1 Path Integrals and Their Application to Dissipative Quantum Systems

Gert-Ludwig Ingold

Institut für Physik, Universität Augsburg, D-86135 Augsburg, Germany

1.1 Introduction

The coupling of a system to its environment is a recurrent subject in this collection of lecture notes. The consequences of such a coupling are threefold. First of all, energy may irreversibly be transferred from the system to the environment thereby giving rise to the phenomenon of *dissipation*. In addition, the fluctuating force exerted by the environment on the system causes *fluctuations* of the system degree of freedom which manifest itself for example as Brownian motion. While these two effects occur both for classical as well as quantum systems, there exists a third phenomenon which is specific to the quantum world. As a consequence of the entanglement between system and environmental degrees of freedom a coherent superposition of quantum states may be destroyed in a process referred to as *decoherence*. This effect is of major concern if one wants to implement a quantum computer. Therefore, decoherence is discussed in detail in Chap. 5.

Quantum computation, however, is by no means the only topic where the coupling to an environment is relevant. In fact, virtually no real system can be considered as completely isolated from its surroundings. Therefore, the phenomena listed in the previous paragraph play a role in many areas of physics and chemistry and a series of methods has been developed to address this situation. Some approaches like the master equations discussed in Chap. 2 are particularly well suited if the coupling to the environment is weak, a situation desired in quantum computing. On the other hand, in many solid state systems, the environmental coupling can be so strong that weak coupling theories are no longer valid. This is the regime where the path integral approach has proven to be very useful.

It would be beyond the scope of this chapter even to attempt to give a complete overview of the use of path integrals in the description of dissipative quantum systems. In particular for a two-level system coupled to harmonic oscillator degrees of freedom, the so-called spin-boson model, quite a number of approximations have been developed which are useful in their respective parameter regimes. This chapter rather attempts to give an introduction to path integrals for readers unfamiliar with but interested in this method and its application to dissipative quantum systems.

In this spirit, Sect. 1.2 gives an introduction to path integrals. Some aspects discussed in this section are not necessarily closely related to the problem of dissipative systems. They rather serve to illustrate the path integral approach and to convey to the reader the beauty and power of this approach. In Sect. 1.3

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we elaborate on the general idea of the coupling of a system to an environment. The path integral formalism is employed to eliminate the environmental degrees of freedom and thus to obtain an effective description of the system degree of freedom. The results provide the basis for a discussion of the damped harmonic oscillator in Sect. 1.4. Starting from the partition function we will examine several aspects of this dissipative quantum system.

Readers interested in a more in-depth treatment of the subject of quantum dissipation are referred to existing textbooks. In particular, we recommend the book by U. Weiss [1] which provides an extensive presentation of this topic together with a comprehensive list of references. Chapter 4 of [2] may serve as a more concise introduction complementary to the present chapter. Path integrals are discussed in a whole variety of textbooks with an emphasis either on the physical or the mathematical aspects. We only mention the book by H. Kleinert [3] which gives a detailed discussion of path integrals and their applications in different areas.

1.2 Path Integrals

1.2.1 Introduction

The most often used and taught approach to nonrelativistic quantum mechanics is based on the Schrödinger equation which possesses strong ties with the the Hamiltonian formulation of classical mechanics. The nonvanishing Poisson brackets between position and momentum in classical mechanics lead us to introduce noncommuting operators in quantum mechanics. The Hamilton function turns into the Hamilton operator, the central object in the Schrödinger equation. One of the most important tasks is to find the eigenfunctions of the Hamilton operator and the associated eigenvalues. Decomposition of a state into these eigenfunctions then allows us to determine its time evolution.

As an alternative, there exists a formulation of quantum mechanics based on the Lagrange formalism of classical mechanics with the action as the central concept. This approach, which was developed by Feynman in the 1940's [4,5], avoids the use of operators though this does not necessarily mean that the solution of quantum mechanical problems becomes simpler. Instead of finding eigenfunctions of a Hamiltonian one now has to evaluate a functional integral which directly yields the propagator required to determine the dynamics of a quantum system. Since the relation between Feynman's formulation and classical mechanics is very close, the path integral formalism often has the important advantage of providing a much more intuitive approach as we will try to convey to the reader in the following sections.

1.2.2 Propagator

In quantum mechanics, one often needs to determine the solution $|\psi(t)\rangle$ of the time-dependent Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial|\psi\rangle}{\partial t} = H|\psi\rangle\ , \tag{1.1}$$

where H is the Hamiltonian describing the system. Formally, the solution of (1.1) may be written as

$$|\psi(t)\rangle = \mathcal{T} \exp\left(-\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t' H(t')\right)|\psi(0)\rangle \; . \tag{1.2}$$

Here, the time ordering operator $\mathcal{T}$ is required because the operators corresponding to the Hamiltonian at different times do not commute in general. In the following, we will restrict ourselves to time-independent Hamiltonians where (1.2) simplifies to

$$|\psi(t)\rangle = \exp\left(-\frac{\mathrm{i}}{\hbar}Ht\right)|\psi(0)\rangle \; . \tag{1.3}$$

As the inspection of (1.2) and (1.3) demonstrates, the solution of the time-dependent Schrödinger equation contains two parts: the initial state $|\psi(0)\rangle$ which serves as an initial condition and the so-called propagator, an operator which contains all information required to determine the time evolution of the system.

Writing (1.3) in position representation one finds

$$\langle x|\psi(t)\rangle = \int \mathrm{d}x' \langle x| \exp\left(-\frac{\mathrm{i}}{\hbar}Ht\right)|x'\rangle\langle x'|\psi(0)\rangle \tag{1.4}$$

or

$$\psi(x,t) = \int \mathrm{d}x' K(x,t,x',0)\psi(x',0) \tag{1.5}$$

with the propagator

$$K(x,t,x',0) = \langle x| \exp\left(-\frac{\mathrm{i}}{\hbar}Ht\right)|x'\rangle \; . \tag{1.6}$$

It is precisely this propagator which is the central object of Feynman's formulation of quantum mechanics. Before discussing the path integral representation of the propagator, it is therefore useful to take a look at some properties of the propagator.

Instead of performing the time evolution of the state $|\psi(0)\rangle$ into $|\psi(t)\rangle$ in one step as was done in equation (1.3), one could envisage to perform this procedure in two steps by first propagating the initial state $|\psi(0)\rangle$ up to an intermediate time t_1 and taking the new state $|\psi(t_1)\rangle$ as initial state for a propagation over the time $t - t_1$. This amounts to replacing (1.3) by

$$|\psi(t)\rangle = \exp\left(-\frac{\mathrm{i}}{\hbar}H(t-t_1)\right)\exp\left(-\frac{\mathrm{i}}{\hbar}Ht_1\right)|\psi(0)\rangle \tag{1.7}$$

or equivalently

$$\psi(x,t) = \int \mathrm{d}x' \int \mathrm{d}x'' K(x,t,x'',t_1)K(x'',t_1,x',0)\psi(x',0) \; . \tag{1.8}$$

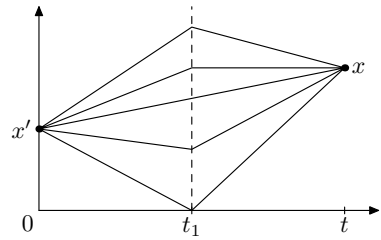

Fig. 1.1. According to the semigroup property (1.9) the propagator $K(x,t,x',0)$ may be decomposed into propagators arriving at some time t_1 at an intermediate point x'' and propagators continuing from there to the final point x

Comparing (1.5) and (1.8), we find the semigroup property of the propagator

$$K(x,t,x',0) = \int \mathrm{d}x'' K(x,t,x'',t_1) K(x'',t_1,x',0) \; . \tag{1.9}$$

This result is visualized in Fig. 1.1 where the propagators between space-time points are depicted by straight lines connecting the corresponding two points. At the intermediate time t_1 one has to integrate over all positions x''. This insight will be of use when we discuss the path integral representation of the propagator later on.

The propagator contains the complete information about the eigenenergies E_n and the corresponding eigenstates $|n\rangle$. Making use of the completeness of the eigenstates, one finds from (1.6)

$$K(x,t,x',0) = \sum_n \exp\left(-\frac{\mathrm{i}}{\hbar} E_n t\right) \psi_n(x) \psi_n(x')^* \; . \tag{1.10}$$

Here, the star denotes complex conjugation. Not only does the propagator contain the eigenenergies and eigenstates, this information may also be extracted from it. To this end, we introduce the retarded Green function

$$G_\mathrm{r}(x,t,x',0) = K(x,t,x',0)\Theta(t) \tag{1.11}$$

where $\Theta(t)$ is the Heaviside function which equals 1 for positive argument t and is zero otherwise. Performing a Fourier transformation, one ends up with the spectral representation

$$\begin{aligned} G_\mathrm{r}(x,x',E) &= -\frac{\mathrm{i}}{\hbar} \int_0^\infty \mathrm{d}t \exp\left(\frac{\mathrm{i}}{\hbar} E t\right) G_\mathrm{r}(t) \\ &= \sum_n \frac{\psi_n(x)\psi_n(x')^*}{E - E_n + \mathrm{i}\varepsilon} \; , \end{aligned} \tag{1.12}$$

where ε is an infinitely small positive quantity. According to (1.12), the poles of the energy-dependent retarded Green function indicate the eigenenergies while the corresponding residua can be factorized into the eigenfunctions at positions x and x'.

1.2.3 Free Particle

An important step towards the path integral formulation of quantum mechanics can be made by considering the propagator of a free particle of mass m. The eigenstates of the corresponding Hamiltonian

$$H = \frac{p^2}{2m} \tag{1.13}$$

are momentum eigenstates

$$\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} \exp\left(\frac{\mathrm{i}}{\hbar} px\right) \tag{1.14}$$

with a momentum eigenvalue p out of a continuous spectrum. Inserting these eigenstates into the representation (1.10) of the propagator, one finds by virtue of

$$\int_{-\infty}^{\infty} \mathrm{d}x \exp(-\mathrm{i}ax^2) = \sqrt{\frac{\pi}{\mathrm{i}a}} = \sqrt{\frac{\pi}{a}} \exp\left(-\mathrm{i}\frac{\pi}{4}\right) \tag{1.15}$$

for the propagator of the free particle the result

$$\begin{aligned} K(x_\mathrm{f}, t, x_\mathrm{i}, 0) &= \frac{1}{2\pi\hbar} \int \mathrm{d}p \exp\left(-\frac{\mathrm{i}}{\hbar}\frac{p^2}{2m}t\right) \exp\left(\frac{\mathrm{i}}{\hbar}p(x_\mathrm{f} - x_\mathrm{i})\right) \\ &= \sqrt{\frac{m}{2\pi\mathrm{i}\hbar t}} \exp\left(\frac{\mathrm{i}}{\hbar}\frac{m(x_\mathrm{f} - x_\mathrm{i})^2}{2t}\right) . \end{aligned} \tag{1.16}$$

It was already noted by Dirac [6] that the quantum mechanical propagator and the classical properties of a free particle are closely related. In order to demonstrate this, we evaluate the action of a particle moving from x_i to x_f in time t. From the classical path

$$x_\mathrm{cl}(s) = x_\mathrm{i} + (x_\mathrm{f} - x_\mathrm{i})\frac{s}{t} \tag{1.17}$$

obeying the boundary conditions $x_\mathrm{cl}(0) = x_\mathrm{i}$ and $x_\mathrm{cl}(t) = x_\mathrm{f}$, the corresponding classical action is found as

$$S_\mathrm{cl} = \frac{m}{2}\int_0^t \mathrm{d}s \dot{x}_\mathrm{cl}^2 = \frac{m}{2}\frac{(x_\mathrm{f} - x_\mathrm{i})^2}{t} . \tag{1.18}$$

This result enables us to express the propagator of a free particle entirely in terms of the classical action as

$$K(x_\mathrm{f}, t, x_\mathrm{i}, 0) = \left(-\frac{1}{2\pi\mathrm{i}\hbar}\frac{\partial^2 S_\mathrm{cl}(x_\mathrm{f}, t, x_\mathrm{i}, 0)}{\partial x_\mathrm{f}\partial x_\mathrm{i}}\right)^{1/2} \exp\left(\frac{\mathrm{i}}{\hbar}S_\mathrm{cl}(x_\mathrm{f}, t, x_\mathrm{i}, 0)\right) . \tag{1.19}$$

This result is quite remarkable and one might suspect that it is due to a peculiarity of the free particle. However, since the propagation in a general potential (in the absence of delta function contributions) may be decomposed into a series of short-time propagations of a free particle, the result (1.19) may indeed be employed to construct a representation of the propagator where the classical action appears in the exponent. In the prefactor, the action appears in the form shown in (1.19) only within the semiclassical approximation (cf. Sect. 1.2.8) or for potentials where this approximation turns out to be exact.

1.2.4 Path Integral Representation of Quantum Mechanics

While avoiding to go too deeply into the mathematical details, we nevertheless want to sketch the derivation of the path integral representation of the propagator. The main idea is to decompose the time evolution over a finite time t into N slices of short time intervals $\Delta t = t/N$ where we will eventually take the limit $N \to \infty$. Denoting the operator of the kinetic and potential energy by T and V, respectively, we thus find

$$\exp\left(-\frac{\mathrm{i}}{\hbar}Ht\right) = \left[\exp\left(-\frac{\mathrm{i}}{\hbar}(T+V)\Delta t\right)\right]^N . \tag{1.20}$$

For simplicity, we will assume that the Hamiltonian is time-independent even though the following derivation may be generalized to the time-dependent case. We now would like to decompose the short-time propagator in (1.20) into a part depending on the kinetic energy and another part containing the potential energy. However, since the two operators do not commute, we have to exercise some caution. From an expansion of the Baker-Hausdorff formula one finds

$$\exp\left(-\frac{\mathrm{i}}{\hbar}(T+V)\Delta t\right) \approx \exp\left(-\frac{\mathrm{i}}{\hbar}T\Delta t\right)\exp\left(-\frac{\mathrm{i}}{\hbar}V\Delta t\right) + \frac{1}{\hbar^2}[T,V](\Delta t)^2 \tag{1.21}$$

where terms of order $(\Delta t)^3$ and higher have been neglected. Since we are interested in the limit $\Delta t \to 0$, we may neglect the contribution of the commutator and arrive at the Trotter formula

$$\exp\left(-\frac{\mathrm{i}}{\hbar}(T+V)t\right) = \lim_{N\to\infty}\left[U(\Delta t)\right]^N \tag{1.22}$$

with the short time evolution operator

$$U(\Delta t) = \exp\left(-\frac{\mathrm{i}}{\hbar}T\Delta t\right)\exp\left(-\frac{\mathrm{i}}{\hbar}V\Delta t\right) . \tag{1.23}$$

What we have presented here is, of course, at best a motivation and certainly does not constitute a mathematical proof. We refer readers interested in the details of the proof and the conditions under which the Trotter formula holds to the literature [7].

In position representation one now obtains for the propagator

$$K(x_\mathrm{f},t,x_\mathrm{i},0) = \lim_{N\to\infty}\int_{-\infty}^{\infty}\left(\prod_{j=1}^{N-1}\mathrm{d}x_j\right)\langle x_\mathrm{f}|U(\Delta t)|x_{N-1}\rangle\ldots \times\langle x_1|U(\Delta t)|x_\mathrm{i}\rangle . \tag{1.24}$$

Since the potential is diagonal in position representation, one obtains together with the expression (1.16) for the propagator of the free particle for the matrix

element

$$\begin{aligned}\langle x_{j+1}\,|U(\Delta t)|\,x_j\rangle &= \left\langle x_{j+1}\left|\exp\left(-\frac{\mathrm{i}}{\hbar}T\Delta t\right)\right|x_j\right\rangle \exp\left(-\frac{\mathrm{i}}{\hbar}V(x_j)\Delta t\right)\\ &= \sqrt{\frac{m}{2\pi\mathrm{i}\hbar\Delta t}}\exp\left[\frac{\mathrm{i}}{\hbar}\left(\frac{m}{2}\frac{(x_{j+1}-x_j)^2}{\Delta t}-V(x_j)\Delta t\right)\right]\ .\end{aligned} \tag{1.25}$$

We thus arrive at our final version of the propagator

$$\begin{aligned}K(x_\mathrm{f},t,x_\mathrm{i},0) = \lim_{N\to\infty}\sqrt{\frac{m}{2\pi\mathrm{i}\hbar\Delta t}}\int_{-\infty}^{\infty}\left(\prod_{j=1}^{N-1}\mathrm{d}x_j\sqrt{\frac{m}{2\pi\mathrm{i}\hbar\Delta t}}\right)\\ \times\exp\left[\frac{\mathrm{i}}{\hbar}\sum_{j=0}^{N-1}\left(\frac{m}{2}\left(\frac{x_{j+1}-x_j}{\Delta t}\right)^2-V(x_j)\right)\Delta t\right]\end{aligned} \tag{1.26}$$

where x_0 and x_N should be identified with x_i and x_f, respectively. The discretization of the propagator used in this expression is a consequence of the form (1.21) of the Baker-Hausdorff relation. In lowest order in Δt, we could have used a different decomposition which would have led to a different discretization of the propagator. For a discussion of the mathematical subtleties we refer the reader to [8].

Remarking that the exponent in (1.26) contains a discretized version of the action

$$S[x] = \int_0^t \mathrm{d}s\left(\frac{m}{2}\dot{x}^2 - V(x)\right)\ , \tag{1.27}$$

we can write this result in short notation as

$$K(x_\mathrm{f},t,x_\mathrm{i},0) = \int \mathcal{D}x\exp\left(\frac{\mathrm{i}}{\hbar}S[x]\right)\ . \tag{1.28}$$

The action (1.27) is a functional which takes as argument a function $x(s)$ and returns a number, the action $S[x]$. The integral in (1.28) therefore is a functional integral where one has to integrate over all functions satisfying the boundary conditions $x(0) = x_\mathrm{i}$ and $x(t) = x_\mathrm{f}$. Since these functions represent paths, one refers to this kind of functional integrals also as path integral.

The three lines shown in Fig. 1.2 represent the infinity of paths satisfying the boundary conditions. Among them the thicker line indicates a special path corresponding to an extremum of the action. According to the principal of least action such a path is a solution of the classical equation of motion. It should be noted, however, that even though sometimes there exists a unique extremum, in general there may be more than one or even none. A demonstration of this fact will be provided in Sect. 1.2.7 where we will discuss the driven harmonic oscillator.

The other paths depicted in Fig. 1.2 may be interpreted as quantum fluctuations around the classical path. As we will see in Sect. 1.2.8, the amplitude of

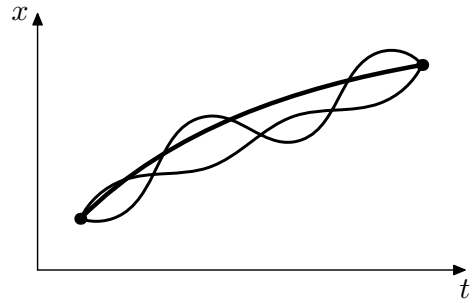

Fig. 1.2. The thick line represents a classical path satisfying the boundary conditions. The thinner lines are no solutions of the classical equation of motion and may be associated with quantum fluctuations

these fluctuations is typically of the order of $\sqrt{\hbar}$. In the classical limit $\hbar \to 0$ therefore only the classical paths survive as one should expect.

Before explicitly evaluating a path integral, we want to discuss two examples which will give us some insight into the difference of the approaches offered by the Schrödinger and Feynman formulation of quantum mechanics.

