature expectation. This decomposition is proved in Appendix 18C, where it is also generalized to products of more than two operators.

Let us also go to the Keldysh basis here:

$$\tilde\eta_{\rm P} = Q\eta_{\rm P} = \frac{1}{\sqrt 2}\left(\begin{array}{cc} 1 & -1 \\ 1 & 1 \end{array}\right)\hat\eta_{\rm P}. \tag{18B.11}$$

Then the generating functional becomes [instead of (18.180)]:

$$\begin{aligned} Z_0[\eta^*_{\rm P},\eta_{\rm P}] &= \exp\left[-\int dt \int dt'\,(\eta^*_+, -\eta^*_-)Q^{-1}\left(\begin{array}{cc} 0 & G^A_\Omega \\ G^R_\Omega & A \end{array}\right) Q \left(\begin{array}{c} \eta_+ \\ -\eta_- \end{array}\right)\right] \\ &= \exp\Big\{ -\frac12 \int dt \int dt' \,\big[(\eta^*_+ - \eta^*_-)(t) G^R_\Omega(t-t')(\eta_+ + \eta_-)(t') \\ &\qquad + (\eta^*_+ + \eta^*_-)(t) G^A_\Omega(t-t')(\eta_+ - \eta_-)(t') \\ &\qquad + (\eta^*_- - \eta^*_-)(t) A_\Omega(t-t')(\eta_+ - \eta_-)(t')\big]\Big\}, \end{aligned} \tag{18B.12}$$

where we have used the notation

$$\eta_+(t) \equiv \eta(t_+), \quad \eta_-(t) \equiv \eta(t_-). \tag{18B.13}$$

Expression (18B.12) can be simplified [as before (18.180)] using the time reversal relation (18.62) in the form

$$A_\Omega(t,t') = \Theta(t,t')A_\Omega(t,t') \pm \Theta(t'-t)A_\Omega(t',t), \tag{18B.14}$$

leading to

$$\begin{aligned} Z_0[\eta^*_{\rm P},\eta_{\rm P}] = \exp\Big\{ &-\frac12 \int_{-\infty}^{\infty} dt \int_{-\infty}^{t} dt' \\ &\times \Big[(\eta_+ - \eta_-)^*(t) G^R_\Omega(t,t')(\eta_+ + \eta_-)(t') \\ &- (\eta_+ - \eta_-)(t) G^R_\Omega(t,t')^*(\eta_+ + \eta_-)^*(t') \\ &+ (\eta_+ - \eta_-)^*(t) A_\Omega(t,t')(\eta_+ - \eta_-)(t') \\ &+ (\eta_+ - \eta_-)(t) A_\Omega(t,t')^*(\eta_+ - \eta_-)^*(t')\Big]\Big\}. \end{aligned} \tag{18B.15}$$

For the case of a second-quantized field, this is the most useful generating functional.

The expression (18B.15) can be used to derive the generating functional for correlation functions between one or more $\varphi(t)$ and the associated canonically-conjugate momenta. As an example, consider immediately a harmonic oscillator with $\varphi(t) = x(t)$ and the momentum $p(t)$. We would like to find the generating functional

$$Z[j_{\rm P}, k_{\rm P}] = {\rm Tr}\left(\hat\rho\, \hat T_{\rm P} \exp\left\{i\int_{\rm P} dx\, [j_{\rm P}(t)x_{\rm P}(t) + k_{\rm P}(t)p_{\rm P}(t)]\right\}\right). \tag{18B.16}$$

The position variable $x(t)$ is decomposed as in (18.92) into a sum of creation and an annihilation operators:

$$\hat x(t) = \sqrt{\frac{\hbar}{2M\Omega}}\left[\hat a e^{-i\Omega t} + \hat a^\dagger e^{i\Omega t}\right]. \tag{18B.17}$$

The inverse of this decomposition is

$$\left\{\begin{array}{c}\hat a\\ \hat a^\dagger\end{array}\right\} = (M\Omega\,\hat\varphi \pm i\hat p)/\sqrt{2M\Omega\hbar}, \tag{18B.18}$$

and there is an analogous relation of the complex sources:

$$\left\{\begin{array}{c}\eta\\ \eta^\dagger\end{array}\right\} = (j \pm iM\Omega\, k)\,/\sqrt{2M\Omega\hbar}. \tag{18B.19}$$

