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Dissipative Quantum Systems

4.1 Introduction

Dissipation is a ubiquitous phenomenon in real physical systems. Its nature is made clear by considering the damped harmonic oscillator, a paradigm for dissipative systems in the classical as well as the quantum regime. After starting at a nonequilibrium position, the system will perform damped oscillations and end up in the equilibrium position. Looking closely, one will notice that even in equilibrium the oscillator coordinate fluctuates. This effect is related to the Brownian motion of a free particle. Damping and fluctuations are both caused by the coupling of the harmonic oscillator to other degrees of freedom. A pendulum's motion is damped because of collisions with molecules in the air during the oscillations. For the same reason the pendulum will fluctuate around its equilibrium position. The identical origin of both effects manifests itself in the fluctuation-dissipation theorem which will be discussed later in this chapter.

Another system where the coupling to other degrees of freedom plays a prominent role, is the decay of a metastable state. At not too low temperatures a state in a potential minimum, which is separated by a barrier from an energetically lower region, may decay by thermal activation. Here, the other degrees of freedom, which are also collectively called heat bath or reservoir, provide the system with the necessary energy to surmount the barrier. At low enough temperatures, the decay of the metastable state will be dominated by quantum tunneling through the barrier, and one might ask how the other degrees of freedom influence the tunneling rate.

In this chapter, we will specifically consider the damped harmonic oscillator, the damped free particle, and the decay of a metastable state to illustrate the techniques introduced to describe dissipation in quantum mechanics. Of course, there are other interesting problems like the damped motion in a periodic potential and the dissipative two-level system [1]. For a more complete discussion of many aspects of quantum dissipation, we refer the reader e.g. to the textbook by Weiss [2] which may also serve as a guide to the literature.

A rather recent area of research activities is concerned with the interplay between quantum dissipation and chaos which is discussed in Chapter 6. In this context, techniques for the treatment of driven systems discussed in Chapter 5 are required.

4.2 Description of dissipation in quantum mechanics

In classical physics damping may often be described by introducing a velocity propor-
tional term in the equation of motion. For a damped harmonic oscillator with mass M
and frequency ω_0 one has

$$M\left(\ddot{q} + \gamma\dot{q} + \omega_0^2 q\right) = 0, \tag{4.1}$$

where q is the position of the oscillator and γ is the damping constant. By including a
fluctuating force $\xi(t)$ on the right-hand-side one arrives at a so-called Langevin equation
which not only describes the damped average motion but also the fluctuations around it.
The velocity proportional damping term is often referred to as Ohmic damping because
an electrical circuit containing a resistance R, an inductance L, and a capacitance C
in series is described by (4.1), where q is the charge on the capacitor, $\omega_0 = (LC)^{-1/2}$,
and $\gamma = R/L$. Obviously, in a classical description, damping may be introduced in a
rather phenomenological way without necessarily knowing the microscopic details of
the other degrees of freedom and their coupling to the degree of freedom of interest.

   In quantum mechanics, the inclusion of dissipation requires more care because
quantum systems are described by a Hamilton operator which in the absence of time-
dependent external forces ensures conservation of energy. Several approaches have
been developed to circumvent this problem [3]. The most successful and rather general
approach, which also catches the physics discussed above, is based on the concept of a
reservoir of other degrees of freedom which will be discussed in the following section.
It will turn out that again knowledge of the microscopic details of the heat bath is
not necessarily needed. Although the system including the reservoir is described by
a time-independent Hamiltonian, the elimination of the bath degrees of freedom gives
rise to dissipation.

4.2.1 Hamiltonian for system and heat bath

We start out with one degree of freedom called system (S) which we view as a particle
of mass M moving in a potential $V(q)$. The corresponding Hamiltonian reads

$$H_{\mathrm{S}} = \frac{p^2}{2M} + V(q), \tag{4.2}$$

where p is the momentum conjugate to the position q of the particle. The bath (B) is
described by a set of harmonic oscillators

$$H_{\mathrm{B}} = \sum_{i=1}^{N}\left(\frac{p_i^2}{2m_i} + \frac{m_i}{2}\omega_i^2 x_i^2\right). \tag{4.3}$$

System and bath positions are coupled bilinearly according to

$$H_{\mathrm{SB}} = -q\sum_{i=1}^{N} c_i x_i + q^2 \sum_{i=1}^{N} \frac{c_i^2}{2m_i\omega_i^2}. \tag{4.4}$$

Here, the last term, which does not depend on the bath coordinates, has to be included for $V(q)$ to be the bare potential. This can be seen by considering a free damped particle, i.e. $V(q) = 0$, for which the Hamiltonian should be translationally invariant. It is easy to check that this is indeed the case if we set $c_i = m_i \omega_i^2$. This definition of the coupling constants leaves sufficient free parameters as we will see later. Omission of the last term in (4.4) would lead to a potential renormalization which would turn the free particle into a harmonically bound one.

The total Hamiltonian

$$H = H_{\mathrm{S}} + H_{\mathrm{B}} + H_{\mathrm{SB}} \tag{4.5}$$

was used by various authors to study dissipative quantum systems for the special case of a harmonic potential $V(q)$ [4]. Probably the first proof that (4.5) in this case leads to dissipation can be found in the lucid paper by Magalinskiĭ [5]. Later, Zwanzig [6] within a classical description generalized the approach to nonlinear potentials. Most of the early work was aimed at applications in quantum optics and spin relaxation where the coupling to the heat bath is usually weak. More recently, Caldeira and Leggett [7] emphasized that the Hamiltonian (4.5) is also applicable to strongly damped systems and used it to describe dissipative tunnel systems. In the solid state physics community it is therefore often referred to as Caldeira-Leggett Hamiltonian.

While the Hamiltonian (4.5) incorporates in some sense the microscopic origin of dissipation, it does not really represent a microscopic model. For example, we could treat the LCR-circuit mentioned above quantum mechanically without a microscopic model of a resistor. Instead, as will become clear from the following discussion, we may choose the parameters in (4.3) and (4.4) in such a way that we effectively model the damping term in (4.1) by means of the virtual bath oscillators. However, there are cases where a microscopic derivation is feasible. As an example, we mention the dissipation caused by quasiparticles in a superconducting tunnel junction [8] which is discussed in Chapter 3.

Of course, not every dissipative system may be described in terms of the Hamiltonian (4.5). On the other hand, this model gives a correct description for a wide variety of quantum dissipative systems, and maybe equally important, it allows for an analytical treatment.

4.2.2   Elimination of the heat bath

We now want to prove that the Hamiltonian (4.5) indeed describes dissipation if we are interested in the system degree of freedom only. To this end, we first write down the Heisenberg equations of motion which we solve for the reservoir degrees of freedom. This gives us an effective equation of motion which may then be compared with the classical damped equation of motion. Employing the Heisenberg equation of motion

$$\frac{\mathrm{d}A}{\mathrm{d}t} = \frac{\mathrm{i}}{\hbar}[H, A], \tag{4.6}$$

we obtain the (operator) equations of motion

$$\ddot{q} + \frac{1}{M}\left(\frac{\mathrm{d}V}{\mathrm{d}q} + q\sum_{i=1}^{N}\frac{c_i^2}{m_i\omega_i^2}\right) = \frac{1}{M}\sum_{i=1}^{N}c_ix_i \tag{4.7}$$

for the system and

$$\ddot{x}_i + \omega_i^2 x_i = \frac{c_i}{m_i}q \tag{4.8}$$

for the bath degrees of freedom. Considering $q(t)$ as given, (4.8) is formally solved by

$$x_i(t) = x_i(0)\cos(\omega_i t) + \frac{p_i(0)}{m_i\omega_i}\sin(\omega_i t) + \int_0^t \mathrm{d}s\frac{c_i}{m_i\omega_i}\sin\left(\omega_i(t-s)\right)q(s). \tag{4.9}$$

We eliminate the bath degrees of freedom by inserting this solution into the inhomogeneity of (4.7) and arrive at an effective operator equation for our system. By partial integration we obtain

$$M\ddot{q} + M\int_0^t \mathrm{d}s\gamma(t-s)\dot{q}(s) + \frac{\mathrm{d}V}{\mathrm{d}q} = \xi(t) \tag{4.10}$$

where the damping kernel is given by

$$\gamma(t) = \frac{1}{M}\sum_{i=1}^{N}\frac{c_i^2}{m_i\omega_i^2}\cos(\omega_i t). \tag{4.11}$$

The inhomogeneity

$$\xi(t) = \sum_{i=1}^{N}c_i\left[\left(x_i(0) - \frac{c_i}{m_i\omega_i^2}q(0)\right)\cos(\omega_i t) + \frac{p_i(0)}{m_i\omega_i}\sin(\omega_i t)\right] \tag{4.12}$$

represents a fluctuating force and depends on the initial conditions of both the system and the bath. Its equilibrium expectation value (for the definition see (4.38) below) with respect to the heat bath including the coupling to the system, i.e. $H_{\mathrm{B}} + H_{\mathrm{SB}}$, vanishes.

4.2.3   Spectral density of bath modes

So far, we have considered a heat bath with a finite number of harmonic oscillators. If the system is also a harmonic oscillator, we may choose a normal mode representation and convince ourselves that the whole system will return to its initial state after a finite time, the Poincaré recurrence time [9]. In order to actually describe dissipation, this time has to be very long which certainly is the case for a continuous distribution of bath modes. We therefore take the limit $N \to \infty$ and replace sums by integrals. It is convenient to introduce the spectral density of bath modes as

$$J(\omega) = \pi\sum_{i=1}^{N}\frac{c_i^2}{2m_i\omega_i}\delta(\omega - \omega_i). \tag{4.13}$$

This quantity contains information on the frequencies of the modes and their coupling to the system and is in fact sufficient to characterize the heat bath. By appropriately choosing the parameters c_i, m_i, and ω_i we may model any spectral density of bath modes. This is even true if we set $c_i = m_i\omega_i^2$ as we did on page 215. In Section 3.4.1 it is shown how for an electrical circuit the impedance is related to the spectral density $J(\omega)$.

With (4.11) and (4.13) we may relate the spectral density of bath modes to the damping kernel by

$$\gamma(t) = \frac{2}{M} \int_0^\infty \frac{\mathrm{d}\omega}{\pi} \frac{J(\omega)}{\omega} \cos(\omega t). \tag{4.14}$$

Setting $J(\omega) = M\gamma\omega$, we obtain the Ohmic damping kernel $\gamma(t) = 2\gamma\delta(t)$. Since the integral in (4.10) ends at $s = t$, the delta function counts only half, and we thus obtain the damping term introduced in (4.1). The Ohmic model represents the prototype for damping and is therefore often used. However, it is not very realistic in its strict form because the spectral density of bath modes diverges for large frequencies. In practice, one always has a cutoff which may take different forms. One possibility is the so-called Drude model where the spectral density

$$J(\omega) = M\gamma\omega\frac{\omega_\mathrm{D}^2}{\omega^2 + \omega_\mathrm{D}^2} \tag{4.15}$$

behaves like in the Ohmic case for small frequencies but goes smoothly to zero above the Drude frequency ω_D. Together with (4.14), we get for the damping kernel at times $t > 0$

$$\gamma(t) = \gamma\omega_\mathrm{D}\mathrm{e}^{-\omega_\mathrm{D}t}. \tag{4.16}$$

The damping strength defined as the integral over the damping kernel

$$\gamma_0 = \int_0^\infty \mathrm{d}t\,\gamma(t) \tag{4.17}$$

yields $\gamma_0 = \gamma$ like in the Ohmic case. However, the damping kernel (4.16) exhibits memory on the time scale

$$\tau_\mathrm{c} = \frac{1}{\gamma_0} \int_0^\infty \mathrm{d}t\,t\gamma(t) \tag{4.18}$$

with $\tau_\mathrm{c} = \omega_\mathrm{D}^{-1}$ in the Drude model. If we are not interested in time scales shorter than τ_c, which usually is the case if ω_D represents the largest frequency scale, these memory effects may often be neglected, and the Ohmic model may be employed instead.