1.2.5 Particle on a Ring

We confine a particle of mass m to a ring of radius R and denote its angular degree of freedom by ϕ. This system is described by the Hamiltonian

$$H = -\frac{\hbar^2}{2mR^2}\frac{\partial^2}{\partial\phi^2} \; . \tag{1.29}$$

Requiring the wave function to be continuous and differentiable, one finds the stationary states

$$\psi_\ell(\phi) = \frac{1}{\sqrt{2\pi}} \exp\left(\mathrm{i}\ell\phi\right) \tag{1.30}$$

with $\ell = 0, \pm 1, \pm 2, \ldots$ and the eigenenergies

$$E_\ell = \frac{\hbar^2\ell^2}{2mR^2} \; . \tag{1.31}$$

These solutions of the time-independent Schrödinger equation allow us to construct the propagator

$$K(\phi_\mathrm{f}, t, \phi_\mathrm{i}, 0) = \frac{1}{2\pi}\sum_{\ell=-\infty}^{\infty} \exp\left(\mathrm{i}\ell(\phi_\mathrm{f} - \phi_\mathrm{i}) - \mathrm{i}\frac{\hbar\ell^2}{2mR^2}t\right) \; . \tag{1.32}$$

We now want to derive this result within the path integral formalism. To this end we will employ the propagator of the free particle. However, an important difference between a free particle and a particle on a ring deserves our attention.

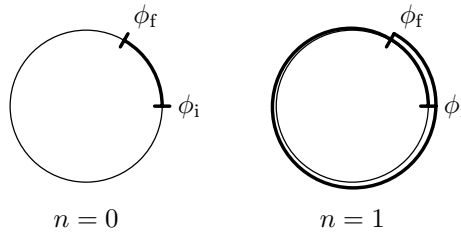

Fig. 1.3. On a ring, the angles ϕ_f and $\phi_\mathrm{f} + 2\pi n$ have to be identified. As a consequence, there exist infinitely many classical paths connecting two points on a ring, which may be identified by their winding number n

Due to the ring topology we have to identify all angles $\phi + 2\pi n$, where n is an integer, with the angle ϕ. As a consequence, there exist infinitely many classical paths connecting ϕ_i and ϕ_f. All these paths are topologically different and can be characterized by their winding number n. As an example, Fig. 1.3 shows a path for $n = 0$ and $n = 1$. Due to their different topology, these two paths (and any two paths corresponding to different winding numbers) cannot be continuously transformed into each other. This implies that adding a fluctuation to one of the classical paths will never change its winding number.

Therefore, we have to sum over all winding numbers in order to account for all possible paths. The propagator thus consists of a sum over free propagators corresponding to different winding numbers

$$K(\phi_\mathrm{f}, t, \phi_\mathrm{i}, 0) = \sum_{n=-\infty}^{\infty} R\sqrt{\frac{m}{2\pi\mathrm{i}\hbar t}}\exp\left(\frac{\mathrm{i}}{\hbar}\frac{mR^2}{2}\frac{(\phi_\mathrm{f} - \phi_\mathrm{i} - 2\pi n)^2}{t}\right) . \tag{1.33}$$

Here, the factor R accounts for the fact that, in contrast to the free particle, the coordinate is given by an angle instead of a position.

The propagator (1.33) is 2π-periodic in $\phi_\mathrm{f} - \phi_\mathrm{i}$ and can therefore be expressed in terms of a Fourier series

$$K(\phi_\mathrm{f}, t, \phi_\mathrm{i}, 0) = \sum_{\ell=-\infty}^{\infty} c_\ell \exp\left[\mathrm{i}\ell(\phi_\mathrm{f} - \phi_\mathrm{i})\right] . \tag{1.34}$$

The Fourier coefficients are found to read

$$c_\ell = \frac{1}{2\pi}\exp\left(-\mathrm{i}\frac{\hbar\ell^2}{2mR^2}t\right) \tag{1.35}$$

which proves the equivalence of (1.33) with our previous result (1.32). We thus have obtained the propagator of a free particle on a ring both by solving the Schrödinger equation and by employing path integral methods. These two approaches make use of complementary representations. In the first case, this is the angular momentum representation while in the second case, one works in the phase representation and sums over winding numbers.

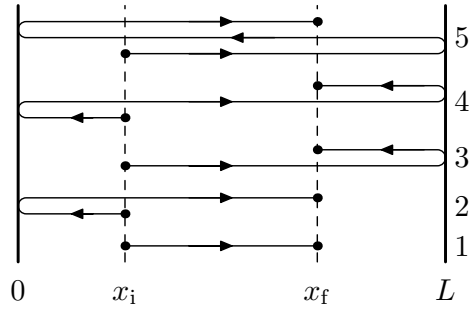

Fig. 1.4. The reflection at the walls of a box leads to an infinite number of possible trajectories connecting two points in the box

1.2.6 Particle in a Box

Another textbook example in standard quantum mechanics is the particle in a box of length L confined by infinitely high walls at $x = 0$ and $x = L$. From the eigenvalues

$$E_j = \frac{\hbar^2\pi^2 j^2}{2mL^2} \tag{1.36}$$

with $j = 1, 2, \ldots$ and the corresponding eigenfunctions

$$\psi_j(x) = \sqrt{\frac{2}{L}} \sin\left(\pi j \frac{x}{L}\right) \tag{1.37}$$

the propagator is immediately obtained as

$$K(x_\mathrm{f}, t, x_\mathrm{i}, 0) = \frac{2}{L} \sum_{j=1}^{\infty} \exp\left(-\mathrm{i}\frac{\hbar\pi^2 j^2}{2mL^2} t\right) \sin\left(\pi j \frac{x_\mathrm{f}}{L}\right) \sin\left(\pi j \frac{x_\mathrm{i}}{L}\right) \ . \tag{1.38}$$

It took some time until this problem was solved within the path integral approach [9,10]. Here, we have to consider all paths connecting the points x_i and x_f within a period of time t. Due to the reflecting walls, there again exist infinitely many classical paths, five of which are depicted in Fig. 1.4. However, in contrast to the case of a particle on a ring, these paths are no longer topologically distinct. As a consequence, we may deform a classical path continuously to obtain one of the other classical paths.

If, for the moment, we disregard the details of the reflections at the wall, the motion of the particle in a box is equivalent to the motion of a free particle. The fact that paths are folded back on themselves can be accounted for by taking into account replicas of the box as shown in Fig. 1.5. Now, the path does not necessarily end at $x_\mathrm{f}^{(0)} = x_\mathrm{f}$ but at one of the mirror images $x_\mathrm{f}^{(n)}$ where n is an arbitrary integer. In order to obtain the propagator, we will have to sum over all replicas. Due to the different geometry we need to distinguish between those paths arising from an even and an odd number of reflections. From Fig. 1.5 one

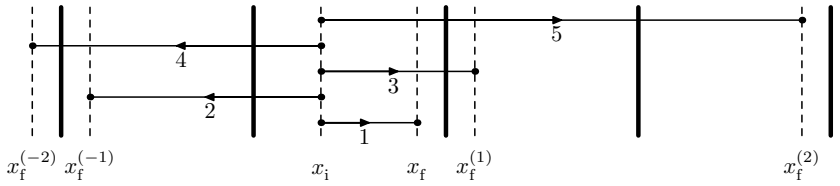

Fig. 1.5. Instead of a particle getting reflected at the walls of the box one may think of a free particle moving from the starting point in the box to the end point in one of the replicas of the box

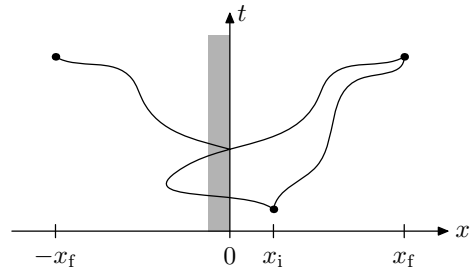

Fig. 1.6. A path crossing the wall is cancelled by a path running to the mirror point of the end point

can see that for an odd number $2n-1$ of reflections, the end point lies at $2nL-x_{\rm f}$ and the contribution to the full propagator therefore is given by

$$K^{(2n-1)}(x_{\rm f},t,x_{\rm i},0)=\sqrt{\frac{m}{2\pi{\rm i}\hbar t}}\exp\!\left(\frac{\rm i}{\hbar}\frac{m(2nL-x_{\rm f}-x_{\rm i})^2}{2t}\right)\,. \tag{1.39}$$

On the other hand, for an even number $2n$ of reflections, the end point is located at $2nL+x_{\rm f}$ and we find

$$K^{(2n)}(x_{\rm f},t,x_{\rm i},0)=\sqrt{\frac{m}{2\pi{\rm i}\hbar t}}\exp\!\left(\frac{\rm i}{\hbar}\frac{m(2nL+x_{\rm f}-x_{\rm i})^2}{2t}\right)\,. \tag{1.40}$$

However, it is not obvious that just summing up the propagators (1.39) and (1.40) for all n will do the job.

In order to clarify this point, we start with the somewhat simpler situation of just one wall and take a look at all paths running between $x_{\rm i}$ and $x_{\rm f}$ in time t. As can be seen from the space-time diagram in Fig. 1.6 there are paths which do not cross the wall and which therefore contribute to the path integral. On the other hand, there exist also paths which cross the wall an even number of times. Since these paths spend some time in the forbidden region, they do not contribute to the path integral.

It requires some thinking to ensure that only paths not crossing the wall are taken into account. Our strategy will consist in first writing down a propagator $K_{\rm free}$ which disregards the wall. Then, we have to subtract off the contributions of all the paths which cross the wall. This can be done by constructing a path

with the same action as the original path. To this end we take the original path up to the last crossing with the wall and then continue along the mirror image of the original path. We thus end up at the mirror image $-x_\mathrm{f}$ of the original end point x_f. Note that a path running from x_i to $-x_\mathrm{f}$ necessarily crosses the wall at least once. As a consequence, subtracting the propagator between these two points eliminates all original paths which do not remain in the region $x > 0$. We therefore obtain our desired result, the propagator K_wall in the presence of a wall, by subtracting a propagator going to the reflected end point from the unconstrained propagator to the original end point [9,10,11]

$$K_\mathrm{wall}(x_\mathrm{f},t,x_\mathrm{i},0) = K_\mathrm{free}(x_\mathrm{f},t,x_\mathrm{i},0) - K_\mathrm{free}(-x_\mathrm{f},t,x_\mathrm{i},0)\,. \tag{1.41}$$

This result bears much resemblance with the method of image charges in electrostatics. After giving it some thought, this should not be too surprising since the free Schrödinger equation and the Poisson equation are formally equivalent. According to the method of image charges one may account for a metallic plate (i.e. the wall) by putting a negative charge (i.e. the mirrored end point) complementing the positive charge (i.e. the original end point). For the propagator this results in the difference appearing in (1.41).

Let us now come back to our infinitely deep potential well with two walls. This problem corresponds to the electrostatics of a charge between two parallel metal plates. In this case, the method of image charges leads to an infinite number of charges of alternating signs. The original positive charge gives rise to two negative charges which are each an image corresponding to one of the two metal plates. In addition, however, these images have mirror images corresponding to the other metal plate and this process has to be carried on ad infinitum.

Expressing the propagator of the particle in the box in terms of the free propagator works in exactly the same way. A path intersecting both walls is subtracted twice, i.e. one time too often. Therefore, one contribution has to be restored which is done by adding another end point. Continuing the procedure one ends up with an infinite number of end points, some of which we have shown in Fig. 1.5. As a consequence, we can attribute a sign to each end point in this figure. The general rule which follows from these considerations is that each reflection at a wall leads to factor -1. The propagator therefore can be written as

$$\begin{aligned} K(x_\mathrm{f},t,x_\mathrm{i},0) = \sqrt{\frac{m}{2\pi\mathrm{i}\hbar t}} \sum_{n=-\infty}^{\infty} \Bigg[&\exp\left(\frac{\mathrm{i}}{\hbar}\frac{m(2nL+x_\mathrm{f}-x_\mathrm{i})^2}{2t}\right) \\ &- \exp\left(\frac{\mathrm{i}}{\hbar}\frac{m(2nL-x_\mathrm{f}-x_\mathrm{i})^2}{2t}\right)\Bigg]\,. \end{aligned} \tag{1.42}$$

The symmetries

$$K(x_\mathrm{f}+2L,t,x_\mathrm{i},0) = K(x_\mathrm{f},t,x_\mathrm{i},0) \tag{1.43}$$

$$K(-x_\mathrm{f},t,x_\mathrm{i},0) = -K(x_\mathrm{f},t,x_\mathrm{i},0) \tag{1.44}$$

suggest to expand the propagator into the Fourier series

$$K(x_\mathrm{f},t,x_\mathrm{i},0)=\sum_{j=1}^{\infty}a_j(x_\mathrm{i},t)\sin\left(\pi j\frac{x_\mathrm{f}}{L}\right)\ . \tag{1.45}$$

Its Fourier coefficients are obtained from (1.42) as

$$\begin{aligned}a_j(x_\mathrm{i},t)&=\frac{1}{L}\int_{-L}^{L}\mathrm{d}x_\mathrm{f}\sin\left(\pi j\frac{x_\mathrm{f}}{L}\right)K(x_\mathrm{f},t,x_\mathrm{i},0)\\&=\frac{2}{L}\sin\left(\pi j\frac{x_\mathrm{i}}{L}\right)\exp\left(-\frac{\mathrm{i}}{\hbar}E_jt\right)\end{aligned} \tag{1.46}$$

where the energies E_j are the eigenenergies of the box defined in (1.36). Inserting (1.46) into (1.45) we thus recover our previous result (1.38).

1.2.7 Driven Harmonic Oscillator

Even though the situations dealt with in the previous two sections have been conceptually quite interesting, we could in both cases avoid the explicit calculation of a path integral. In the present section, we will introduce the basic techniques needed to evaluate path integrals. As an example, we will consider the driven harmonic oscillator which is simple enough to allow for an exact solution. In addition, the propagator will be of use in the discussion of damped quantum systems in later sections.

Our starting point is the Lagrangian

$$L=\frac{m}{2}\dot{x}^2-\frac{m}{2}\omega^2x^2+xf(t) \tag{1.47}$$

of a harmonic oscillator with mass m and frequency ω. The force $f(t)$ may be due to an external field, e.g. an electric field coupling via dipole interaction to a charged particle. In the context of dissipative quantum mechanics, the harmonic oscillator could represent a degree of freedom of the environment under the influence of a force exerted by the system.

According to (1.28) we obtain the propagator $K(x_\mathrm{f},t,x_\mathrm{i},0)$ by calculating the action for all possible paths starting at time zero at x_i and ending at time t at x_f. It is convenient to decompose the general path

$$x(s)=x_\mathrm{cl}(s)+\xi(s) \tag{1.48}$$

into the classical path x_cl satisfying the boundary conditions $x_\mathrm{cl}(0)=x_\mathrm{i}$, $x_\mathrm{cl}(t)=x_\mathrm{f}$ and a fluctuating part ξ vanishing at the boundaries, i.e. $\xi(0)=\xi(t)=0$. The classical path has to satisfy the equation of motion

$$m\ddot{x}_\mathrm{cl}+m\omega^2x_\mathrm{cl}=f(s) \tag{1.49}$$

obtained from the Lagrangian (1.47).

For an exactly solvable problem like the driven harmonic oscillator, we could replace $x_{\rm cl}$ by any path satisfying $x(0) = x_{\rm i}$, $x(t) = x_{\rm f}$. We leave it as an exercise to the reader to perform the following calculation with $x_{\rm cl}(s)$ of the driven harmonic oscillator replaced by $x_{\rm i} + (x_{\rm f} - x_{\rm i})s/t$. However, it is important to note that within the semiclassical approximation discussed in Sect. 1.2.8 an expansion around the classical path is essential since this path leads to the dominant contribution to the path integral.

With (1.48) we obtain for the action

$$\begin{aligned} S &= \int_0^t {\rm d}s \left(\frac{m}{2}\dot{x}^2 - \frac{m}{2}\omega^2 x^2 + x f(s)\right) \\ &= \int_0^t {\rm d}s \left(\frac{m}{2}\dot{x}_{\rm cl}^2 - \frac{m}{2}\omega^2 x_{\rm cl}^2 + x_{\rm cl} f(s)\right) + \int_0^t {\rm d}s \left(m\dot{x}_{\rm cl}\dot{\xi} - m\omega^2 x_{\rm cl}\xi + \xi f(s)\right) \\ &\quad + \int_0^t {\rm d}s \left(\frac{m}{2}\dot{\xi}^2 - \frac{m}{2}\omega^2\xi^2\right). \end{aligned} \tag{1.50}$$

For our case of a harmonic potential, the third term is independent of the boundary values $x_{\rm i}$ and $x_{\rm f}$ as well as of the external driving. The second term vanishes as a consequence of the expansion around the classical path. This can be seen by partial integration and by making use of the fact that $x_{\rm cl}$ is a solution of the classical equation of motion:

$$\int_0^t {\rm d}s\big(m\dot{x}_{\rm cl}\dot{\xi} - m\omega^2 x_{\rm cl}\xi + \xi f(s)\big) = -\int_0^t {\rm d}s\big(m\ddot{x}_{\rm cl} + m\omega^2 x_{\rm cl} - f(s)\big)\xi = 0\,. \tag{1.51}$$

We now proceed in two steps by first determining the contribution of the classical path and then addressing the fluctuations. The solution of the classical equation of motion satisfying the boundary conditions reads

$$\begin{aligned} x_{\rm cl}(s) &= x_{\rm f}\frac{\sin(\omega s)}{\sin(\omega t)} + x_{\rm i}\frac{\sin(\omega(t-s))}{\sin(\omega t)} \\ &\quad + \frac{1}{m\omega}\left[\int_0^s {\rm d}u \sin(\omega(s-u)) f(u) - \frac{\sin(\omega s)}{\sin(\omega t)}\int_0^t {\rm d}u \sin(\omega(t-u)) f(u)\right]. \end{aligned} \tag{1.52}$$

A peculiarity of the harmonic oscillator in the absence of driving is the appearance of conjugate points at times $T_n = (\pi/\omega)n$ where n is an arbitrary integer. Since the frequency of the oscillations is independent of the amplitude, the position of the oscillator at these times is determined by the initial position: $x(T_{2n+1}) = -x_{\rm i}$ and $x(T_{2n}) = x_{\rm i}$, see Fig. 1.7. This also illustrates the fact mentioned on p. 7, that depending on the boundary conditions there may be more than one or no classical solution.