Inserting these sources into (18B.15), we obtain the generating functional

$$\begin{aligned} Z_0[j_{\rm P}, k_{\rm P}] = \exp\Bigg\{ &-\frac{1}{2M\Omega}\int_{-\infty}^{\infty} dt \int_{-\infty}^{t} dt'\,(j_+ - j_-)(t)\\ &\qquad\times\left\{[{\rm Re}\,A_\Omega(t,t') + i{\rm Im}\,G^R_\Omega(t,t')]j_+(t')\right.\\ &\qquad\left. -\ [{\rm Re}\,A_\Omega(t,t') - i{\rm Im}\,G^R_\Omega(t,t')]j_-(t')\right\}\\ &-\frac{1}{2}\int_{-\infty}^{\infty} dt\int_{-\infty}^{t} dt'\,(k_+ - k_-)(t)\ \{[{\rm Im}\,A_\Omega(t,t') - i{\rm Re}\,G^R_\Omega(t,t')]j_+(t')\\ &\qquad -\ [{\rm Im}\,A_\Omega(t,t') + i{\rm Re}\,G^R_\Omega(t,t')]j_-(t')\} + (j \leftrightarrow kM\Omega)\Bigg\}. \end{aligned} \tag{18B.20}$$

Here it is useful to introduce the quantities

$$\begin{aligned} \alpha(t,t') &= \frac{1}{2M\Omega}\left[{\rm Re}\,A_\Omega(t,t') + i{\rm Im}\,G^R_\Omega(t,t')\right],\\ \beta(t,t') &= \frac{1}{2M\Omega}\left[{\rm Im}\,A_\Omega(t,t') - i{\rm Re}\,G^R_\Omega(t,t')\right]. \end{aligned} \tag{18B.21}$$

Then the generating functional reads

$$\begin{aligned} Z_0[j_+, j_-, k_+, k_-] = \exp\Bigg\{&-\int_{-\infty}^{\infty} dt\int_{-\infty}^{t} dt'\,(j_+ - j_-)(t)\,[\alpha(t,t')j_+(t') - \alpha^*(t,t')j_-(t')] + (j \leftrightarrow kM\Omega)\\ &-M\Omega\int_{-\infty}^{\infty} dt\int_{-\infty}^{t} dt'\,(k_+ - k_-)(t)\,[\beta(t,t')j_+(t') - \beta^*(t,t')j_-(t')] + (j \leftrightarrow kM\Omega)\Bigg\}. \end{aligned} \tag{18B.22}$$

If the oscillator is coupled only to the real source j, i.e., if its generating functional reads

$$Z[j_{\rm P}] = {\rm Tr}\left\{\hat\rho\, \hat T_{\rm P} \exp\left[i\int_{\rm P} dx\, j_{\rm P}(t)\hat x_{\rm P}(t)\right]\right\}, \tag{18B.23}$$

we can drop all but the first line in the exponent of (18B.22) and have

$$Z_0[j_+,j_-]=\exp\left\{-\int_{-\infty}^{\infty}dt\int_{-\infty}^{t}dt'\,(j_+-j_-)(t)\,[\alpha(t,t')j_+(t')-\alpha^*(t,t')j_-(t')]\right\}. \tag{18B.24}$$

Since (18B.22) and (18B.24) contain only the causal temporal order $t>t'$, the retarded Green function $G^R_\Omega(t,t')$ in (18B.21) can be replaced by the expectation value of the commutator [see (18.40), (18.41), and (18.42)]. Thus, for $t>t'$, the functions $\alpha(t,t')$ and $\beta(t,t')$ are equal to[11]

$$\begin{aligned}\alpha(t,t') &= \frac{1}{2M\Omega}\left[\mathrm{Re}\,A_\Omega(t,t')+i\mathrm{Im}\,C_\Omega(t,t')\right], \qquad t>t',\\ \beta(t,t') &= \frac{1}{2M\Omega}\left[\mathrm{Im}\,A_\Omega(t,t')-i\mathrm{Re}\,C_\Omega(t,t')\right], \qquad t>t'.\end{aligned} \tag{18B.25}$$