4.2.4   Rubin model

A rather nontrivial damping kernel is obtained by considering a heavy particle (the system) of mass M coupled to two semi-infinite chains of harmonic oscillators (the
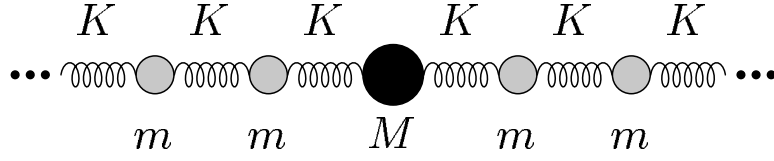
Fig. 4.1: Mechanical realization of the Rubin model.

heat bath) with masses m and coupling constants K, the so-called Rubin model [10] shown in Fig. 4.1. The corresponding Hamiltonian is given by

$$H = \frac{p^2}{2M} + V(q) + \sum_{n=1}^{\infty} \frac{p_n^2}{2m} + \frac{K}{2} \sum_{n=1}^{\infty} (x_{n+1} - x_n)^2 + \frac{K}{2}(q - x_1)^2 \qquad (4.19)$$

where we have taken into consideration only the right part of the oscillator chain. Due to the symmetry the left chain may later be accounted for in the spectral density $J(\omega)$ by an additional factor of two. The Hamiltonian (4.19) couples the bath oscillators and is therefore not of the form (4.5). However, the reservoir contribution may be diagonalized by means of the ansatz

$$x_n = \sqrt{\frac{2}{\pi}} \int_0^{\pi} dk \sin(kn) \widetilde{x}(k). \qquad (4.20)$$

Together with the relation

$$\sum_{n=-\infty}^{+\infty} e^{ink} = 2\pi \sum_{n=-\infty}^{+\infty} \delta(k - 2\pi n), \qquad (4.21)$$

we arrive at the transformed Hamiltonian

$$H = \frac{p^2}{2M} + V(q) + \frac{1}{2m} \int_0^{\pi} dk \, \widetilde{p}(k)^2 + 2K \int_0^{\pi} dk \, \widetilde{x}(k)^2 \sin^2(k/2)$$

$$-q\sqrt{\frac{2}{\pi}} K \int_0^{\pi} dk \, \widetilde{x}(k) \sin(k) + \frac{K}{2}q^2 \qquad (4.22)$$

where $\widetilde{p}(k)$ denotes the momentum conjugate to $\widetilde{x}(k)$. For the coupling constant corresponding to c_i we obtain by comparison with (4.4)

$$c(k) = \sqrt{\frac{2}{\pi}} K \sin(k). \qquad (4.23)$$

The frequencies of the bath oscillators form a continuous spectrum with

$$\omega(k) = \omega_{\mathrm{L}} \sin(k/2) \qquad (4.24)$$

and a maximum frequency

$$\omega_{\mathrm{L}} = 2\sqrt{\frac{K}{m}}. \tag{4.25}$$

Inserting these results into (4.13) and accounting also for the left oscillator chain, we find for the spectral density of bath oscillators

$$J(\omega) = \frac{2K^2}{m\omega_{\mathrm{L}}} \int_0^\pi \mathrm{d}k \, \frac{\sin^2(k)}{\sin(k/2)} \delta(\omega - \omega_{\mathrm{L}} \sin(k/2)). \tag{4.26}$$

With (4.14), we obtain for the damping kernel

$$\gamma(t) = \frac{4K}{M\pi} \int_0^\pi \mathrm{d}k \, \cos^2(k/2) \cos\left(\omega_{\mathrm{L}} t \sin(k/2)\right). \tag{4.27}$$

The integral may be expressed in terms of a Bessel function of the first kind

$$\gamma(t) = r\omega_{\mathrm{L}} \frac{J_1(\omega_{\mathrm{L}} t)}{t} \tag{4.28}$$

where we introduced the mass ratio $r = m/M$. Making use of the asymptotic expansion of the Bessel function, we get for the damping kernel at long times

$$\gamma(t) = r\sqrt{\frac{2\omega_{\mathrm{L}}}{\pi}} \frac{\sin(\omega_{\mathrm{L}} t - \pi/4)}{t^{3/2}} \quad \text{for } t \to \infty \tag{4.29}$$

which in contrast to the Drude case decays only algebraically. In addition, the damping kernel is not always positive. Nevertheless, the integrated damping strength, which equals $r\omega_{\mathrm{L}}$, is positive, indicating that the two chains of oscillators indeed cause dissipation. The memory introduced by coupling to the chains is determined by the characteristic frequency of the chains with $\tau_{\mathrm{c}} = \omega_{\mathrm{L}}^{-1}$ as can be seen by evaluating (4.18) for the damping kernel (4.28).

4.3   Density matrices

Before we can continue by considering specific systems, we have to remind ourselves of some facts from quantum statistical mechanics. In ordinary quantum mechanics a state is described by a state vector $|\psi\rangle$. In quantum statistics this is no longer sufficient, and one has to introduce density matrices of the general form

$$\rho = \sum_{n,m} \rho_{nm} |n\rangle\langle m| \tag{4.30}$$

where the states $|n\rangle$ form a complete set. The density matrix should be normalized according to

$$\mathrm{tr}(\rho) = \sum_k \langle k|\rho|k\rangle = 1. \tag{4.31}$$

Again, the sum runs over a complete set of states. A pure state would be represented by $\rho = |\psi\rangle\langle\psi|$. However, often only probabilities p_n are known with which the states $|n\rangle$ are found. The lack of phase information then makes it impossible to describe the state by a state vector. Instead we have to use the density matrix

$$\rho = \sum_n p_n |n\rangle\langle n|. \tag{4.32}$$

One can show that $\text{tr}(\rho^2) \le 1$, where the equality only holds for density matrices describing pure states.

The most prominent example of a density matrix is the equilibrium density matrix

$$\rho_\beta = \frac{1}{Z_\beta} e^{-\beta H} = \frac{1}{Z_\beta} \sum_n e^{-\beta E_n} |n\rangle\langle n| \tag{4.33}$$

where $|n\rangle$ are energy eigenstates and the probabilities p_n are given by Boltzmann weights at inverse temperature $\beta = 1/k_B T$. The normalization is provided by the partition function

$$Z_\beta = \text{tr}\left(e^{-\beta H}\right). \tag{4.34}$$

The equation of motion for a density matrix is obtained by differentiating (4.30) with respect to time and employing the time-dependent Schrödinger equation. This leads us to

$$\dot{\rho}(t) = -i\mathcal{L}(t)\rho(t) \tag{4.35}$$

where the Liouville operator

$$\mathcal{L}X = \frac{1}{\hbar}[H, X] \tag{4.36}$$

represents a superoperator acting on an operator X. At first sight, (4.35) looks like a Heisenberg equation of motion. However, there is an extra minus sign and in fact (4.35) was derived within the Schrödinger picture.

Finally, we may express expectation values of observables through the density matrix as

$$\langle A \rangle = \text{tr}(\rho A) \tag{4.37}$$

where the equilibrium expectation value

$$\langle A \rangle_\beta = \text{tr}(\rho_\beta A) \tag{4.38}$$

taken with respect to the equilibrium density matrix as indicated by the subscript β plays an important role.

4.4   Linear damped systems

As a first example we discuss one of the simplest dissipative quantum systems, the damped harmonic oscillator. The corresponding Hamiltonian is given by (4.2)–(4.5) with the potential

$$V(q) = \frac{M}{2}\omega_0^2 q^2. \tag{4.39}$$

Because of its linear equation of motion, the problem may be solved exactly not only in the classical but also the quantum case.

   We start out by recapitulating some facts from linear response theory. In particular, we introduce the response function (Section 4.4.1) and derive the fluctuation-dissipation theorem (Section 4.4.2). While linear response theory is exact for linear systems like the damped harmonic oscillator, the concepts presented here may also be useful when considering nonlinear systems.

   The fluctuation-dissipation theorem will allow us to make a connection between the damped motion as given by the response function and the fluctuations described by correlation functions. In Section 4.4.3 we discuss in some detail the equilibrium correlation functions of the damped harmonic oscillator while paying special attention to the low temperature properties. The free damped particle is obtained as a limiting case in Section 4.4.4.

4.4.1   Response function

In linear response theory one considers the influence of an external force on the system to first order in this force. The starting point therefore is the Hamiltonian

$$H(t) = H - h_G(t)G \tag{4.40}$$

which in general may depend on time and where the first part is given by (4.5). G is an operator acting only in the Hilbert space of the system while h_G is a c-number which should vanish for negative times. Such a situation was already discussed in Section 1.2.3 where the Kubo-Greenwood formula for the conductivity was derived within linear response theory.

   Our aim is now to calculate the deviation

$$\Delta\langle F(t)\rangle = \langle F(t)\rangle - \langle F\rangle_\beta \tag{4.41}$$

of the expectation value of the system operator F in presence of an applied force from its equilibrium value $\langle F\rangle_\beta$ taken for $h_G = 0$. The time evolution of the expectation value $\langle F(t)\rangle$ in the Schrödinger picture is governed by the time evolution of the density matrix according to (4.35). Decomposing the Liouville operator

$$\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_1 \tag{4.42}$$

with

$$\mathcal{L}_0 X = \frac{1}{\hbar}[H, X] \tag{4.43}$$

and

$$\mathcal{L}_1 X = -\frac{1}{\hbar}[G, X]h_G(t), \tag{4.44}$$

we may formally solve the equation of motion for the density matrix as

$$\rho(t) = e^{-i\mathcal{L}_0 t}\rho(0) - i\int_0^t ds\, e^{-i\mathcal{L}_0(t-s)}\mathcal{L}_1(s)\rho(s). \tag{4.45}$$

Assuming that the external force has been absent for negative times, we may replace the initial density matrix $\rho(0)$ by the equilibrium density matrix. Iteration of the integral equation then yields [11]

$$\rho(t) = \rho_\beta - i\int_0^t ds\, e^{-i\mathcal{L}_0(t-s)}\mathcal{L}_1(s)\rho_\beta + \mathcal{O}(h_G^2). \tag{4.46}$$

Within linear response theory the iteration is carried out only up to first order. As already mentioned this is exact for linear systems and otherwise represents a good approximation for sufficiently weak forces, i.e. small h_G.

With (4.46) we get for the time dependence of the expectation value of F up to first order in h_G

$$\langle F(t)\rangle = \langle F\rangle_\beta + \frac{i}{\hbar}\int_0^t ds\, \text{tr}\left(Fe^{-i\mathcal{L}_0(t-s)}[G, \rho_\beta]\right)h_G(s). \tag{4.47}$$

By means of the relation

$$\exp(-i\mathcal{L}_0 t)X = \exp\left(-\frac{i}{\hbar}H_0 t\right)X\exp\left(\frac{i}{\hbar}H_0 t\right) \tag{4.48}$$

and the cyclic invariance of the trace, we may switch from the Schrödinger to the Heisenberg picture by letting the exponential containing the Liouville operator generate the time dependence of the operator F. This leaves us finally with

$$\Delta\langle F(t)\rangle = \frac{i}{\hbar}\int_0^t ds\, \text{tr}([F(t-s), G]\rho_\beta)h_G(s). \tag{4.49}$$

This result, which establishes a linear relation between the external force h_G conjugate to the system operator G and the response of the observable F, allows us to define a response function χ_{FG} as

$$\Delta\langle F(t)\rangle = \int_0^t ds\chi_{FG}(t-s)h_G(s). \tag{4.50}$$

Comparison with (4.49) finally yields [11]

$$\chi_{FG}(t) = \frac{i}{\hbar}\langle [F(t), G]\rangle_\beta\Theta(t) \tag{4.51}$$

where we introduced a step function $\Theta(t)$ which makes causality manifest.