The task of evaluating the action of the classical path may be simplified by a partial integration

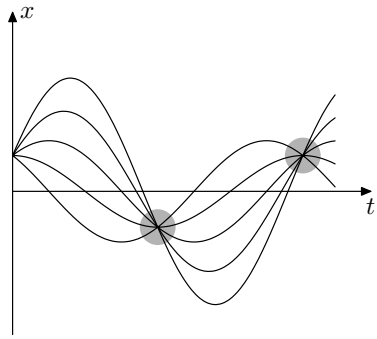

Fig. 1.7. In a harmonic potential all trajectories emerging from the same starting point converge at conjugate points at multiples of half an oscillation period

$$\begin{aligned} S_{\rm cl} &= \int_0^t {\rm d}s \left(\frac{m}{2}\dot{x}_{\rm cl}^2 - \frac{m}{2}\omega^2 x_{\rm cl}^2 + x_{\rm cl} f(s) \right) \\ &= \frac{m}{2} x_{\rm cl}\dot{x}_{\rm cl}\Big|_0^t - \int_0^t {\rm d}s \left(\frac{m}{2} x_{\rm cl}\ddot{x}_{\rm cl} + \frac{m}{2}\omega^2 x_{\rm cl}^2 - x_{\rm cl} f(s) \right) \\ &= \frac{m}{2}\left(x_{\rm f}\dot{x}_{\rm cl}(t) - x_{\rm i}\dot{x}_{\rm cl}(0) \right) + \frac{1}{2}\int_0^t {\rm d}s\, x_{\rm cl}(s) f(s) \end{aligned} \tag{1.53}$$

where we have made use of the classical equation of motion to obtain the third line. From the solution (1.52) of the classical equation of motion we get

$$\dot{x}_{\rm cl}(0) = \omega \frac{x_{\rm f} - x_{\rm i}\cos(\omega t)}{\sin(\omega t)} - \frac{1}{m\sin(\omega t)} \int_0^t {\rm d}s \sin(\omega(t-s)) f(s) \tag{1.54}$$

$$\dot{x}_{\rm cl}(t) = \omega \frac{x_{\rm f}\cos(\omega t) - x_{\rm i}}{\sin(\omega t)} + \frac{1}{m\sin(\omega t)} \int_0^t {\rm d}s \sin(\omega s) f(s)\ . \tag{1.55}$$

Inserting initial and final velocity into (1.53) we find for the classical action

$$\begin{aligned} S_{\rm cl} =& \frac{m\omega}{2\sin(\omega t)} \left[(x_{\rm i}^2 + x_{\rm f}^2)\cos(\omega t) - 2x_{\rm i}x_{\rm f} \right] \\ &+ \frac{x_{\rm f}}{\sin(\omega t)} \int_0^t {\rm d}s \sin(\omega s) f(s) + \frac{x_{\rm i}}{\sin(\omega t)} \int_0^t {\rm d}s \sin(\omega(t-s)) f(s) \\ &- \frac{1}{m\omega\sin(\omega t)} \int_0^t {\rm d}s \int_0^s {\rm d}u \sin(\omega u) \sin(\omega(t-s)) f(s) f(u)\ . \end{aligned} \tag{1.56}$$

As a second step, we have to evaluate the contribution of the fluctuations which is determined by the third term in (1.50). After partial integration this term becomes

$$S^{(2)} = \int_0^t {\rm d}s \left(\frac{m}{2}\dot{\xi}^2 - \frac{m}{2}\omega^2\xi^2 \right) = -\int_0^t {\rm d}s \frac{m}{2}\xi \left(\frac{{\rm d}^2}{{\rm d}s^2} + \omega^2 \right) \xi\ . \tag{1.57}$$

Here, the superscript '(2)' indicates that this term corresponds to the contribution of second order in ξ. In view of the right-hand side it is appropriate to expand the fluctuation

$$\xi(s) = \sum_{n=1}^{\infty} a_n \xi_n(s) \tag{1.58}$$

into eigenfunctions of

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}s^2} + \omega^2\right) \xi_n = \lambda_n \xi_n \tag{1.59}$$

with $\xi_n(0) = \xi_n(t) = 0$. As eigenfunctions of a selfadjoint operator, the ξ_n are complete and may be chosen orthonormal. Solving (1.59) yields the eigenfunctions

$$\xi_n(s) = \sqrt{\frac{2}{t}} \sin\left(\pi n \frac{s}{t}\right) \tag{1.60}$$

and corresponding eigenvalues

$$\lambda_n = -\left(\frac{\pi n}{t}\right)^2 + \omega^2 \,. \tag{1.61}$$

We emphasize that (1.58) is not the usual Fourier series on an interval of length t. Such an expansion could be used in the form

$$\xi(s) = \sqrt{\frac{2}{t}} \sum_{n=1}^{\infty} \left[a_n \left(\cos\left(2\pi n \frac{s}{t}\right) - 1\right) + b_n \sin\left(2\pi n \frac{s}{t}\right)\right] \tag{1.62}$$

which ensures that the fluctuations vanish at the boundaries. We invite the reader to redo the following calculation with the expansion (1.62) replacing (1.58). While at the end the same propagator should be found, it will become clear why the expansion in terms of eigenfunctions satisfying (1.59) is preferable.

The integration over the fluctuations now becomes an integration over the expansion coefficients a_n. Inserting the expansion (1.58) into the action one finds

$$S^{(2)} = -\frac{m}{2} \sum_{n=1}^{\infty} \lambda_n a_n^2 = \frac{m}{2} \sum_{n=1}^{\infty} \left(\left(\frac{\pi n}{t}\right)^2 - \omega^2\right) a_n^2 \,. \tag{1.63}$$

As this result shows, the classical action is only an extremum of the action but not necessarily a minimum although this is the case for short time intervals $t < \pi/\omega$. The existence of conjugate points at times $T_n = n\pi/\omega$ mentioned above manifests itself here as vanishing of the eigenvalue λ_n. Then the action is independent of a_n which implies that for a time interval T_n all paths $x_{\mathrm{cl}} + a_n \xi_n$ with arbitrary coefficient a_n are solutions of the classical equation of motion.

After expansion of the fluctuations in terms of the eigenfunctions (1.60), the propagator takes the form

$$K(x_{\mathrm{f}}, t, x_{\mathrm{i}}, 0) \sim \exp\left(\frac{\mathrm{i}}{\hbar} S_{\mathrm{cl}}\right) \int \left(\prod_{n=1}^{\infty} \mathrm{d}a_n\right) \exp\left(-\frac{\mathrm{i}}{\hbar} \frac{m}{2} \sum_{n=1}^{\infty} \lambda_n a_n^2\right) \,. \tag{1.64}$$

In principle, we need to know the Jacobi determinant of the transformation from the path integral to the integral over the Fourier coefficients. However, since this Jacobi determinant is independent of the oscillator frequency ω, we may also compare with the free particle. Evaluating the Gaussian fluctuation integrals, we find for the ratio between the prefactors of the propagators K_ω and K_0 of the harmonic oscillator and the free particle, respectively,

$$\frac{K_\omega \exp[-(\mathrm{i}/\hbar)S_{\mathrm{cl},\omega}]}{K_0 \exp[-(\mathrm{i}/\hbar)S_{\mathrm{cl},0}]} = \sqrt{\frac{D_0}{D}} \,. \tag{1.65}$$

Here, we have introduced the fluctuation determinants for the harmonic oscillator

$$D = \det\left(\frac{\mathrm{d}^2}{\mathrm{d}s^2} + \omega^2\right) = \prod_{n=1}^{\infty} \lambda_n \tag{1.66}$$

and the free particle

$$D_0 = \det\left(\frac{\mathrm{d}^2}{\mathrm{d}s^2}\right) = \prod_{n=1}^{\infty} \lambda_n^0 \,. \tag{1.67}$$

The eigenvalues for the free particle

$$\lambda_n^0 = -\left(\frac{\pi n}{t}\right)^2 \tag{1.68}$$

are obtained from the eigenvalues (1.61) of the harmonic oscillator simply by setting the frequency ω equal to zero. With the prefactor of the propagator of the free particle

$$K_0 \exp\left(-\frac{\mathrm{i}}{\hbar} S_{\mathrm{cl},0}\right) = \sqrt{\frac{m}{2\pi \mathrm{i}\hbar t}} \tag{1.69}$$

and (1.65), the propagator of the harmonic oscillator becomes

$$K(x_\mathrm{f}, t, x_\mathrm{i}, 0) = \sqrt{\frac{m}{2\pi \mathrm{i}\hbar t}} \sqrt{\frac{D_0}{D}} \exp\left(\frac{\mathrm{i}}{\hbar} S_{\mathrm{cl}}\right) \,. \tag{1.70}$$

For readers unfamiliar with the concept of determinants of differential operators we mention that we may define matrix elements of an operator by projection onto a basis as is familiar from standard quantum mechanics. The operator represented in its eigenbasis yields a diagonal matrix with the eigenvalues on the diagonal. Then, as for finite dimensional matrices, the determinant is the product of these eigenvalues.

Each of the determinants (1.66) and (1.67) by itself diverges. However, we are interested in the ratio between them which is well-defined [12]

$$\frac{D}{D_0} = \prod_{n=1}^{\infty} \left(1 - \left(\frac{\omega t}{\pi n}\right)^2\right) = \frac{\sin(\omega t)}{\omega t} \,. \tag{1.71}$$

Inserting this result into (1.70) leads to the propagator of the driven harmonic oscillator in its final form

$$\begin{aligned} K(x_\mathrm{f},t,x_\mathrm{i},0) &= \sqrt{\frac{m\omega}{2\pi\mathrm{i}\hbar\sin(\omega t)}}\exp\left[\frac{\mathrm{i}}{\hbar}S_\mathrm{cl}\right] \\ &= \sqrt{\frac{m\omega}{2\pi\hbar|\sin(\omega t)|}}\exp\left[\frac{\mathrm{i}}{\hbar}S_\mathrm{cl}-\mathrm{i}\left(\frac{\pi}{4}+n\frac{\pi}{2}\right)\right] \end{aligned} \tag{1.72}$$

with the classical action defined in (1.56). The Morse index n in the phase factor is given by the integer part of $\omega t/\pi$. This phase accounts for the changes in sign of the sine function [13]. Here, one might argue that it is not obvious which sign of the square root one has to take. However, the semigroup property (1.9) allows to construct propagators across conjugate points by joining propagators for shorter time intervals. In this way, the sign may be determined unambiguously [14].

It is interesting to note that the phase factor $\exp(-\mathrm{i}n\pi/2)$ in (1.72) implies that $K(x_\mathrm{f},2\pi/\omega,x_\mathrm{i},0) = -K(x_\mathrm{f},0,x_\mathrm{i},0) = -\delta(x_\mathrm{f}-x_\mathrm{i})$, i.e. the wave function after one period of oscillation differs from the original wave function by a factor -1. The oscillator thus returns to its original state only after two periods very much like a spin-1/2 particle which picks up a sign under rotation by 2π and returns to its original state only after a 4π-rotation. This effect might be observed in the case of the harmonic oscillator by letting interfere the wave functions of two oscillators with different frequency [15].

1.2.8 Semiclassical Approximation

The systems considered so far have been special in the sense that an exact expression for the propagator could be obtained. This is a consequence of the fact that the potential was at most quadratic in the coordinate. Unfortunately, in most cases of interest the potential is more complicated and apart from a few exceptions an exact evaluation of the path integral turns out to be impossible. To cope with such situations, approximation schemes have been devised. In the following, we will restrict ourselves to the most important approximation which is valid whenever the quantum fluctuations are small or, equivalently, when the actions involved are large compared to Planck's constant so that the latter may be considered to be small.

The decomposition of a general path into the classical path and fluctuations around it as employed in (1.48) in the previous section was merely a matter of convenience. For the exactly solvable case of a driven harmonic oscillator it is not really relevant how we express a general path satisfying the boundary conditions. Within the semiclassical approximation, however, it is decisive to expand around the path leading to the dominant contribution, i.e. the classical path. From a more mathematical point of view, we have to evaluate a path integral over $\exp(\mathrm{i}S/\hbar)$ for small $\hbar$. This can be done in a systematic way by the method of stationary phase where the exponent has to be expanded around the extrema of the action S.

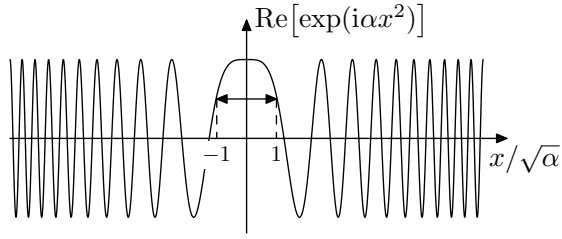

Fig. 1.8. In stationary phase approximation only a small region around the extremum contributes to the integral. For the example shown here, the extremum lies at $x = 0$

At this point it may be useful to give a brief reminder of the method of stationary phase. Suppose we want to evaluate the integral

$$I(\alpha) = \int_{-\infty}^{\infty} \mathrm{d}x g(x) \exp\bigl(\mathrm{i}\alpha f(x)\bigr) \tag{1.73}$$

in the limit of very large α. Inspection of Fig. 1.8, where $f(x) = x^2$, suggests that the dominant contribution to the integral comes from a region, in our example of size $1/\sqrt{\alpha}$, around the extremal (or stationary) point of the function $f(x)$. Outside of this region, the integrand is rapidly oscillating and therefore gives to leading order a negligible contribution. Since for large α, the region determining the integral is very small, we may expand the function $f(x)$ locally around the extremum x_0

$$f(x) \approx f(x_0) + \frac{1}{2} f''(x_0)(x - x_0)^2 + \dots \tag{1.74}$$

and replace $g(x)$ by $g(x_0)$. Neglecting higher order terms, which is allowed if $f''(x_0)$ is of order one, we are left with the Gaussian integral

$$\begin{aligned} I(\alpha) &\approx g(x_0) \exp\bigl(\mathrm{i}\alpha f(x_0)\bigr) \int_{-\infty}^{\infty} \mathrm{d}x \exp\left(\frac{\mathrm{i}}{2} f''(x_0)(x - x_0)^2\right) \\ &= \sqrt{\frac{2\pi}{|f''(x_0)|}} g(x_0) \exp\Bigl[\mathrm{i}\alpha f(x_0) + \mathrm{i}\frac{\pi}{4} \mathrm{sgn}\bigl(f''(x_0)\bigr)\Bigr] \ , \end{aligned} \tag{1.75}$$

where $\mathrm{sgn}(f''(x_0))$ denotes the sign of $f''(x_0)$. If $f(x)$ possesses more than one extremum, one has to sum over the contributions of all extrema unless one extremum can be shown to be dominant.

We now apply the stationary phase approximation to path integrals where $1/\hbar$ plays the role of the large parameter. Since the action is stationary at classical paths, we are obliged to express the general path as

$$x(s) = x_{\mathrm{cl}}(s) + \xi(s) \ , \tag{1.76}$$

where x_{cl} is the classical path (or one of several possible paths) satisfying the boundary conditions and ξ represents the fluctuations around the classical path.

With this decomposition the action becomes

$$\begin{aligned} S &= \int_0^t \mathrm{d}s \left(\frac{m}{2}\dot{x}^2 - V(x)\right) \\ &= \int_0^t \mathrm{d}s \left(\frac{m}{2}\dot{x}_{\mathrm{cl}}^2 - V(x_{\mathrm{cl}})\right) + \int_0^t \mathrm{d}s \left(m\dot{x}_{\mathrm{cl}}\dot{\xi} - V'(x_{\mathrm{cl}})\xi\right) \\ &\qquad + \int_0^t \mathrm{d}s \left(\frac{m}{2}\dot{\xi}^2 - \frac{1}{2}V''(x_{\mathrm{cl}})\xi^2\right) + \ldots \end{aligned} \tag{1.77}$$

It is instructive to compare this result with the action (1.50) for the driven harmonic oscillator. Again, the first term represents the classical action. The second term vanishes as was shown explicitly in (1.51) for the driven oscillator. In the general case, one can convince oneself by partial integration of the kinetic part and comparison with the classical equation of motion that this term vanishes again. This is of course a consequence of the fact that the classical path, around which we expand, corresponds to an extremum of the action. The third term on the right-hand-side of (1.77) is the leading order term in the fluctuations as was the case in (1.50). There is however an important difference since for anharmonic potentials the second derivative of the potential V'' is not constant and therefore the contribution of the fluctuations depends on the classical path. Finally, in general there will be higher order terms in the fluctuations as indicated by the dots in (1.77). The semiclassical approximation consists in neglecting these higher order terms so that after a partial integration, we get for the action

$$S_{\mathrm{sc}} = S_{\mathrm{cl}} - \frac{1}{2}\int_0^t \mathrm{d}s\, \xi\left(m\frac{\mathrm{d}^2}{\mathrm{d}s^2} + V''(x_{\mathrm{cl}})\right)\xi \tag{1.78}$$

where the index 'sc' indicates the semiclassical approximation.

Before deriving the propagator in semiclassical approximation, we have to discuss the regime of validity of this approximation. Since the first term in (1.78) gives only rise to a global phase factor, it is the second term which determines the magnitude of the quantum fluctuations. For this term to contribute, we should have $\xi^2/\hbar \lesssim 1$ so that the magnitude of typical fluctuations is at most of order $\sqrt{\hbar}$. The term of third order in the fluctuations is already smaller than the second order term by a factor $(\sqrt{\hbar})^3/\hbar = \sqrt{\hbar}$. If Planck's constant can be considered to be small, we may indeed neglect the fluctuation contributions of higher than second order except for one exception: It may happen that the second order term does not contribute, as has been the case at the conjugate points for the driven harmonic oscillator in Sect. 1.2.7. Then, the leading nonvanishing contribution becomes dominant. For the following discussion, we will not consider this latter case.

In analogy to Sect. 1.2.7 we obtain for the propagator in semiclassical approximation

$$K(x_{\mathrm{f}}, t, x_{\mathrm{i}}, 0) = \sqrt{\frac{m}{2\pi\mathrm{i}\hbar t}}\sqrt{\frac{D_0}{D}}\exp\left(\frac{\mathrm{i}}{\hbar}S_{\mathrm{cl}}\right) \tag{1.79}$$

where

$$D = \det\left(\frac{\mathrm{d}^2}{\mathrm{d}s^2} + V''(x_{\mathrm{cl}})\right) \tag{1.80}$$

and D_0 is the fluctuation determinant (1.67) of the free particle.

Even though it may seem that determining the prefactor is a formidable task since the fluctuation determinant for a given potential has to be evaluated, this task can be greatly simplified. In addition, the following considerations offer the benefit of providing a physical interpretation of the prefactor. In our evaluation of the prefactor we follow Marinov [16]. The main idea is to make use of the semigroup property (1.9) of the propagator

$$\begin{aligned} &C(x_{\mathrm{f}}, t, x_{\mathrm{i}}, 0) \exp\left[\frac{\mathrm{i}}{\hbar} S_{\mathrm{cl}}(x_{\mathrm{f}}, t, x_{\mathrm{i}}, 0)\right] \\ &= \int \mathrm{d}x' C(x_{\mathrm{f}}, t, x', t') C(x', t', x_{\mathrm{i}}, 0) \exp\left[\frac{\mathrm{i}}{\hbar}\left[S_{\mathrm{cl}}(x_{\mathrm{f}}, t, x', t') + S_{\mathrm{cl}}(x', t', x_{\mathrm{i}}, 0)\right]\right] \end{aligned} \tag{1.81}$$

where the prefactor C depends on the fluctuation contribution. We now have to evaluate the x'-integral within the semiclassical approximation. According to the stationary phase requirement discussed above, the dominant contribution to the integral comes from $x' = x_0(x_{\mathrm{f}}, x_{\mathrm{i}}, t, t')$ satisfying

$$\left.\frac{\partial S_{\mathrm{cl}}(x_{\mathrm{f}}, t, x', t')}{\partial x'}\right|_{x'=x_0} + \left.\frac{\partial S_{\mathrm{cl}}(x', t', x_{\mathrm{i}}, 0)}{\partial x'}\right|_{x'=x_0} = 0\,. \tag{1.82}$$

According to classical mechanics these derivatives are related to initial and final momentum by [17]

$$\left(\frac{\partial S_{\mathrm{cl}}}{\partial x_{\mathrm{i}}}\right)_{x_{\mathrm{f}}, t_{\mathrm{f}}, t_{\mathrm{i}}} = -p_{\mathrm{i}} \qquad \left(\frac{\partial S_{\mathrm{cl}}}{\partial x_{\mathrm{f}}}\right)_{x_{\mathrm{i}}, t_{\mathrm{f}}, t_{\mathrm{i}}} = p_{\mathrm{f}} \tag{1.83}$$

so that (1.82) can expressed as

$$p(t' - \varepsilon) = p(t' + \varepsilon)\,. \tag{1.84}$$

The point x_0 thus has to be chosen such that the two partial classical paths can be joined with a continuous momentum. Together they therefore yield the complete classical path and in particular

$$S_{\mathrm{cl}}(x_{\mathrm{f}}, t, x_{\mathrm{i}}, 0) = S_{\mathrm{cl}}(x_{\mathrm{f}}, t, x_0, t') + S_{\mathrm{cl}}(x_0, t', x_{\mathrm{i}}, 0)\,. \tag{1.85}$$

This relation ensures that the phase factors depending on the classical actions on both sides of (1.81) are equal.

