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QUANTUM BROWNIAN MOTION: THE FUNCTIONAL INTEGRAL APPROACH

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Abstract:
The quantum mechanical dynamics of a particle coupled to a heat bath is treated by functional integral methods and a generalization of the Feynman–Vernon influence functional is derived. The extended theory describes the time evolution of nonfactorizing initial states and of equilibrium correlation functions. The theory is illuminated through exactly solvable models.

1. Introduction

In the last four or five years there has been renewed interest in the problem of describing damping of a quantum system. Since Pauli's seminal work in 1928 [1] a great variety of approaches aiming at a consistent quantum mechanical description of dissipation were developed. The most common approaches are based on quantum mechanical Langevin equations [2–4] or associated quantum master equations [5] which were successfully used to describe damping phenomena, e.g. in quantum optics [6] and spin relaxation theory [7, 8]. This and related theories are available through various review articles [9–11].

Unfortunately, the formal simplicity of quantum Langevin and master equations is paid for by the fact that concrete results can only be obtained for systems which allow for a perturbative treatment of the coupling to the environmental heat bath. Basically this restricts the approach to weakly damped systems, where the relaxation time is large compared with the longest time scale of undamped motion and also large compared with the "thermal" time $\hbar/k_B T$. These conditions are easily violated for low temperature systems, in particular if their dynamics involves tunnelling transitions [12–15].

In part because of its relevance to those problems, the functional integral description of damped quantum systems pioneered by Feynman and Vernon [16, 17] has seen a remarkable resurgence recently [18–21]. The method allows for a study of the quantum mechanical dynamics at arbitrarily low temperatures and for arbitrarily strong damping. In particular, Schmid [18] and Caldeira and Leggett [19] have presented a detailed study of quantum Brownian motion in the case of frequency-independent (Ohmic) dissipation. At present, however, the theory is still of limited applicability due to a factorization assumption for the initial condition introduced by Feynman and Vernon [16]. Subsequent authors have mostly adhered to this assumption.

In this article we present an approach which overcomes these limitations. The correlations between the system and the heat bath in the initial state are described by an additional Euclidean functional integral. This apparent complication of the theory is compensated for by the fact that symmetries of the equilibrium process are incorporated exactly in the functional integral representation. Apart from the relaxation of nonequilibrium initial states, the extended theory also allows for the calculation of equilibrium correlation and response functions. The theory was developed in Stuttgart since 1985 and some results were already given elsewhere [22–24]. Here we give a detailed and systematic account of the approach. Results are given for a specific mechanical model: A quantum particle moving in a potential field interacts linearly with a heat bath represented by an infinite set of harmonic oscillators. Apart from the general treatment within the functional integral approach exactly solvable cases of the model are discussed.

In part I of this paper the problems underlying an exact functional integral representation of

quantum Brownian motion in a field of force are explained and analyzed starting from first principles. The time evolution of experimentally attainable initial states is thoroughly discussed and no factorization assumption is made. The environmental oscillators are eliminated exactly and the functional integral representation of the reduced dynamics of the damped particle is obtained. We then examine the minimal action paths and relate the quantities characterizing the functional integral to quantities familiar from the phenomenological theory of Brownian motion.

In Part II the results are specified for a particle moving in a harmonic potential. Contrary to earlier work employing functional integral techniques, our analysis does not stop at a formal level inasmuch as frequency integrals over environmental modes are evaluated explicitly and related to measurable quantities. Besides the relaxation of nonequilibrium initial states we also study the evolution under the influence of a time-dependent external force. Moreover, equilibrium correlation functions and response functions are calculated within the functional integral approach. The method is developed for systems with a linear dissipative mechanism of arbitrary frequency dependence, thus providing a complete description of quantum mechanical Gaussian processes in terms of functional integrals.

Part III examines the quantum dynamics of a damped free particle. Previously, Hakim and Ambegaokar [20] have studied the time evolution of nonfactorizing initial states of a free particle with Ohmic damping. We extend this work in various directions. Studying environmental spectral densities with arbitrary frequency dependence we find a rich variety of dynamical behaviour. For a large density of low frequency environmental modes a dissipative phase transition to localized states occurs at $T = 0$. We also discuss models leading to subdiffusive or superdiffusive spreading of the state.

PART I. GENERAL THEORY

2. Microscopic model and preparation of the initial state

The motion of a particle in a potential field is the general theme underlying the theoretical approaches to many problems in physical and chemical sciences. Brownian motion theory has led to an understanding of such varied phenomena as interstitial diffusion in solids [25, 26], reaction rates in chemical physics [27], macroscopic quantum tunnelling in Josephson systems [12–15, 28], and fission in nuclear physics [29]. In many applications the coordinate and momentum of the Brownian particle represent the value and time rate of change of a general coordinate characterizing the kinetic process under study. Here, we shall consider a concrete mechanical model where the calculations are most transparent.

2.1. The model Hamiltonian

We consider a Brownian particle of mass M moving in a potential $V(q, t)$ which may depend explicitly on time. The Brownian motion of the particle arises because of its interaction with a heat bath environment. Many authors [2, 3, 14, 18–20, 30–34] have used a model where the environment consists of a set of harmonic oscillators coupled linearly to the coordinate q of the Brownian particle. The system under study is then governed by the Hamiltonian

$$H = H_0 + H_R + H_{0R}\,, \tag{2.1}$$

where

$$H_0 = p^2/2M + V(q, t) \tag{2.2}$$

is the Hamiltonian of the undamped particle,

$$H_R = \sum_{n=1}^{N} \tfrac{1}{2}(p_n^2/m_n + m_n\omega_n^2 x_n^2) \tag{2.3}$$

describes the reservoir consisting of N harmonic oscillators, and

$$H_{0R} = -q\sum_{n=1}^{N} c_n x_n + q^2 \sum_{n=1}^{N} c_n^2/2m_n\omega_n^2 \tag{2.4}$$

introduces the coupling. The last term in eq. (2.4) compensates for the coupling-induced renormalization of the potential (see below) and it is introduced here as a matter of convenience. Naturally, such a term can always be split off from $V(q, t)$ in eq. (2.2).

The Hamiltonian given by (2.1–2.4) has widely been used to model dissipation for more than twenty years. Early studies of this or related models for harmonic potential $V(q)$ include the work by Rubin [31] and Hemmer [32] for classical systems, and Senitzky [2], Ford et al. [3] and Ullersma [33] for quantum systems. While these authors discussed the form of the equations of motion, explicit results for measurable quantities in the quantum regime were worked out only within perturbation theory. A great body of related work for the harmonic case was reviewed by Dekker [11]. Zwanzig [34] treated the classical statistical mechanics of the model with nonlinear potential and showed that under appropriate assumptions for the spectrum of the reservoir oscillators the Hamiltonian (2.1–2.4) leads to a Langevin equation with Ohmic dissipation.

While most of the work from the sixties and seventies envisaged applications, e.g., in quantum optics and spin relaxation theory and involved approximations appropriate to those fields, more recent work [14, 18–20, 35–37] has focussed on the effect of low temperatures and/or strong damping. In their study of the quantum mechanics of the model Caldeira and Leggett [14] pointed out that a reservoir consisting of harmonic oscillators is rather general and often provides a suitable description of a realistic environment at sufficiently low temperatures. For instance even the coupling to a Fermionic heat bath may be related to the Bosonic environment considered here [26, 38].

2.2. Initial states and preparation function

The model defined by the Hamiltonian (2.1–2.4) has to be supplemented by information concerning the initial state. In earlier work [2, 3, 8, 18, 19, 21, 33] it was frequently assumed that the initial density matrix W_0 of the system consisting of Brownian particle and environmental heat bath factorizes according to

$$W_0 = \rho_0 W_R \tag{2.5}$$

where ρ_0 is the density matrix of the particle, while $W_R = Z_R^{-1}\exp(-\beta H_R)$ is the canonical density matrix of the unperturbed heat bath at inverse temperature $\beta = 1/k_B T$. The factorization is based on

the assumption that there are no correlations between the particle and the reservoir at time $t = 0$ which is the case if the interaction is switched on for $t > 0$ only. Unfortunately, in most applications of Brownian motion theory the coordinate q and the environmental degrees of freedom are integral parts of the same system and their interaction is not at the disposal of the experimentalist.

A class of initial states including many initial conditions resulting from experimentally feasible preparations is of the form

$$W_0 = \sum_j O_j W_\beta O_j' , \tag{2.6}$$

where

$$W_\beta = Z_\beta^{-1} \exp(-\beta H) \tag{2.7}$$

is the canonical density matrix describing the equilibrium of the interacting systems in the presence of a time-independent potential V. The operators O_j, O_j' act upon the particle only and leave the reservoir coordinates unchanged but they may be chosen arbitrarily otherwise. Incidentally we note that there are certain constraints on these operators if W_0 is asked to be a proper density matrix. However, this is not necessarily required for the following analysis to be useful, and physical examples where W_0 is not a density matrix will explicitly be given below.

The simplest initial state of the form (2.6) is the equilibrium density matrix W_β itself. It can be prepared by waiting sufficiently long so that the system has reached equilibrium at $t = 0$. Then the response of the particle to a time-dependent external force acting at times $t > 0$ may be studied.