As an example, we consider the response function χ_{qq} of the damped harmonic oscillator which may now be obtained by taking the commutator of the equation of motion (4.10) with $q(0)$. Since the commutator with the noise term (4.12) vanishes, we find that the response function obeys the differential equation

$$\ddot{\chi}_{qq}(t) + \int_0^t ds \gamma(t-s)\dot{\chi}_{qq}(s) + \omega_0^2 \chi_{qq}(t) = 0 \qquad (4.52)$$

with the initial conditions

$$\chi_{qq}(0) = \frac{i}{\hbar}\langle[q(0), q(0)]\rangle_\beta = 0 \qquad (4.53)$$

and

$$\dot{\chi}_{qq}(0) = \frac{i}{M\hbar}\langle[p(0), q(0)]\rangle_\beta = \frac{1}{M}. \qquad (4.54)$$

Two comments are now in order. Firstly, (4.52) could have been obtained more directly by making use of (4.50) and (4.10). However, our derivation has lead to the relation (4.51) which will be of importance later on. Secondly, (4.52) is identical to the corresponding classical equation for the response function. Thus, the classical response function for the damped harmonic oscillator and its quantum version are identical. This is a direct consequence of the Ehrenfest theorem.

Unfortunately, it is not possible to evaluate the response function for arbitrary damping kernel in closed form. However, we may determine the corresponding dynamic susceptibility

$$\tilde{\chi}_{qq}(\omega) = \int_{-\infty}^{+\infty} dt\, \chi_{qq}(t) e^{i\omega t} = \hat{\chi}_{qq}(-i\omega) \qquad (4.55)$$

where we introduced the Laplace transform

$$\hat{\chi}_{qq}(z) = \int_0^\infty dt\, e^{-zt} \chi_{qq}(t) \qquad (4.56)$$

and made use of causality. From (4.52) together with the initial conditions (4.53) and (4.54) we find

$$\tilde{\chi}_{qq}(\omega) = \frac{1}{M} \frac{1}{-\omega^2 - i\omega\tilde{\gamma}(\omega) + \omega_0^2}. \qquad (4.57)$$

A valid damping kernel will lead to poles of (4.57) in the lower half plane to ensure causality of the response function.

For Ohmic damping with $\tilde{\gamma}(\omega) = \gamma$ the inverse Fourier transform may be performed, and one obtains the response function

$$\chi_{qq}(t) = \frac{1}{M\bar{\omega}} e^{-\gamma t/2} \sin(\bar{\omega}t)\, \Theta(t) \qquad (4.58)$$

with a frequency

$$\bar{\omega} = \sqrt{\omega_0^2 - \frac{\gamma^2}{4}} \qquad (4.59)$$

shifted due to the damping.

4.4.2   Fluctuation-dissipation theorem

We now calculate the power

$$P = \sum_F h_F(t) \frac{\mathrm{d}}{\mathrm{d}t} \Delta \langle F(t) \rangle \tag{4.60}$$

dissipated due to all external forces $h_F(t)$ in order to relate the response function to dissipation. The change in the expectation value of the observable F is induced by external forces conjugate to all observables G

$$h_G(t) = \widetilde{h}_G(\omega) \mathrm{e}^{-\mathrm{i}\omega t} + \widetilde{h}_G^*(\omega) \mathrm{e}^{\mathrm{i}\omega t} \tag{4.61}$$

which we take to be monochromatic for convenience. From (4.50) we obtain together with (4.55)

$$\frac{\mathrm{d}}{\mathrm{d}t} \Delta \langle F(t) \rangle = - \sum_G \mathrm{i}\omega \left[\widetilde{h}_G(\omega) \mathrm{e}^{-\mathrm{i}\omega t} \widetilde{\chi}_{FG}(\omega) - \widetilde{h}_G^*(\omega) \mathrm{e}^{\mathrm{i}\omega t} \widetilde{\chi}_{FG}(-\omega) \right]. \tag{4.62}$$

For the dissipated power (4.60) averaged over one period of the driving forces we thus find

$$\bar{P} = \sum_{F,G} 2\omega \widetilde{h}_F^*(\omega) \widetilde{h}_G(\omega) \widetilde{\chi}_{FG}^{\mathrm{d}}(\omega). \tag{4.63}$$

This expression contains the dissipative part of the dynamic susceptibility

$$\widetilde{\chi}_{FG}^{\mathrm{d}}(\omega) = \frac{1}{2\mathrm{i}} \left(\widetilde{\chi}_{FG}(\omega) - \widetilde{\chi}_{GF}(-\omega) \right) \tag{4.64}$$

which depending on the time reversal symmetry of the observables is given by the imaginary or real part of the dynamic susceptibility.

Equilibrium fluctuations may be described by equilibrium correlation functions

$$C_{FG}(t) = \langle F(t) G(0) \rangle_\beta \tag{4.65}$$

which are defined according to (4.38). The definition may be used to show stationarity

$$\langle F(t) G(0) \rangle_\beta = \langle F(0) G(-t) \rangle_\beta \tag{4.66}$$

by exploiting the cyclic invariance of the trace. Using the same technique one can derive the symmetry

$$C_{FG}(t) = C_{GF}(-t - \mathrm{i}\hbar\beta). \tag{4.67}$$

Introducing the spectral function

$$\widetilde{C}_{FG}(\omega) = \int_{-\infty}^{+\infty} \mathrm{d}t \, C_{FG}(t) \mathrm{e}^{\mathrm{i}\omega t}, \tag{4.68}$$

this relation turns into

$$\widetilde{C}_{FG}(\omega) = \widetilde{C}_{GF}(-\omega)\mathrm{e}^{\beta\hbar\omega}. \tag{4.69}$$

It is convenient to introduce the symmetrized and the antisymmetrized equilibrium correlation functions

$$S_{FG}(t) = \frac{1}{2}\langle F(t)G(0) + G(0)F(t)\rangle_\beta \tag{4.70}$$

and

$$A_{FG}(t) = \frac{1}{2\mathrm{i}}\langle F(t)G(0) - G(0)F(t)\rangle_\beta, \tag{4.71}$$

respectively. For the Fourier transform of the antisymmetrized equilibrium correlation function we then find with (4.69)

$$\widetilde{A}_{FG}(\omega) = \frac{1}{2\mathrm{i}}(1 - \mathrm{e}^{-\hbar\beta\omega})\widetilde{C}_{FG}(\omega). \tag{4.72}$$

Making use of the result (4.51) of linear response theory, our expression (4.64) for the dissipative part of the dynamic susceptibility becomes

$$\widetilde{\chi}^{\mathrm{d}}_{FG}(\omega) = \frac{\mathrm{i}}{\hbar}\widetilde{A}_{FG}(\omega) \tag{4.73}$$

or in view of (4.72)

$$\widetilde{\chi}^{\mathrm{d}}_{FG}(\omega) = \frac{1}{2\hbar}(1 - \mathrm{e}^{-\hbar\beta\omega})\widetilde{C}_{FG}(\omega). \tag{4.74}$$

This relation is called fluctuation-dissipation theorem [12] because it relates the dissipative part $\widetilde{\chi}^{\mathrm{d}}_{FG}(\omega)$ of the dynamic susceptibility to the equilibrium fluctuations described by its spectral function $\widetilde{C}_{FG}(\omega)$.

4.4.3   Correlation functions of the damped harmonic oscillator

The fluctuation-dissipation theorem was derived within linear response theory and is therefore an exact relation for the damped harmonic oscillator. Following Ref. [13] we may thus use the theorem to determine the equilibrium correlation functions for this system. It is sufficient to calculate the position autocorrelation function

$$C_{qq}(t) = \langle q(t)q(0)\rangle_\beta \tag{4.75}$$

from which we may obtain the other correlation functions

$$C_{pq}(t) = -C_{qp}(t) = M\frac{\mathrm{d}}{\mathrm{d}t}C_{qq}(t) \tag{4.76}$$

$$C_{pp}(t) = -M^2\frac{\mathrm{d}^2}{\mathrm{d}t^2}C_{qq}(t) \tag{4.77}$$

by differentiation with respect to time. These expressions may be derived by using $p = M\dot{q}$ and the stationarity (4.66) of equilibrium correlation functions.

The fluctuation-dissipation theorem allows us to express the equilibrium position autocorrelation function in terms of the imaginary part of the dynamical susceptibility (4.57). We consider specifically the case of Ohmic damping for which analytical results may be obtained. After a Fourier transformation the fluctuation-dissipation theorem reads

$$C_{qq}(t) = \frac{\hbar}{M\pi} \int_{-\infty}^{+\infty} d\omega \frac{\gamma\omega}{(\omega^2 - \omega_0^2)^2 + \gamma^2\omega^2} \frac{e^{-i\omega t}}{1 - e^{-\beta\hbar\omega}}. \tag{4.78}$$

Making use of the relation

$$\frac{1}{1 - e^{-\beta\hbar\omega}} = \frac{1}{2} + \frac{1}{2}\coth\left(\frac{\hbar\beta\omega}{2}\right), \tag{4.79}$$

we decompose the correlation function $C_{qq}(t) = S_{qq}(t) + iA_{qq}(t)$ into its symmetric part

$$S_{qq}(t) = \frac{\hbar}{2\pi M} \int_{-\infty}^{+\infty} d\omega \frac{\gamma\omega}{(\omega^2 - \omega_0^2)^2 + \gamma^2\omega^2} \coth\left(\frac{1}{2}\beta\hbar\omega\right)\cos(\omega t) \tag{4.80}$$

and its antisymmetric part

$$A_{qq}(t) = -\frac{\hbar}{2\pi M} \int_{-\infty}^{+\infty} d\omega \frac{\gamma\omega}{(\omega^2 - \omega_0^2)^2 + \gamma^2\omega^2}\sin(\omega t) \tag{4.81}$$

which agree with the definitions (4.70) and (4.71), respectively. The antisymmetric correlation function may be evaluated by complex contour integration yielding

$$A_{qq}(t) = -\frac{\hbar}{2M\bar{\omega}}e^{-\gamma|t|/2}\sin(\bar{\omega}t). \tag{4.82}$$

According to (4.71), this correlation function is related to a commutator which should be zero in the classical limit. This is indeed the case as one can readily see by taking the limit $\hbar \to 0$. It should be noted, however, that (4.82) does not contain specific quantum effects but is directly related to the classical response function (4.58) by

$$\chi_{qq}(t) = -\frac{2}{\hbar}A_{qq}(t)\Theta(t) \tag{4.83}$$

which is a consequence of (4.51) and (4.71).

For the evaluation of the symmetric correlation function (4.80), we first decompose the hyperbolic cotangent as

$$\coth\left(\frac{1}{2}\hbar\beta\omega\right) = \frac{2}{\beta\hbar\omega}\left(1 + 2\sum_{n=1}^{\infty}\frac{\omega^2}{\nu_n^2 + \omega^2}\right) \tag{4.84}$$

where we have introduced the so-called Matsubara frequencies

$$\nu_n = \frac{2\pi}{\hbar\beta}n. \tag{4.85}$$

It is interesting at this point to discuss the physical significance of the terms appearing in (4.84). The $\hbar$ in the prefactor cancels with the prefactor of the integral (4.80) so that the first term in the brackets of (4.84) is independent of $\hbar$ and proportional to the temperature. It therefore represents the classical result. The sum in (4.84), on the other hand, gives rise to quantum corrections which are present here in contrast to the antisymmetric correlation function.