After having identified the stationary path, we have to evaluate the integral over x' in (1.81). Within semiclassical approximation this Gaussian integral leads to

$$\begin{aligned} &\frac{C(x_{\mathrm{f}}, t, x_{\mathrm{i}}, 0)}{C(x_{\mathrm{f}}, t, x_0, t') C(x_0, t', x_{\mathrm{i}}, 0)} \\ &\qquad = \left(\frac{1}{2\pi\mathrm{i}\hbar} \frac{\partial^2}{\partial x_0^2}\left[S_{\mathrm{cl}}(x_{\mathrm{f}}, t, x_0, t') + S_{\mathrm{cl}}(x_0, t', x_{\mathrm{i}}, 0)\right]\right)^{-1/2}. \end{aligned} \tag{1.86}$$

In order to make progress, it is useful to take the derivative of (1.85) with respect to x_f and x_i. Keeping in mind that x_0 depends on these two variables one finds

$$\begin{aligned}\frac{\partial^2 S_\mathrm{cl}(x_\mathrm{f},t,x_\mathrm{i},0)}{\partial x_\mathrm{f}\partial x_\mathrm{i}} &= \frac{\partial^2 S_\mathrm{cl}(x_\mathrm{f},t,x_0,t')}{\partial x_\mathrm{f}\partial x_0}\frac{\partial x_0}{\partial x_\mathrm{i}} + \frac{\partial^2 S_\mathrm{cl}(x_0,t',x_\mathrm{i},0)}{\partial x_\mathrm{i}\partial x_0}\frac{\partial x_0}{\partial x_\mathrm{f}} \\ &\quad + \frac{\partial^2}{\partial x_0^2}\big[S_\mathrm{cl}(x_\mathrm{f},t,x_0,t') + S_\mathrm{cl}(x_0,t',x_\mathrm{i},t)\big]\frac{\partial x_0}{\partial x_\mathrm{i}}\frac{\partial x_0}{\partial x_\mathrm{f}}\,.\end{aligned} \tag{1.87}$$

Similarly, one finds by taking derivatives of the stationary phase condition (1.82)

$$\frac{\partial x_0}{\partial x_\mathrm{f}} = -\frac{\dfrac{\partial^2}{\partial x_\mathrm{f}x_0}S_\mathrm{cl}(x_\mathrm{f},t,x_0,t')}{\dfrac{\partial^2}{\partial x_0^2}\big[S_\mathrm{cl}(x_\mathrm{f},t,x_0,t') + S_\mathrm{cl}(x_0,t',x_\mathrm{i},0)\big]} \tag{1.88}$$

and

$$\frac{\partial x_0}{\partial x_\mathrm{i}} = -\frac{\dfrac{\partial^2}{\partial x_\mathrm{i}x_0}S_\mathrm{cl}(x_0,t',x_\mathrm{i},0)}{\dfrac{\partial^2}{\partial x_0^2}\big[S_\mathrm{cl}(x_\mathrm{f},t,x_0,t') + S_\mathrm{cl}(x_0,t',x_\mathrm{i},0)\big]}\,. \tag{1.89}$$

These expressions allow to eliminate the partial derivatives of x_0 with respect to x_i and x_f appearing in (1.87) and one finally obtains

$$\begin{aligned}&\left(\frac{\partial^2}{\partial x_0^2}\big[S_\mathrm{cl}(x_\mathrm{f},t,x_0,t') + S_\mathrm{cl}(x_0,t',x_\mathrm{i},0)\big]\right)^{-1} \\ &\qquad = -\frac{\dfrac{\partial^2}{\partial x_\mathrm{i}\partial x_\mathrm{f}}S_\mathrm{cl}(x_\mathrm{f},t,x_\mathrm{i},0)}{\dfrac{\partial^2 S_\mathrm{cl}(x_\mathrm{f},t,x_0,t')}{\partial x_\mathrm{f}\partial x_0}\dfrac{\partial^2 S_\mathrm{cl}(x_0,t',x_\mathrm{i},0)}{\partial x_\mathrm{i}\partial x_0}}\,.\end{aligned} \tag{1.90}$$

Inserting this result into (1.86), the prefactor can be identified as the so-called van Vleck–Pauli–Morette determinant [18,19,20]

$$C(x_\mathrm{f},t,x_\mathrm{i},0) = \left[\frac{1}{2\pi\mathrm{i}\hbar}\left(-\frac{\partial^2 S_\mathrm{cl}(x_\mathrm{f},t,x_\mathrm{i},0)}{\partial x_\mathrm{f}\partial x_\mathrm{i}}\right)\right]^{1/2} \tag{1.91}$$

so that the propagator in semiclassical approximation finally reads

$$\begin{aligned}&K(x_\mathrm{f},t,x_\mathrm{i},0) \\ &\quad = \left(\frac{1}{2\pi\hbar}\left|-\frac{\partial^2 S_\mathrm{cl}(x_\mathrm{f},t,x_\mathrm{i},0)}{\partial x_\mathrm{f}\partial x_\mathrm{i}}\right|\right)^{1/2}\exp\left[\frac{\mathrm{i}}{\hbar}S_\mathrm{cl}(x_\mathrm{f},t,x_\mathrm{i},0) - \mathrm{i}\left(\frac{\pi}{4}+n\frac{\pi}{2}\right)\right]\end{aligned} \tag{1.92}$$

where the Morse index n denotes the number of sign changes of $\partial^2 S_\mathrm{cl}/\partial x_\mathrm{f}\partial x_\mathrm{i}$ [13]. We had encountered such a phase factor before in the propagator (1.72) of the harmonic oscillator.

As we have already mentioned above, derivatives of the action with respect to position are related to momenta. This allows to give a physical interpretation of the prefactor of the propagator as the change of the end point of the path as a function of the initial momentum

$$\left(-\frac{\partial^2 S_{\rm cl}}{\partial x_{\rm i}\partial x_{\rm f}}\right)^{-1} = \frac{\partial x_{\rm f}}{\partial p_{\rm i}} \,. \tag{1.93}$$

A zero of this expression, or equivalently a divergence of the prefactor of the propagator, indicates a conjugate point where the end point does not depend on the initial momentum.

To close this section, we compare the semiclassical result (1.92) with exact results for the free particle and the harmonic oscillator. In our discussion of the free particle in Sect. 1.2.3 we already mentioned that the propagator can be expressed entirely in terms of classical quantities. Indeed, the expression (1.19) for the propagator of the free particle agrees with (1.92).

For the harmonic oscillator, we know from Sect. 1.2.7 that the prefactor does not depend on a possibly present external force. We may therefore consider the action (1.56) in the absence of driving $f(s) = 0$ which then reads

$$S_{\rm cl} = \frac{m\omega}{2\sin(\omega t)}\left[\left(x_{\rm i}^2 + x_{\rm f}^2\right)\cos(\omega t) - 2x_{\rm i}x_{\rm f}\right] \,. \tag{1.94}$$

Taking the derivative with respect to $x_{\rm i}$ and $x_{\rm f}$ one finds for the prefactor

$$C(x_{\rm f}, t, x_{\rm i}, 0) = \left(\frac{m\omega}{2\pi{\rm i}\hbar\sin(\omega t)}\right)^{1/2} \tag{1.95}$$

which is identical with the prefactor in our previous result (1.72). As expected, for potentials at most quadratic in the coordinate the semiclassical propagator agrees with the exact expression.

1.2.9 Imaginary Time Path Integral

In the discussion of dissipative systems we will be dealing with a system coupled to a large number of environmental degrees of freedom. In most cases, the environment will act like a large heat bath characterized by a temperature T. The state of the environment will therefore be given by an equilibrium density matrix. Occasionally, we may also be interested in the equilibrium density matrix of the system itself. Such a state may be reached after equilibration due to weak coupling with a heat bath.

In order to describe such thermal equilibrium states and the dynamics of the system on a unique footing, it is desirable to express equilibrium density matrices in terms of path integrals. This is indeed possible as one recognizes by writing the equilibrium density operator in position representation

$$\rho_\beta(x, x') = \frac{1}{\mathcal{Z}}\langle x|\exp(-\beta H)|x'\rangle \tag{1.96}$$

with the partition function

$$\mathcal{Z} = \int \mathrm{d}x \langle x| \exp(-\beta H)|x\rangle \ . \tag{1.97}$$

Comparing with the propagator in position representation

$$K(x,t,x',0) = \langle x| \exp\left(-\frac{\mathrm{i}}{\hbar}Ht\right)|x'\rangle \tag{1.98}$$

one concludes that apart from the partition function the equilibrium density matrix is equivalent to a propagator in imaginary time $t = -\mathrm{i}\hbar\beta$.

After the substitution $\sigma = \mathrm{i}s$ the action in imaginary time $-\mathrm{i}\hbar\beta$ reads

$$\int_0^{-\mathrm{i}\hbar\beta} \mathrm{d}s \left[\frac{m}{2}\left(\frac{\mathrm{d}x}{\mathrm{d}s}\right)^2 - V(x)\right] = \mathrm{i}\int_0^{\hbar\beta} \mathrm{d}\sigma \left[\frac{m}{2}\left(\frac{\mathrm{d}x}{\mathrm{d}\sigma}\right)^2 + V(x)\right] \ . \tag{1.99}$$

Here and in the following, we use greek letters to indicate imaginary times. Motivated by the right-hand side of (1.99) we define the so-called Euclidean action

$$S^{\mathrm{E}}[x] = \int_0^{\hbar\beta} \mathrm{d}\sigma \left[\frac{m}{2}\dot{x}^2 + V(x)\right] \ . \tag{1.100}$$

Even though one might fear a lack of intuition for motion in imaginary time, this results shows that it can simply be thought of as motion in the inverted potential in real time. With the Euclidean action (1.100) we now obtain as an important result the path integral expression for the (unnormalized) equilibrium density matrix

$$\langle x| \exp(-\beta H)|x'\rangle = \int_{\bar{x}(0)=x'}^{\bar{x}(\hbar\beta)=x} \mathcal{D}\bar{x} \exp\left(-\frac{1}{\hbar}S^{\mathrm{E}}[\bar{x}]\right) \ . \tag{1.101}$$

This kind of functional integral was discussed as early as 1923 by Wiener [21] in the context of classical Brownian motion.

As an example we consider the (undriven) harmonic oscillator. There is actually no need to evaluate a path integral since we know already from Sect. 1.2.7 the propagator

$$\begin{aligned} &K(x_{\mathrm{f}},t,x_{\mathrm{i}},0) \\ &\quad = \sqrt{\frac{m\omega}{2\pi\mathrm{i}\hbar\sin(\omega t)}} \exp\left[-\mathrm{i}\frac{m\omega}{2\hbar}\frac{(x_{\mathrm{i}}^2 + x_{\mathrm{f}}^2)\cos(\omega t) - 2x_{\mathrm{i}}x_{\mathrm{f}}}{\sin(\omega t)}\right] \ . \end{aligned} \tag{1.102}$$

Transforming the propagator into imaginary time $t \to -\mathrm{i}\hbar\beta$ and renaming x_{i} and x_{f} into x' and x, respectively, one obtains the equilibrium density matrix

$$\begin{aligned} &\rho_\beta(x,x') \\ &\quad = \frac{1}{\mathcal{Z}}\sqrt{\frac{m\omega}{2\pi\hbar\sinh(\hbar\beta\omega)}} \exp\left[-\frac{m\omega}{2\hbar}\frac{(x^2 + x'2)\cosh(\hbar\beta\omega) - 2xx'}{\sinh(\hbar\beta\omega)}\right] \ . \end{aligned} \tag{1.103}$$

The partition function is obtained by performing the trace as

$$\mathcal{Z} = \int \mathrm{d}x \langle x| \exp(-\beta H)|x\rangle = \frac{1}{2\sinh(\hbar\beta\omega/2)} \tag{1.104}$$

which agrees with the expression

$$\mathcal{Z} = \sum_{n=0}^{\infty} \exp\left[-\beta\hbar\omega\left(n+\frac{1}{2}\right)\right] \tag{1.105}$$

based on the energy levels of the harmonic oscillator.

Since the partition function often serves as a starting point for the calculation of thermodynamic properties, it is instructive to take a closer at how this quantity may be obtained within the path integral formalism. A possible approach is the one we just have sketched. By means of an imaginary time path integral one first calculates $\langle x| \exp(-\beta H)|x\rangle$ which is proportional to the probability to find the system at position x. Subsequent integration over coordinate space then yields the partition function.

However, the partition function may also be determined in one step. To this end, we expand around the periodic trajectory with extremal Euclidean action which in our case is given by $x(\sigma) = 0$. Any deviation will increase both the kinetic and potential energy and thus increase the Euclidean action. All other trajectories contributing to the partition function are generated by a Fourier series on the imaginary time interval from 0 to $\hbar\beta$

$$x(\sigma) = \frac{1}{\sqrt{\hbar\beta}}\left[a_0 + \sqrt{2}\sum_{n=1}^{\infty}\left(a_n\cos(\nu_n\sigma) + b_n\sin(\nu_n\sigma)\right)\right] \tag{1.106}$$

where we have introduced the so-called Matsubara frequencies

$$\nu_n = \frac{2\pi}{\hbar\beta}n\,. \tag{1.107}$$

This ansatz should be compared with (1.62) for the fluctuations where a_0 was fixed because the fluctuations had to vanish at the boundaries. For the partition function this requirement is dropped since we have to integrate over all periodic trajectories. Furthermore, we note that indeed with the ansatz (1.106) only the periodic trajectories contribute. All other paths cost an infinite amount of action due to the jump at the boundary as we will see shortly.

Inserting the Fourier expansion (1.106) into the Euclidean action of the harmonic oscillator

$$S^{\mathrm{E}} = \int_0^{\hbar\beta} \mathrm{d}\sigma \frac{m}{2}\left(\dot{x}^2 + \omega^2 x^2\right) \tag{1.108}$$

we find

$$S^{\mathrm{E}} = \frac{m}{2}\left[\omega^2 a_0^2 + \sum_{n=1}^{\infty}(\nu_n^2+\omega^2)(a_n^2+b_n^2)\right]\,. \tag{1.109}$$

As in Sect. 1.2.7 we do not want to go into the mathematical details of integration measures and Jacobi determinants. Unfortunately, the free particle cannot serve as a reference here because its partition function does not exist. We therefore content ourselves with remarking that because of

$$\frac{1}{\omega}\prod_{n=1}^{\infty}\frac{1}{\nu_n^2+\omega^2}=\frac{\hbar\beta}{\sum_{n=1}^{\infty}\nu_n^2}\frac{1}{2\sinh(\hbar\beta\omega/2)} \tag{1.110}$$

the result of the Gaussian integral over the Fourier coefficients yields the partition function up to a frequency independent factor. This enables us to determine the partition function in more complicated cases by proceeding as above and using the partition function of the harmonic oscillator as a reference.

Returning to the density matrix of the harmonic oscillator we finally obtain by inserting the partition function (1.104) into the expression (1.103) for the density matrix

$$\begin{aligned}\rho_\beta(x,x')=&\sqrt{\frac{m\omega}{\pi\hbar}\frac{\cosh(\hbar\beta\omega)-1}{\sinh(\hbar\beta\omega)}}\\&\times\exp\left[-\frac{m\omega}{2\hbar}\frac{(x^2+x'^2)\cosh(\hbar\beta\omega)-2xx'}{\sinh(\hbar\beta\omega)}\right].\end{aligned} \tag{1.111}$$

Without path integrals, this result would require the evaluation of sums over Hermite polynomials.

The expression for the density matrix (1.111) can be verified in the limits of high and zero temperature. In the classical limit of very high temperatures, the probability distribution in real space is given by

$$P(x)=\rho_\beta(x,x)=\sqrt{\frac{\beta m\omega^2}{2\pi}}\exp\left(-\beta\frac{m\omega^2}{2}x^2\right)\sim\exp[-\beta V(x)]\,. \tag{1.112}$$

We thus have obtained the Boltzmann distribution which depends only on the potential energy. The fact that the kinetic energy does not play a role can easily be understood in terms of the path integral formalism. Excursions in a very short time $\hbar\beta$ cost too much action and are therefore strongly suppressed.

In the opposite limit of zero temperature the density matrix factorizes into a product of ground state wave functions of the harmonic oscillator

$$\lim_{\beta\to\infty}\rho_\beta(x,x')=\left[\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega}{2\hbar}x^2\right)\right]\left[\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega}{2\hbar}x'^2\right)\right] \tag{1.113}$$

as should be expected.

1.3 Dissipative Systems

1.3.1 Introduction

In classical mechanics dissipation can often be adequately described by including a velocity dependent damping term into the equation of motion. Such a phenomenological approach is no longer possible in quantum mechanics where the Hamilton formalism implies energy conservation for time-independent Hamiltonians. Then, a better understanding of the situation is necessary in order to arrive at an appropriate physical model.

A damped pendulum may help us to understand the mechanism of dissipation. The degree of freedom of interest, the elongation of the pendulum, undergoes a damped motion because it interacts with other degrees of freedom, the molecules in the air surrounding the pendulum's mass. We may consider the pendulum and the air molecules as one large system which, if assumed to be isolated from further degrees of freedom, obeys energy conservation. The energy of the pendulum alone, however, will in general not be conserved. This single degree of freedom is therefore subject to dissipation arising from the coupling to other degrees of freedom.

This insight will allow us in the following section to introduce a model for a system coupled to an environment and to demonstrate explicitly its dissipative nature. In particular, we will introduce the quantities needed for a description which focuses on the system degree of freedom. We are then in a position to return to the path integral formalism and to demonstrate how it may be employed to study dissipative systems. Starting from the model of system and environment, the latter will be eliminated to obtain a reduced description for the system alone. This leaves us with an effective action which forms the basis of the path integral description of dissipation.

1.3.2 Environment as a Collection of Harmonic Oscillators

A suitable model for dissipative quantum systems should both incorporate the idea of a coupling between system and environment and be amenable to an analytic treatment of the environmental coupling. These requirements are met by a model which nowadays is often referred to as Caldeira–Leggett model [22,23] even though it has been discussed in the literature under various names before for harmonic systems [24,25,26,27] and anharmonic systems [28]. The Hamiltonian

$$H = H_{\mathrm{S}} + H_{\mathrm{B}} + H_{\mathrm{SB}} \tag{1.114}$$

consists of three contributions. The Hamiltonian of the system degree of freedom

$$H_{\mathrm{S}} = \frac{p^2}{2m} + V(q) \tag{1.115}$$

models a particle of mass m moving in a potential V. Here, we denote the coordinate by q to facilitate the distinction from the environmental coordinates x_n which we will introduce in a moment. Of course, the system degree of freedom does not have to be associated with a real particle but may be quite abstract. In

fact, a substantial part of the calculations to be discussed in the following does not depend on the detailed form of the system Hamiltonian.