A modification of this problem is the following. The system may be displaced from equilibrium by applying a constant external force F and W_0 describes the modified equilibrium in the presence of this force. When the external force is switched off at time $t = 0_+$ we can study the relaxation towards nonconstrained equilibrium. This relaxation problem reduces to the determination of the response of a system with a Hamiltonian including the external force to the special perturbation $F(t) = -F\Theta(t)$ where $\Theta(t)$ is the unit step function.

Further, for a system in equilibrium at time $t = 0_-$ we may perform a measurement of a dynamical variable of the Brownian particle. This leads to a reduction of the density matrix. The state W_0 after the measurement will be of the form (2.6) where the operators O_j, O_j' describe the effect of the measuring device [39]. For instance an ideal position measurement with the outcome $q_0 - \delta/2 < q < q_0 + \delta/2$ leads to

$$W_0 = P_q W_\beta P_q , \tag{2.8}$$

where

$$P_q = N^{-1/2} \int_{q_0-\delta/2}^{q_0+\delta/2} \mathrm{d}q \, |q\rangle\langle q| \tag{2.9}$$

projects on the measured interval, and where N is a normalization factor.

Thirdly, we may perform a scattering experiment in which the cross section is related to an equilibrium correlation function of the Brownian particle [40]. Now, an equilibrium correlation function $\langle A(t)B \rangle$ may formally be viewed as the expectation value of A at time t in the "initial ensemble" $W_0 = BW_\beta$. Clearly BW_β is not a proper density matrix, however, it is again of the form (2.6).

In coordinate representation (2.6) reads

$$W_0(q, x_n, q', x_n') = \langle q, x_n | W_0 | q', x_n' \rangle$$
$$= \sum_j \int \mathrm{d}\bar{q} \int \mathrm{d}\bar{q}'\, O_j(q, \bar{q}) O_j'(\bar{q}', q') W_\beta(\bar{q}, x_n, \bar{q}', x_n') \tag{2.10}$$

where $O_j(q, \bar{q}) = \langle q | O_j | \bar{q} \rangle$ and $O_j'(\bar{q}', q') = \langle \bar{q}' | O_j' | q' \rangle$. Hence, the initial states studied are of the form

$$W_0(q, x_n, q', x_n') = \int \mathrm{d}\bar{q} \int \mathrm{d}\bar{q}'\, \lambda(q, \bar{q}, q', \bar{q}') W_\beta(\bar{q}, x_n, \bar{q}', x_n') \tag{2.11}$$

where

$$\lambda(q, \bar{q}, q', \bar{q}') = \sum_j O_j(q, \bar{q}) O_j'(\bar{q}', q') \tag{2.12}$$

is a *preparation function* describing the deviation from the equilibrium distribution. This function can be quite arbitrary since a decomposition into a sum of products of the form (2.12) is always possible. In the sequel we study the time evolution of initial states of the form (2.11).

3. Functional integral representation of the density matrix and elimination of the environment

We are interested in a reduced description of the system and focus on the time evolution of the Brownian particle only. Hence, we want to eliminate the environmental degrees of freedom. To that end it is convenient to employ the functional integral representation of quantum mechanics [17] introduced by Feynman. Since for our model integrals over environmental coordinates are Gaussian, they can be done exactly.

3.1. Euclidean functional integral

The coordinate representation of the equilibrium density matrix W_β of the entire system may be written as a so-called Euclidean functional integral [17]

$$W_\beta(\bar{q}, \bar{x}_n, \bar{q}', \bar{x}_n') = Z_\beta^{-1} \int \mathcal{D}\bar{q} \mathcal{D}\bar{x}_n \exp\left(-\frac{1}{\hbar} S^{\mathrm{E}}[\bar{q}, \bar{x}_n]\right), \tag{3.1}$$

where the integral is over all paths $\bar{q}(\tau)$, $\bar{x}_n(\tau)$, $0 \le \tau \le \hbar\beta$ with $\bar{q}(0) = \bar{q}'$, $\bar{x}_n(0) = \bar{x}_n'$, and $\bar{q}(\hbar\beta) = \bar{q}$, $\bar{x}_n(\hbar\beta) = \bar{x}_n$. The path probability is weighted according to Euclidean action

$$S^{\mathrm{E}}[\bar{q}, \bar{x}_n] = S_0^{\mathrm{E}}[\bar{q}] + S_{\mathrm{R}}^{\mathrm{E}}[\bar{x}_n] + S_{0\mathrm{R}}^{\mathrm{E}}[\bar{q}, \bar{x}_n], \tag{3.2}$$

where

$$S_0^{\mathrm{E}}[\bar{q}] = \int_0^{\hbar\beta} \mathrm{d}\tau\, \mathcal{L}_0^{\mathrm{E}}(\bar{q}, \dot{\bar{q}}) = \int_0^{\hbar\beta} \mathrm{d}\tau\, (\tfrac{1}{2} M \dot{\bar{q}}^2 + V(\bar{q})) \tag{3.3}$$

is the Euclidean action of the undamped particle moving in the time-independent potential $V(\bar{q})$ effective during the preparation of the initial state,

$$S_{\mathrm{R}}^{\mathrm{E}}[\bar{x}_n] = \int_0^{\hbar\beta} \mathrm{d}\tau\, \mathscr{L}_{\mathrm{R}}^{\mathrm{E}}(\bar{x}_n, \dot{\bar{x}}_n) = \sum_{n=1}^{N} \int_0^{\hbar\beta} \mathrm{d}\tau\, (\tfrac{1}{2} m_n \dot{\bar{x}}_n^2 + \tfrac{1}{2} m_n \omega_n^2 \bar{x}_n^2) \tag{3.4}$$

describes the reservoir, and

$$S_{0\mathrm{R}}^{\mathrm{E}}[\bar{q}, \bar{x}_n] = \int_0^{\hbar\beta} \mathrm{d}\tau\, \mathscr{L}_{0\mathrm{R}}^{\mathrm{E}}(\bar{q}, \bar{x}_n) = \sum_{n=1}^{N} \int_0^{\hbar\beta} \mathrm{d}\tau \left(-c_n \bar{q} \bar{x}_n + \bar{q}^2 \frac{c_n^2}{2 m_n \omega_n^2} \right) \tag{3.5}$$

the interaction. Finally Z_β normalizes the state. If eq. (3.1) is inserted into eq. (2.11) we obtain a functional integral representation of the initial state W_0.

3.2. Real time functional integral

A pure state $\Psi(q_i, x_{n_i}, 0)$ of the entire system evolves in time according to

$$\Psi(q_{\mathrm{f}}, x_{n_{\mathrm{f}}}, t) = \int \mathrm{d}q_{\mathrm{i}}\, \mathrm{d}x_{n_{\mathrm{i}}} K(q_{\mathrm{f}}, x_{n_{\mathrm{f}}}, t; q_{\mathrm{i}}, x_{n_{\mathrm{i}}}, 0) \Psi(q_{\mathrm{i}}, x_{n_{\mathrm{i}}}, 0)\,, \tag{3.6}$$

where $K(q, x_n, t; q', x_n', 0)$ is the coordinate representation of the time evolution operator $\exp(-\mathrm{i}Ht/\hbar)$ of the entire system which may again be represented as a functional integral [17]

$$K(q_{\mathrm{f}}, x_{n_{\mathrm{f}}}, t; q_{\mathrm{i}}, x_{n_{\mathrm{i}}}, 0) = \int \mathscr{D}q\, \mathscr{D}x_n \exp\left(\frac{\mathrm{i}}{\hbar} S[q, x_n] \right), \tag{3.7}$$

where the integral is over all paths $q(s), x_n(s)$, $0 \le s \le t$ with $q(0) = q_i$, $x_n(0) = x_{n_i}$, and $q(t) = q_{\mathrm{f}}$, $x_n(t) = x_{n_{\mathrm{f}}}$. Here the path probability is weighted according to the usual action

$$S[q, x_n] = \int_0^t \mathrm{d}s\, \mathscr{L}(q, \dot{q}, x_n, \dot{x}_n, s)\,, \tag{3.8}$$

where $\mathscr{L}$ is the Lagrangian associated with the Hamiltonian (2.1). Hence

$$\mathscr{L}_0(q, \dot{q}) = \tfrac{1}{2} M \dot{q}^2 - V(q, s)\,, \tag{3.9}$$

$$\mathscr{L}_{\mathrm{R}}(x_n, \dot{x}_n) = \sum_{n=1}^{N} [\tfrac{1}{2} m_n \dot{x}_n^2 - \tfrac{1}{2} m_n \omega_n^2 x_n^2]\,, \tag{3.10}$$

$$\mathscr{L}_{0\mathrm{R}}(q, x_n) = \sum_{n=1}^{N} \left[c_n q x_n - q^2 \frac{c_n^2}{2 m_n \omega_n^2} \right]. \tag{3.11}$$

Note that in the Euclidean action functional (3.2) kinetic and potential energies are added, while the potential energy is subtracted from the kinetic term in the familiar action (3.8). The canonical density matrix may be viewed as a time evolution operator for imaginary time $t = -i\hbar\beta$ and the functional integral (3.1) is just an imaginary time version of integral (3.7) provided that the potential is independent of time. The rotation to imaginary time changes the sign of the kinetic term and transforms $iS[q, x_n]$ into $-S^E[q, x_n]$. In the sequel, however, we will allow for a potential which depends explicitly on time for $t > 0$.