For a single oscillator of frequency Ω, we use the spectral function (18.74) properties (18.44) and (18.53) of $A_\Omega(t,t')$ and $C_\Omega(t,t')$, and find the simple expressions:

$$\begin{aligned}\alpha(t,t') &= \frac{1}{2M\Omega}\left[\mathrm{Re}\,e^{-i\Omega(t-t')}\left\{\begin{array}{c}\coth\frac{\Omega}{2T}\\ \tanh\frac{\Omega}{2T}\end{array}\right\}+i\mathrm{Im}\,e^{-i\Omega(t-t')}\right]\\ &= \frac{1}{2M\Omega}\left[\cos\Omega(t-t')\left\{\begin{array}{c}\coth\frac{\Omega}{2T}\\ \tanh\frac{\Omega}{2T}\end{array}\right\}-i\sin\Omega(t-t')\right],\end{aligned} \tag{18B.26}$$

$$\begin{aligned}\beta(t,t') &= \frac{1}{2M\Omega}\left[\mathrm{Im}\,e^{-i\Omega(t-t')}\left\{\begin{array}{c}\coth\frac{\Omega}{2T}\\ \tanh\frac{\Omega}{2T}\end{array}\right\}-i\mathrm{Re}\,e^{-i\Omega(t-t')}\right]\\ &= -\frac{1}{2M\Omega}\left[\sin\Omega(t-t')\left\{\begin{array}{c}\coth\frac{\Omega}{2T}\\ \tanh\frac{\Omega}{2T}\end{array}\right\}+i\cos\Omega(t-t')\right].\end{aligned} \tag{18B.27}$$

Note that real and imaginary parts of the functions $\bar\alpha(t-t')$ can be combined into a single expression ($\beta=1/T$)

$$\bar\alpha(t-t')=\frac{1}{2M\Omega}\left\{\begin{array}{ll}\dfrac{\cosh[\Omega(\beta/2-i(t-t')]}{\sinh(\Omega\beta/2)} & \text{for}\quad \text{bosons},\\[2mm] \dfrac{\sinh[\Omega(\beta/2-i(t-t')]}{\cosh(\Omega\beta/2)} & \text{for}\quad \text{fermions}.\end{array}\right. \tag{18B.28}$$

The bosonic function agrees with the time-ordered Green function (18.101) for $t>t'$ and continues it analytically to $t<t'$.

In Fourier space, the functions (18B.26) and (18B.27) correspond to

$$\begin{aligned}\alpha(\omega') &= \frac{\pi}{2M\Omega}\left(\coth^{\pm1}\frac{\omega'}{2T}+1\right)[\delta(\omega'-\Omega)-\delta(\omega'+\Omega)],\\ \beta(\omega') &= -\frac{i\pi}{2M\Omega}\left(\coth^{\pm1}\frac{\omega'}{2T}+1\right)[\delta(\omega'-\Omega)+\delta(\omega'+\Omega)].\end{aligned}$$

Let us split these functions into a zero-temperature contribution plus a remainder

$$\begin{aligned}\alpha(\omega') &= \frac{\pi}{M\Omega}\left\{\delta(\omega'-\Omega)\pm\frac{1}{e^{\Omega/T}\mp1}[\delta(\omega'-\Omega)+\delta(\omega'+\Omega)]\right\},\\ \beta(\omega') &= \frac{\pi}{M\Omega}\left\{\delta(\omega'-\Omega)\pm\frac{1}{e^{\Omega/T}\mp1}[\delta(\omega'-\Omega)-\delta(\omega'+\Omega)]\right\}.\end{aligned}$$

[11] Note that $\alpha(t,t')=\langle x(t)x(t')\rangle_T$.