The integrand of (4.80) has poles at

$$\omega = \pm \left(\bar{\omega} \pm \mathrm{i}\frac{\gamma}{2} \right) \tag{4.86}$$

with $\bar{\omega}$ defined by (4.59). In view of (4.84), there are additional poles at $\omega = \pm \mathrm{i}\nu_n$. Evaluating the integral by complex contour integration one obtains after some straightforward calculation for the symmetric correlation function

$$S_{qq}(t) = \frac{\hbar}{2M\bar{\omega}} \frac{\exp\left(-\frac{\gamma}{2}|t|\right)}{\cosh(\hbar\beta\bar{\omega}) - \cos(\hbar\beta\gamma/2)} \left[\sinh(\hbar\beta\bar{\omega})\cos(\bar{\omega}t) + \sin(\hbar\beta\gamma/2)\sin(\bar{\omega}|t|)\right]$$

$$- \frac{2\gamma}{M\beta} \sum_{n=1}^{\infty} \frac{\nu_n \mathrm{e}^{-\nu_n|t|}}{(\nu_n^2 + \omega_0^2)^2 - \gamma^2\nu_n^2}. \tag{4.87}$$

In the classical limit $\hbar \to 0$, which here is equivalent to the high temperature limit, this becomes

$$S_{qq}(t) = \frac{1}{M\beta\omega_0^2} \exp(-\frac{\gamma}{2}|t|) \left[\cos(\bar{\omega}t) + \frac{\gamma}{2\bar{\omega}}\sin(\bar{\omega}|t|)\right]. \tag{4.88}$$

According to (4.75) and (4.77), the classical second moments of position and momentum are then obtained as

$$\langle q^2 \rangle_\beta = \frac{k_{\mathrm{B}}T}{M\omega_0^2} \tag{4.89}$$

$$\langle p^2 \rangle_\beta = M k_{\mathrm{B}}T. \tag{4.90}$$

Quantum effects come into play if we lower the temperature so that no longer $k_{\mathrm{B}}T \gg \hbar\omega_0$. Since these effects already exist in the undamped case, it is more interesting to consider another regime which is present for finite damping only. Comparing the exponential decay of the different terms in (4.87), we notice that the first term determines the long time behavior only if $\hbar\gamma/4\pi k_{\mathrm{B}}T \ll 1$, i.e. for sufficiently weak damping or for sufficiently high temperatures. Otherwise, the exponential decay with a time constant given by the Matsubara frequency ν_1 will dominate the long time behavior. In contrast to the assumption made in standard weak coupling theories, the decay of the correlation function is then no longer governed by the damping constant. This becomes especially apparent at zero temperature. With decreasing temperature

the Matsubara frequencies ν_n get closer to each other and at zero temperature all of them contribute. We may then replace the sum in (4.87) by an integral

$$\lim_{\beta \to \infty} \frac{2\gamma}{M\beta} \sum_{n=1}^{\infty} \frac{\nu_n e^{-\nu_n t}}{(\nu_n^2 + \omega_0^2)^2 - \gamma^2 \nu_n^2} = \frac{\hbar\gamma}{\pi M} \int_0^{\infty} dx \frac{x e^{-xt}}{(x^2 + \omega_0^2)^2 - \gamma^2 x^2} \qquad (4.91)$$

which may be expressed in terms of exponential integral functions. The leading long time behavior, however, may easily be obtained by replacing the integrand by its behavior for small values of the integration variable. One thus finds that all exponential terms act together to produce an algebraic decay of the correlation function

$$S_{qq}(t) = -\frac{\hbar\gamma}{\pi M \omega_0^4} \frac{1}{t^2} \quad \text{for } t \to \infty. \qquad (4.92)$$

This behavior is not purely academic because it can be found at low but finite temperatures at intermediate times before the exponential decay takes over [14].

After the long time behavior we now take a look at the second moments of position and momentum, i.e. the correlation functions at time zero, at zero temperature. With (4.87) and (4.91) one finds after evaluation of the integral at $t = 0$

$$\langle q^2 \rangle_\beta = \frac{\hbar}{2M\bar{\omega}} \left[1 - \frac{2}{\pi} \arctan\left(\frac{\gamma}{2\bar{\omega}}\right) \right] \qquad (4.93)$$

which for $\gamma \to 0$ reduces to the correct quantum mechanical result for the undamped oscillator $\langle q^2 \rangle_\beta = \hbar/2M\omega_0$. In contrast, the second moment of the momentum diverges for any finite damping as can be seen from (4.80) by differentiating twice with respect to time. This ultraviolet divergence is due to the spectral density which for Ohmic damping increases proportional to frequency. Therefore, one has to introduce a cutoff for the spectral density like in the Drude model (4.15). The memoryfree Ohmic damping kernel is then broadened and the divergence removed.

4.4.4 Free damped particle

A free damped particle can be viewed as a particle subject to damping moving in a harmonic potential with $\omega_0 \to 0$. In contrast to the damped harmonic oscillator discussed in the previous section, the particle is no longer bounded and exhibits diffusive motion.

From (4.80) it is obvious, that the second moment of the position $S_{qq}(0)$ does not exist since for the free particle the integrand diverges at small frequencies. This is of course a consequence of the fact that the particle is not bounded but may be found everywhere. Therefore, we introduce the mean square displacement

$$s(t) = \langle (q(t) - q(0))^2 \rangle_\beta \qquad (4.94)$$

which is related to the symmetric position autocorrelation function by

$$s(t) = 2 \left[\langle q^2 \rangle_\beta - S_{qq}(t) \right]. \qquad (4.95)$$

For any finite temperature, the long time behavior of $s(t)$ is given by the first term in (4.87). In the limit $\omega_0 \to 0$, one finds

$$s(t) = \frac{2}{M\beta\gamma}t \quad \text{for } t \to \infty \tag{4.96}$$

with the leading corrections being time-independent. This represents the classical diffusive behavior for which a diffusion constant can be defined as

$$D = \frac{1}{2}\lim_{t\to\infty}\frac{s(t)}{t}. \tag{4.97}$$

From (4.96) we thus get the so-called Einstein relation [15]

$$D = \frac{k_\mathrm{B}T}{M\gamma} \tag{4.98}$$

which in slightly different form appeared already in (1.6). Quantum fluctuations do not affect this result even for very low temperatures except that the time after which (4.96) is valid may become quite large. For zero temperature, however, the diffusion constant vanishes, and thus the mean square displacement no longer increases linearly for long times. In this case the infinite sum in (4.87) determines the long time behavior. The latter is obtained from the integral representation (4.91) in the limit $\omega_0 \to 0$. For long times the integral is again dominated by small values of the integration variable. We obtain

$$s(t) = \frac{2\hbar}{\pi M\gamma}\log(\gamma t) \quad \text{for } t \to \infty. \tag{4.99}$$

In the absence of thermal fluctuations the mean square displacement thus grows only logarithmically [16].

4.5   Short introduction to path integrals

The path-integral formalism has been quite successful in recent years in the context of quantum dissipative systems. This formalism was originally invented by Feynman [17] as an alternative formulation of quantum mechanics which can be shown to be equivalent to the more familiar Schrödinger equation approach. Here, we do not want to go into the mathematical subtleties of path integrals but give a more practical introduction as far as it will be needed in the following.

The time evolution of a state $|\Psi\rangle$ of an undamped quantum system is governed by the time-dependent Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\Psi\rangle = H|\Psi\rangle \tag{4.100}$$

where H is the Hamiltonian describing the system. For a time-independent Hamiltonian we may formally integrate (4.100) to obtain the time evolution of the initial state $|\Psi(0)\rangle$ according to

$$|\Psi(t)\rangle = \exp\left(-\frac{i}{\hbar}Ht\right)|\Psi(0)\rangle. \tag{4.101}$$

Introducing the propagator in coordinate representation from the initial position q_i to the final position q_f

$$G(q_f, q_i, t) = \langle q_f| \exp\left(-\frac{i}{\hbar}Ht\right)|q_i\rangle, \tag{4.102}$$

which was already encountered in the discussion of Green functions in Section 1.2.2, we may express the time evolution of a state as

$$\Psi(q_f, t) = \int dq_i\, G(q_f, q_i, t)\Psi(q_i, 0) \tag{4.103}$$

where we have to integrate over all initial positions.

One of the advantages of the path-integral formulation of quantum mechanics is the absence of operators. Instead, one uses the classical action $S[q]$ which is defined by the classical Lagrange function $L(q, \dot{q}, t)$ as

$$S[q] = \int_0^t ds\, L(q, \dot{q}, s). \tag{4.104}$$

In contrast to a function like the Lagrange function L which relates a number to a number, the action is a functional which relates a function to a number. Here, the function is the path $q(s)$ starting at time $s = 0$ and ending at $s = t$. According to Feynman the propagator (4.102) may now be written as

$$G(q_f, q_i, t) = \int_{q(0)=q_i}^{q(t)=q_f} \mathcal{D}q\, \exp\left(\frac{i}{\hbar}S[q]\right). \tag{4.105}$$

The right-hand-side represents a path integral or functional integral. In analogy to the difference between a function and a functional, this integral does not run over an interval as usual, but one has to integrate over all paths satisfying the boundary conditions $q(0) = q_i$ and $q(t) = q_f$. To distinguish between integrals and path integrals, we have replaced the "d" by a "$\mathcal{D}$". We do not want to prove the validity of (4.105) here, but refer the reader to the literature [18].

The physical meaning of (4.105) becomes clear by first considering the classical limit $\hbar \to 0$. In this case, the integrand will oscillate very rapidly and the contributions of neighboring paths will cancel. The only exception are extrema of the action, i.e. paths where its first variation vanishes. This is of course equivalent to Hamilton's principle of classical mechanics. Hence, in the classical limit, only the classical paths contribute to the propagator. In the quantum regime, other paths also contribute and the most important contributions come from fluctuations around the classical paths. In the remainder of this section we assume for simplicity that there is just one classical path.

Although we do not have to deal with operators anymore, it can be quite hard to evaluate the path integral and to get an exact result for the propagator. However, it is often possible to make a so-called semiclassical approximation where fluctuations around the classical path are treated up to second order. According to our above discussion, the classical path q_{cl} gives the dominant contribution to the path integral. It therefore makes sense to expand the paths around the classical path according to

$$q(s) = q_{\mathrm{cl}}(s) + \xi(s). \tag{4.106}$$

Since the classical path satisfies the boundary conditions, the fluctuations $\xi(s)$ have to vanish at times $s = 0$ and t. Accordingly, we expand the action

$$S[q] = S[q_{\mathrm{cl}}] + \int_0^t \mathrm{d}s \; \frac{\delta S}{\delta q(s)}\bigg|_{q_{\mathrm{cl}}} \xi(s)$$

$$+ \frac{1}{2} \int_0^t \mathrm{d}s \int_0^t \mathrm{d}u \; \frac{\delta^2 S}{\delta q(s)\delta q(u)}\bigg|_{q_{\mathrm{cl}}} \xi(s)\xi(u) + \dots \tag{4.107}$$

where δ denotes the functional derivative. Since the classical path is a stationary point of the action, the second term on the right-hand-side of (4.107) vanishes. The first quantum corrections are thus described by the term which is quadratic in the fluctuations. For actions which are at most quadratic in the path, e.g. for the free particle and the harmonic oscillator, the expansion will break off after the second term. Therefore, taking into account only the terms given in (4.107) will then yield an exact result. In general, however, there will be higher order terms. If $\hbar$ can be taken to be small, the exponential in (4.105) represents a Gaussian in the vicinity of the classical path. Its width $\hbar$ limits the possible fluctuations to be of order $\sqrt{\hbar}$ or less. The quadratic term in (4.107) is therefore of order 1 while higher order terms are smaller by at least a factor $\sqrt{\hbar}$. As a consequence, restriction to the quadratic term implies a semiclassical approximation.