The Hamiltonian of the environmental degrees of freedom

$$H_{\mathrm{B}} = \sum_{n=1}^{N} \left(\frac{p_n^2}{2m_n} + \frac{m_n}{2} \omega_n^2 x_n^2 \right) \tag{1.116}$$

describes a collection of harmonic oscillators. While the properties of the environment may in some cases be chosen on the basis of a microscopic model, this does not have to be the case. Often, a phenomenological approach is sufficient as we will see below. As an example we mention an Ohmic resistor which as a linear electric element should be well described by a Hamiltonian of the form (1.116). On the other hand, the underlying mechanism leading to dissipation, e.g. in a resistor, may be much more complicated than that implied by the model of a collection of harmonic oscillators.

The coupling defined by the Hamiltonian

$$H_{\mathrm{SB}} = -q \sum_{n=1}^{N} c_n x_n + q^2 \sum_{n=1}^{N} \frac{c_n^2}{2m_n \omega_n^2} \tag{1.117}$$

is bilinear in the position operators of system and environment. There are cases where the bilinear coupling is realistic, e.g. for an environment consisting of a linear electric circuit like the resistor just mentioned or for a dipolar coupling to electromagnetic field modes encountered in quantum optics. Within a more general scope, this Hamiltonian may be viewed as linearization of a nonlinear coupling in the limit of weak coupling to the environmental degrees of freedom. As was first pointed out by Caldeira and Leggett, an infinite number of degrees of freedom still allows for strong damping even if each environmental oscillator couples only weakly to the system [22,23].

An environment consisting of harmonic oscillators as in (1.116) might be criticized. If the potential $V(q)$ is harmonic, one may pass to normal coordinates and thus demonstrate that after some time a revival of the initial state will occur. For sufficiently many environmental oscillators, however, this so-called Poincaré recurrence time tends to infinity [29]. Therefore, even with a linear environment irreversibility becomes possible at least for all practical purposes.

The reader may have noticed that in the coupling Hamiltonian (1.117) a term is present which only contains an operator acting in the system Hilbert space but depends on the coupling constants c_n. The physical reason for the inclusion of this term lies in a potential renormalization introduced by the first term in (1.117). This becomes clear if we consider the minimum of the Hamiltonian with respect to the system and environment coordinates. From the requirement

$$\frac{\partial H}{\partial x_n} = m_n \omega_n^2 x_n - c_n q \stackrel{!}{=} 0 \tag{1.118}$$

we obtain

$$x_n = \frac{c_n}{m_n \omega_n^2} q \,. \tag{1.119}$$

Using this result to determine the minimum of the Hamiltonian with respect to the system coordinate we find

$$\frac{\partial H}{\partial q} = \frac{\partial V}{\partial q} - \sum_{n=1}^{N} c_n x_n + q \sum_{n=1}^{N} \frac{c_n^2}{m_n \omega_n^2} = \frac{\partial V}{\partial q} \; . \tag{1.120}$$

The second term in (1.117) thus ensures that this minimum is determined by the bare potential $V(q)$.

After having specified the model, we now want to derive an effective description of the system alone. It was first shown by Magalinskiĭ [24] that the elimination of the environmental degrees of freedom leads indeed to a damped equation of motion for the system coordinate. We perform the elimination within the Heisenberg picture where the evolution of an operator A is determined by

$$\frac{\mathrm{d}A}{\mathrm{d}t} = \frac{\mathrm{i}}{\hbar}[H, A] \; . \tag{1.121}$$

From the Hamiltonian (1.114) we obtain the equations of motion for the environmental degrees of freedom

$$\begin{aligned} \dot{p}_n &= -m_n \omega_n^2 x_n + c_n q \\ \dot{x}_n &= \frac{p_n}{m_n} \end{aligned} \tag{1.122}$$

and the system degree of freedom

$$\begin{aligned} \dot{p} &= -\frac{\partial V}{\partial q} + \sum_{n=1}^{N} c_n x_n - q \sum_{n=1}^{N} \frac{c_n^2}{m_n \omega_n^2} \\ \dot{x} &= \frac{p}{m} \; . \end{aligned} \tag{1.123}$$

The trick for solving the environmental equations of motion (1.122) consists in treating the system coordinate $q(t)$ as if it were a given function of time. The inhomogeneous differential equation then has the solution

$$x_n(t) = x_n(0)\cos(\omega_n t) + \frac{p_n(0)}{m_n \omega_n}\sin(\omega_n t) + \frac{c_n}{m_n \omega_n}\int_0^t \mathrm{d}s \sin\big(\omega_n(t-s)\big) q(s) \; . \tag{1.124}$$

Inserting this result into (1.123) one finds an effective equation of motion for the system coordinate

$$\begin{aligned} m\ddot{q} - \int_0^t \mathrm{d}s \sum_{n=1}^{N} \frac{c_n^2}{m_n \omega_n} \sin\big(\omega_n(t-s)\big) q(s) + \frac{\partial V}{\partial q} + q \sum_{n=1}^{N} \frac{c_n^2}{m_n \omega_n^2} \\ = \sum_{n=1}^{N} c_n \left[x_n(0)\cos(\omega_n t) + \frac{p_n(0)}{m_n \omega_n}\sin(\omega_n t) \right] . \end{aligned} \tag{1.125}$$

By a partial integration of the second term on the left-hand side this equation of motion can be cast into its final form

$$m\ddot{q} + m\int_0^t \mathrm{d}s\gamma(t-s)\dot{q}(s) + \frac{\partial V}{\partial q} = \xi(t) \tag{1.126}$$

with the damping kernel

$$\gamma(t) = \frac{1}{m}\sum_{n=1}^{N}\frac{c_n^2}{m_n\omega_n^2}\cos(\omega_n t) \tag{1.127}$$

and the operator-valued fluctuating force

$$\xi(t) = \sum_{n=1}^{N} c_n\left[\left(x_n(0) - \frac{c_n}{m_n\omega_n^2}q(0)\right)\cos(\omega_n t) + \frac{p_n(0)}{m_n\omega_n}\sin(\omega_n t)\right] . \tag{1.128}$$

The fluctuating force vanishes if averaged over a thermal density matrix of the environment including the coupling to the system

$$\langle\xi(t)\rangle_{\mathrm{B+SB}} = \frac{\mathrm{Tr}_{\mathrm{B}}\left[\xi(t)\exp\bigl(-\beta(H_{\mathrm{B}}+H_{\mathrm{SB}})\bigr)\right]}{\mathrm{Tr}_{\mathrm{B}}\left[\exp\bigl(-\beta(H_{\mathrm{B}}+H_{\mathrm{SB}})\bigr)\right]} = 0 . \tag{1.129}$$

For weak coupling, one may want to split off the transient term $m\gamma(t)q(0)$ which is of second order in the coupling and write the fluctuating force as [30]

$$\xi(t) = \zeta(t) - m\gamma(t)q(0) . \tag{1.130}$$

The so defined force $\zeta(t)$ vanishes if averaged over the environment alone

$$\langle\zeta(t)\rangle_{\mathrm{B}} = \frac{\mathrm{Tr}_{\mathrm{B}}\left[\zeta(t)\exp(-\beta H_{\mathrm{B}})\right]}{\mathrm{Tr}_{\mathrm{B}}\left[\exp(-\beta H_{\mathrm{B}})\right]} = 0 . \tag{1.131}$$

An important quantity to characterize the fluctuating force is the correlation function which again can be evaluated for ξ with respect to $H_{\mathrm{B}} + H_{\mathrm{SB}}$ or equivalently for ζ with respect to H_{B} alone. With (1.128) and (1.130) we get the correlation function

$$\langle\zeta(t)\zeta(0)\rangle_{\mathrm{B}} = \sum_{n,l} c_n c_l\left\langle\left(x_n(0)\cos(\omega_n t) + \frac{p_n(0)}{m_n\omega_i}\sin(\omega_n t)\right)x_l(0)\right\rangle_{\mathrm{B}} . \tag{1.132}$$

In thermal equilibrium the second moments are given by

$$\langle x_n(0)x_l(0)\rangle_{\mathrm{B}} = \delta_{nl}\frac{\hbar}{2m_n\omega_n}\coth\left(\frac{\hbar\beta\omega_n}{2}\right) \tag{1.133}$$

$$\langle p_n(0)x_l(0)\rangle_{\mathrm{B}} = -\frac{\mathrm{i}\hbar}{2}\delta_{nl} , \tag{1.134}$$

so that the noise correlation function finally becomes

$$\langle\zeta(t)\zeta(0)\rangle_{\mathrm{B}} = \sum_{n=1}^{N} \frac{\hbar c_n^2}{2m_n\omega_n} \left[\coth\left(\frac{\hbar\beta\omega_n}{2}\right)\cos(\omega_n t) - \mathrm{i}\sin(\omega_n t)\right] . \tag{1.135}$$

The imaginary part appearing here is a consequence of the fact that the operators $\zeta(t)$ and $\zeta(0)$ in general do not commute. The correlation function (1.135) appears as an integral kernel both in master equations as well as in the effective action derived below (cf. (1.168) and (1.169)).

It is remarkable that within a reduced description for the system alone all quantities characterizing the environment may be expressed in terms of the spectral density of bath oscillators

$$J(\omega) = \pi \sum_{n=1}^{N} \frac{c_n^2}{2m_n\omega_n}\delta(\omega - \omega_n) . \tag{1.136}$$

As an example, the damping kernel may be expressed in terms of this spectral density as

$$\gamma(t) = \frac{1}{m}\sum_{n=1}^{N} \frac{c_n^2}{m_n\omega_n^2}\cos(\omega_n t) = \frac{2}{m}\int_0^\infty \frac{\mathrm{d}\omega}{\pi}\frac{J(\omega)}{\omega}\cos(\omega t) . \tag{1.137}$$

For practical calculations, it is therefore unnecessary to specify all parameters m_n, ω_n and c_n appearing in (1.116) and (1.117). It rather suffices to define the spectral density $J(\omega)$.

The most frequently used spectral density

$$J(\omega) = m\gamma\omega \tag{1.138}$$

is associated with the so-called Ohmic damping. This term is sometimes employed to indicate a proportionality to frequency merely at low frequencies instead of over the whole frequency range. In fact, in any realistic situation the spectral density will not increase like in (1.138) for arbitrarily high frequencies. It is justified to use the term "Ohmic damping" even if (1.138) holds only below a certain frequency provided this frequency is much higher than the typical frequencies appearing in the system dynamics.

From (1.137) one finds the damping kernel for Ohmic damping

$$\gamma(t) = 2\gamma\delta(t) , \tag{1.139}$$

which renders (1.126) memory-free. We thus recover the velocity proportional damping term familiar from classical damped systems. It should be noted that the factor of two in (1.139) disappears upon integration in (1.126) since (1.137) implies that the delta function is symmetric around zero.

At this point, we want to briefly elucidate the origin of the term "Ohmic damping". Let us consider the electric circuit shown in Fig. 1.9 consisting of a

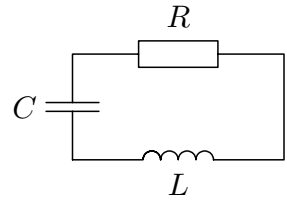

Fig. 1.9. LC oscillator with Ohmic damping due to a resistor R

resistance R, a capacitance C and an inductance L. Summing up the voltages around the loop, one obtains as equation of motion for the charge Q on the capacitor

$$L\ddot{Q} + R\dot{Q} + \frac{Q}{C} = 0 \,, \tag{1.140}$$

which shows that an Ohmic resistor leads indeed to memoryless damping. These considerations demonstrate that even without knowledge of the microscopic origin of dissipation in a resistor, we may employ the Ohmic spectral density (1.138) to account for its dissipative nature.

The spectral density (1.138) for Ohmic damping unfortunately diverges at high frequencies which, as already mentioned, cannot be the case in practice. Even in theoretical considerations this feature of strict Ohmic damping may lead to divergencies and a cutoff is needed for regularization. One possibility is the Drude cutoff, where the spectral density

$$J(\omega) = m\gamma\omega \frac{\omega_{\mathrm{D}}^2}{\omega^2 + \omega_{\mathrm{D}}^2} \tag{1.141}$$

above frequencies of the order of ω_{D} is suppressed. The corresponding damping kernel reads

$$\gamma(t) = \gamma\omega_{\mathrm{D}} \exp(-\omega_{\mathrm{D}}|t|) \,. \tag{1.142}$$

This leads to memory effects in (1.126) for short times $t < \omega_{\mathrm{D}}^{-1}$. For the long-time behaviour, however, only the Ohmic low frequency behaviour of the spectral density (1.141) is relevant. If a Drude cutoff is introduced for technical reasons, the cutoff frequency ω_{D} should be much larger than all other frequencies appearing in the problem in order to avoid spurious effects.

The relation (1.136) between the spectral density and the "microscopic" parameters implies that one may set $c_n = m_n\omega_n^2$ without loss of generality since the frequencies ω_n and the oscillator strengths $c_n^2/2m_n\omega_n$ can still be freely chosen. This special choice for the coupling constants has the advantage of a translationally invariant coupling [31]

$$H = H_S + \sum_{n=1}^{N} \left(\frac{p_n^2}{2m_n} + \frac{m_n}{2}\omega_n^2 (x_n - q)^2 \right) \,. \tag{1.143}$$

Furthermore, we now can determine the total mass of environmental oscillators

$$\sum_{n=1}^{N} m_n = \frac{2}{\pi} \int_0^\infty \mathrm{d}\omega \frac{J(\omega)}{\omega^3} \,. \tag{1.144}$$

If the spectral density of bath oscillators at small frequencies takes the form $J(\omega) \sim \omega^\alpha$, the total mass of bath oscillators is infinite for $\alpha \leq 2$. In particular, this includes the case of Ohmic damping where a free damped particle executes a diffusive motion. In contrast, for $\alpha > 2$, the total mass is finite. In this case, the particle will behave for long times like it were free albeit possessing a renormalized mass due to the environmental coupling [32]. We emphasize that the divergence of the total mass for $\alpha \leq 2$ is due to an infrared divergence and therefore independent of a high-frequency cutoff.

It is also useful to express the potential renormalization introduced in (1.117) in terms of the spectral density of bath oscillators. From (1.136) it is straightforward to obtain

$$q^2 \sum_{n=1}^{N} \frac{c_n^2}{2m_n\omega_n^2} = \frac{q^2}{\pi} \int_0^\infty \mathrm{d}\omega \frac{J(\omega)}{\omega} \,. \tag{1.145}$$

This term is infinite for strictly Ohmic damping but becomes finite when a high-frequency cutoff is introduced.

Finally, one finds for the noise correlation function (1.132)

$$\begin{aligned} K(t) &= \langle \zeta(t)\zeta(0) \rangle_\mathrm{B} \\ &= \hbar \int_0^\infty \frac{\mathrm{d}\omega}{\pi} J(\omega) \left[\coth\left(\frac{\hbar\beta\omega}{2}\right) \cos(\omega t) - \mathrm{i}\sin(\omega t) \right] \,. \end{aligned} \tag{1.146}$$

In the classical limit, $\hbar \to 0$, this correlation function reduces to the real-valued expression

$$K(t) = m k_\mathrm{B} T \gamma(t) \,, \tag{1.147}$$

where we have made use of (1.137). For Ohmic damping this implies delta correlated, i.e. white, noise.

In the quantum case, the noise correlation function is complex and can be decomposed into its real and imaginary part

$$K(t) = K'(t) + \mathrm{i}K''(t) \,. \tag{1.148}$$

Employing once more (1.137), one immediately finds that the imaginary part is related to the time derivative of the damping kernel by

$$K''(t) = \frac{m\hbar}{2} \frac{\mathrm{d}\gamma}{\mathrm{d}t} \,. \tag{1.149}$$

For Ohmic damping, the real part reads

$$K'(t) = -\frac{\pi m \gamma}{(\hbar\beta)^2} \frac{1}{\sinh^2\left(\dfrac{\pi t}{\hbar\beta}\right)} \tag{1.150}$$

which implies that at zero temperature the noise is correlated even for long times. The noise correlation then only decays algebraically like $1/t^2$ much in contrast to the classical result (1.147).

1.3.3 Effective Action

In the previous section we had eliminated the environmental degrees of freedom to obtain the effective equation of motion (1.126) for the system degree of freedom alone. This section will be devoted to a discussion of the corresponding procedure within the path integral formalism.

We start to illustrate the basic idea by considering the time evolution of the full density matrix of system and environment

$$W(q_\mathrm{f}, x_{n\mathrm{f}}, q'_\mathrm{f}, x'_{n\mathrm{f}}, t) = \int \mathrm{d}q_\mathrm{i}\mathrm{d}q'_\mathrm{i}\mathrm{d}x_{n\mathrm{i}}\mathrm{d}x'_{n\mathrm{i}} K(q_\mathrm{f}, x_{n\mathrm{f}}, t, q_\mathrm{i}, x_{n\mathrm{i}}, 0) \times W(q_\mathrm{i}, x_{n\mathrm{i}}, q'_\mathrm{i}, x'_{n\mathrm{i}}, 0) K^*(q'_\mathrm{f}, x'_{n\mathrm{f}}, t, q'_\mathrm{i}, x'_{n\mathrm{i}}, 0) \tag{1.151}$$

which is induced by the two propagators K. Here, the coordinates q and x_n refer again to the system and bath degrees of freedom, respectively. The environment is assumed to be in thermal equilibrium described by the density matrix W_β^B while the system may be in a nonequilibrium state ρ. If we neglect initial correlations between system and environment, i.e. if we switch on the coupling after preparation of the initial state, the initial density matrix may be written in factorized form

$$W(q_\mathrm{i}, x_{n\mathrm{i}}, q'_\mathrm{i}, x'_{n\mathrm{i}}, 0) = \rho(q_\mathrm{i}, q'_\mathrm{i}) W_\beta^\mathrm{B}(x_{n\mathrm{i}}, x'_{n\mathrm{i}}) \,. \tag{1.152}$$

Since we are only interested in the dynamics of the system degree of freedom, we trace out the environment. Then the time evolution may be expressed as

$$\rho(q_\mathrm{f}, q'_\mathrm{f}, t) = \int \mathrm{d}q_\mathrm{i}\mathrm{d}q'_\mathrm{i} J(q_\mathrm{f}, q'_\mathrm{f}, t, q_\mathrm{i}, q'_\mathrm{i}, 0) \rho(q_\mathrm{i}, q'_\mathrm{i}) \tag{1.153}$$

with the propagating function

$$J(q_\mathrm{f}, q'_\mathrm{f}, t, q_\mathrm{i}, q'_\mathrm{i}, 0) = \int \mathrm{d}x_{n\mathrm{f}}\mathrm{d}x_{n\mathrm{i}}\mathrm{d}x'_{n\mathrm{i}} K(q_\mathrm{f}, x_{n\mathrm{f}}, t, q_\mathrm{i}, x_{n\mathrm{i}}, 0) \times W_\beta^\mathrm{B}(x_{n\mathrm{i}}, x'_{n\mathrm{i}}) K^*(q'_\mathrm{f}, x_{n\mathrm{f}}, t, q'_\mathrm{i}, x'_{n\mathrm{i}}, 0) \,. \tag{1.154}$$

Here, the trace has been performed by setting $x_{n\mathrm{f}} = x'_{n\mathrm{f}}$ and integrating over these coordinates. The propagators may be expressed as real time path integrals while the equilibrium density matrix of the bath is given by a path integral in imaginary time. Performing the path integrals and the conventional integrals appearing in (1.154) one finds a functional depending on the system path. The important point is that this functional contains all information about the environment required to determine the system dynamics.