On the basis of this formula, Einstein first explained the induced emission and absorption of light by atoms which he considered as harmonically oscillating dipoles in contact with a thermal reservoir. He imagined them to be harmonically oscillating dipole moments coupled to a thermal bath consisting of the Fourier components of the electromagnetic field in thermal equilibrium. Such a thermal bath is called a *black body*. The first purely dissipative and temperature-independent term in $\alpha(\omega')$ was attributed by Einstein to the *spontaneous emission* of photons. The second term is caused by the bath fluctuations, making energy go in and out via *induced emission and absorption* of photons. It is proportional to the occupation number of the oscillator state $n_\Omega = (e^{-\Omega/T} \mp 1)^{-1}$. The equality of the prefactors in front of the two terms is the important manifestation of the fluctuation-dissipation theorem found earlier [see (18.53)].

Appendix 18C Wick Decomposition of Operator Products

Consider two operators $\hat{A}(t)$ and $\hat{B}(t)$ which are linear combinations of creation and annihilation operators

$$\begin{aligned} \hat{A}(t) &= \alpha_1 \hat{a}(t) + \alpha_2 \hat{a}^\dagger(t), \\ \hat{B}(t) &= \beta_1 \hat{a}(t) + \beta_2 \hat{a}^\dagger(t). \end{aligned} \tag{18C.1}$$

We want to show that the time-ordered product of two operators has the decomposition quoted in Eq. (18B.10):

$$\hat{T}\hat{A}(t)\hat{B}(t) = \langle \hat{T}\hat{A}(t)\hat{B}(t)\rangle_0 + \hat{N}\hat{A}(t)\hat{B}(t). \tag{18C.2}$$

The first term on the right-hand side is the thermal expectation of the time-ordered product at zero temperature; the second term is the normal product of the two operators.

If $\hat{A}$ and $\hat{B}$ are both creation or annihilation operators, the statement is trivial with $\langle \hat{T}\hat{A}\hat{B}\rangle_0 = 0$. If one of the two, say $\hat{A}(t)$, is a creation operator and the other, $\hat{B}(t)$, an annihilation operator, then

$$\begin{aligned} \hat{T}\hat{a}(t)\hat{a}^\dagger(t') &= \Theta(t-t')\hat{a}(t)\hat{a}^\dagger(t') \pm \Theta(t'-t)\hat{a}^\dagger(t')\hat{a}(t) \\ &= \Theta(t-t')[\hat{a}(t)\hat{a}^\dagger(t')]_\mp \pm \hat{a}^\dagger(t')\hat{a}(t). \end{aligned} \tag{18C.3}$$

Due to the commutator (anticommutator) the first term is a c-number. As such it is equal to the expectation value of the time-ordered product at zero temperature. The second term is a normal product, so that we can write

$$\hat{T}\hat{a}(t)\hat{a}^\dagger(t') = \langle \hat{T}\hat{a}(t)\hat{a}^\dagger(t')\rangle_0 + \hat{N}\hat{a}(t)\hat{a}^\dagger(t'). \tag{18C.4}$$

The same thing is true if a and $a^\dagger$ are interchanged (such an interchange produces merely a sign change on both sides of the equation). The general statement for $\hat{A}(t)\hat{B}(t')$ follows from the bilinearity of the product.

The decomposition (18C.2) of the time-ordered product of two operators can be extended to a product of n operators, where it reads

$$\hat{T}\hat{A}(t_1)\dots\hat{A}(t_n) = \sum_{i=2}^{n} \hat{N}\dot{\hat{A}}(t_1)\dots\dot{\hat{A}}(t_i)\dots\hat{A}(t_n). \tag{18C.5}$$

A common pair of dots on top of a pair of operators denotes a *Wick contraction* of Section 3.10. It indicates that the pair of operators has been replaced by the expectation $\langle \hat{T}\hat{A}(t_1)\hat{A}(t_i)\rangle_0$, multiplied by a factor $(-)^F$, if F = fermion permutations were necessary to bring the contracted operator to the adjacent positions. The remaining factors are contracted further in the same way. In this way, any time-ordered product

$$\hat{T}\hat{A}(t_1)\cdots\hat{A}(t_n) \tag{18C.6}$$

can be expanded into a sum of normal products of these operators containing successively one, two, three, etc. pairs of contracted operators.