We are now in the position to write down the density matrix W of the entire system at time t. Using the time evolution operator we have

$$W(q_f, x_{n_f}, q'_f, x'_{n_f}, t) = \int dq_i\, dq'_i\, dx_{n_i}\, dx'_{n_i}\, K(q_f, x_{n_f}, t; q_i, x_{n_i}, 0) \times W(q_i, x_{n_i}, q'_i, x'_{n_i}, 0) K^*(q'_f, x'_{n_f}, t; q'_i, x'_{n_i}, 0)\,, \tag{3.12}$$

which is just the coordinate representation of the familiar operator equation $W(t) = \exp(-iHt/\hbar)\, W_0 \exp(iHt/\hbar)$. Inserting the functional integral representations (3.1) and (3.7) and the general expression (2.11) for the initial state, we obtain a representation of the density matrix at time t in terms of a $3(N+1)$-fold functional integral

$$W(q_f, x_{n_f}, q'_f, x'_{n_f}, t) = \int dq_i\, dq'_i\, d\bar{q}\, d\bar{q}'\, dx_{n_i}\, dx'_{n_i}\, \lambda(q_i, \bar{q}, q'_i, \bar{q}') Z_\beta^{-1} \times \int \mathcal{D}q\, \mathcal{D}x_n\, \mathcal{D}q'\, \mathcal{D}x'_n\, \mathcal{D}\bar{q}\, \mathcal{D}\bar{x}_n \exp\left\{\frac{i}{\hbar}\left(S[q, x_n] - S[q', x'_n]\right) - \frac{1}{\hbar} S^E[\bar{q}, \bar{x}_n]\right\}, \tag{3.13}$$

which sums over all paths $q(s)$, $x_n(s)$, $q'(s)$, $x'_n(s)$, $0 \le s \le t$, with

$$q(0) = q_i\,, \quad x_n(0) = x_{n_i}\,, \quad q'(0) = q'_i\,, \quad x'_n(0) = x'_{n_i}\,,$$

$$q(t) = q_f\,, \quad x_n(t) = x_{n_f}\,, \quad q'(t) = q'_f\,, \quad x'_n(t) = x'_{n_f}$$

in real time and over all paths $\bar{q}(\tau)$, $\bar{x}_n(\tau)$, $0 \le \tau \le \hbar\beta$, with

$$\bar{q}(0) = \bar{q}'\,, \quad \bar{x}_n(0) = x'_{n_i}\,, \qquad \bar{q}(\hbar\beta) = \bar{q}\,, \quad \bar{x}_n(\hbar\beta) = x_{n_i}$$

in imaginary time. Note that for the reservoir the endpoints x_{n_f} and x'_{n_f} are connected by a continuous path which goes from x'_{n_f} to $x'_{n_i} = \bar{x}_n(0)$, then follows $\bar{x}_n(\tau)$ to $\bar{x}_n(\hbar\beta) = x_{n_i}$ from where it runs to x_{n_f} (fig. 1). Contrary to this path the one connecting q'_f and q_f is interrupted since $q'(0) \neq \bar{q}(0)$ and $q(0) \neq \bar{q}(\hbar\beta)$ in general. These intermediate points are connected by the function $\lambda(q_i, \bar{q}, q'_i, \bar{q}')$ describing the deviation of the initial state from equilibrium.

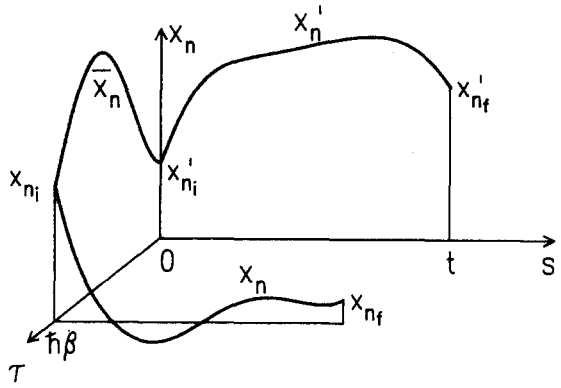

Fig. 1. A continuous path defined on a contour in the complex time plane connects the final coordinates of the nth environmental oscillator.

3.3. Integration over the environmental coordinates and influence functional

The expression (3.13) for the density matrix still describes the entire system consisting of Brownian particle and environment. The state of the Brownian particle is characterized by the reduced density matrix $\rho = \mathrm{tr}_R W$ where tr_R is the trace over the reservoir. In coordinate representation we have

$$\rho(q_f, q_f', t) = \int \mathrm{d}x_{n_f} W(q_f, x_{n_f}, q_f', x_{n_f}, t) . \tag{3.14}$$

Since only the part of W diagonal in the environmental coordinates contributes to this integral, the reduced density matrix ρ involves only integrations over closed paths of the environment. By virtue of (3.13) we find

$$\rho(q_f, q_f', t) = \int \mathrm{d}q_i \, \mathrm{d}q_i' \, \mathrm{d}\bar{q} \, \mathrm{d}\bar{q}' \, \lambda(q_i, \bar{q}, q_i', \bar{q}') \, Z^{-1}$$
$$\times \int \mathscr{D}q \, \mathscr{D}q' \, \mathscr{D}\bar{q} \exp\left\{ \frac{\mathrm{i}}{\hbar} (S_0[q] - S_0[q']) - \frac{1}{\hbar} S_0^E[\bar{q}] \right\} \tilde{F}[q, q', \bar{q}] , \tag{3.15}$$

where the functional integration is over the set of paths $q(s)$, $q'(s)$, $\bar{q}(\tau)$ of the Brownian particle described above, and where

$$\tilde{F}[q, q', \bar{q}] = \int \mathrm{d}x_{n_f} \mathrm{d}x_{n_i} \mathrm{d}x_{n_i}' \, Z_R^{-1} \int \mathscr{D}x_n \, \mathscr{D}x_n' \, \mathscr{D}\bar{x}_n \exp\left\{ \frac{\mathrm{i}}{\hbar} (S_R[x_n] + S_{0R}[q, x_n] - S_R[x_n'] \right.$$
$$\left. - S_{0R}[q', x_n']) - \frac{1}{\hbar} (S_R^E[\bar{x}_n] + S_{0R}^E[\bar{q}, \bar{x}_n]) \right\} \tag{3.16}$$

is a functional integral over all closed paths $x_n(s)$, $x_n'(s)$, $\bar{x}_n(\tau)$ of the environment with

$$x_n(t) = x_n'(t) = x_{n_f} , \quad x_n(0) = \bar{x}_n(\hbar\beta) = x_{n_i} , \quad \bar{x}_n(0) = x_n'(0) = x_{n_i}' .$$

This integral depends on the trajectory of the Brownian particle as a functional. Z_R normalizes $\tilde{F}$ so that

$\tilde{F} = 1$ for vanishing interaction, i.e., Z_R is the partition function of the unperturbed bath. The new normalization factor Z in eq. (3.15) is given by $Z = Z_\beta / Z_R$. In eq. (3.15) the influence of the reservoir is described completely by the functional $\tilde{F}$. Hence, the elimination of the environmental degrees of freedom is reduced to the determination of this so-called *influence functional.*

From eq. (3.16) we see that $\tilde{F}$ may be decomposed according to

$$\tilde{F}[q, q', \bar{q}] = \int \mathrm{d}x_{n_f}\, \mathrm{d}x_{n_i}\, \mathrm{d}x'_{n_i}\, F[q, x_{n_f}, x_{n_i}] F^{E}[\bar{q}, x_{n_i}, x'_{n_i}] F^{*}[q', x_{n_f}, x'_{n_i}], \tag{3.17}$$

where

$$F[q, x_{n_f}, x_{n_i}] = \int \mathcal{D}x_n \exp\left\{\frac{\mathrm{i}}{\hbar}\left(S_R[x_n] + S_{0R}[q, x_n]\right)\right\} \tag{3.18}$$

is a real time functional integral over all paths $x_n(s)$ of the environment connecting $x_n(0) = x_{n_i}$ with $x_n(t) = x_{n_f}$, and where

$$F^{E}[\bar{q}, x_{n_i}, x'_{n_i}] = Z_R^{-1} \int \mathcal{D}\bar{x}_n \exp\left\{-\frac{1}{\hbar}\left(S_R^{E}[\bar{x}_n] + S_{0R}^{E}[\bar{q}, \bar{x}_n]\right)\right\} \tag{3.19}$$

is an imaginary time functional integral over all paths $\bar{x}_n(\tau)$ connecting $\bar{x}_n(0) = x'_{n_i}$ with $\bar{x}_n(\hbar\beta) = x_{n_i}$. So far the analysis carried out is independent of a particular model for the environment.

At this point it seems worth mentioning that the influence functional $\tilde{F}$ defined in eq. (3.16) differs from the influence functional discussed in previous work [16, 18, 19] based on the factorization assumption. In our approach the Euclidean part F^E of the influence functional describes initial correlations between particle and reservoir. In the conventional approach the imaginary time functional integral is absent and the two real time parts $F[q, x_{n_f}, x_{n_i}]$ and $F^*[q', x_{n_f}, x'_{n_i}]$ of the influence functional are averaged over the unperturbed reservoir distribution $W_R(x_{n_i}, x'_{n_i})$.