For damped quantum systems it is not sufficient to consider the propagator because we do not deal with pure states. We rather have to treat density matrices, the most important of which is of course the equilibrium density matrix introduced in (4.33). If we write the equilibrium density matrix in its coordinate representation

$$\rho_\beta(q, q') = \frac{1}{Z_\beta} \langle q | \mathrm{e}^{-\beta H} | q' \rangle, \tag{4.108}$$

we notice that this is quite similar to the expression (4.102) for the propagator. A comparison of the two exponents suggests to interpret the temperature as an imaginary time $t = -\mathrm{i}\hbar\beta$. By further exploiting this analogy, we may express the equilibrium density matrix in terms of a path integral. We call this an imaginary-time path integral in order to distinguish it from the real-time path integral (4.105).

We convert the real-time path integral into an imaginary-time path integral by considering the action, which for a particle of mass M moving in a potential $V(q)$ is

given by

$$S[q, t] = \int_0^t ds \left[\frac{M}{2} \left(\frac{dq}{ds} \right)^2 - V(q) \right] \tag{4.109}$$

where we specified the final time t as argument of S explicitly for sake of clarity. Replacing t by $-i\hbar\beta$ and substituting s by $-i\tau$ we obtain

$$S[q, -i\hbar\beta] = i \int_0^{\hbar\beta} d\tau \left[\frac{M}{2} \left(\frac{dq}{d\tau} \right)^2 + V(q) \right]. \tag{4.110}$$

It is convenient to rewrite this equation as

$$S[q, -i\hbar\beta] = iS^{\mathrm{E}}[q, \hbar\beta] \tag{4.111}$$

by introducing the so-called Euclidean action

$$S^{\mathrm{E}}[q, \hbar\beta] = \int_0^{\hbar\beta} d\tau \left[\frac{M}{2} \left(\frac{dq}{d\tau} \right)^2 + V(q) \right]. \tag{4.112}$$

While this looks formally like an action, we note that the Euclidean action describes the motion of a particle in the inverted potential $-V(q)$. Given the analogy between the coordinate representations of the propagator (4.102) and the equilibrium density matrix (4.108), we obtain together with (4.111) the imaginary-time path-integral representation of the equilibrium density matrix

$$\rho_\beta(q, q') = \frac{1}{Z_\beta} \int_{\bar{q}(0)=q'}^{\bar{q}(\hbar\beta)=q} \mathcal{D}\bar{q} \exp\left(-\frac{1}{\hbar} S^{\mathrm{E}}[\bar{q}] \right). \tag{4.113}$$

Here and in the following, we drop again the time argument of the action.

4.6   Dissipation within the path-integral formalism

4.6.1   Influence functional

In Section 4.2.2 we have shown how damping arises from a Hamiltonian description by coupling to a heat bath. The presence of damping became apparent after eliminating the bath degrees of freedom and considering the system degree of freedom alone. This elimination may also be carried out within the path-integral formalism [17].

In the following, we discuss the elimination procedure by considering the equilibrium density matrix for an Hamiltonian of the form (4.5)

$$W_\beta = \frac{1}{Z_\beta} \exp\left[-\beta \left(H_{\mathrm{S}} + H_{\mathrm{B}} + H_{\mathrm{SB}} \right) \right]. \tag{4.114}$$

For N bath oscillators we may express the position representation of the density matrix in terms of an $(N+1)$-fold imaginary-time path integral

$$W_\beta(q, x_i, q', x_i') = \frac{1}{Z_\beta} \int \mathcal{D}\bar{q} \prod_{i=1}^{N} \mathcal{D}\bar{x}_i \exp\left(-\frac{1}{\hbar} S^{\mathrm{E}}[\bar{q}, \bar{x}_i]\right) \qquad (4.115)$$

where the paths run from $\bar{q} = q'$ and $\bar{x}_i = x_i'$ within the imaginary-time interval $\hbar\beta$ to $\bar{q} = q$ and $\bar{x}_i = x_i$, respectively. In view of (4.2), (4.3), and (4.4) the Euclidean action may be decomposed according to

$$S^{\mathrm{E}}[\bar{q}, \bar{x}_i] = S_{\mathrm{S}}^{\mathrm{E}}[\bar{q}] + S_{\mathrm{B}}^{\mathrm{E}}[\bar{x}_i] + S_{\mathrm{SB}}^{\mathrm{E}}[\bar{q}, \bar{x}_i] \qquad (4.116)$$

with

$$S_{\mathrm{S}}^{\mathrm{E}}[\bar{q}] = \int_0^{\hbar\beta} \mathrm{d}\tau \left[\frac{M}{2}\dot{\bar{q}}^2 + V(\bar{q})\right], \qquad (4.117)$$

$$S_{\mathrm{B}}^{\mathrm{E}}[\bar{x}_i] = \int_0^{\hbar\beta} \mathrm{d}\tau \sum_{i=1}^{N} \frac{m_i}{2}\left(\dot{\bar{x}}_i^2 + \omega_i^2 \bar{x}_i^2\right), \qquad (4.118)$$

and

$$S_{\mathrm{SB}}^{\mathrm{E}}[\bar{q}, \bar{x}_i] = \int_0^{\hbar\beta} \mathrm{d}\tau \left[-\bar{q}\sum_{i=1}^{N} c_i \bar{x}_i + \bar{q}^2 \sum_{i=1}^{N} \frac{c_i^2}{2m_i\omega_i^2}\right]. \qquad (4.119)$$

We obtain the reduced equilibrium density matrix of the system by tracing out the bath degrees of freedom

$$\rho_\beta(q, q') = \mathrm{tr}_{\mathrm{B}}\left(W_\beta(q, x_i, q', x_i')\right)$$

$$= \frac{1}{Z} \int \mathcal{D}\bar{q} \int \prod_{i=1}^{N} \mathrm{d}x_i \oint \prod_{i=1}^{N} \mathcal{D}\bar{x}_i \exp\left(-\frac{1}{\hbar} S^{\mathrm{E}}[\bar{q}, \bar{x}_i]\right) \qquad (4.120)$$

thereby retaining the correlations between system and bath. The symbol $\oint$ implies an integral over paths having the same starting and end point x_{i}. Together with the integration over x_{i} this indeed amounts to taking the trace over the bath variables. The partition function appearing in (4.120) is given by $Z = Z_\beta / Z_{\mathrm{R}}$ where

$$Z_{\mathrm{R}} = \prod_{i=1}^{N} Z_i \qquad (4.121)$$

is the partition function of the uncoupled bath and

$$Z_i = \frac{1}{2\sinh(\hbar\beta\omega_i/2)} \qquad (4.122)$$

the partition function of a single bath oscillator.

We now have to carry out N path integrals and subsequently N integrations which can be done since the bath consists of harmonic oscillators coupled linearly to the system. Note that the following calculation may also be performed if the coupling is nonlinear in the system coordinate as long as the bath coordinates appear only linearly. Since the oscillators are not coupled among each other, it is sufficient to carry out the elimination procedure for one oscillator only and take the product over all oscillators at the very end. It is thus convenient to rewrite the system density matrix as

$$\rho_\beta(q, q') = \frac{1}{Z} \int \mathcal{D}\bar{q} \exp\left(-\frac{1}{\hbar} S_{\mathrm{S}}^{\mathrm{E}}[\bar{q}]\right) F[\bar{q}] \tag{4.123}$$

where we introduced

$$F[\bar{q}] = \prod_{i=1}^{N} \frac{1}{Z_i} F_i[\bar{q}] \tag{4.124}$$

and

$$F_i[\bar{q}] = \int \mathrm{d}x_i \oint \mathcal{D}\bar{x}_i \exp\left(-\frac{1}{\hbar} S_i^{\mathrm{E}}[\bar{q}, \bar{x}_i]\right) \tag{4.125}$$

with the action

$$S_i^{\mathrm{E}}[\bar{q}, \bar{x}_i] = \int_0^{\hbar\beta} \mathrm{d}\tau \frac{m_i}{2}\left[\dot{\bar{x}}_i^2 + \omega_i^2\left(\bar{x}_i - \frac{c_i}{m_i\omega_i^2}\bar{q}\right)^2\right]. \tag{4.126}$$

The functional (4.124) is called influence functional because it contains the complete information of the influence of the heat bath on the system. In the uncoupled case we should have $F[\bar{q}] = 1$ which is indeed the case because for $c_i = 0$ we have $F_i[\bar{q}] = Z_i$.

In general, one is not simply interested in the equilibrium density matrix but in the time evolution of a nonequilibrium density matrix. There the concept of an influence functional still applies, and it is rather straightforward to appropriately modify the calculations outlined below. In the simplest case, one neglects the initial correlations between system and heat bath by assuming that the initial density matrix factorizes into a nonequilibrium density matrix of the system and the equilibrium density matrix of the heat bath [19]. More realistic situations including initial correlations may be treated as well [20]. In any case the calculations will become more tedious compared to the one which we are going to perform now.

4.6.2   Elimination of the heat bath

We begin the calculation of the influence functional by evaluating the functional integral in (4.125). One approach to evaluate the trace is to express the most general path in terms of a Fourier series

$$\bar{x}_i(\tau) = \sum_{n=-\infty}^{+\infty} \xi_n \mathrm{e}^{\mathrm{i}\nu_n\tau}. \tag{4.127}$$

The fact that this generates also nonperiodic paths which should not be taken into account does not represent a problem because a jump in $\bar{x}_i(\tau)$ will cause an infinite contribution to the kinetic term in the action. Unwanted paths are therefore automatically suppressed.

Here, we take another approach which allows us to demonstrate the general procedure of evaluating a path integral within the semiclassical approximation as explained in Section 4.5. It should be stressed however, that since the action (4.126) is harmonic, the following calculation is exact.