For factorizing initial conditions, the propagating function J has been calculated by Feynman and Vernon [33] on the basis of the Hamiltonian (1.114).

More general initial conditions taking into account correlations between system and environment may be considered as well [34].

Instead of deriving the propagating function we will demonstrate how to trace the environment out of the equilibrium density matrix of system plus environment. While this task is conceptually similar and leads to the same physical insight, it is considerably less tedious.

We start from the imaginary time path integral representation of the full equilibrium density matrix

$$W_\beta(q, x_n, q', x_n') = \frac{1}{\mathcal{Z}_\beta} \int \mathcal{D}\bar{q} \left(\prod_{n=1}^{N} \mathcal{D}\bar{x}_n \right) \exp\left(-\frac{1}{\hbar} S^{\mathrm{E}}[\bar{q}, \bar{x}_n] \right) \tag{1.155}$$

where the paths run from $\bar{q}(0) = q'$ and $\bar{x}_n(0) = x_n'$ to $\bar{q}(\hbar\beta) = q$ and $\bar{x}_n(\hbar\beta) = x_n$. The Euclidean action corresponding to the model Hamiltonian (1.114) reads in imaginary time

$$S^{\mathrm{E}}[\bar{q}, \bar{x}_n] = S_{\mathrm{S}}^{\mathrm{E}}[\bar{q}] + S_{\mathrm{B}}^{\mathrm{E}}[\bar{x}_n] + S_{\mathrm{SB}}^{\mathrm{E}}[\bar{q}, \bar{x}_n] \tag{1.156}$$

with

$$S_{\mathrm{S}}^{\mathrm{E}}[\bar{q}] = \int_0^{\hbar\beta} \mathrm{d}\tau \left(\frac{m}{2} \dot{\bar{q}}^2 + V(\bar{q}) \right) \tag{1.157}$$

$$S_{\mathrm{B}}^{\mathrm{E}}[\bar{x}_n] = \int_0^{\hbar\beta} \mathrm{d}\tau \sum_{n=1}^{N} \frac{m_n}{2} \left(\dot{\bar{x}}_n^2 + \omega_n^2 \bar{x}_n^2 \right) \tag{1.158}$$

$$S_{\mathrm{SB}}^{\mathrm{E}}[\bar{q}, \bar{x}_n] = \int_0^{\hbar\beta} \mathrm{d}\tau \left(-\bar{q} \sum_{n=1}^{N} c_n \bar{x}_n + \bar{q}^2 \sum_{n=1}^{N} \frac{c_n^2}{2 m_n \omega_n^2} \right) . \tag{1.159}$$

The reduced density matrix of the system is obtained by tracing over the environmental degrees of freedom

$$\begin{aligned} \rho_\beta(q, q') &= \mathrm{tr}_{\mathrm{B}} \left(W_\beta(q, x_n, q', x_n') \right) \\ &= \frac{1}{\mathcal{Z}_\beta} \int \mathcal{D}\bar{q} \int \prod_{n=1}^{N} \mathrm{d}x_n \oint \prod_{n=1}^{N} \mathcal{D}\bar{x}_n \exp\left(-\frac{1}{\hbar} S^{\mathrm{E}}[\bar{q}, \bar{x}_n] \right) \end{aligned} \tag{1.160}$$

where the circle on the second functional integral sign indicates that one has to integrate over closed paths $\bar{x}_n(0) = \bar{x}_n(\hbar\beta) = x_n$ when performing the trace. The dependence on the environmental coupling may be made explicit by writing

$$\rho_\beta(q, q') = \frac{1}{\mathcal{Z}} \int \mathcal{D}\bar{q} \exp\left(-\frac{1}{\hbar} S_{\mathrm{S}}^{\mathrm{E}}[\bar{q}] \right) \mathcal{F}[\bar{q}] \tag{1.161}$$

where the influence functional $\mathcal{F}[\bar{q}]$ describes the influence of the environment on the system. Here, the partition function $\mathcal{Z}$ should not be confused with the partition function $\mathcal{Z}_\beta$ of system plus environment. The relation between the two quantities will be discussed shortly.

Since the bath oscillators are not coupled among each other, the influence functional may be decomposed into factors corresponding to the individual bath oscillators

$$\mathcal{F}[\bar{q}] = \prod_{n=1}^{N} \frac{1}{\mathcal{Z}_n} \mathcal{F}_n[\bar{q}] \tag{1.162}$$

where

$$\mathcal{Z}_n = \frac{1}{2\sinh\left(\hbar\beta\omega_n/2\right)} \tag{1.163}$$

is the partition function of a single bath oscillator. The influence functional of a bath oscillator can be expressed as

$$\mathcal{F}_n[\bar{q}] = \int \mathrm{d}x_n \oint \mathcal{D}\bar{x}_n \exp\left(-\frac{1}{\hbar} S_n^{\mathrm{E}}[\bar{q}, \bar{x}_n]\right) \tag{1.164}$$

with the action

$$S_n^{\mathrm{E}}[\bar{q}, \bar{x}_n] = \int_0^{\hbar\beta} \mathrm{d}\tau \frac{m_n}{2} \left[\dot{\bar{x}}_n^2 + \omega_n^2 \left(\bar{x}_n - \frac{c_n}{m_n\omega_n^2}\bar{q}\right)^2\right] . \tag{1.165}$$

The partition function $\mathcal{Z}$ of the damped system is related to the full partition function $\mathcal{Z}_\beta$ by the partition function of the environmental oscillators $\mathcal{Z}_{\mathrm{B}} = \prod_{n=1}^{N} \mathcal{Z}_n$ according to $\mathcal{Z} = \mathcal{Z}_\beta/\mathcal{Z}_{\mathrm{B}}$. In the limit of vanishing coupling, $c_n = 0$, the influence functional becomes $\mathcal{F}[\bar{q}] = 1$ so that (1.161) reduces to the path integral representation of the density matrix of an isolated system as it should.

Apart from the potential renormalization term proportional to $\bar{q}^2$, the action (1.165) describes a driven harmonic oscillator. We may therefore make use of our results from Sect. 1.2.7. After analytic continuation $t \to -\mathrm{i}\hbar\beta$ in (1.56) and setting $x_{\mathrm{i}} = x_{\mathrm{f}} = x_n$ one finds for the classical Euclidean action

$$\begin{aligned} S_n^{\mathrm{E,cl}}[\bar{q}] = {} & m_n\omega_n \frac{\cosh(\hbar\beta\omega_n) - 1}{\sinh(\hbar\beta\omega_n)} x_n^2 \\ & - c_n \int_0^{\hbar\beta} \mathrm{d}\tau \frac{\sinh(\omega_n\tau) + \sinh(\omega_n(\hbar\beta - \tau))}{\sinh(\hbar\beta\omega_n)} x_n \bar{q}(\tau) \\ & - \frac{c_n^2}{m_n\omega_n} \int_0^{\hbar\beta} \mathrm{d}\tau \int_0^{\tau} \mathrm{d}\sigma \frac{\sinh(\omega_n(\hbar\beta - \tau))\sinh(\omega_n\sigma)}{\sinh(\hbar\beta\omega_n)} \bar{q}(\tau)\bar{q}(\sigma) \\ & + \frac{c_n^2}{2m_n\omega_n^2} \int_0^{\hbar\beta} \mathrm{d}\tau \bar{q}^2(\tau) . \end{aligned} \tag{1.166}$$

In view of the required integration over x_n one completes the square

$$\begin{aligned} S_n^{\mathrm{E,cl}}[\bar{q}] = {} & m_n\omega_n \frac{\cosh(\hbar\beta\omega_n) - 1}{\sinh(\hbar\beta\omega_n)} (x_n - x_n^{(0)})^2 - \int_0^{\hbar\beta} \mathrm{d}\tau \int_0^{\tau} \mathrm{d}\sigma K_n(\tau - \sigma)\bar{q}(\tau)\bar{q}(\sigma) \\ & + \frac{c_n^2}{2m_n\omega_n^2} \int_0^{\hbar\beta} \mathrm{d}\tau \bar{q}^2(\tau) \end{aligned} \tag{1.167}$$

where $x_n^{(0)}$ does not need to be specified since it drops out after integration.

The integral kernel appearing in (1.167) follows from (1.166) as

$$K_n(\tau) = \frac{c_n^2}{2m_n\omega_n} \frac{\cosh\left(\omega_n\left(\frac{\hbar\beta}{2} - \tau\right)\right)}{\sinh\left(\frac{\hbar\beta\omega_n}{2}\right)} = K_n(\hbar\beta - \tau) \tag{1.168}$$

and therefore can be identified as the noise correlation function (1.135) in imaginary time

$$K_n(\tau) = \frac{1}{\hbar}\langle\zeta_n(-\mathrm{i}\tau)\zeta_n(0)\rangle_{\mathrm{B}} \,. \tag{1.169}$$

The term in (1.167) containing this kernel is quite unusual for an action. The double integral describes a nonlocal contribution where the system trajectory interacts with itself. This self-interaction is mediated by the environment as can be seen from the factor c_n^2 in (1.168).

The integral kernel $K_n(\tau)$ is only needed in an interval of length $\hbar\beta$. Periodic continuation outside of this interval therefore allows us to expand the kernel into a Fourier series

$$\begin{aligned} K_n(\tau) &= \frac{c_n^2}{\hbar\beta m_n\omega_n} \sum_{l=-\infty}^{\infty} \frac{\omega_n}{\omega_n^2 + \nu_l^2} \exp(\mathrm{i}\nu_l\tau) \\ &= \frac{c_n^2}{\hbar\beta m_n\omega_n^2} \sum_{l=-\infty}^{\infty} \exp(\mathrm{i}\nu_l\tau) - \frac{c_n^2}{\hbar\beta m_n\omega_n^2} \sum_{l=-\infty}^{\infty} \frac{\nu_l^2}{\omega_n^2 + \nu_l^2} \exp(\mathrm{i}\nu_l\tau) \\ &= \frac{c_n^2}{m_n\omega_n^2} \sum_{j=-\infty}^{\infty} \delta(\tau - j\hbar\beta) - k_n(\tau) \,, \end{aligned} \tag{1.170}$$

where the Matsubara frequencies ν_l have been defined in (1.107). In (1.170), we split the kernel into two parts. The first term contains delta functions which lead to a local contribution to the action. Noting that due to the region of integration in (1.167) only half of the delta function contributes, this local term just cancels the potential renormalization (1.145). We are therefore left with the nonlocal kernel

$$k_n(\tau) = \frac{c_n^2}{\hbar\beta m_n\omega_n^2} \sum_{l=-\infty}^{\infty} \frac{\nu_l^2}{\omega_n^2 + \nu_l^2} \exp(\mathrm{i}\nu_l\tau) \,. \tag{1.171}$$

It can be shown that this kernel no longer contains a local contribution by writing

$$\begin{aligned} &\int_0^{\hbar\beta} \mathrm{d}\tau \int_0^{\tau} \mathrm{d}\sigma k_n(\tau - \sigma)\bar{q}(\tau)\bar{q}(\sigma) \\ &\qquad = -\frac{1}{2}\int_0^{\hbar\beta} \mathrm{d}\tau \int_0^{\tau} \mathrm{d}\sigma k_n(\tau - \sigma)\left[\left(\bar{q}(\tau) - \bar{q}(\sigma)\right)^2 - \left(\bar{q}(\tau)^2 + \bar{q}(\sigma)^2\right)\right] \,. \end{aligned} \tag{1.172}$$

The first term is manifestly nonlocal because it contains the difference $\bar{q}(\tau)-\bar{q}(\sigma)$. Exploiting the symmetry of $k_n(\tau)$, the second term can be expressed as

$$\frac{1}{2}\int_0^{\hbar\beta}\mathrm{d}\tau\int_0^{\tau}\mathrm{d}\sigma k_n(\tau-\sigma)\left(\bar{q}(\tau)^2+\bar{q}(\sigma)^2\right)=\int_0^{\hbar\beta}\mathrm{d}\tau\bar{q}(\tau)^2\int_0^{\hbar\beta}\mathrm{d}\sigma k_n(\sigma)\;. \quad (1.173)$$

Therefore, this term potentially could result in a local contribution. However, the time integral over the interval from 0 to $\hbar\beta$ corresponds to the $l=0$ Fourier component which vanishes for $k_n(\tau)$. As a consequence, the kernel $k_n(\tau)$ indeed gives rise to a purely nonlocal contribution to the action.

Now, we can carry out the Gaussian integral over x_n appearing in the influence functional (1.164). With the action (1.167) we find

$$\mathcal{F}_n[\bar{q}]=\mathcal{Z}_n\exp\left(-\frac{1}{2\hbar}\int_0^{\hbar\beta}\mathrm{d}\tau\int_0^{\hbar\beta}\mathrm{d}\sigma k_n(\tau-\sigma)\bar{q}(\tau)\bar{q}(\sigma)\right)\;. \quad (1.174)$$

The partition function $\mathcal{Z}_n$ arises from the fluctuation contribution and may be shown to be given by (1.163) for example by comparison with the uncoupled case $c_n=0$.

With (1.162) we finally obtain the influence functional

$$\mathcal{F}[\bar{q}]=\exp\left(-\frac{1}{2\hbar}\int_0^{\hbar\beta}\mathrm{d}\tau\int_0^{\hbar\beta}\mathrm{d}\sigma k(\tau-\sigma)\bar{q}(\tau)\bar{q}(\sigma)\right) \quad (1.175)$$

with

$$\begin{aligned}k(\tau)=\sum_{n=1}^{N}k_n(\tau)&=\sum_{n=1}^{N}\frac{c_n^2}{\hbar\beta m_n\omega_n^2}\sum_{l=-\infty}^{\infty}\frac{\nu_l^2}{\omega_n^2+\nu_l^2}\exp(\mathrm{i}\nu_l\tau)\\&=\frac{2}{\hbar\beta}\int_0^{\infty}\frac{\mathrm{d}\omega}{\pi}\frac{J(\omega)}{\omega}\sum_{l=-\infty}^{\infty}\frac{\nu_l^2}{\omega^2+\nu_l^2}\exp(\mathrm{i}\nu_l\tau)\end{aligned} \quad (1.176)$$

where we have made use of the spectral density of bath oscillators (1.136) to obtain the last line.

The kernel $k(\tau)$ may be related to the damping kernel $\gamma(t)$ by observing that the Laplace transform of the latter is given by

$$\begin{aligned}\hat{\gamma}(z)=\int_0^{\infty}\mathrm{d}t\exp(-zt)\gamma(t)&=\frac{2}{m}\int_0^{\infty}\frac{\mathrm{d}\omega}{\pi}\frac{J(\omega)}{\omega}\int_0^{\infty}\mathrm{d}t\exp(-zt)\cos(\omega t)\\&=\frac{2}{m}\int_0^{\infty}\frac{\mathrm{d}\omega}{\pi}\frac{J(\omega)}{\omega}\frac{z}{z^2+\omega^2}\;.\end{aligned} \quad (1.177)$$

In the first line we have employed the relation (1.137) between the damping kernel and the spectral density of bath oscillators. In view of (1.176) and (1.177) we can finally express the kernel as

$$k(\tau)=\frac{m}{\hbar\beta}\sum_{l=-\infty}^{\infty}|\nu_l|\hat{\gamma}(|\nu_l|)\exp(\mathrm{i}\nu_l\tau)\;. \quad (1.178)$$

For strictly Ohmic damping, this kernel is highly singular and we therefore introduce a Drude cutoff. The Laplace transform of the corresponding damping kernel is obtained from (1.142) as

$$\hat{\gamma}(z) = \frac{\gamma\omega_{\mathrm{D}}}{\omega_{\mathrm{D}} + z} \tag{1.179}$$

which reduces to $\hat{\gamma}(z) = \gamma$ for strictly Ohmic damping. Keeping the leading terms in the cutoff frequency ω_{D}, the kernel now reads

$$k(\tau) = m\gamma\omega_{\mathrm{D}} \sum_{n=-\infty}^{\infty} \delta(\tau - n\hbar\beta) - \frac{\pi m\gamma}{(\hbar\beta)^2} \frac{1}{\sin^2\left(\dfrac{\pi\tau}{\hbar\beta}\right)} + O(\omega_{\mathrm{D}}^{-1}) \,. \tag{1.180}$$

For low temperatures, this gives rise to a long range interaction between different parts of the system trajectory. This reminds us of the algebraic decay of the real part (1.150) of the noise correlation function $K(t)$ and in fact it follows from our previous discussion that up to the periodic delta function appearing in (1.180) the kernel $k(\tau)$ equals $-K(-\mathrm{i}\tau)$.

Summarizing this calculation we obtain the important result that the influence of the environment on the system may be taken into account by adding a nonlocal contribution to the action. We then obtain the effective action

$$S_{\mathrm{eff}}^{\mathrm{E}}[\bar{q}] = S_{\mathrm{S}}^{\mathrm{E}}[\bar{q}] + \frac{1}{2}\int_0^{\hbar\beta} \mathrm{d}\tau \int_0^{\hbar\beta} \mathrm{d}\sigma\, k(\tau - \sigma)\bar{q}(\tau)\bar{q}(\sigma) \tag{1.181}$$

with $k(\tau)$ given by (1.178). The elimination of the environment within the real time path integral formalism, e.g. along the lines of the calculation by Feynman and Vernon [33] mentioned at the beginning of this section, would have led to an effective action of a structure similar to (1.181). An important difference consists in the fact that the propagation of a density matrix involves two paths instead of one. In addition, the integral kernel then of course appears in its real time version.

1.4 Damped Harmonic Oscillator

1.4.1 Partition Function

In this final section we will apply the results of the previous sections to the damped harmonic oscillator where exact results may be obtained analytically. The Hamiltonian describing system and environment is given by (1.114)–(1.117) with the potential

$$V(q) = \frac{m}{2}\omega_0^2 q^2 \,. \tag{1.182}$$

As we have seen in Sect. 1.3.2, there is no point in dealing with all the microscopic parameters present in the Hamiltonians (1.116) and (1.117). Instead, it

is sufficient to specify the spectral density of bath oscillators (1.136). In the following, we will mostly assume Ohmic damping, i.e. $J(\omega) = m\gamma\omega$, and introduce a high-frequency cutoff of the Drude type (1.141) when necessary.

In the general discussion of dissipative quantum systems we have concentrated on imaginary time calculations and we will therefore try to take this approach as a starting point of the following considerations. Probably the most important quantity which can be obtained in imaginary time is the partition function which in statistical mechanics can be viewed as a generating function for expectation values. Based on our previous discussion of the partition function of the undamped harmonic oscillator in Sect. 1.2.9 and the effective action in imaginary time in Sect. 1.3.3, it is rather straightforward to obtain the partition function of the damped harmonic oscillator.