For the harmonic oscillator model of the reservoir discussed previously the functionals (3.18) and (3.19) factorize into independent contributions from each reservoir oscillator. By virtue of eqs. (2.3) and (2.4) the functional (3.18) may be written

$$F[q, x_{n_f}, x_{n_i}] = \prod_{k=1}^{N} F_k[q, x_{k_f}, x_{k_i}], \tag{3.20}$$

where

$$F_n[q, x_{n_f}, x_{n_i}] = \int \mathcal{D}x_n \exp\left[\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}s \left\{\frac{1}{2} m_n(\dot{x}_n^2 - \omega_n^2 x_n^2) + q c_n x_n - q^2 \frac{c_n^2}{2 m_n \omega_n^2}\right\}\right] \tag{3.21}$$

describes the influence of the nth oscillator. Equation (3.21) is a Gaussian functional integral over all paths $x_n(s)$, $0 \le s \le t$ with $x_n(0) = x_{n_i}$, $x_n(t) = x_{n_f}$ which can be evaluated exactly [17]. A brief outline of the calculation is given in appendix A. One finds

$$F_n[q, x_{n_f}, x_{n_i}] = \left(\frac{m_n \omega_n}{2\pi\mathrm{i}\hbar \sin(\omega_n t)}\right)^{1/2} \exp\left(\frac{\mathrm{i}}{\hbar} \Phi_n[q, x_{n_f}, x_{n_i}]\right), \tag{3.22}$$

where

$$\Phi_n[q, x_{n_f}, x_{n_i}] = \frac{m_n\omega_n}{2\sin(\omega_n t)}\{(x_{n_i}^2 + x_{n_f}^2)\cos(\omega_n t) - 2x_{n_i}x_{n_f}\}$$
$$+ \frac{x_{n_i}c_n}{\sin(\omega_n t)}\int_0^t \mathrm{d}s\,\sin(\omega_n(t-s))\,q(s) + \frac{x_{n_f}c_n}{\sin(\omega_n t)}\int_0^t \mathrm{d}s\,\sin(\omega_n s)\,q(s)$$
$$- \frac{c_n^2}{m_n\omega_n\sin(\omega_n t)}\int_0^t \mathrm{d}s\int_0^s \mathrm{d}u\,\sin(\omega_n(t-s))\sin(\omega_n u)\,q(s)q(u)$$
$$- \frac{c_n^2}{2m_n\omega_n^2}\int_0^t \mathrm{d}s\,q^2(s)\,. \tag{3.23}$$

The functional (3.19) may also be decomposed according to

$$F^{\mathrm{E}}[\bar{q}, x_{n_i}, x'_{n_i}] = Z_{\mathrm{R}}^{-1}\prod_{k=1}^{N} F_k^{\mathrm{E}}[\bar{q}, x_{k_i}, x'_{k_i}]\,, \tag{3.24}$$

where

$$F_n^{\mathrm{E}}[\bar{q}, x_{n_i}, x'_{n_i}] = \left(\frac{m_n\omega_n}{2\pi\hbar\sinh(\omega_n\hbar\beta)}\right)^{1/2}\exp\left(-\frac{1}{\hbar}\,\Phi_n^{\mathrm{E}}[\bar{q}, x_{n_i}, x'_{n_i}]\right), \tag{3.25}$$

in which

$$\Phi_n^{\mathrm{E}}[\bar{q}, x_{n_i}, x'_{n_i}] = \frac{m_n\omega_n}{2\sinh(\omega_n\hbar\beta)}\{(x_{n_i}^2 + x'^2_{n_i})\cosh(\omega_n\hbar\beta) - 2x_{n_i}x'_{n_i}\}$$
$$- \frac{x'_{n_i}c_n}{\sinh(\omega_n\hbar\beta)}\int_0^{\hbar\beta} \mathrm{d}\tau\,\sinh(\omega_n(\hbar\beta-\tau))\,\bar{q}(\tau) - \frac{x_{n_i}c_n}{\sinh(\omega_n\hbar\beta)}\int_0^{\hbar\beta} \mathrm{d}\tau\,\sinh(\omega_n\tau)\,\bar{q}(\tau)$$
$$- \frac{c_n^2}{m_n\omega_n\sinh(\omega_n\hbar\beta)}\int_0^{\hbar\beta} \mathrm{d}\tau\int_0^{\tau} \mathrm{d}\sigma\,\sinh(\omega_n(\hbar\beta-\tau))\sinh(\omega_n\sigma)\,\bar{q}(\tau)\bar{q}(\sigma)$$
$$+ \frac{c_n^2}{2m_n\omega_n^2}\int_0^{\hbar\beta} \mathrm{d}\tau\,\bar{q}^2(\tau)\,. \tag{3.26}$$

The exponents Φ_n and Φ_n^{E} are quadratic functions of the endpoints of the bath oscillator. They are related by an analytic continuation from real to imaginary time.

Collecting the results (3.20–3.26), the integrand of the functional (3.17) may be written down explicitly. The remaining evaluation of the Gaussian integrals over the intermediate coordinates x_{n_i}, x'_{n_i},

x_{n_f} is straightforward but tedious. After some algebra one obtains

$$\tilde{F}[q, q', \bar{q}] = \exp\Big(-\frac{1}{\hbar}\,\tilde{\Phi}[q, q', \bar{q}]\Big)\,, \tag{3.27}$$

where the exponent is given by

$$\begin{aligned}\tilde{\Phi}[q, q', \bar{q}] = &-\int_0^{\hbar\beta} \mathrm{d}\tau \int_0^{\tau} \mathrm{d}\sigma\, K(-\mathrm{i}\tau + \mathrm{i}\sigma)\bar{q}(\tau)\bar{q}(\sigma) + \int_0^{\hbar\beta} \mathrm{d}\tau \tfrac{1}{2}\mu\bar{q}^2(\tau) \\ &-\mathrm{i}\int_0^{\hbar\beta} \mathrm{d}\tau \int_0^{t} \mathrm{d}s\, K^*(s - \mathrm{i}\tau)\bar{q}(\tau)\{q(s) - q'(s)\} \\ &+\int_0^{t} \mathrm{d}s \int_0^{s} \mathrm{d}u\, \{q(s) - q'(s)\}\{K(s-u)q(u) - K^*(s-u)q'(u)\} \\ &+\mathrm{i}\int_0^{t} \mathrm{d}s\, \tfrac{1}{2}\mu\{q^2(s) - q'^2(s)\}\,.\end{aligned} \tag{3.28}$$

Here we have introduced the kernel

$$K(\theta) = \sum_{n=1}^{N} \frac{c_n^2}{2m_n\omega_n} \frac{\cosh[\omega_n(\frac{1}{2}\hbar\beta - \mathrm{i}\theta)]}{\sinh(\frac{1}{2}\omega_n\hbar\beta)} \tag{3.29}$$

which is defined for complex times $\theta = s - \mathrm{i}\tau$, $0 \le \tau \le \hbar\beta$ and describes the influence of the environment. The terms with

$$\mu = \sum_{n=1}^{N} \frac{c_n^2}{m_n\omega_n^2} \tag{3.30}$$

arise from the second (counter-)term in eq. (2.4). We note that the pre-exponential factors from eqs. (3.22) and (3.25) and the partition function of the unperturbed reservoir

$$Z_{\mathrm{R}} = \prod_{n=1}^{N} \{2\sinh(\tfrac{1}{2}\omega_n\hbar\beta)\}^{-1} \tag{3.31}$$

combine with the coupling-independent factors arising from the Gaussian integrals over x_{n_i}, x'_{n_i} and x_{n_f} to give 1. This is necessary in order that the influence functional becomes equal to 1 for vanishing coupling.

The influence functional (3.27) may be written in a more compact form by introducing the contour $\mathscr{C}$ in the complex plane depicted in fig. 2 and defining a path $\tilde{q}(z)$ on this contour through

$$\tilde{q}(z) = \begin{cases} q'(s) & \text{for } z = s\,, \quad 0 \le s \le t\,, \\ \bar{q}(\tau) & \text{for } z = -\mathrm{i}\tau\,, \quad 0 \le \tau \le \hbar\beta\,, \\ q(s) & \text{for } z = -\mathrm{i}\hbar\beta + s\,, \quad 0 \le s \le t\,. \end{cases} \tag{3.32}$$

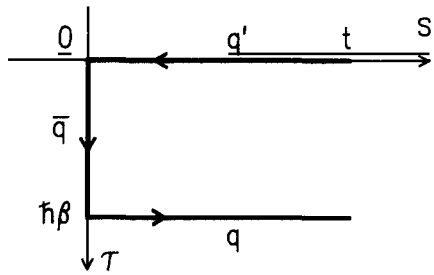

Fig. 2. The integration contour $\mathscr{C}$ in the complex time plane $z = s + i\tau$ along which the exponent $\tilde{\Phi}[q(z)]$ of the influence functional has to be evaluated.

Then the exponent (3.28) can be rewritten as

$$\tilde{\Phi}[\tilde{q}] = \int \mathrm{d}z \int_{z>z'} \mathrm{d}z'\, K(z-z')\tilde{q}(z)\tilde{q}(z') + \frac{\mathrm{i}}{2}\,\mu \int \mathrm{d}z\, \tilde{q}^2(z)\,, \tag{3.33}$$

where the integrals over z and z' are along the contour $\mathscr{C}$ and where $z > z'$ means that z follows z' in the direction of the arrows in fig. 2.