The expansion rule can be phrased most compactly by means of a generating functional

$$\hat{T}e^{i\int_{-\infty}^{\infty}dt\hat{A}(t)j(t)} = e^{-\frac{1}{2}\int_{-\infty}^{\infty}dtdt'j(t)\langle\hat{T}\hat{A}(t)\hat{A}(t')\rangle_0 j(t')}\;\hat{N}\left(e^{i\int_{-\infty}^{\infty}dt\hat{A}(t)j(t)}\right). \tag{18C.7}$$

Differentiations with respect to the source $j(t)$ on both sides produce precisely the above decompositions.

By going to thermal expectation values of (18C.7) at a temperature T, we find

$$\left\langle \hat{T}e^{i\int_{-\infty}^{\infty}dt\hat{A}(t)j(t)}\right\rangle_T = e^{-\frac{i}{2}\int_{-\infty}^{\infty}dtdt'j(t)G(t,t')j(t')}, \tag{18C.8}$$

with

$$G(t,t') = \langle\hat{T}\hat{A}(t)\hat{A}(t')\rangle_0 + \langle\hat{N}\hat{A}(t)\hat{A}(t')\rangle_T. \tag{18C.9}$$

The first term on the right-hand side is calculated at zero temperature. All finite temperature effects reside in the second term.

Notes and References

The fluctuation-dissipation theorem was first formulated by
H.B. Callen and T.A. Welton, Phys. Rev. **83**, 34 (1951).
It generalizes the relation between the diffusion constant and the viscosity discovered by
A. Einstein, Ann. Phys. (Leipzig) **17**, 549 (1905),
and an analogous relation for induced light emission in
A. Einstein, "Strahlungs-Emission und -Absorption nach der Quantentheorie", Verhandlungen der Deutschen Physikalischen Gesellschaft **18**, 318 (1916),
where he derived Planck's black-body formula. See also the functioning of this theorem in the thermal noise in a resistor:
H. Nyquist, Phys. Rev. **32**, 110 (1928).

K.V. Keldysh, Z. Eksp. Teor. Fiz. **47**, 1515 (1964); Sov. Phys. JETP **20**, 1018 (1965).
See also
V. Korenman, Ann. Phys. (N. Y.) **39**, 72 (1966);
D. Dubois, in *Lectures in Theoretical Physics*, Vol. IX C, ed. by W.E. Brittin, Gordon and Breach, New York, 1967;
D. Langreth, in *Linear and Nonlinear Electronic Transport in Solids*, ed. by J.T. Devreese and V. Van Doren, Plenum, New York, 1976;
A.M. Tremblay, B. Patton, P.C. Martin, and P. Maldague, Phys. Rev. A **19**, 1721 (1979).
For the derivation of the Langevin equation from the forward–backward path integral see
S.A. Adelman, Chem. Phys. Lett. **40**, 495 (1976);
and especially
A. Schmid, J. Low Temp. Phys. **49**, 609 (1982).
To solve the operator ordering problem, Schmid assumes that a time-sliced derivation of the forward–backward path integral would yield a sliced version of the stochastic differential equation (18.317) $\eta_n \equiv (M/\epsilon)(x_n - 2x_{n-1} + x_{n-2}) + +(M\gamma/2)(x_n - x_{n-2}) + \epsilon V'(x_{n-1}$. The matrix $\partial\eta/\partial x$ has a constant determinant $(M/\epsilon)^N(1+\epsilon\gamma/2)^N$. His argument [cited also in the textbook by
U. Weiss, *Quantum Dissipative Systems*, World Scientific, 1993,
in the discussion following Eq. (5.93)] is unacceptable for two reasons: First, his slicing is not derived. Second, the resulting determinant has the wrong continuum limit proportional to

$\exp\left[\int dt\,\gamma/2\right]$ for $\epsilon \to 0$, $N = (t_b - t_a)/\epsilon \to \infty$, corresponding to the unretarded functional determinant (18.274), whereas the correct limit should be γ-independent, by Eq. (18.282).
The above textbook by U. Weiss contains many applications of nonequilibrium path integrals.