The first step is to find a solution of the classical equation of motion

$$\ddot{\bar{x}}_i^{\text{cl}} - \omega_i^2 \bar{x}_i^{\text{cl}} = -\frac{c_i}{m_i}\bar{q} \tag{4.128}$$

which is obtained by variation of the action (4.126) with respect to $\bar{x}_i$. This is of course just the imaginary-time version of the equation of motion (4.8). The boundary conditions $\bar{x}_i^{\text{cl}}(0) = \bar{x}_i^{\text{cl}}(\hbar\beta) = x_i$ select the paths needed for tracing out the environment, leading to the solution of (4.128)

$$\bar{x}_i^{\text{cl}}(\tau) = \frac{\sinh(\omega_i\tau)}{\sinh(\hbar\beta\omega_i)} \left[x_i + \frac{c_i}{m_i\omega_i} \int_\tau^{\hbar\beta} d\sigma \, \sinh[\omega_i(\hbar\beta - \sigma)]\bar{q}(\sigma) \right]$$

$$+ \frac{\sinh[\omega_i(\hbar\beta - \tau)]}{\sinh(\hbar\beta\omega_i)} \left[x_i + \frac{c_i}{m_i\omega_i} \int_0^\tau d\sigma \, \sinh(\omega_i\sigma)\bar{q}(\sigma) \right]. \tag{4.129}$$

Given this solution, we may calculate the classical action. The number of integrals may be reduced somewhat in the presence of quadratic terms in the potential. We partially integrate the kinetic energy and make use of the equation of motion (4.128) to obtain

$$S_i^{\text{E,cl}}[\bar{q}, x_i] = \frac{m_i}{2} \left[\bar{x}_i^{\text{cl}}(\hbar\beta)\dot{\bar{x}}_i^{\text{cl}}(\hbar\beta) - \bar{x}_i^{\text{cl}}(0)\dot{\bar{x}}_i^{\text{cl}}(0) \right]$$

$$+ \int_0^{\hbar\beta} d\tau \, \frac{m_i}{2}\left[-\frac{c_i}{m_i}\bar{q}\bar{x}_i^{\text{cl}} + \frac{c_i^2}{m_i^2\omega_i^2}\bar{q}^2 \right]. \tag{4.130}$$

Inserting (4.129), we get after some algebra

$$S_i^{\text{E,cl}}[\bar{q}, x_i] = m_i\omega_i\frac{\cosh(\hbar\beta\omega_i) - 1}{\sinh(\hbar\beta\omega_i)}x_i^2$$

$$-c_i \int_0^{\hbar\beta} d\tau \frac{\sinh(\omega_i\tau) + \sinh[\omega_i(\hbar\beta - \tau)]}{\sinh(\hbar\beta\omega_i)}x_i\bar{q}(\tau)$$

$$-\frac{c_i^2}{m_i\omega_i} \int_0^{\hbar\beta} d\tau \int_0^\tau d\sigma \frac{\sinh[\omega_i(\hbar\beta - \tau)]\sinh(\omega_i\sigma)}{\sinh(\hbar\beta\omega_i)}\bar{q}(\tau)\bar{q}(\sigma)$$

$$+\frac{c_i^2}{2m_i\omega_i^2} \int_0^{\hbar\beta} d\tau \bar{q}^2(\tau). \tag{4.131}$$

Since according to (4.125) we later on have to integrate over x_i, it is useful to rewrite (4.131) as

$$S_i^{\mathrm{E,cl}}[\bar{q}, x_i] = m_i \omega_i \frac{\cosh(\hbar\beta\omega_i) - 1}{\sinh(\hbar\beta\omega_i)}(x_i - x^{(0)})^2$$

$$- \int_0^{\hbar\beta} \mathrm{d}\tau \int_0^\tau \mathrm{d}\sigma K_i(\tau - \sigma)\bar{q}(\tau)\bar{q}(\sigma) \qquad (4.132)$$

$$+ \frac{c_i^2}{2m_i\omega_i^2} \int_0^{\hbar\beta} \mathrm{d}\tau \bar{q}^2(\tau)$$

where we made frequent use of relations between hyperbolic functions. The quantity $x^{(0)}$, which depends on the path $\bar{q}(\tau)$, will drop out in the integration over x_i and is therefore not needed explicitly. The integral kernel is defined as

$$K_i(\tau) = \frac{c_i^2}{2m_i\omega_i} \frac{\cosh\left[\omega_i\left(\dfrac{\hbar\beta}{2} - \tau\right)\right]}{\sinh\left(\dfrac{\hbar\beta\omega_i}{2}\right)} = K_i(\hbar\beta - \tau). \qquad (4.133)$$

The action (4.132) contains local as well as nonlocal terms in the system path $\bar{q}(\tau)$. In order to show that the local terms cancel, it is convenient to expand the kernel (4.133) into a Fourier series

$$\frac{\cosh\left[\omega_i\left(\dfrac{\hbar\beta}{2} - \tau\right)\right]}{\sinh\left(\dfrac{\hbar\beta\omega_i}{2}\right)} = \frac{2}{\hbar\beta} \sum_{n=-\infty}^{+\infty} \frac{\omega_i}{\omega_i^2 + \nu_n^2} e^{i\nu_n\tau} \qquad (4.134)$$

in the interval $0 \leq \tau \leq \hbar\beta$ which we are interested in. The local contribution to the double integral in the action can be identified by using the identity

$$\bar{q}(\tau)\bar{q}(\sigma) = -\frac{1}{2}\left(\bar{q}(\tau) - \bar{q}(\sigma)\right)^2 + \frac{1}{2}\left(\bar{q}(\tau)^2 + \bar{q}(\sigma)^2\right) \qquad (4.135)$$

where the first term on the right hand side represents the nonlocal part while the second term gives rise to a local part. In the double integral the latter can be written as

$$\int_0^{\hbar\beta} \mathrm{d}\tau \int_0^\tau \mathrm{d}\sigma K_i(\tau - \sigma)\left(\bar{q}(\tau)^2 + \bar{q}(\sigma)^2\right) = \int_0^{\hbar\beta} \mathrm{d}\tau \bar{q}(\tau)^2 \int_0^{\hbar\beta} \mathrm{d}\sigma K_i(\sigma) \qquad (4.136)$$

from which it becomes clear that the strength of the local part is given by the $n = 0$ Fourier component in (4.134). We therefore decompose the kernel $K_i(\tau)$ into a periodic delta function

$$\frac{c_i^2}{m_i\omega_i^2} \sum_{n=-\infty}^{\infty} \delta(\tau - n\hbar\beta) = \frac{c_i^2}{\hbar\beta m_i\omega_i^2} \sum_{n=-\infty}^{\infty} e^{i\nu_n\tau} \qquad (4.137)$$

and a new kernel

$$k_i(\tau) = \frac{c_i^2}{\hbar\beta m_i\omega_i^2} \sum_{n=-\infty}^{+\infty} \frac{\nu_n^2}{\nu_n^2 + \omega_i^2} e^{i\nu_n\tau} = k_i(-\tau) \tag{4.138}$$

which results in a nonlocal contribution to the classical action. The delta function only gives rise to a local contribution to the second term of (4.132) which could be interpreted as potential renormalization but cancels exactly with the third term. This is in agreement with the reasoning which lead us to include the second term on the right hand side of (4.4).

After this discussion of the classical path, we should consider the fluctuations around it according to the decomposition (4.106). As mentioned before, the expansion (4.107) for our problem terminates after the second order and the first order term vanishes because we expand around the classical path. The second order contribution to the action is given by

$$S_i^{\mathrm{E},(2)}[\xi_i] = \int_0^{\hbar\beta} d\tau \frac{m_i}{2} \left(\dot{\xi}_i^2 + \omega_i^2\xi_i^2\right) \tag{4.139}$$

where $\xi_i(\tau)$ represents a fluctuation around the classical path. However, this contribution is independent of $\bar{x}_i$ and the fluctuations just lead to a numerical factor. This advantage of expanding around the classical path allows us to proceed by performing the x_i-integration required in (4.125) to obtain

$$F_i[\bar{q}] = F_i^\xi \sqrt{\frac{\hbar\pi \sinh(\hbar\beta\omega_i)}{m_i\omega_i(\cosh(\hbar\beta\omega_i) - 1)}}$$

$$\times \exp\left(-\frac{1}{2\hbar} \int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\sigma k_i(\tau - \sigma)\bar{q}(\tau)\bar{q}(\sigma)\right) \tag{4.140}$$

where F_i^ξ is the contribution of the fluctuations which is independent of $\bar{q}$ and the coupling constant c_i. We may determine this factor without explicitly performing the path integral over the fluctuations by considering the uncoupled case where $c_i = 0$ and therefore $k_i(\tau) = 0$. According to our discussion on page 234, $F_i[\bar{q}]$ should then reduce to the partition function Z_i defined in (4.122). This leads us to

$$F_i[\bar{q}] = Z_i \exp\left(-\frac{1}{2\hbar} \int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\sigma k_i(\tau - \sigma)\bar{q}(\tau)\bar{q}(\sigma)\right) \tag{4.141}$$

which describes the influence of one bath oscillator on the system.

4.6.3   Evaluation of the fluctuations

While we did not need to evaluate the fluctuation integral to obtain the result (4.141), it is nevertheless instructive to see how it could be done. We first note that since the

fluctuation vanishes at times $t = 0$ and $\hbar\beta$ the second order contribution (4.139) may be written as

$$S_i^{\mathrm{E},(2)} = \int_0^{\hbar\beta} \mathrm{d}\tau \frac{m_i}{2} \xi_i \mathcal{S}_i \xi_i \tag{4.142}$$

with the linear operator

$$\mathcal{S}_i = -\frac{\mathrm{d}2}{\mathrm{d}t^2} + \omega_i^2. \tag{4.143}$$

The normalized eigenfunctions of $\mathcal{S}_i$ satisfying the boundary conditions are given by

$$\xi_{i,n}(\tau) = \sqrt{\frac{2}{\hbar\beta}} \sin\left(\frac{\nu_n}{2}\tau\right) \tag{4.144}$$

with the corresponding eigenvalues

$$\lambda_{i,n} = \frac{\nu_n^2}{4} + \omega_i^2 \tag{4.145}$$

where the Matsubara frequencies ν_n have been defined in (4.85). Expanding the fluctuation in these eigenfunctions

$$\xi_i(\tau) = \sum_{n=1}^{\infty} a_n \xi_{i,n}(\tau) \tag{4.146}$$

and exploiting their orthogonality, we immediately obtain

$$S_i^{\mathrm{E},(2)} = \frac{m_i}{2} \sum_{n=1}^{\infty} \lambda_{i,n} a_n^2. \tag{4.147}$$

The functional integral over all fluctuations can now be rewritten in terms of a conventional integral over the expansion coefficients

$$F_i^\xi = \oint \mathcal{D}\xi_i \exp\left(-\frac{1}{\hbar} S_i^{\mathrm{E},(2)}[\xi_i]\right)$$

$$= J \int_{-\infty}^{+\infty} \prod_{j=1}^{\infty} \mathrm{d}a_j \exp\left[-\frac{m_i}{2\hbar} \sum_{n=1}^{\infty} \lambda_{i,n} a_n^2\right] \tag{4.148}$$

where J is the Jacobian of the transformation.

While J may be determined [18], it is often useful to take the free particle as a sort of reference system. The propagator of the free particle

$$G(q_{\mathrm{f}}, q_{\mathrm{i}}, t) = \left(\frac{-\mathrm{i}m}{2\pi\hbar t}\right)^{1/2} \exp\left(\frac{\mathrm{i}}{\hbar} \frac{m}{2t} (q_{\mathrm{f}} - q_{\mathrm{i}})^2\right) \tag{4.149}$$

may be derived in a number of different ways. Switching to imaginary times, we get the fluctuation contribution for the free particle

$$F_0^\xi = \left(\frac{m}{2\pi\hbar^2\beta}\right)^{1/2}. \tag{4.150}$$

On the other hand, we may rewrite (4.148) for the free particle by replacing the eigenvalues $\lambda_{i,n}$ by $\lambda_{0,n} = \nu_n^2/4$. Performing the Gaussian integrals we get

$$F_i^\xi = \left(\frac{m}{2\pi\hbar^2\beta}\right)^{1/2} \prod_{n=1}^{\infty} \left(\frac{\lambda_{0,n}}{\lambda_{i,n}}\right)^{1/2}. \tag{4.151}$$

The products of eigenvalues appearing in this result are often referred to in the literature as determinants of the corresponding operators as a generalization of the case of finite dimensional matrices. For the interpretation of determinants in the semiclassical approximation of path integrals it is also instructive to take a look at (6.22).

The infinite product in (4.151) may be evaluated with the help of

$$\prod_{n=1}^{\infty} \left(1 + \frac{x^2}{\pi^2 n^2}\right) = \frac{\sinh(x)}{x}. \tag{4.152}$$

Inserting the result

$$F_i^\xi = \left(\frac{m\omega_i}{2\pi\hbar\sinh(\hbar\beta\omega_i)}\right)^{1/2} \tag{4.153}$$

into (4.140) yields (4.141) as expected.