3.4. Reduced dynamics and propagating function

The result (3.27) for the influence functional may now be inserted into the expression (3.15) for the reduced density matrix of the Brownian particle at time t. We then find

$$\rho(q_\mathrm{f}, q'_\mathrm{f}, t) = \int \mathrm{d}q_\mathrm{i}\, \mathrm{d}q'_\mathrm{i}\, \mathrm{d}\bar{q}\, \mathrm{d}\bar{q}'\, J(q_\mathrm{f}, q'_\mathrm{f}, t, q_\mathrm{i}, q'_\mathrm{i}, \bar{q}, \bar{q}')\lambda(q_\mathrm{i}, \bar{q}, q'_\mathrm{i}, \bar{q}') \tag{3.34}$$

where $J(q_\mathrm{f}, q'_\mathrm{f}, t, q_\mathrm{i}, q'_\mathrm{i}, \bar{q}, \bar{q}')$ is a *propagating function* describing the time evolution of the state. The reservoir is eliminated since

$$J(q_\mathrm{f}, q'_\mathrm{f}, t, q_\mathrm{i}, q'_\mathrm{i}, \bar{q}, \bar{q}') = \frac{1}{Z}\int \mathscr{D}q\, \mathscr{D}q'\, \mathscr{D}\bar{q}\, \exp\Big\{\frac{\mathrm{i}}{\hbar}\,(S_0[q] - S_0[q']) - \frac{1}{\hbar}\,S_0^\mathrm{E}[\bar{q}]\Big\}$$
$$\times \exp\Big(-\frac{1}{\hbar}\,\tilde{\Phi}[q, q', \bar{q}]\Big) \tag{3.35}$$

is a functional integral over paths $q(s)$, $q'(s)$, $\bar{q}(\tau)$ of the Brownian particle satisfying the boundary conditions

$$q(0) = q_\mathrm{i}\,, \quad q(t) = q_\mathrm{f}\,, \quad q'(0) = q'_\mathrm{i}\,, \quad q'(t) = q'_\mathrm{f}\,, \quad \bar{q}(0) = \bar{q}'\,, \quad \bar{q}(\hbar\beta) = \bar{q}\,.$$

Equation (3.34) determines the time evolution of the density matrix starting from the initial state

$$\rho_0(q, q') = \int \mathrm{d}\bar{q}\, \mathrm{d}\bar{q}'\, \lambda(q, \bar{q}, q', \bar{q}')\rho_\beta(\bar{q}, \bar{q}')\,, \tag{3.36}$$

where

$$\rho_\beta = \mathrm{tr}_R(W_\beta) \tag{3.37}$$

is the reduced density matrix of the Brownian particle in equilibrium. Relation (3.36) is readily obtained by integrating eq. (2.11) over the reservoir coordinates. On the other hand, eq. (3.36) follows from eq. (3.34) if we note that eq. (3.35) gives for $t = 0$

$$J(q_f, q_f', 0, q_i, q_i', \bar{q}, \bar{q}') = \delta(q_f - q_i)\delta(q_f' - q_i')\rho_\beta(\bar{q}, \bar{q}'), \tag{3.38}$$

where

$$\rho_\beta(\bar{q}, \bar{q}') = \frac{1}{Z}\int \mathcal{D}\bar{q}\, \exp\Big[-\frac{1}{\hbar}S_0^E(\bar{q}) + \frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \int_0^{\tau} d\sigma\, K(-i\tau + i\sigma)\bar{q}(\tau)\bar{q}(\sigma) - \frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\, \frac{\mu}{2}\bar{q}^2(\tau)\Big] \tag{3.39}$$

is an explicit representation of the reduced equilibrium density matrix as a Euclidean functional integral running over all imaginary time paths $\bar{q}(\tau)$ with $\bar{q}(0) = \bar{q}'$ and $\bar{q}(\hbar\beta) = \bar{q}$. It should be noted that the function $\lambda(q, \bar{q}, q', \bar{q}')$ characterizing the preparation of the initial state is not uniquely determined by the reduced density matrix $\rho_0(q, q')$ through relation (3.36). Rather $\lambda(q, \bar{q}, q', \bar{q}')$ is only specified by the density matrix of the entire system through relation (2.11). (See also section 6.8.)

4. Minimal action paths and damping kernel

So far, we have considered a particle coupled to a finite number of reservoir oscillators. However, the environment can only be considered as a proper heat bath causing dissipation if the spectrum of environmental oscillators is quasi-continuous. Hence, we introduce a spectral density of the environment through

$$I(\omega) = \pi \sum_{n=1}^{N} \frac{c_n^2}{2m_n\omega_n}\delta(\omega - \omega_n). \tag{4.1}$$

Then sums of the form (3.29, 3.30) may be written as integrals. Using the general relation

$$\sum_{n=1}^{N} \frac{c_n^2}{2m_n\omega_n} f(\omega_n) = \int_0^{\infty} \frac{d\omega}{\pi} I(\omega) f(\omega), \tag{4.2}$$

we find

$$K(\theta) = \int_0^{\infty} \frac{d\omega}{\pi} I(\omega) \frac{\cosh[\omega(\frac{1}{2}\hbar\beta - i\theta)]}{\sinh(\frac{1}{2}\omega\hbar\beta)} \tag{4.3}$$

and

$$\mu = \int_0^\infty \frac{d\omega}{\pi} I(\omega) \frac{2}{\omega} . \tag{4.4}$$

In the following we shall first transform the exponent (3.28) of the influence functional into a form particularly suitable for further evaluation. The result of this calculation is the transformed exponent (4.29). Subsequently, we discuss the equations of motion for those paths for which the action is minimal. This will allow us to relate the influence kernel to the phenomenological damping kernel.

4.1. The potential renormalization

The kernel $K(\theta)$ defined for complex times $\theta = s - i\tau$ still contains a purely reversible renormalization of the potential [14, 19] which will be split off in the sequel. Let us first decompose $K(\theta)$ into its real and imaginary parts

$$K(s - i\tau) = K'(s - i\tau) + iK''(s - i\tau) , \tag{4.5}$$

where

$$K'(s - i\tau) = \int_0^\infty \frac{d\omega}{\pi} I(\omega) \frac{\cosh[\omega(\frac{1}{2}\hbar\beta - \tau)]}{\sinh(\frac{1}{2}\omega\hbar\beta)} \cos(\omega s) \tag{4.6}$$

and

$$K''(s - i\tau) = -\int_0^\infty \frac{d\omega}{\pi} I(\omega) \frac{\sinh[\omega(\frac{1}{2}\hbar\beta - \tau)]}{\sinh(\frac{1}{2}\omega\hbar\beta)} \sin(\omega s) . \tag{4.7}$$

Since the imaginary part of the argument varies only within the interval $0 \le \tau \le \hbar\beta$, it is convenient to expand these kernels into a Fourier series with respect to τ. Introducing the characteristic frequencies ν_n of the interval $\hbar\beta$ given by

$$\nu_n = 2\pi n/\hbar\beta , \tag{4.8}$$

we find for $0 \le \tau \le \hbar\beta$

$$\frac{\cosh[\omega(\frac{1}{2}\hbar\beta - \tau)]}{\sinh(\frac{1}{2}\omega\hbar\beta)} = \frac{2}{\hbar\beta} \sum_{n=-\infty}^{\infty} \omega \frac{\exp(i\nu_n\tau)}{\omega^2 + \nu_n^2} \tag{4.9}$$

and

$$\frac{\sinh[\omega(\frac{1}{2}\hbar\beta - \tau)]}{\sinh(\frac{1}{2}\omega\hbar\beta)} = -\frac{2}{\hbar\beta} \sum_{n=-\infty}^{\infty} i\nu_n \frac{\exp(i\nu_n\tau)}{\omega^2 + \nu_n^2} \tag{4.10}$$

by virtue of which eqs. (4.6) and (4.7) take the form

$$K'(s-\mathrm{i}\tau)=\frac{M}{\hbar\beta}\sum_{n=-\infty}^{\infty}g_n(s)\exp(\mathrm{i}\nu_n\tau) \tag{4.11}$$

and

$$K''(s-\mathrm{i}\tau)=\frac{M}{\hbar\beta}\sum_{n=-\infty}^{\infty}\mathrm{i}f_n(s)\exp(\mathrm{i}\nu_n\tau) \tag{4.12}$$

with the Fourier components

$$g_n(s)=\frac{1}{M}\int_0^{\infty}\frac{\mathrm{d}\omega}{\pi}\,I(\omega)\,\frac{2\omega}{\omega^2+\nu_n^2}\cos(\omega s)\,, \tag{4.13}$$

$$f_n(s)=\frac{1}{M}\int_0^{\infty}\frac{\mathrm{d}\omega}{\pi}\,I(\omega)\,\frac{2\nu_n}{\omega^2+\nu_n^2}\sin(\omega s)\,. \tag{4.14}$$

Since the real part $K'(s-\mathrm{i}\tau)$ of the influence kernel has the symmetry $K'(s-\mathrm{i}\hbar\beta+\mathrm{i}\tau)=K'(s-\mathrm{i}\tau)$ its Fourier coefficients are real and satisfy $g_{-n}(s)=g_n(s)$. On the other hand, the imaginary part $K''(s-\mathrm{i}\tau)$ has the symmetry $K''(s-\mathrm{i}\hbar\beta+\mathrm{i}\tau)=-K''(s-\mathrm{i}\tau)$ which leads to imaginary Fourier coefficients $\mathrm{i}f_n(s)$ with $f_{-n}(s)=-f_n(s)$.