More on Langevin and Fokker-Planck equations can be found in
S. Chandrasekhar, Rev. Mod. Phys. **15**, 1 (1943);
N.G. van Kampen, *Stochastic Processes in Physics and Chemistry*, North-Holland, Amsterdam, 1981;
P. Hänggi and H. Thomas, Phys. Rep. **88**, 207 (1982);
C.W. Gardiner, *Handbook of Stochastic Methods*, Springer Series in Synergetics, 1983, Vol. 13;
H. Risken, *The Fokker-Planck Equation*, *ibid.*, 1983, Vol. 18;
R. Kubo, M. Toda, and N. Hashitsume, *Statistical Physics II*, Springer, Berlin, 1985;
H. Grabert, P. Schramm, and G.-L. Ingold, Phys. Rep. **168**, 116 (1988).

The stochastic Schrödinger equation with the Hamiltonian operator (18.521) was derived by
A.O. Caldeira and A.J. Leggett, Physica A **121**, 587 (1983); A **130** 374(E) (1985).
See also
A.O. Caldeira and A.J. Leggett, Phys. Rev. A **31**, 1059 (1985).
A recent discussion of the relation between time slicing and Itō versus Stratonovich calculus can be found in
H. Nakazato, K. Okano, L. Schülke, and Y. Yamanaka, Nucl. Phys. B **346**, 611 (1990).
For the Heisenberg operator approach to stochastic calculus see
N. Saito and M. Namiki, Progr. Theor. Phys. **16**, 71 (1956).
Recent applications of the Langevin equation to decay problems and quantum fluctuations are discussed in
U. Eckern, W. Lehr, A. Menzel-Dorwarth, F. Pelzer, A. Schmid, J. Stat. Phys. **59**, 885-934 (1990).
See also their references and those quoted at the end of Chapter 3.

The quantum Langevin equation is discussed in
G.W. Ford, J.T. Lewis und R.F. O'Connell, Phys. Rev. Lett. **55**, 42273 (1985); Phys. Rev. A **37**, 4419 (1988); Ann. of Phys. **185**, 270 (1988).

Deterministic models for Schrödinger wave functions are discussed in
G. 't Hooft, Class. Quant. Grav. **16**, 3263 (1999) (gr-gc/9903084); hep-th/0003005; Int. J. Theor. Phys. **42**, 355 (2003) (hep-th/0104080); hep-th/0105105; Found. Phys. Lett. **10**, 105 (1997) (quant-ph/9612018).
See also the Lecture Ref. [37].
The representation in Section 18.24 is due to
Z. Haba and H. Kleinert, Phys. Lett. A **294**, 139 (2002) (quant-ph/0106095).
See also
F. Haas, *Stochastic Quantization of the Time-Dependent Harmonic Oscillator*, Int. J. Theor. Phys. **44**, 1 (2005) (quant/ph-0406062).
M. Blasone, P. Jizba, and H. Kleinert, Phys. Rev. A **71**, 2005; Braz. J. Phys. **35**, 479 (2005) (quant/ph-0504047); Annals Phys. **320**, 468 (2005) (quant/ph-0504200).
Another improvement is due to
M. Blasone, P. Jizba, G. Vitiello, Phys. Lett. A **287**, 205 (2001) (hep-th/0007138);
M. Blasone, E. Celeghini, P. Jizba, G. Vitiello, *Quantization, Group Contraction and Zero-Point Energy*, Phys. Lett. A **310**, 393 (2003) (quant-ph/0208012).

The individual citations refer to

[1] Some authors define $G_{12}(\tau)$ as having an extra minus sign and the retarded Green function with a factor $-i$, so that the relation is more direct: $G_{12}^R(\omega) = G_{12}(\omega_m = -i\omega + \eta)$. See

A.A. Abrikosov, L.P. Gorkov, and I.E. Dzyaloshinski, Sov. Phys. JETP **9**, 636 (1959); or *Methods of Quantum Field Theory in Statistical Physics*, Dover, New York, 1975; also A.L. Fetter and J.D. Walecka, *Quantum Theory of Many-Particle Systems*, McGraw-Hill, New York, 1971.
Our definition (18.20) without a minus sign conforms with the definition of the fixed-energy amplitude in Chapter 9, Eq. (1.325), which is also a retarded Green function.