According to (1.104) and (1.110) we can express the partition function of the undamped harmonic oscillator as

$$\mathcal{Z}_{\mathrm{u}} = \frac{1}{\hbar\beta\omega_0} \prod_{n=1}^{\infty} \frac{\nu_n^2}{\nu_n^2 + \omega_0^2} \,. \tag{1.183}$$

We remind the reader that the denominator of the product stems from the fluctuation determinant associated with the Euclidean action

$$S^{\mathrm{E}}[q] = \int_0^{\hbar\beta} \mathrm{d}\tau \left(\frac{m}{2}\dot{q}^2 + \frac{m}{2}\omega_0^2 q^2 \right) \,. \tag{1.184}$$

As we have seen in Sect. 1.3.3, the coupling to the environment leads to an additional, nonlocal term to the action. Expanding the fluctuations in a Fourier series as we did on p. 25 and making use of the Fourier decomposition (1.178) of the integral kernel $k(\tau)$, we conclude that an additional term $\nu_n\hat{\gamma}(\nu_n)$ appears in the fluctuation determinant. Modifying (1.183) accordingly, we find for the partition function of the damped harmonic oscillator

$$\mathcal{Z} = \frac{1}{\hbar\beta\omega_0} \prod_{n=1}^{\infty} \frac{\nu_n^2}{\nu_n^2 + \nu_n\hat{\gamma}(\nu_n) + \omega_0^2} \,. \tag{1.185}$$

For strictly Ohmic damping, we have $\hat{\gamma}(\nu_n) = \gamma$. Since infinite products over terms of the form $1 + a/n$ for large n do not converge, we are forced to introduce a high-frequency cutoff in order to obtain a finite result. One possibility is the Drude cutoff (1.142) with $\hat{\gamma}$ given by (1.179).

In the following section we will try to extract some interesting information from the partition function and in the process will get an idea of where the difficulties for strictly Ohmic damping arise from.

1.4.2 Ground State Energy and Density of States

A thermodynamic quantity directly related to the partition function is the free energy which can be obtained from the former by means of

$$F = -\frac{1}{\beta} \ln(\mathcal{Z}) \,. \tag{1.186}$$

In the limit of zero temperature, the free energy becomes the ground state energy of the undamped oscillator shifted due to the coupling to the environment. For the free energy, we find with (1.185)

$$F = \frac{1}{\beta}\ln(\hbar\beta\omega_0) + \frac{1}{\beta}\sum_{n=1}^{\infty}\ln\left(1 + \frac{\hat{\gamma}(\nu_n)}{\nu_n} + \frac{\omega_0^2}{\nu_n^2}\right) . \tag{1.187}$$

In the limit $\beta \to \infty$ the spacing between the Matsubara frequencies ν_n goes to zero and the sum turns into the ground state energy of the damped oscillator given by the integral

$$\varepsilon_0 = \frac{\hbar}{2\pi}\int_0^{\infty} \mathrm{d}\nu \ln\left(1 + \frac{\hat{\gamma}(\nu)}{\nu} + \frac{\omega_0^2}{\nu^2}\right) . \tag{1.188}$$

It is particularly interesting to consider the case of weak coupling where connection can be made to results of perturbation theory. This will also help to understand the physical meaning of a ground state energy of a dissipative system derived from a free energy. An expansion of (1.188) including terms of order γ yields

$$\varepsilon_0 = \frac{\hbar}{2\pi}\int_0^{\infty} \mathrm{d}\nu \ln\left(1 + \frac{\omega_0^2}{\nu^2}\right) + \frac{\hbar}{2\pi}\int_0^{\infty} \mathrm{d}\nu \frac{\nu}{\nu^2 + \omega_0^2}\hat{\gamma}(\nu) . \tag{1.189}$$

Evaluation of the first integral yields the expected result $\hbar\omega_0/2$, i.e. the ground state energy of the undamped harmonic oscillator. The second integral represents the shift due to the coupling to the environmental oscillators and can be expressed in terms of the spectral density of bath oscillators $J(\omega)$. Recalling (1.177) one can perform the integral over ν and the ground state energy (1.189) in the presence of damping becomes

$$\varepsilon_0 = \frac{\hbar\omega_0}{2} + \frac{\hbar}{2\pi m}\int_0^{\infty} \mathrm{d}\omega J(\omega)\frac{1}{\omega(\omega_0 + \omega)} . \tag{1.190}$$

In order to facilitate the physical interpretation, we rewrite this result as

$$\varepsilon_0 = \frac{\hbar\omega_0}{2} - \frac{\hbar}{2\pi m\omega_0}\int_0^{\infty} \mathrm{d}\omega J(\omega)\left(\frac{1}{\omega_0 + \omega} - \frac{1}{\omega}\right) . \tag{1.191}$$

The first term of order γ may be interpreted in analogy to the Lamb shift. There, an atomic level is shifted by creation and subsequent annihilation of a virtual photon as a consequence of the coupling to the electromagnetic vacuum. In our case, the atomic level is replaced by the ground state of the harmonic oscillator and the environmental oscillators are completely equivalent to the modes of the electromagnetic field. The pictorial representation of this process is shown in Fig. 1.10. The coupling Hamiltonian (1.117) allows a transition from the ground state into the first excited state $|1\rangle$ by excitation of the j-th environmental oscillator into its first excited state $|1_j\rangle$.

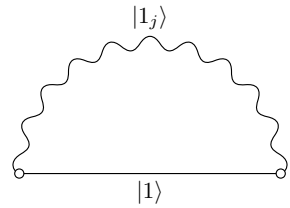

Fig. 1.10. The ground state energy of the harmonic oscillator is shifted by a transition to the first excited state accompanied by a virtual excitation of the j-th environmental mode

The energy shift associated with the diagram depicted in Fig. 1.10 is given by second order perturbation theory as

$$\Delta_0 = \sum_{j=1}^{N} \frac{|\langle 1, 1_j|c_j q x_j|0, 0\rangle|^2}{-\hbar\omega_0 - \hbar\omega_j} \tag{1.192}$$

where the denominator is determined by the energy of the intermediate state $|1, 1_j\rangle$. With the matrix element

$$\langle 1, 1_j|qx_j|0, 0\rangle = \frac{\hbar}{2(mm_j\omega_0\omega_j)^{1/2}} \tag{1.193}$$

and the relation (1.136) for the spectral density of bath oscillators we get

$$\Delta_0 = -\frac{\hbar}{2\pi m\omega_0} \int_0^\infty \mathrm{d}\omega J(\omega) \frac{1}{\omega_0 + \omega} \tag{1.194}$$

which is just the first term of order γ in (1.191). As we know, the bilinear coupling Hamiltonian appearing in (1.192) gives rise to a renormalization of the potential which has been taken care of by the second term in the Hamiltonian (1.117). The result (1.194) contains this potential renormalization since only the bilinear coupling term has been considered. In (1.191), which results from the full Hamiltonian, this effect is subtracted off by the second term under the integral in (1.191) as can be verified by comparison with (1.145).

It is obvious that for strictly Ohmic damping with $J(\omega) = m\gamma\omega$ the correction (1.194) and with it the ground state energy (1.191) will display an ultraviolet divergence which is due to the unphysical behaviour of the spectral density $J(\omega)$ at large frequencies. Assuming a Drude cutoff we find with (1.141) to leading order in the cutoff frequency ω_D the finite result

$$\Delta_0 = -\frac{\hbar\gamma\omega_\mathrm{D}}{4\omega_0} + \frac{\hbar\gamma}{2\pi} \ln\left(\frac{\omega_\mathrm{D}}{\omega_0}\right) + O(\omega_\mathrm{D}^{-1}) \,. \tag{1.195}$$

The negative first term corresponds to the potential renormalization which is no longer present in the ground state energy ε_0. The second term, on the other hand, is positive and thus leads to an increase of the ground state energy.

Not only the ground state energy can be derived from the partition function but one may also formally introduce a density of states $\rho(E)$ of the damped system according to [35]

$$\mathcal{Z}(\beta) = \int_0^\infty \mathrm{d}E \rho(E) \exp(-\beta E) \; . \tag{1.196}$$

Inversion of the Laplace transformation allows to determine $\rho(E)$ from the partition function according to

$$\rho(E) = \frac{1}{2\pi \mathrm{i}} \int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} \mathrm{d}\beta \mathcal{Z}(\beta) \exp(\beta E) \tag{1.197}$$

where the constant c has to be chosen such that the line of integration is to the right of all poles of $\mathcal{Z}(\beta)$.

Once a high-frequency cutoff for the spectral density of bath oscillators is specified, the inverse Laplace transform in (1.197) may be evaluated either numerically or by contour integration. The second approach leads to a series which again has to be evaluated numerically [35]. However, it is not necessary to introduce a cutoff provided we shift the energy by the ground state energy ε_0 which in fact is the only divergent quantity in this problem. Such a shift may be performed by considering $\mathcal{Z} \exp(\beta\varepsilon_0)$ instead of $\mathcal{Z}$ itself. To demonstrate that this procedure renders the cutoff irrelevant, we will restrict ourselves to the limit of weak damping and large cutoff considered before even though a more general treatment is feasible.

In a first step we decompose the infinite product appearing in the partition function (1.185) with Drude cutoff (1.179) into a factor where the limit $\omega_\mathrm{D} \to \infty$ can safely be taken and a factor still containing the cutoff frequency

$$\mathcal{Z} = \frac{1}{\hbar\beta\omega_0} \prod_{n=1}^\infty \frac{\nu_n^2 + \gamma\nu_n}{\nu_n^2 + \gamma\nu_n + \omega_0^2} \prod_{n=1}^\infty \frac{1}{1 + \dfrac{\gamma\omega_\mathrm{D}}{\nu_n(\nu_n + \omega_\mathrm{D})}} \; . \tag{1.198}$$

It is the last product which has to be analyzed with care because it vanishes in the limit $\omega_D \to \infty$. To leading order in γ one finds

$$\begin{aligned} \ln\left(\prod_{n=1}^\infty 1 + \frac{\gamma\omega_\mathrm{D}}{\nu_n(\nu_n + \omega_\mathrm{D})} \right) &= \sum_{n=1}^\infty \frac{\gamma\omega_\mathrm{D}}{\nu_n(\nu_n + \omega_\mathrm{D})} \\ &= \frac{\hbar\beta\gamma}{2\pi} \psi\left(1 + \frac{\hbar\beta\omega_\mathrm{D}}{2\pi} \right) \end{aligned} \tag{1.199}$$

where we have introduced the digamma function [36]

$$\psi(1+z) = -\mathcal{C} + \sum_{n=1}^\infty \frac{z}{n(n+z)} \; . \tag{1.200}$$

Here, $\mathcal{C} = 0.577\ldots$ is the Euler constant. With the leading asymptotic behaviour $\psi(1+z) \sim \ln(z)$ for large arguments z, the partition function for large cutoff

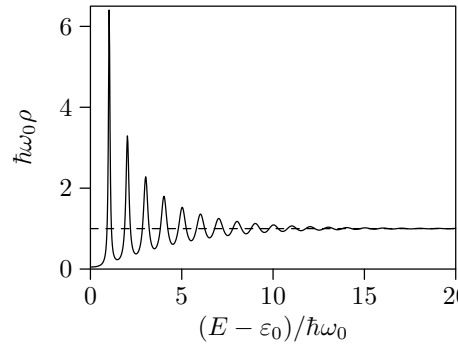

Fig. 1.11. The density of states (1.197) of the damped harmonic oscillator is shown for $\gamma/2\omega_0 = 0.05$. A delta function contribution at $E = \varepsilon_0$ has been omitted. The dashed line marks the average density of states $1/\hbar\omega_0$

frequency becomes

$$\mathcal{Z} = \frac{1}{\hbar\beta\omega_0}\prod_{n=1}^{\infty}\frac{\nu_n^2+\gamma\nu_n}{\nu_n^2+\gamma\nu_n+\omega_0^2}\left(\frac{\hbar\beta\omega_\mathrm{D}}{2\pi}\right)^{-\hbar\beta\gamma/2\pi}. \tag{1.201}$$

On the other hand, we know from our result (1.195) that the ground state energy diverges to leading order with $(\hbar\gamma/2\pi)\ln(\omega_\mathrm{D})$. Therefore, multiplication of the partition function with $\exp(\beta\varepsilon_0)$ leads indeed to an expression with a finite value in the limit of infinite cutoff frequency.

Before taking a look at numerical results, we remark that the partition function contains a pole at $\beta = 0$ with residue $1/\hbar\omega_0$. This pole represents the Laplace transform of the constant $1/\hbar\omega_0$ and therefore is related to the average density of states which takes the value of the undamped case where the energy spacing between adjacent levels is $\hbar\omega_0$. In Fig. 1.11 we present the density of states for weak damping, $\gamma/2\omega_0 = 0.05$. A delta function contribution at $E = \varepsilon_0$ has been omitted. Due to the weak damping we find well defined peaks which are close to the energies expected for an undamped oscillator. With increasing energy the levels become broader. For stronger damping, only the lowest levels can be resolved and a level shift induced by the damping becomes visible.

The behaviour of the level widths shown in Fig. 1.11 is consistent with the result of a perturbative treatment. According to Fermi's golden rule, the width of the n-th level is given by

$$\begin{aligned}\Gamma_n = \frac{2\pi}{\hbar^2}\sum_{j=1}^{\infty}\Big[&\big|\langle n+1,1_j|c_jqx_j|n,0\rangle\big|^2\delta(-\omega_0-\omega_j)\\ &+\big|\langle n-1,1_j|c_jqx_j|n,0\rangle\big|^2\delta(\omega_0-\omega_j)\Big]\end{aligned} \tag{1.202}$$

where we have already taken into account that the matrix element of the dipole-type coupling connects the state n only to its nearest neighbors. Because of

energy conservation the first part of the sum never contributes. With the matrix elements

$$\langle n-1,1_j|qx_j|n,0\rangle = \frac{\hbar}{2(mm_j\omega_0\omega_j)^{1/2}}n^{1/2} \tag{1.203}$$

we thus find for the width of the n-th level in terms of the spectral density of bath oscillators

$$\Gamma_n = \frac{n}{m\omega_0}J(\omega_0)\ . \tag{1.204}$$

For Ohmic damping, $J(\omega) = m\gamma\omega$, we finally get

$$\Gamma_n = n\gamma\ . \tag{1.205}$$

As observed before, the levels broaden with increasing damping strength γ and level number n. We remark that one can demonstrate by a semiclassical analysis of other one-dimensional potentials that it is indeed the level number and not the energy which is decisive for the level width [37].

1.4.3 Position Autocorrelation Function

In the introduction we have mentioned fluctuations as one of the effects arising from the coupling to an environment. Even if a system is in thermal equilibrium with its environment, fluctuations due to the noise term (1.128) will be present. The appropriate quantity to describe this phenomenon are equilibrium correlation functions like the position autocorrelation function

$$C(t) = \langle q(t)q(0)\rangle = \mathrm{Tr}(q(t)q(0)\rho_\beta)\ . \tag{1.206}$$

From this quantity one can derive all other equilibrium correlation functions of the damped harmonic oscillator as is discussed in [38].

We now want to determine this correlation function by first calculating its imaginary time version and start with the Euclidean action

$$\begin{aligned} S^{\mathrm{E}}[q] = \int_0^{\hbar\beta}\mathrm{d}\tau\left(\frac{m}{2}\dot{q}^2+\frac{m}{2}\omega_0^2q^2\right)+\frac{1}{2}\int_0^{\hbar\beta}\mathrm{d}\tau\int_0^{\hbar\beta}\mathrm{d}\sigma k(\tau-\sigma)q(\tau)q(\sigma) \\ +\int_0^{\hbar\beta}\mathrm{d}\tau F(\tau)q(\tau)\ . \end{aligned} \tag{1.207}$$

The second term accounts for the coupling to the environment as we have shown in Sect. 1.3.3. In addition, we have included the third term corresponding to an external force in imaginary time. This constitutes a useful trick which will allow us to determine the correlation function by variation with respect to this force

$$\langle q(\tau)q(\sigma)\rangle = \hbar^2\mathrm{Tr}\left(\frac{\delta}{\delta F(\tau)}\frac{\delta}{\delta F(\sigma)}\rho\right)\Big|_{F=0}\ . \tag{1.208}$$

As we know already from Sect. 1.2.7, the force does not appear in the fluctuation part. It is therefore sufficient, to restrict our attention to the classical path.

The classical equation of motion following from variation of the action (1.207)

$$m\ddot{q}(\tau) - \int_0^{\hbar\beta} \mathrm{d}\sigma k(\tau-\sigma)q(\sigma) - m\omega_0^2 q(\tau) = F(\tau) \tag{1.209}$$

is most conveniently solved by Fourier transformation on the interval from 0 to $\hbar\beta$. Introducing the Fourier transforms

$$q(\tau) = \frac{1}{\hbar\beta}\sum_{n=-\infty}^{\infty} q_n \exp(\mathrm{i}\nu_n\tau) \tag{1.210}$$

and

$$F(\tau) = \frac{m}{\hbar\beta}\sum_{n=-\infty}^{\infty} f_n \exp(\mathrm{i}\nu_n\tau) \tag{1.211}$$

and making use of the Fourier representation (1.178) of $k(\tau)$ for Ohmic damping, we find for the Fourier coefficients of the classical solution

$$q_n^{\mathrm{cl}} = -\frac{f_n}{\nu_n^2 + \gamma|\nu_n| + \omega_0^2}\ . \tag{1.212}$$

Inserting this result into the Fourier representation of the action (1.207)

$$S^{\mathrm{E}}[q] = \frac{m}{2\hbar\beta}\sum_{n=-\infty}^{\infty}\left[(\nu_n^2 + \gamma|\nu_n| + \omega_0^2)q_n q_{-n} + f_n q_{-n} + f_{-n}q_n\right] \tag{1.213}$$

yields the classical Euclidean action

$$S_{\mathrm{cl}}^{\mathrm{E}} = -\frac{m}{2\hbar\beta}\sum_{n=-\infty}^{\infty}\frac{f_n f_{-n}}{\nu_n^2 + \gamma|\nu_n| + \omega_0^2} \tag{1.214}$$

or equivalently

$$\begin{aligned} S_{\mathrm{cl}}^{\mathrm{E}} = -\frac{1}{2m\hbar\beta}\sum_{n=-\infty}^{\infty}&\frac{1}{\nu_n^2 + \gamma|\nu_n| + \omega_0^2} \\ &\times\int_0^{\hbar\beta}\mathrm{d}\tau\int_0^{\hbar\beta}\mathrm{d}\sigma F(\tau)F(\sigma)\exp\left(\mathrm{i}\nu_n(\tau-\sigma)\right)\ . \end{aligned} \tag{1.215}$$

Since the external force appears only through this action in the exponent of the equilibrium density matrix, we may easily evaluate the functional derivatives according to (1.208). For the position autocorrelation function in imaginary time we thus find

$$C(\tau) = \frac{1}{m\beta}\sum_{n=-\infty}^{\infty}\frac{\exp(\mathrm{i}\nu_n\tau)}{\nu_n^2 + \gamma|\nu_n| + \omega_0^2}\ . \tag{1.216}$$

Unfortunately, the real time correlation function cannot be obtained simply by replacing the imaginary time τ by $\mathrm{i}t$ where t is a real time. For negative times t,

the sum in (1.216) would not converge. We therefore have to perform an analytic continuation to real times in a more elaborate way.