Now, the first term in the exponent (3.28) of the influence functional only involves $K(\theta)$ for imaginary times $\theta=-\mathrm{i}\tau$. Noting that $K''(s-\mathrm{i}\tau)$ vanishes for $s=0$ we find

$$K(-\mathrm{i}\tau)=\frac{M}{\hbar\beta}\sum_{n=-\infty}^{\infty}g_n\exp(\mathrm{i}\nu_n\tau)\,, \tag{4.15}$$

where $g_n=g_n(s=0)$. Using eq. (4.4) it is readily seen that g_n may be written as

$$g_n=\mu/M-\zeta_n\,, \tag{4.16}$$

where

$$\zeta_n=\frac{1}{M}\int_0^{\infty}\frac{\mathrm{d}\omega}{\pi}\,\frac{I(\omega)}{\omega}\,\frac{2\nu_n^2}{\omega^2+\nu_n^2}\,. \tag{4.17}$$

Since

$$\frac{1}{\hbar\beta}\sum_{n=-\infty}^{\infty}\exp(\mathrm{i}\nu_n\tau)=:\delta(\tau):=\sum_{n=-\infty}^{\infty}\delta(\tau-n\hbar\beta) \tag{4.18}$$

is a δ-function periodically repeated at times $\tau=\pm n\hbar\beta$, the decomposition (4.16) of g_n splits the imaginary time kernel (4.15) into a local and a nonlocal part. Accordingly, the first term of the exponent $\tilde{\Phi}[q, q', \bar{q}]$ defined in eq. (3.28) may be written as

$$-\int_0^{\hbar\beta} d\tau \int_0^{\tau} d\sigma\, K(-i\tau + i\sigma)\bar{q}(\tau)\bar{q}(\sigma) = -\int_0^{\hbar\beta} d\tau\, \tfrac{1}{2}\mu\dot{\bar{q}}^2(\tau) + \tfrac{1}{2}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\sigma\, k(\tau-\sigma)\bar{q}(\tau)\bar{q}(\sigma)\,, \tag{4.19}$$

where

$$k(\tau) = \frac{M}{\hbar\beta}\sum_{n=-\infty}^{\infty} \zeta_n \exp(i\nu_n\tau)\,. \tag{4.20}$$

The first term of eq. (4.19) now exactly cancels the second term in eq. (3.28). For a model without a counterterm in eq. (2.4) the first term in eq. (4.19) would lead to a renormalization of the potential $V(\bar{q})$ in the action $S_0^E[\bar{q}]$ [cf. eq. (3.15)]. Hence, the counterterm simply removes the frequency shift such that the potential in the Hamiltonian (2.2) is the physically observable potential [14]. The last term in eq. (4.19) does not contain a further potential renormalization. This becomes obvious if it is transformed into the form

$$\tfrac{1}{2}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\sigma\, k(\tau-\sigma)\bar{q}(\tau)\bar{q}(\sigma) = -\frac{1}{4}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\sigma\, k(\tau-\sigma)\{\bar{q}(\tau)-\bar{q}(\sigma)\}^2\,, \tag{4.21}$$

clearly displaying its nonlocal character. Equation (4.21) is readily verified by performing the square and noting that

$$\int_0^{\hbar\beta} d\tau\, k(\tau) = M\zeta_0 = 0\,. \tag{4.22}$$

For real times the real and imaginary parts of the kernel (4.3) read [cf. (4.6), (4.7)]

$$K'(s) = \int_0^{\infty} \frac{d\omega}{\pi}\, I(\omega)\coth(\tfrac{1}{2}\omega\hbar\beta)\cos(\omega s) \tag{4.23}$$

and

$$K''(s) = -\int_0^{\infty} \frac{d\omega}{\pi}\, I(\omega)\sin(\omega s)\,. \tag{4.24}$$

Now, the fourth term of the exponent (3.28) of the influence functional splits into

$$\begin{aligned}
&\int_0^t ds \int_0^s du\{q(s)-q'(s)\}\{K(s-u)q(u) - K^*(s-u)q'(u)\} \\
&\quad = \int_0^t ds \int_0^s du\, K'(s-u)\{q(s)-q'(s)\}\{q(u)-q'(u)\} \\
&\qquad + i\int_0^t ds \int_0^s du\, K''(s-u)\{q(s)-q'(s)\}\{q(u)+q'(u)\}\,.
\end{aligned} \tag{4.25}$$

The imaginary part $K''(s)$ of the kernel again contains a reversible renormalization of the potential and may be written

$$K''(s) = \tfrac{1}{2}\, \mathrm{d}\eta(s)/\mathrm{d}s\,, \tag{4.26}$$

where

$$\eta(s) = 2\int_0^\infty \frac{\mathrm{d}\omega}{\pi}\,\frac{I(\omega)}{\omega}\cos(\omega s)\,. \tag{4.27}$$

By virtue of eq. (4.26) the second term of eq. (4.25) may be integrated by parts with respect to u to yield

$$\begin{aligned}
\mathrm{i}\int_0^t \mathrm{d}s \int_0^s \mathrm{d}u\, K''(s-u)\{q(s)-q'(s)\}\{q(u)+q'(u)\} &= -\frac{\mathrm{i}}{2}\int_0^t \mathrm{d}s\,\eta(0)\{q^2(s)-q'^2(s)\} \\
&+ \frac{\mathrm{i}}{2}\{q(0)+q'(0)\}\int_0^t \mathrm{d}s\,\eta(s)\{q(s)-q'(s)\} \\
&+ \frac{\mathrm{i}}{2}\int_0^t \mathrm{d}s \int_0^s \mathrm{d}u\,\eta(s-u)\{q(s)-q'(s)\}\{\dot{q}(u)+\dot{q}'(u)\}\,.
\end{aligned} \tag{4.28}$$

Because of $\eta(0) = \mu$ the first term in eq. (4.28) just cancels the last term in eq. (3.28). Hence, the potential renormalization implicit in $K(s)$ is again eliminated by the counterterm. The last term in eq. (4.28) contains no further potential renormalization since it does not have the structure of a potential energy contribution due to its dependence on the particle velocity.

Collecting the results (4.19), (4.25), and (4.28), the exponent (3.28) of the influence functional now takes the form

$$\begin{aligned}
\tilde{\Phi}[q, q', \bar{q}] = \frac{1}{2}\int_0^{\hbar\beta} \mathrm{d}\tau \int_0^{\hbar\beta} \mathrm{d}\sigma\, k(\tau-\sigma)\bar{q}(\tau)\bar{q}(\sigma) - \mathrm{i}\int_0^{\hbar\beta} \mathrm{d}\tau \int_0^t \mathrm{d}s\, K^*(s-\mathrm{i}\tau)\bar{q}(\tau)\{q(s)-q'(s)\} \\
+ \int_0^t \mathrm{d}s \int_0^s \mathrm{d}u\, K'(s-u)\{q(s)-q'(s)\}\{q(u)-q'(u)\} \\
+ \frac{\mathrm{i}}{2}\int_0^t \mathrm{d}s \int_0^s \mathrm{d}u\,\eta(s-u)\{q(s)-q'(s)\}\{\dot{q}(u)+\dot{q}'(u)\} \\
+ \frac{\mathrm{i}}{2}\{q(0)+q'(0)\}\int_0^t \mathrm{d}s\,\eta(s)\{q(s)-q'(s)\}\,.
\end{aligned} \tag{4.29}$$

The first two terms describe the effect of initial correlations between the environment and the Brownian particle on the subsequent time evolution of the particle. The remaining three terms just constitute the exponent of the influence functional of the conventional Feynman–Vernon theory [16] which neglects correlations between the particle and the environment in the initial state. We remark that Caldeira and

Leggett [19] omitted the last term in eq. (4.29) in their treatment of the conventional theory.