4.6.4   Effective action

From (4.124) we obtain together with (4.141) the influence functional

$$F[\bar{q}] = \exp\left(-\frac{1}{2\hbar}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\sigma k(\tau-\sigma)\bar{q}(\tau)\bar{q}(\sigma)\right). \tag{4.154}$$

The nonlocal kernel $k(\tau)$ is given by the sum over all kernels $k_i(\tau)$ defined in (4.138). Introducing the Laplace transform of the damping kernel (4.14)

$$\widehat{\gamma}(z) = \int_0^\infty dz e^{-zt}\gamma(t) = \frac{2}{M}\int_0^\infty \frac{d\omega}{\pi}\frac{J(\omega)}{\omega}\frac{z}{z^2+\omega^2} \tag{4.155}$$

and making use of the spectral density of bath oscillators (4.13), we finally obtain the kernel

$$k(\tau) = \frac{M}{\hbar\beta}\sum_{n=-\infty}^{+\infty}|\nu_n|\widehat{\gamma}(|\nu_n|)e^{i\nu_n\tau}. \tag{4.156}$$

As the main result let us note that dissipation may be taken into account within the path-integral formalism by adding a nonlocal term to the action of the system under consideration. In view of (4.123), we get the imaginary-time effective action for a damped system

$$S_{\text{eff}}^{\text{E}}[\bar{q}] = S^{\text{E}}[\bar{q}] + \frac{1}{2}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\sigma k(\tau-\sigma)\bar{q}(\tau)\bar{q}(\sigma). \tag{4.157}$$

We finish this section by discussing the kernel $k(\tau)$ for a specific damping kernel $\gamma(\tau)$. Since Ohmic damping corresponds to $\widehat{\gamma}(z) = \gamma$, we encounter problems with the convergence of the sum in (4.156). We therefore consider the damping kernel of the Drude model which according to (4.16) is described by $\widehat{\gamma}(|\nu_n|) = \gamma\omega_D/(\omega_D+|\nu_n|)$. Since the Fourier coefficients of the kernel approach a constant for $n \to \infty$, it is reasonable to split off a periodic delta function which we defined in (4.137). Expressing the numerator of $\widehat{\gamma}(|\nu_n|)$ as an integral over an exponential function, the summation over n leads to a geometric sum. This leaves us with

$$k(\tau) = M\gamma\omega_D \sum_{n=-\infty}^{+\infty} \delta(\tau - n\hbar\beta) - \frac{M\gamma\omega_D^2}{\hbar\beta} \int_0^\infty ds \frac{\sinh(\nu s)}{\cosh(\nu s) - \cos(\nu\tau)} e^{-\omega_D s} \quad (4.158)$$

where $\nu = 2\pi/\hbar\beta$ is the first Matsubara frequency. Since we are only interested in the case of very large cutoff frequency ω_D, we expand the integral asymptotically by partial integration. The kernel then becomes

$$k(\tau) = M\gamma\omega_D \sum_{n=-\infty}^{+\infty} \delta(\tau - n\hbar\beta) - \frac{\pi M\gamma}{(\hbar\beta)^2} \frac{1}{\sin^2\left(\dfrac{\nu\tau}{2}\right)} + O(\omega_D^{-1}). \quad (4.159)$$

In the limit of Ohmic damping ($\omega_D \to \infty$), the delta function contribution diverges in order to ensure nonlocality. This corresponds to the divergence of the potential renormalization in (4.4). The second term leads to an interaction between paths at different times. Taking the limit of zero temperature, we find a long range interaction decaying algebraically like $k(\tau) = -(M\gamma/\pi)\tau^{-2}$.

4.7   Decay of a metastable state

We now want to make use of what we have discussed in the last two sections by applying it to the decay of a metastable state in the presence of dissipation. A comprehensive treatment would be beyond the scope of this chapter. We rather try to convey some of the key ideas. For details we refer the reader to the literature, e.g. to the review by Hänggi et al. [21], and mention that other aspects of tunneling are addressed in various sections of Chapter 3 as well as in Sections 5.6 and 6.3.1.

To be specific, we consider the cubic potential shown in Fig. 4.2 which may be expressed in the form

$$V(q) = \frac{M}{2}\omega_0^2 q^2 \left(1 - \frac{q}{q_0}\right). \quad (4.160)$$

This potential possesses a minimum at $q = 0$ with a frequency ω_0 for small oscillations around this minimum. At $q_b = 2q_0/3$ there is a barrier of height $V_b = (2/27)M\omega_0^2 q_0^2$. A harmonic approximation around the barrier yields $V(q) = V_b - (M/2)\omega_b^2 q^2$ with a barrier frequency $\omega_b = \omega_0$. Where it is possible we will distinguish between the two frequencies in order to make the physical origin of the results more transparent.
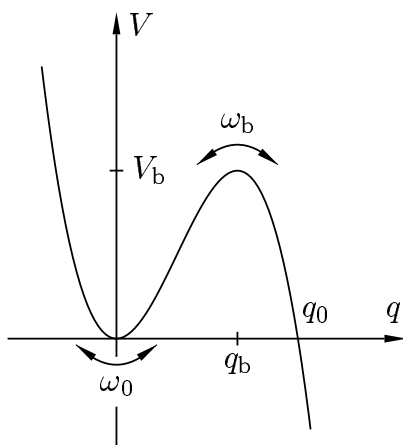
Fig. 4.2: Cubic potential as defined by (4.160).

We are now interested in the decay of a metastable state initially prepared in the potential well at $q = 0$. As we will see below, the decay rate may be calculated from the partition function. Unfortunately, for a cubic potential the partition function may not be obtained exactly. We therefore have to resort to the semiclassical approximation. In principle, we could proceed as in Section 4.6 and first evaluate the action of all paths starting and ending at a certain point and then integrate over all these points. However, for our nonlinear problem this would imply that we include contributions beyond the semiclassical approximation. Rather it is sufficient to look for extrema of the action among arbitrary paths and take into account fluctuations around these extremal paths semiclassically. Then the fluctuations do not have to vanish at the initial and final time.

4.7.1   Crossover temperature

The classical equation of motion for a cubic potential in the presence of dissipation is given by

$$M\ddot{q}_{\mathrm{cl}} - M\omega_0^2 q_{\mathrm{cl}} + \frac{3}{2}M\omega_0^2\frac{q_{\mathrm{cl}}^2}{q_0} - \int_0^{\hbar\beta} \mathrm{d}\sigma\, k(\tau - \sigma)q_{\mathrm{cl}}(\sigma) = 0 \qquad (4.161)$$

where the dissipative kernel $k(\tau)$ was defined in (4.156). Since the integral over $k(\tau)$ vanishes, it is clear that constant solutions at the extrema of the potential, i.e. $q = 0$ and $q = q_{\mathrm{b}}$, are solutions of (4.161). For high temperatures (corresponding to short imaginary times) these two paths are the stationary points of the action. Let us first consider the path which remains in the potential minimum, i.e. at $q = 0$. Fluctuations around this path may be described by a Fourier series

$$\xi(\tau) = \sum_{n=-\infty}^{+\infty} \xi_n \mathrm{e}^{\mathrm{i}\nu_n\tau} \qquad (4.162)$$

where ξ_n and ξ_{-n} are complex conjugate in order to ensure a real path. The semiclassical action

$$S^{\mathrm{E}}[q] = \int_0^{\hbar\beta} \mathrm{d}\tau \left[\frac{M}{2}\dot{q}_{\mathrm{cl}}^2 + \frac{M}{2}\omega_0^2 q_{\mathrm{cl}}^2 \left(1 - \frac{q_{\mathrm{cl}}}{q_0}\right) + \frac{1}{2}\int_0^{\hbar\beta}\mathrm{d}\sigma k(\tau-\sigma)q_{\mathrm{cl}}(\tau)q_{\mathrm{cl}}(\sigma) \right.$$

$$\left. + \frac{M}{2}\dot{\xi}^2 + \frac{M}{2}\omega_0^2 \left(1 - 3\frac{q_{\mathrm{cl}}}{q_0}\right)\xi^2 + \frac{1}{2}\int_0^{\hbar\beta}\mathrm{d}\sigma k(\tau-\sigma)\xi(\tau)\xi(\sigma) \right] \quad (4.163)$$

then becomes

$$S^{\mathrm{E}} = \frac{M\hbar\beta}{2}\sum_{n=-\infty}^{+\infty} (\nu_n^2 + |\nu_n|\hat{\gamma}(|\nu_n|) + \omega_0^2)|\xi_n|^2. \quad (4.164)$$

Obviously, any deviation from the classical path will increase the action and $q = 0$ represents a minimum of the action.

The same analysis may be performed for $q = q_{\mathrm{b}}$ which yields

$$S^{\mathrm{E}} = \hbar\beta V_{\mathrm{b}} + \frac{M\hbar\beta}{2}\sum_{n=-\infty}^{+\infty} \left(\nu_n^2 + |\nu_n|\hat{\gamma}(|\nu_n|) - \omega_{\mathrm{b}}^2\right)|\xi_n|^2. \quad (4.165)$$

Again, the expression is quadratic in the Fourier components ξ_n but there is one fluctuation mode, ξ_0, which decreases the action. Therefore, $q = q_{\mathrm{b}}$ corresponds to a saddle point of the action. This should not come as a surprise since this classical path lies at the top of the barrier. With decreasing temperature one reaches a point where

$$\nu_1^2 + |\nu_1|\hat{\gamma}(|\nu_1|) - \omega_{\mathrm{b}}^2 = 0. \quad (4.166)$$

Below this temperature another fluctuation mode becomes unstable indicating the appearance of an additional solution.

The solution of (4.166) defines a temperature which depends on the damping strength. For Ohmic damping one obtains

$$T_0 = \frac{\hbar}{2\pi k_{\mathrm{B}}}\left(\sqrt{\frac{\gamma^2}{4} + \omega_{\mathrm{b}}^2} - \frac{\gamma}{2}\right) \quad (4.167)$$

which decreases with increasing damping strength γ. In the case of zero damping this becomes

$$T_0 = \frac{\hbar\omega_{\mathrm{b}}}{2\pi k_{\mathrm{B}}}. \quad (4.168)$$

The latter result can be understood by realizing that a periodic path traversing the minimum of the inverted potential needs at least the time $2\pi/\omega_{\mathrm{b}}$ corresponding to one period in the harmonically approximated potential. Translating this into temperature, one immediately obtains (4.168). Since the anharmonicity of the potential will increase the period of finite oscillations, the new solution at temperatures just below T_0 will be a harmonic oscillation of small amplitude.

On the other hand, at zero temperature the periodic path may take infinite time. In this case one can solve (4.161) in the absence of dissipation to obtain

$$q_{\mathrm{B}}(\tau) = q_0 \frac{1}{\cosh^2(\omega_0\tau/2)}. \qquad (4.169)$$

This zero-energy path starts at $q = 0$, traverses the minimum of the inverted potential to reach $q = q_0$ where it is reflected and retraces its path. Because of the reflection this solution is often referred to as "bounce". In the vicinity of $q = 0$ the motion is exponentially slow. Therefore, it is not possible to express this solution on the time interval from $t = 0$ to ∞. Instead, one uses the time interval starting at $t = -\infty$ which is obtained by shifting the finite imaginary time interval by $-\hbar\beta/2$ and letting $\hbar\beta \to \infty$.

The temperature T_0 leads to a division into two regimes and is therefore often referred to as crossover temperature. For high temperatures the decay mechanism is mainly thermal activation. As temperature is lowered, quantum effects become visible to a certain extent as we will see below. The appearance of the bounce solution below the crossover temperature is interpreted in terms of a new decay channel, namely quantum tunneling which is the dominant effect at very low temperatures.