[2] E.S. Fradkin, *The Green's Function Method in Quantum Statistics*, Sov. Phys. JETP **9**, 912 (1959).

[3] G. Baym and D. Mermin, J. Math. Phys. **2**, 232 (1961).
One extrapolation uses Padé approximations:
H.J. Vidberg and J.W. Serene, J. Low Temp. Phys. **29**, 179 (1977); W.H. Press, S.A. Teukolsky, W.T. Vetterling, and B.P. Flannery, *Numerical Recipes in Fortran*, Cambridge Univ. Press (1992), Chapter 12.5.
Since the thermal Green function are usually known only approximately, the continuation is not unique. A maximal-entropy method by
R.N. Silver, D.S. Sivia, and J.E. Gubernatis, Phys. Rev. B **41**, 2380 (1990)
selects the most reliable result.

[4] J. Schwinger, J. Math. Phys. **2**, 407 (1961).

[5] K.V. Keldysh, Z. Eksp. Teor. Fiz. **47**, 1515 (1964); Sov. Phys. JETP **20**, 1018 (1965).

[6] K.-C. Chou, Z.-B. Su, B.-L. Hao, and L. Yu, Phys. Rep. **118**, 1 (1985);
also K.-C. Chou et al., Phys. Rev. B **22**, 3385 (1980).

[7] R.P. Feynman and F.L. Vernon, Ann. Phys. **24**, 118 (1963);
R.P. Feynman and A.R. Hibbs, *Quantum Mechanics and Path Integrals*, McGraw-Hill, New York, 1965, Sections 12.8 and 12.9.

[8] The solution of path integrals with second time derivatives in the Lagrangian is given in
H. Kleinert, J. Math. Phys. **27**, 3003 (1986) (`http://www.physik.fu-berlin.de/~kleinert/144`).

[9] H. Kleinert, *Gauge Fields in Condensed Matter*, op. cit., Vol. II, Section 17.3 (*ibid.*`http/b2`), and references therein.

[10] See the review paper by
S. Chandrasekhar, Rev. Mod. Phys. **15**, 1 (1943), or the original papers:
A.A. Fokker, Ann. Phys. (Leipzig) **43**, 810 (1914);
M. Planck, Sitzber. Preuss. Akad. Wiss. p. 324 (1917);
O. Klein, Arkiv Mat. Astr. Fysik **16**, No. 5 (1922);
H.A. Kramers, Physica **7**, 284 (1940);
M. Smoluchowski, Ann. Phys. (Leipzig) **48** , 1103 (1915).

[11] H. Kleinert, A. Chervyakov, Phys. Lett. B **464**, 257 (1999) (hep-th/9906156); Phys. Lett. B **477**, 373 (2000) (quant-ph/9912056); Eur. Phys. J. C **19**, 743-747 (2001) (quant-ph/0002067); Phys. Lett. A **273**, 1 (2000) (quant-ph/0003095); Int. J. Mod. Phys. A **17**, 2019 (2002) (quant-ph/0208067); Phys. Lett. A **308**, 85 (2003) (quant-ph/0204067); Int. J. Mod. Phys. A **18**, 5521 (2003) (quant-ph/0301081) .

[12] In a first attempt to show that this functional the determinant is unity,
A. Schmid, J. Low Temp. Phys. **49**, 609 (1982). contrived a suitable time slicing of the differential operator in (18.326) to achieve this goal. However, since this was not derived from a time slicing of the initial forward–backwards path integral (18.230), this procedure cannot be considered as a proof.

[13] The operator-ordering problem was first solved by
H. Kleinert, Ann. of Phys. **291**, 14 (2001) (quant-ph/0008109).

[14] R. Benguria and M. Kac, Phys. Rev. Lett. **46**, 1 (1981);
Y.C. Chen, M.P.A. Fisher and A.J. Leggett, J. Appl. Phys. **64**, 3119 (1988).