The result (4.29) suggests the introduction of sum and difference coordinates of the Brownian particle, i.e.

$$x = q - q' , \qquad r = (q + q')/2 \tag{4.30}$$

with initial and final values defined accordingly. The functional integral representation (3.34) of the density matrix is then recast into

$$\rho(x_f, r_f, t) = \int \mathrm{d}x_i \, \mathrm{d}r_i \, \mathrm{d}\bar{q} \, \mathrm{d}\bar{q}' \, J(x_f, r_f, t, x_i, r_i, \bar{q}, \bar{q}') \lambda(x_i, r_i, \bar{q}, \bar{q}') , \tag{4.31}$$

where the propagating function

$$J(x_f, r_f, t, x_i, r_i, \bar{q}, \bar{q}') = Z^{-1} \int \mathscr{D}x \, \mathscr{D}r \, \mathscr{D}\bar{q} \exp\Big\{ \frac{\mathrm{i}}{\hbar} (S_0[r + x/2] - S_0[r - x/2]) - \frac{1}{\hbar} S_0^{\mathrm{E}}[\bar{q}] \Big\} \tilde{F}[x, r, \bar{q}] \tag{4.32}$$

is a functional integral over all paths $x(s)$, $r(s)$, $0 \le s \le t$ in real time with

$$x(0) = x_i , \quad r(0) = r_i , \qquad x(t) = x_f , \quad r(t) = r_f$$

and over all paths $\bar{q}(\tau)$, $0 \le \tau \le \hbar\beta$ in imaginary time with $\bar{q}(0) = \bar{q}'$, $\bar{q}(\hbar\beta) = \bar{q}$. The influence functional now becomes

$$\tilde{F}[x, r, \bar{q}] = \exp\Big(- \frac{1}{\hbar} \tilde{\Phi}[x, r, \bar{q}] \Big) , \tag{4.33}$$

where the exponent is given by eq. (4.29) expressed in terms of the new variables (4.30). The functional integral (4.32) can thus be written

$$J(x_f, r_f, t, x_i, r_i, \bar{q}, \bar{q}') = Z^{-1} \int \mathscr{D}x \, \mathscr{D}r \, \mathscr{D}\bar{q} \exp\Big(\frac{\mathrm{i}}{\hbar} \Sigma[x, r, \bar{q}] \Big) \tag{4.34}$$

where $\Sigma[x, r, \bar{q}]$ is an effective action given by

$$\begin{aligned} \Sigma[x, r, \bar{q}] = \mathrm{i} \int_0^{\hbar\beta} \mathrm{d}\tau \Big[\frac{M}{2} \dot{\bar{q}}^2 + V(\bar{q}) + \frac{1}{2} \int_0^{\hbar\beta} \mathrm{d}\sigma \, k(\tau - \sigma) \bar{q}(\tau) \bar{q}(\sigma) \Big] + \int_0^{\hbar\beta} \mathrm{d}\tau \int_0^t \mathrm{d}s \, K^*(s - \mathrm{i}\tau) \bar{q}(\tau) x(s) \\ + \int_0^t \mathrm{d}s \, [M\dot{x}\dot{r} - V(r + x/2, s) + V(r - x/2, s) - r_i \eta(s) x(s)] \\ - \int_0^t \mathrm{d}s \Big[\int_0^s \mathrm{d}u \, \eta(s - u) x(s) \dot{r}(u) + \frac{\mathrm{i}}{2} \int_0^t \mathrm{d}u \, K'(s - u) x(s) x(u) \Big] . \end{aligned} \tag{4.35}$$

The kernels occurring in eq. (4.35) have been defined in eqs. (4.3), (4.20), (4.23), and (4.27). Note that the potential may depend explicitly on time only for $t > 0$.

4.2. Minimal action paths

Frequently, the dominant contribution to the functional integral (4.34) comes from paths for which the action Σ is extremal. The equations of motion satisfied by the minimal action paths are obtained in the usual way by variation of the effective action (4.35). Variation with respect to $\bar{q}(\tau)$ with fixed endpoints $\bar{q}(0) = \bar{q}'$, $\bar{q}(\hbar\beta) = \bar{q}$ leads to

$$M\ddot{\bar{q}} - \int_0^{\hbar\beta} \mathrm{d}\sigma\, k(\tau - \sigma)\bar{q}(\sigma) - \frac{\mathrm{d}V(\bar{q})}{\mathrm{d}\bar{q}} = f(\tau)\,, \tag{4.36}$$

where the inhomogeneity

$$f(\tau) = -\mathrm{i}\int_0^t \mathrm{d}s\, K^*(s - \mathrm{i}\tau)x(s) \tag{4.37}$$

depends on the real time path $x(s)$. Accordingly, we find by variation of $\Sigma[x, r, \bar{q}]$ with respect to $x(s)$ with fixed endpoints $x(0) = x_\mathrm{i}$, $r(0) = r_\mathrm{i}$, $x(t) = x_\mathrm{f}$, $r(t) = r_\mathrm{f}$ an equation of motion for $r(s)$ of the form

$$\begin{aligned} &M\ddot{r} + \int_0^s \mathrm{d}u\, \eta(s-u)\dot{r}(u) + \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}r}\{V(r + x/2, s) + V(r - x/2, s)\} \\ &\quad = -r_\mathrm{i}\eta(s) + \mathrm{i}\int_0^t \mathrm{d}u\, K'(s-u)x(u) + \int_0^{\hbar\beta} \mathrm{d}\tau\, K^*(s - \mathrm{i}\tau)\bar{q}(\tau)\,. \end{aligned} \tag{4.38}$$

Note that $r(s)$ is coupled to both the real time path $x(s)$ and to the imaginary time path $\bar{q}(\tau)$. Carrying out the same variation with respect to $r(s)$ we get the equation of motion for $x(s)$

$$M\ddot{x} - \int_s^t \mathrm{d}u\, \eta(u-s)\dot{x}(u) + 2\frac{\mathrm{d}}{\mathrm{d}x}\{V(r + x/2, s) + V(r - x/2, s)\} = -x_\mathrm{f}\eta(t-s)\,, \tag{4.39}$$

where the inhomogeneity arises from the variation of the term proportional to $\dot{r}(u)$ in eq. (4.35) as a boundary term after a partial integration. For later convenience we rewrite the real time equations of motion (4.38) and (4.39) in the form

$$\begin{aligned} &M\ddot{r} + \frac{\mathrm{d}}{\mathrm{d}s}\int_0^s \mathrm{d}u\, \eta(s-u)r(u) + \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}r}\{V(r + x/2, s) + V(r - x/2, s)\} \\ &\quad = \mathrm{i}\int_0^t \mathrm{d}u\, K'(s-u)x(u) + \int_0^{\hbar\beta} \mathrm{d}\tau\, K^*(s - \mathrm{i}\tau)\bar{q}(\tau)\,, \end{aligned} \tag{4.40}$$

$$M\ddot{x} - \frac{\mathrm{d}}{\mathrm{d}s}\int_s^t \mathrm{d}u\,\eta(u-s)x(u) + 2\frac{\mathrm{d}}{\mathrm{d}x}\{V(r+x/2,s)+V(r-x/2,s)\} = 0\,, \tag{4.41}$$

where partial integrations removed the boundary terms in the inhomogeneities of eqs. (4.38) and (4.39).

To gain additional insight in the physical meaning of the influence kernel $K(\theta)$ we study the classical limit of the equations of motion derived above. Consider an initial density matrix which is diagonal in coordinate representation, i.e.

$$\rho(x_\mathrm{i}, r_\mathrm{i}, 0) = \delta(x_\mathrm{i})w(r_\mathrm{i}, 0)\,. \tag{4.42}$$

To determine the probability distribution $w(r_\mathrm{f}, t) = \rho(x_\mathrm{f}=0, r_\mathrm{f}, t)$ evolving from this initial state, we have to evaluate the functional integral (4.34) by summing over all paths satisfying the boundary conditions $x_\mathrm{i} = x_\mathrm{f} = 0$ and $\bar{q} = \bar{q}' = r_\mathrm{i}$. In the limit $\hbar \to 0$ the path probability sharply peaks about the minimal action paths and their equations of motion simplify considerably. The evolution equation (4.39) for $x(s)$ admits for the boundary conditions $x_\mathrm{i} = x_\mathrm{f} = 0$ the trivial solution $x(s) = 0$. Therefore, the equation of motion (4.36) for the imaginary time path $\bar{q}(\tau)$ becomes homogeneous. Further, since the interval $\hbar\beta$ vanishes in the classical limit, the minimal action path $\bar{q}(\tau)$ with boundary conditions $\bar{q}(0) = \bar{q}(\hbar\beta) = r_\mathrm{i}$ just contracts to the point $\bar{q} = r_\mathrm{i}$. The equation of motion (4.38) for $r(s)$ then becomes

$$M\ddot{r} + \int_0^s \mathrm{d}u\,\eta(s-u)\dot{r}(u) + \frac{\mathrm{d}V(r,s)}{\mathrm{d}r} = 0\,, \tag{4.43}$$

where we noted that the inhomogeneity vanishes because of $x(u) = 0$ and

$$\int_0^{\hbar\beta} \mathrm{d}\tau\, K^*(s - \mathrm{i}\tau) = \eta(s)\,. \tag{4.44}$$

It seems worth mentioning that within the conventional theory based on the factorization assumption the classical equation of motion (4.43) does not become homogeneous; rather the term $-r_\mathrm{i}\eta(s)$ survives on the rhs of eq. (4.43). This shows that even classical processes generally depend on the preparation of the initial state [41]. The complete classical theory including thermal noise is obtained from the functional integral (4.34) if one takes Gaussian fluctuations about the classical path into account. The Gaussian approximation becomes exact in the classical limit and eq. (4.43) is replaced by the classical Langevin equation with thermal Gaussian noise.