4.7.2   Imaginary part of the free energy

For temperatures above the crossover temperature we have shown the existence of a saddle point of the action which is related to the fact that we are treating a potential containing a barrier. The existence of this saddle point for lower temperatures will become clear from arguments given in Section 4.7.4. We therefore have to address the question how to properly treat the fluctuations around the saddle point. Fluctuation modes with positive eigenvalues can be treated by evaluating Gaussian integrals as we have seen in Section 4.6.3. This is no longer the case for negative eigenvalues where the Gaussian integral

$$f_0 = \sqrt{\frac{M\beta}{2\pi}} \int_{-\infty}^{+\infty} \mathrm{d}\xi_0 \exp\left(\frac{M\beta\omega_{\mathrm{b}}^2}{2}\xi_0^2\right) \qquad (4.170)$$

does not exist. On the interval from $-\infty$ to zero the problems are due to the semi-classical approximation. Taking into account the anharmonicity of the potential would yield a finite value which to leading order is in fact described by the path $q = 0$ and fluctuations around it. The divergence for positive ξ_0 is more serious because the potential on this side is not bounded from below. This difficulty may be removed by an analytical continuation where one deforms the path of integration in (4.170) to run into the direction of steepest descent, i.e. it continues from zero along the positive imaginary axis. By this procedure the integral acquires an imaginary part

$$\mathrm{Im}f_0 = \mathrm{Im}\left(\sqrt{\frac{M\beta}{2\pi}} \int_0^{\mathrm{i}\infty} \mathrm{d}\xi_0 \exp\left(\frac{M\beta\omega_{\mathrm{b}}^2}{2}\xi_0^2\right)\right) = \frac{\mathrm{i}}{2\omega_{\mathrm{b}}}. \qquad (4.171)$$

Comparing (4.164) and (4.165), we find that for $\beta V_b \gg 1$ the imaginary part of the partition function will be exponentially small compared to the real part. Nevertheless we have to keep it as the leading imaginary term.

As a consequence of the complex partition function, the free energy

$$F = -\frac{1}{\beta}\ln(Z) \tag{4.172}$$

also becomes complex. Since at zero temperature the free energy turns into the energy, this would result in a decay of the probability amplitude of a state proportional to $\exp(2\mathrm{Im}(E)t/\hbar)$. This leads us to conjecture the following expression for the decay rate [22]

$$\Gamma = -\frac{2}{\hbar}\mathrm{Im}F \tag{4.173}$$

which expressed in terms of the free energy should also be valid at finite temperatures. It turns out, however, that above the crossover temperature (4.173) has to be modified into [23]

$$\Gamma = -\frac{2}{\hbar}\frac{T_0}{T}\mathrm{Im}F. \tag{4.174}$$

The additional prefactor ensures correct results for very high temperatures, i.e. in the classical limit. The difference between (4.173) and (4.174) will be motivated in Section 4.7.4. It should be emphasized that the given arguments do not represent a proof of the relation between the decay rate and the imaginary part of the free energy in the dissipative case. However, there exist independent methods employing periodic orbit [21, 24] or real-time path integral techniques [25] which lead to the same results for the decay rates. For details we refer the reader to the literature.

4.7.3   Above crossover

We now want to calculate the decay rate above the crossover temperature using (4.174). Within the semiclassical approximation the partition function consists of two contributions

$$Z = Z_0 + Z_b \tag{4.175}$$

from the potential well and the barrier, respectively. Setting $\xi_n = a_n + \mathrm{i}b_n$ with $a_{-n} = a_n$ and $b_{-n} = -b_n$ to ensure real paths, we obtain by evaluating Gaussian integrals with the action (4.164)

$$Z_0 = N\frac{1}{\omega_0}\prod_{n=1}^{\infty}\frac{1}{\nu_n^2 + \nu_n\widehat{\gamma}(\nu_n) + \omega_0^2} \tag{4.176}$$

where N is a normalization factor which will turn out to be irrelevant. With (4.165) the second contribution to the partition function yields

$$Z_b = N\frac{\mathrm{i}}{2\omega_b}\prod_{n=1}^{\infty}\frac{\mathrm{e}^{-\beta V_b}}{\nu_n^2 + \nu_n\widehat{\gamma}(\nu_n) - \omega_b^2} \tag{4.177}$$

where we made use of (4.171). Using the fact that for $\beta V_b \gg 1$ the imaginary part of the partition function is exponentially small compared to the real part, we obtain for the imaginary part of the free energy

$$\mathrm{Im}F = -\frac{1}{\beta}\frac{\omega_0}{2\omega_\mathrm{b}}\mathrm{e}^{-\beta V_\mathrm{b}}\prod_{n=1}^{\infty}\frac{\nu_n^2 + \nu_n\widehat{\gamma}(\nu_n) + \omega_0^2}{\nu_n^2 + \nu_n\widehat{\gamma}(\nu_n) - \omega_\mathrm{b}^2}. \tag{4.178}$$

This result depends only on the barrier height and the frequencies of small oscillations around $q = 0$ and q_b but not on the specific form of the potential. This is a consequence of the fact that the stationary points of the action do not explore the whole potential and of the semiclassical approximation.

The decay rate according to (4.174) may be expressed as

$$\Gamma = f_\mathrm{q}\Gamma_\mathrm{cl} \tag{4.179}$$

where

$$\Gamma_\mathrm{cl} = \frac{k_\mathrm{B}T_0}{\hbar}\frac{\omega_0}{\omega_\mathrm{b}}\mathrm{e}^{-\beta V_\mathrm{b}} \tag{4.180}$$

is the classical rate derived in 1940 by Kramers [26] for not too weak Ohmic damping so that thermal equilibrium in the well is guaranteed, and

$$f_\mathrm{q} = \prod_{n=1}^{\infty}\frac{\nu_n^2 + \nu_n\widehat{\gamma}(\nu_n) + \omega_0^2}{\nu_n^2 + \nu_n\widehat{\gamma}(\nu_n) - \omega_\mathrm{b}^2} \tag{4.181}$$

represents the quantum corrections. The temperature dependence of the exponential term is the well-known Arrhenius behavior which implies that thermally activated decay becomes strongly suppressed as temperature is lowered. At sufficiently low temperatures quantum tunneling, which is discussed in the following section, therefore becomes the dominant process. The factor (4.181) leads to an enhancement of the thermal decay rate due to quantum corrections to the probability distribution in the potential well and at the barrier. The expression for f_q is diverging as the crossover temperature is approached from above. Close to the crossover temperature a more refined treatment taking into account anharmonicities of the potential is required [27]. Below the crossover temperature one has to deal with the bounce solution as we will discuss in the following section for the example of zero temperature.

4.7.4   Zero temperature

Since we want to elucidate only some keypoints we concentrate on the case of vanishing damping. The bounce solution (4.169) represents a stationary solution which in fact is a saddle point as we will show now. Since the fluctuation contribution to the action follows from (4.163) as

$$S^{\mathrm{E},(2)}[\xi] = \int_{-\infty}^{+\infty}\mathrm{d}\tau\frac{M}{2}\left[\dot{\xi}(\tau)^2 + \omega_0^2\left(1 - 3\frac{q_\mathrm{B}(\tau)}{q_0}\right)\xi(\tau)^2\right], \tag{4.182}$$

we obtain the fluctuation modes as the eigenfunctions of

$$-\ddot{\xi}_n + \omega_0^2 \left(1 - 3\frac{q_B(\tau)}{q_0}\right)\xi_n = \lambda_n \xi_n. \tag{4.183}$$

Taking the time derivative of the undamped version of (4.161) we find by comparison with (4.183) that the time derivative of the bounce

$$\dot{q}_B(\tau) = -q_0\omega_0 \frac{\sinh(\omega_0\tau/2)}{\cosh^3(\omega_0\tau/2)} \tag{4.184}$$

is an eigenfunction with zero eigenvalue. The existence of this zero mode is a consequence of the fact that the position of the bounce in time is arbitrary and that for small ϵ

$$q_B(\tau + \epsilon) = q_B(\tau) + \epsilon\dot{q}_B(\tau). \tag{4.185}$$

After this discussion, we may write the partition function in the form

$$Z = Z_0 \left(1 + i\kappa\hbar\beta e^{-S_b/\hbar}\right) \tag{4.186}$$

where Z_0 according to (4.176) is the contribution of the constant path $q = 0$ and S_b is the action of the bounce. The constant κ is the ratio of the contributions of the fluctuations around $q = q_B(\tau)$ and $q = 0$ which we do not want to evaluate explicitly here. Finally, in writing the factor $\hbar\beta$ we assumed for the moment that the temperature is small but finite. This factor stems from the integration over the possible positions of the bounce solution and can be viewed as arising from the zero mode (4.184). This factor cancels with the temperature factor in the relation between the free energy and the partition function (4.172). It is actually this integration over the zero mode which leads to the additional temperature factor in the rate expression (4.174) above the crossover temperature because in this case a zero mode no longer exists.

From (4.186) one obtains with (4.172) and (4.173) for the decay rate

$$\Gamma = 2\kappa e^{-S_b/\hbar}. \tag{4.187}$$

The calculation of the action of the bounce solution is facilitated by noting that this solution corresponds to zero energy. As a consequence

$$S_b = \int_{-\infty}^{+\infty} d\tau\, M\dot{q}_{cl}^2 = 2\int_0^{q_0} dq_{cl}\sqrt{2MV(q_{cl})}, \tag{4.188}$$

and we thus recover the exponent for the decay rate known from WKB. For the cubic potential (4.160) the action takes the value

$$S_b = \frac{36}{5}\frac{V_b}{\omega_0}. \tag{4.189}$$

The prefactor κ may also be calculated and is found to be in agreement with the standard WKB result. For further details the reader is referred to the literature [28, 29] where also results for the weakly damped case can be found [30].
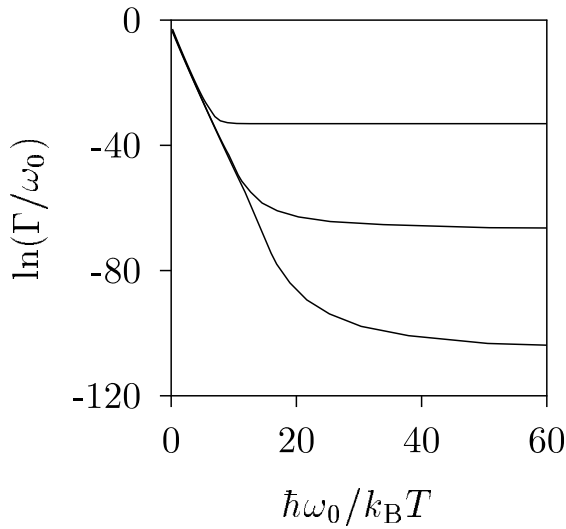
Fig. 4.3: Arrhenius plot for the decay rate Γ of a metastable state. The damping strength from the upper to the lower curve takes the values $\gamma/2\omega_0 = 0, 0.5$, and 1. The low temperature data were derived from the tables given in [27].

We close this chapter by presenting in Fig. 4.3 the decay rate in an Arrhenius plot for three different values of the damping constant. For high temperatures, i.e. on the left side of the plot, the exponential dependence of the rate on the inverse temperature leads to straight line. Below the crossover temperature the curves flatten out indicating that the regime of quantum tunneling is reached. The uppermost curve represents the undamped result while the second and third curve correspond to $\gamma = \omega_0$ and $2\omega_0$, respectively. With increasing damping strength the crossover from the classical to the quantum regime becomes less distinct. More important, the crossover temperature decreases and the quantum tunneling rate is suppressed. The decay rate thus approaches the thermal activation rate and we may conclude that dissipation tends to make the system more classical.

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