[15] G.W. Ford, M. Kac, and P. Mazur, J. Math. Phys. **6**, 504 (1965).
G.W. Ford and M. Kac, J. Stat. Phys. **46**, 803 (1987).

[16] P. Langevin, Comptes Rendues **146**, 530 (1908).

[17] G. Parisi and Y.S. Wu, Scientia Sinica **24**, 483 (1981).

[18] R. Kubo, J.Math.Phys. **4**, 174 (1963);
R. Kubo, M. Toda, and N. Hashitsume, *Statistical Physics II (Nonequilibrium Statistical Mechanics*), Springer-Verlag, Berlin, 1985 (Chap. 2).

[19] J. Zinn-Justin, *Critical Phenomena*, Clarendon, Oxford, 1989.

[20] G. Parisi and N. Sourlas, Phys. Rev. Lett. **43**, 744 (1979); J. de Phys. **41**, L403 (1981); Nucl. Phys. B *206*, 321 (1982);

[21] A.J. McKane, Phys. Lett. A *76*, 22 (1980).

[22] H. Kleinert and S. Shabanov, Phys. Lett. A **235**, 105 (1997) (quant-ph/9705042).

[23] E. Gozzi, Phys. Lett. **B** 201, 525 (1988).

[24] A.O. Caldeira and A.J. Leggett, Physica A **121**, 587 (1983); A *130* 374(E) (1985).

[25] More on this subject is found in the collection of articles
D. Giulini, E. Joos, C. Kiefer, J. Kupsch, I.O. Stamatescu, H.D. Zeh, *Decoherence and the Appearance of a Classical World in Quantum Theory*, Springer, Berlin, 1996.

[26] G. Lindblad, Comm. Math. Phys. **48**, 119 (1976). This paper shows that the form (18.534) of the master equation (18.524) guarantees the positivity of the probabilities derived from the solutions. The right-hand side can be more generally $\sum_{mn} h_{mn} \left(\frac{1}{2} \hat{L}_m \hat{L}_n \hat{\rho} + \frac{1}{2} \hat{\rho} \hat{L}_m \hat{L}_n - \hat{L}_n \hat{\rho} \hat{L}_m \right) + \text{h.c.}$.

[27] L. Diosi, Europhys. Lett. **22**, 1 (1993).

[28] C.W. Gardiner, IBM J. Res. Develop. **32**, 127 (1988).

[29] H. Kleinert and S. Shabanov, Phys. Lett. A **200**, 224 (1995) (quant-ph/9503004);
K. Tsusaka, Phys. Rev. E **59**, 4931 (1999).

[30] H.A. Bethe, Phys. Rev. **72**, 339 (1947).

[31] C. Cohen-Tannoudji, J. Dupont-Roc, G. Grynberg, *Photons and Atoms: Introduction to Quantum Electrodynamics*, Wiley, New York, 1992.

[32] R. Rohrlich, Am. J. Phys. **68**, 1109 (2000).

[33] H. Kleinert and S. Shabanov, J. Phys. A: Math. Gen. **31**, 7005 (1998) (cond-mat/9504121);
R. Bausch, R. Schmitz, and L.A. Turski, Phys. Rev. Lett. **73**, 2382 (1994); Z. Phys. B **97**, 171 (1995).

[34] M. Roncadelli, Europhys. Lett. **16**, 609 (1991); J. Phys. A **25**, L997 (1992);
A. Defendi and M. Roncadelli, Europhys. Lett. **21**, 127 (1993).

[35] Z. Haba, Lett. Math. Phys. **37**, 223 (1996).

[36] G. 't Hooft, Found. Phys. Lett. **10**, 105 (1997) (quant-ph/9612018).

[37] G. 't Hooft, *How Does God Throw Dice?* in *Fluctuating Paths and Fields - Dedicated to Hagen Kleinert on the Occasion of his 60th Birthday*, Eds. W. Janke, A. Pelster, H.-J. Schmidt, and M. Bachmann, World Scientific, Singapore, 2001 (`http://www.physik.fu-berlin.de/~kleinert/fest.html`).