The idea is to express the sum (1.216) as a contour integral in the complex frequency plane. To this end, we need a function with poles at frequencies $\omega = \mathrm{i}\nu_n, n = -\infty, \ldots, \infty$ with a residuum of one. This requirement is satisfied by $\hbar\beta/[1 - \exp(-\hbar\beta\omega)]$. By integration along the contour shown in Fig. 1.12a we find

$$\int_{\mathcal{C}^+} \mathrm{d}\omega \frac{\hbar\beta}{1-\exp(-\hbar\beta\omega)} \frac{\exp(-\omega\tau)}{-\omega^2 + \mathrm{i}\gamma\omega + \omega_0^2} = -\mathrm{i}\frac{\pi}{\omega_0^2} - 2\pi\mathrm{i}\sum_{n=1}^{\infty} \frac{\exp(\mathrm{i}\nu_n\tau)}{\nu_n^2 + \gamma\nu_n + \omega_0^2} \,. \tag{1.217}$$

Similarly, an integration along the contour shown in Fig. 1.12b leads to

$$\int_{\mathcal{C}^-} \mathrm{d}\omega \frac{\hbar\beta}{1-\exp(-\hbar\beta\omega)} \frac{\exp(-\omega\tau)}{-\omega^2 - \mathrm{i}\gamma\omega + \omega_0^2} = \mathrm{i}\frac{\pi}{\omega_0^2} + 2\pi\mathrm{i}\sum_{n=-\infty}^{-1} \frac{\exp(\mathrm{i}\nu_n\tau)}{\nu_n^2 + \gamma\nu_n + \omega_0^2} \tag{1.218}$$

Subtracting (1.218) from (1.217), the imaginary time correlation function can be expressed as

$$\frac{1}{m\beta}\sum_{n=-\infty}^{\infty} \frac{\exp(\mathrm{i}\nu_n\tau)}{\nu_n^2 + \gamma\nu_n + \omega_0^2} = \frac{\hbar}{m\pi}\int_{-\infty}^{\infty} \mathrm{d}\omega \frac{\gamma\omega}{(\omega^2-\omega_0^2)^2 + \gamma^2\omega^2} \frac{\exp(-\omega\tau)}{1-\exp(-\hbar\beta\omega)} \,. \tag{1.219}$$

Now we may pass to real times by the replacement $\tau \to \mathrm{i}t$ to obtain the real time correlation function

$$C(t) = \frac{\hbar}{m\pi}\int_{-\infty}^{\infty} \mathrm{d}\omega \frac{\gamma\omega}{(\omega^2-\omega_0^2)^2 + \gamma^2\omega^2} \frac{\exp(-\mathrm{i}\omega t)}{1-\exp(-\hbar\beta\omega)} \,. \tag{1.220}$$

Physical insight into this result can be gained by considering the Fourier transform of this correlation function

$$\tilde{C}(\omega) = \int_{-\infty}^{\infty} \mathrm{d}t \exp(\mathrm{i}\omega t) C(t) \tag{1.221}$$

which may be related to the dynamic susceptibility $\tilde{\chi}(\omega)$ of the damped harmonic oscillator. According to the Ehrenfest theorem the equation of motion for the expectation value of the position agrees with the corresponding classical equation of motion. In the presence of an external force $F(t)$, the latter reads

$$m\ddot{q} + m\gamma\dot{q} + m\omega_0^2 q = F(t) \,. \tag{1.222}$$

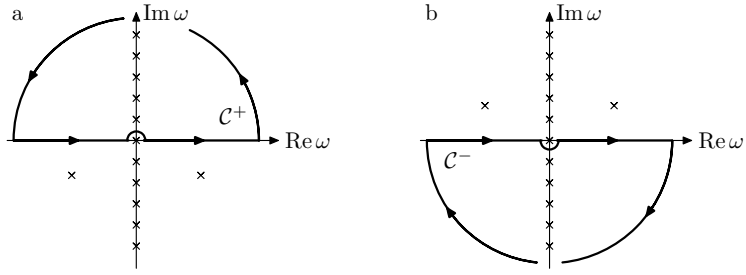

Fig. 1.12. The analytic continuation of the imaginary time correlation function $\langle q(\tau)q(0)\rangle$ to real times makes use of the integration contours depicted in (**a**) and (**b**) to obtain (1.217) and (1.218), respectively

The solution of this equation may be expressed in terms of the response function $\chi(t)$ as

$$q(t) = \int_{-\infty}^{t} \mathrm{d}s\chi(t-s)F(s) \tag{1.223}$$

which by means of a Fourier transformation becomes

$$\tilde{q}(\omega) = \tilde{\chi}(\omega)\tilde{F}(\omega)\ . \tag{1.224}$$

With the equation of motion (1.222) the dynamic susceptibility of the damped harmonic oscillator is then found to read

$$\chi(\omega) = \frac{1}{m}\frac{1}{-\omega^2 - \mathrm{i}\gamma\omega + \omega_0^2}\ . \tag{1.225}$$

Together with (1.220) and (1.221) one finally obtains the relation

$$\tilde{C}(\omega) = \frac{2\hbar}{1-\exp(-\hbar\beta\omega)}\chi''(\omega) \tag{1.226}$$

which represents an example of the so-called fluctuation-dissipation theorem [39]. Here, the position autocorrelation function describes the fluctuations while the imaginary part of the dynamic susceptibility χ'' can be shown to determine the energy dissipated under the influence of the external driving $F(t)$. While the relation (1.226) is exact for linear systems like the damped harmonic oscillator considered here, it still holds for nonlinear systems within linear response theory. There, the response to the external force is considered in leading order perturbation theory [40,41].

It is instructive to consider the real time correlation function (1.220) in more detail. We first decompose the correlation function $C(t)$ into its real and imaginary part, or equivalently, into its symmetric and antisymmetric part

$$C(t) = S(t) + \mathrm{i}A(t)\ , \tag{1.227}$$

with

$$S(t) = \frac{1}{2}\big(\langle q(t)q(0)\rangle + \langle q(0)q(t)\rangle\big) \tag{1.228}$$

and

$$A(t) = -\frac{\mathrm{i}}{2}\big(\langle q(t)q(0)\rangle - \langle q(0)q(t)\rangle\big) \; . \tag{1.229}$$

From (1.220) we find

$$S(t) = \frac{\hbar}{2\pi m}\int_{-\infty}^{\infty} \mathrm{d}\omega \frac{\gamma\omega}{(\omega^2-\omega_0^2)^2+\gamma^2\omega^2}\coth\left(\frac{\hbar\beta\omega}{2}\right)\cos(\omega t) \tag{1.230}$$

and

$$A(t) = -\frac{\hbar}{2\pi m}\int_{-\infty}^{\infty} \mathrm{d}\omega \frac{\gamma\omega}{(\omega^2-\omega_0^2)^2+\gamma^2\omega^2}\sin(\omega t) \; . \tag{1.231}$$

Apart from Planck's constant appearing in the prefactor, the antisymmetric part is purely classical. In fact, one demonstrates within linear response theory the general relation

$$\chi(t) = \frac{\mathrm{i}}{\hbar}\langle[q(t),q(0)]\rangle\Theta(t) = -\frac{2}{\hbar}A(t)\Theta(t) \; . \tag{1.232}$$

Therefore, our statement follows as a consequence of the Ehrenfest theorem which ensures that the response function $\chi(t)$ of the damped harmonic oscillator is classical.

More interesting is the symmetric part (1.230) of the correlation function $C(t)$. There exist two different types of time scales determined by the poles of the integrand in (1.230). One set of four poles at frequencies

$$\omega = \pm\left(\bar{\omega} \pm \mathrm{i}\frac{\gamma}{2}\right) \tag{1.233}$$

corresponds to the characteristic frequencies of a damped harmonic oscillator with the oscillation frequency

$$\bar{\omega} = \left(\omega_0^2 - \frac{\gamma^2}{4}\right)^{1/2} \tag{1.234}$$

shifted by the damping. In addition, there exists an infinite number of poles at imaginary frequencies $\mathrm{i}\nu_n, n = -\infty, \ldots, \infty$ depending on the temperature of the heat bath via the Matsubara frequencies defined in (1.107). With these poles, one can evaluate the integral (1.230) by means of a contour integration to obtain

$$\begin{aligned} S(t) = {} & \frac{\hbar}{2m\bar{\omega}}\exp\left(-\frac{\gamma|t|}{2}\right)\frac{[\sinh(\hbar\beta\bar{\omega})\cos(\bar{\omega}t)+\sin(\hbar\beta\gamma/2)\sin(\bar{\omega}|t|)]}{\cosh(\hbar\beta\bar{\omega})-\cos(\hbar\beta\gamma/2)} \\ & - \frac{2\gamma}{m\beta}\sum_{n=1}^{\infty}\frac{\nu_n\exp(-\nu_n|t|)}{(\nu_n^2+\omega_0^2)^2-\gamma^2\nu_n^2} \; . \end{aligned} \tag{1.235}$$

The sum in the second line becomes important at low temperatures $k_{\mathrm{B}}T \ll \hbar\gamma/4\pi$. In order to discuss this quantum effect, we focus in the following discussion on the case of zero temperature. Then, the poles of the hyperbolic cotangent

in (1.230) become dense and form a cut on the imaginary axis which has consequences for the long-time behaviour of the correlation function. In the limit $\beta \to \infty$ the sum in the second line of (1.235) turns into an integral. Noting that the long-time behaviour is determined by the behaviour of the integrand at small arguments we find

$$S(t) \sim -\frac{\hbar\gamma}{\pi m} \int_0^\infty \mathrm{d}x \frac{x \exp(-x|t|)}{\omega_0^4} = -\frac{\hbar\gamma}{\pi m \omega_0^4} \frac{1}{t^2} \; . \tag{1.236}$$

Instead of the usual exponential decay we thus find an algebraic decay.

In the limit of vanishing damping, the imaginary part of the dynamic susceptibility appearing in the integrand of (1.230) turns into a sum of two delta functions located at ω_0 and $-\omega_0$. For weak but finite damping, the delta functions broaden into Lorentzians

$$\frac{\gamma\omega}{(\omega^2 - \omega_0^2)^2 + \gamma^2\omega^2} = \frac{\gamma}{4\bar{\omega}} \left(\frac{1}{(\omega - \bar{\omega})^2 + \gamma^2/4} - \frac{1}{(\omega + \bar{\omega})^2 + \gamma^2/4} \right) \tag{1.237}$$

corresponding to the four poles (1.233) and one can assume that only the integrand in the neighbourhood of these poles is relevant. Within the so-called Markov approximation, one then replaces the contributions to the integrand which depend only weakly on frequency by their values at $\bar{\omega}$. As we will see, in contrast to (1.236) the correlation function $S(t)$ at zero temperature then no longer decays algebraically. It is interesting to discuss the reason for this discrepancy.

To this end we go back to the integral representation (1.230) of the correlation function $S(t)$. In a first step, we apply the so-called rotating wave approximation (RWA) which consists in neglecting the Lorentzian located at $-\bar{\omega}$, i.e. the second term in (1.237) [42]. Physically speaking, we neglect processes where the system is excited into an energetically higher state by loosing energy to the driving force or where the system decays to a lower state by absorbing energy. For finite temperatures, we now have

$$S_{\mathrm{RWA}}(t) = \frac{\hbar}{8\pi m\bar{\omega}} \int_{-\infty}^\infty \mathrm{d}\omega \frac{\gamma}{(\omega - \bar{\omega})^2 + \gamma^2/4} \coth\left(\frac{\hbar\beta\omega}{2}\right) \cos(\omega t) \; . \tag{1.238}$$

Within the Markov approximation, we replace the hyperbolic cotangent by its value at $\omega = \bar{\omega}$. In the limit of zero temperature this leads to

$$\begin{aligned} S_{\mathrm{RWA,Markov}}(t) &= \frac{\hbar}{8\pi m\bar{\omega}} \int_{-\infty}^\infty \mathrm{d}\omega \frac{\gamma}{(\omega - \bar{\omega})^2 + \gamma^2/4} \cos(\omega t) \\ &= \frac{\hbar}{4m\bar{\omega}} \cos(\bar{\omega}t) \exp\Big(-\frac{\gamma}{2}t\Big) \; . \end{aligned} \tag{1.239}$$

We thus find an oscillation with a frequency shifted due to the environmental coupling and an exponential decay in contrast to the algebraic decay (1.236).

This difference can be understood by taking a closer look at the Markov approximation. In Fig. 1.13 the Lorentzian and the hyperbolic cotangent appearing in (1.238) are schematically shown as full and dashed line, respectively.

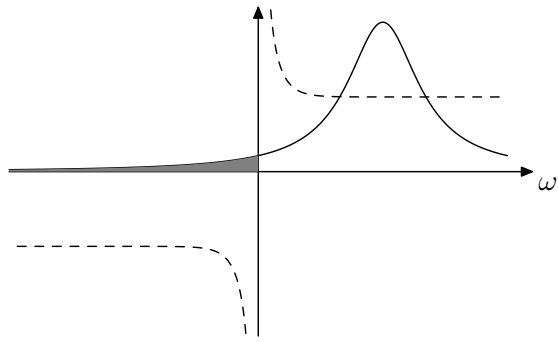

Fig. 1.13. The full and dashed lines represent the Lorentzian and hyperbolic cotangent, respectively, which contribute to the integrand in (1.238)

In order to obtain (1.239), we have approximated the hyperbolic cotangent by a constant. However, in doing this, we have replaced an antisymmetric function by a symmetric one which can only yield a non-vanishing result together with the rotating wave approximation made above. As a consequence, the area shaded in grey has been taken with the wrong sign. The idea was that this difference should be small and arising from frequencies far from $\bar{\omega}$. However, due to the large extent of a Lorentzian, it is of order γ and, in addition, it replaces an exponential decay by an algebraic decay.

At zero temperature the difference between (1.238) and (1.239) becomes

$$\begin{aligned} \Delta &= S_{\mathrm{RWA}}(t) - S_{\mathrm{RWA,Markov}}(t) \\ &= -2\frac{\hbar}{8\pi m}\int_{-\infty}^{0} \mathrm{d}\omega \frac{\gamma}{(\omega-\bar{\omega})^2+\gamma^2/4}\cos(\omega t) \end{aligned} \tag{1.240}$$

which may be expressed in terms of integral sine and integral cosine functions. For our purpose it is sufficient to note that for long times, the difference indeed decays algebraically as

$$\Delta = -\frac{\hbar\gamma}{2\pi m\bar{\omega}_0^4}\frac{1}{t^2}\,. \tag{1.241}$$

We remark that the factor of two relative to the result (1.236) arises because no rotating wave approximation has been made in deriving the latter.

In the previous discussion, we have been concerned with an effect of order γ which in the spirit of the Markov approximation should be considered as small. However, the Markov approximation changes the long-time behaviour of the equilibrium correlation function $S(t)$ qualitatively and the absence of an algebraic decay, even with a small prefactor, may be relevant. For truly weak coupling, the damping constant γ should be the smallest frequency scale. Apart from the usual weak coupling condition $\gamma \ll \omega_0$ we also have to require $\gamma \ll k_{\mathrm{B}}T/\hbar$ which at low temperatures may become difficult to satisfy.

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References

1. U. Weiss: *Quantum Dissipative Systems* (World Scientific 1999)
2. T. Dittrich, P. Hänggi, G.-L. Ingold, B. Kramer, G. Schön, W. Zwerger: *Quantum transport and dissipation* (Wiley-VCH 1998)
3. H. Kleinert: *Path Integrals in Quantum Mechanics, Statistics and Polymer Physics* (World Scientific 1995)
4. R. P. Feynman: Rev. Mod. Phys. **20**, 367 (1948)
5. For a few historical remarks see e.g. D. Derbes: Am. J. Phys. **64**, 881 (1996)
6. P. A. M. Dirac: Phys. Zs. Sowjetunion **3**, 64 (1933)
7. see e.g. E. Nelson, J. Math. Phys. **5**, 332 (1964), Appendix B
8. F. Langouche, D. Roekaerts, E. Tirapegui: *Functional Integration and Semiclassical Expansions*, Mathematics and Its Applications Vol. 10 (D. Reidel 1982)
9. W. Janke, H. Kleinert: Lett. Nuovo Cim. **25**, 297 (1979)
10. M. Goodman: Am. J. Phys. **49**, 843 (1981)
11. A. Auerbach, L. S. Schulman: J. Phys. A **30**, 5993 (1997)
12. I. S. Gradshteyn, I. M. Rhyzik: *Table of Integrals, Series, and Products* (Academic Press 1980)
13. V. P. Maslov, M. V. Fedoriuk: *Semi-classical approximation in quantum mechanics*. Mathematical Physics and Applied Mathematics Vol. 7, ed. by M. Flato et al. (D. Reidel 1981)
14. P. A. Horváthy: Int. J. Theor. Phys. **18**, 245 (1979)
15. D. Rohrlich: Phys. Lett. A **128**, 307 (1988)
16. M. S. Marinov: Phys. Rep. **60**, 1 (1980), Chap. 3.3
17. see e.g. M. Brack, R. K. Bhaduri: *Semiclassical Physics*, Frontiers in Physics Vol. 96 (Addison-Wesley 1997)
18. J. H. van Vleck: Proc. Natl. Acad. Sci. USA **14**, 178 (1928)
19. C. Morette: Phys. Rev. **81**, 848 (1951)
20. W. Pauli: *Selected Topics in Field Quantization*, Pauli Lectures on Physics Vol. 6, ed. by C. P. Enz (Dover 2000)
21. N. Wiener: J. Math. Phys. M.I.T. **2**, 131 (1923)
22. A. O. Caldeira, A. J. Leggett: Phys. Rev. Lett. **46**, 211 (1981)
23. A. O. Caldeira, A. J. Leggett: Ann. Phys. (N.Y.) **149**, 374 (1983)

24. V. B. Magalinskiĭ: Zh. Eksp. Teor. Fiz. **36**, 1942 (1959) [Sov. Phys. JETP **9**, 1381 (1959)]
25. I. R. Senitzky: Phys. Rev. **119**, 670 (1960); **124**, 642 (1961)
26. G. W. Ford, M. Kac, P. Mazur: J. Math. Phys. **6**, 504 (1965)
27. P. Ullersma: Physica **32**, 27, 56, 74, 90 (1966)
28. R. Zwanzig: J. Stat. Phys. **9**, 215 (1973)
29. P. C. Hemmer, L. C. Maximon, H. Wergeland: Phys. Rev. **111**, 689 (1958)
30. P. Hänggi: 'Generalized Langevin Equations: A Useful Tool for the Perplexed Modeller of Nonequilibrium Fluctuations?'. In: *Lecture Notes in Physics Vol. 484*, ed. by L. Schimansky-Geier, T. Pöschel (Springer, Berlin 1997) pp. 15–22
31. V. Hakim, V. Ambegaokar: Phys. Rev. A **32**, 423 (1985)
32. H. Grabert, P. Schramm, G.-L. Ingold: Phys. Rev. Lett. **58**, 1285 (1987)
33. R. P. Feynman, F. L. Vernon, Jr.: Ann. Phys. (N.Y.) **24**, 118 (1963)
34. H. Grabert, P. Schramm, G.-L. Ingold: Phys. Rep. **168**, 115 (1988)
35. A. Hanke, W. Zwerger: Phys. Rev. E **52**, 6875 (1995)
36. M. Abramowitz, I. A. Stegun (eds.): *Handbook of mathematical functions* (Dover 1972)
37. G.-L. Ingold, R. A. Jalabert, K. Richter: Am. J. Phys. **69**, 201 (2001)
38. H. Grabert, U. Weiss, P. Talkner: Z. Phys. B **55**, 87 (1984)
39. H. B. Callen, T. A. Welton: Phys. Rev. **83**, 34 (1951)
40. R. Kubo: J. Phys. Soc. Japan **12**, 570 (1957)
41. R. Kubo: Rep. Progr. Phys. **29**, 255 (1966)
42. R. Loudon: *The Quantum Theory of Light* (Oxford University Press 1983)