4.3. Formulation of the theory in terms of the damping kernel

The classical equation of motion (4.43) shows that $\eta(s)$ is a friction kernel describing the dissipative influence of the environmental oscillators. For later purposes it is convenient to introduce the mass-independent damping kernel

$$\gamma(s) = \eta(s)/M \tag{4.45}$$

in terms of which the classical equation of motion takes the familiar form

$$\ddot{r} + \int_0^s \mathrm{d}u\, \gamma(s-u)\dot{r}(u) + \frac{1}{M}\frac{\mathrm{d}V(r,s)}{\mathrm{d}r} = 0\,. \tag{4.46}$$

We will demonstrate now that for the model under consideration the influence of the environment is characterized by this damping kernel. From (4.27) and (4.45) we see that the damping kernel is related to the spectral density $I(\omega)$ of the environment by

$$\gamma(s) = \frac{2}{M}\int_0^\infty \frac{\mathrm{d}\omega}{\pi}\,\frac{I(\omega)}{\omega}\cos(\omega s)\,. \tag{4.47}$$

The frequency dependence of the dissipative mechanism becomes apparent if we introduce the Laplace transform $\hat{\gamma}(z)$ of the damping kernel

$$\hat{\gamma}(z) = \int_0^\infty \mathrm{d}s\, \gamma(s)\exp(-zs)\,, \tag{4.48}$$

which may be written in terms of $I(\omega)$ as

$$\hat{\gamma}(z) = \frac{1}{M}\int_0^\infty \frac{\mathrm{d}\omega}{\pi}\,\frac{I(\omega)}{\omega}\,\frac{2z}{\omega^2+z^2}\,. \tag{4.49}$$

On the other hand, the damping kernel determines the spectral density $I(\omega)$ by virtue of the relation

$$I(\omega) = M\omega\int_0^\infty \mathrm{d}s\, \gamma(s)\cos(\omega s) = \lim_{\varepsilon\to 0}\tfrac{1}{2}M\omega[\hat{\gamma}(\varepsilon+\mathrm{i}\omega)+\hat{\gamma}(\varepsilon-\mathrm{i}\omega)]\,, \tag{4.50}$$

which is obtained by inversion of eq. (4.47).

Now, we are in the position to re-express the quantities characterizing the functional integral representation of quantum Brownian motion in terms of the phenomenological damping kernel. Combining eqs. (4.3) and (4.50) the influence kernel $K(\theta)$ for complex times $\theta = t - \mathrm{i}\tau$ takes the form

$$\begin{aligned} K(\theta) &= \frac{M}{\hbar\beta}\int_0^\infty \mathrm{d}s\, \gamma(s)\,\frac{\partial}{\partial s}\,\frac{\sinh(\nu s)}{\cosh(\nu s)-\cosh(\nu\theta)} \\ &= -\frac{\pi M}{2(\hbar\beta)^2}\int_0^\infty \mathrm{d}s\, \gamma(s)[\sinh^{-2}\{\tfrac{1}{2}\nu(\theta+s)\}+\sinh^{-2}\{\tfrac{1}{2}\nu(\theta-s)\}]\,, \end{aligned} \tag{4.51}$$

where $\nu = \nu_1 = 2\pi/\hbar\beta$. For real times, that is in the limit $\tau\to 0^+$, this expression gives

$$K(t) = -\frac{\pi M}{2(\hbar\beta)^2}\int_0^\infty \mathrm{d}s\,\gamma(s)[\sinh^{-2}(\tfrac{1}{2}\nu(t+s)) + \sinh^{-2}(\tfrac{1}{2}\nu(t-s))] + \mathrm{i}\,\frac{M}{2}\,\dot{\gamma}(t)\,. \tag{4.52}$$

The integral is regular since in the limit $\tau \to 0^+$ the pole $[\frac{1}{2}\nu(s-t)]^{-2}$ of the integrand at $s=t$ is replaced by

$$(\tfrac{1}{2}\nu)^{-2}\lim_{\tau\to 0}[\{(s-t)^2-\tau^2\}/\{(s-t)^2+\tau^2\}^2]\,.$$

For imaginary times ($t=0$) the kernel is real and reads

$$K(-\mathrm{i}\tau) = \frac{M}{\hbar\beta}\int_0^\infty \mathrm{d}s\,\gamma(s)\,\frac{\partial}{\partial s}\,\frac{\sinh(\nu s)}{\cosh(\nu s)-\cos(\nu\tau)}\,. \tag{4.53}$$

Further, by virtue of eq. (4.19) the transformed kernel $k(\tau)$ may be written

$$\begin{aligned} k(\tau) &= -K(-\mathrm{i}\tau) + \mu{:}\delta(\tau){:} \\ &= \frac{M}{\hbar\beta}\int_0^\infty \mathrm{d}s\,\gamma(s)\,\frac{\partial}{\partial s}\,\frac{\sinh(\nu s)}{\cos(\nu\tau)-\cosh(\nu s)} + M\gamma(0){:}\delta(\tau){:}\,. \end{aligned} \tag{4.54}$$

Here, we used $\mu = M\gamma(0)$ which follows from eqs. (4.4) and (4.47).

For later purposes we also note that the Fourier components (4.13) and (4.14) of the real and imaginary parts of the influence kernel $K(\theta)$ may be transformed by virtue of eq. (4.47) to read

$$g_n(s) = \gamma(s) - \zeta_n(s)\,, \tag{4.55}$$

$$f_n(s) = -\frac{1}{\nu_n}\,\frac{\mathrm{d}}{\mathrm{d}s}\,\zeta_n(s)\,, \tag{4.56}$$

where we introduced

$$\zeta_n(s) = \frac{1}{M}\int_0^\infty \frac{\mathrm{d}\omega}{\pi}\,\frac{I(\omega)}{\omega}\,\frac{2\nu_n^2}{\omega^2+\nu_n^2}\cos(\omega s)\,. \tag{4.57}$$

Now, using eq. (4.50), we can express $\zeta_n(s)$ in terms of the damping kernel as

$$\zeta_n(s) = \tfrac{1}{2}|\nu_n|\int_0^\infty \mathrm{d}u\,\gamma(u)[\exp(-|\nu_n(s+u)|) + \exp(-|\nu_n(s-u)|)]\,. \tag{4.58}$$

Finally, because of eq. (4.17), the $\zeta_n(s=0)$ are just the Fourier components ζ_n of the imaginary time kernel $k(\tau)$. Using eq. (4.48) we obtain

$$\zeta_n = |\nu_n|\hat{\gamma}(|\nu_n|)\,. \tag{4.59}$$

The theory presented so far is determined completely by the mass M, the potential $V(q, t)$ and the spectral density $I(\omega)$. Since $I(\omega)$ is uniquely determined by the damping kernel $\gamma(s)$, the quantum mechanical theory of Brownian motion developed here on the basis of a microscopic model can be formulated entirely in terms of quantities appearing in the classical equation of motion (4.46) [42]. This feature is connected with the fact that the frictional influence of the environment is described by a linear relation, i.e. the damping kernel does not depend on the state of the Brownian particle. Since linear dissipation plays an important role in many areas of physics, the above relations are particularly helpful for a phenomenological modelling of irreversible quantum systems.

PART II. DAMPED HARMONIC OSCILLATOR

5. Time evolution of a damped harmonic oscillator

In this section we discuss the quantum dynamics of a damped harmonic oscillator. Although this problem was investigated extensively in the past [2, 3, 11, 33], new results on anomalous low temperature behaviour were obtained in more recent work [18, 19, 35–37, 43, 44] mostly addressing the case of Ohmic dissipation. Here we employ the methods presented in part I to study the time evolution of the density matrix of a harmonic oscillator interacting with a dissipative mechanism of arbitrary frequency dependence. Hence, we will not use a particular form of the spectral density $I(\omega)$ of the environment. However, in order to avoid unphysical divergencies, we require $I(\omega)$ to vanish for $\omega \to 0$ and to remain bounded for $\omega \to \infty$. Specific forms of the damping will be discussed in subsequent sections.

We consider a Brownian particle in a harmonic potential

$$V(q, t) = \tfrac{1}{2} M\omega_0^2 q^2 - qF(t)\,, \tag{5.1}$$

where we allow for a time-dependent external force $F(t)$ coupled linearly to the particle. As has been stated before, $F(t)$ is assumed not to influence the initial state, i.e.

$$F(t) = 0\,, \qquad \text{for} \quad t \leq 0\,. \tag{5.2}$$

Inserting eq. (5.1), the potential term in the effective action $\Sigma[x, r, \bar{q}]$ becomes [cf. (4.35)]

$$-V(r + x/2, s) + V(r - x/2, s) = -M\omega_0^2 xr + xF(s)\,. \tag{5.3}$$

The equations of motion (4.36–4.41) are now linear and can be solved exactly. Furthermore, the functional integral (4.34) is now Gaussian. Hence it is sufficient to determine the effective action $\Sigma[x, r, \bar{q}]$ along the minimal action paths satisfying (4.36–4.41) because the fluctuations about these paths only contribute a time and temperature dependent factor. Rather than performing the summation over the fluctuation modes explicitly, this latter factor can also be determined from the conservation of the normalization of the density matrix.

5.1. Extremal imaginary time path and reduced equilibrium density matrix

We first consider the equation of motion (4.36) for the path $\bar{q}(\tau)$ in imaginary time

$$M\ddot{\bar{q}} - \int_0^{\hbar\beta} \mathrm{d}\sigma\, k(\tau-\sigma)\bar{q}(\sigma) - M\omega_0^2\bar{q} = f(\tau)\,, \tag{5.4}$$

where the inhomogeneity $f(\tau)$ is given by eq. (4.37). We need a solution in the interval $0 \le \tau \le \hbar\beta$. Therefore it is convenient to use the Fourier series expansion

$$\bar{q}(\tau) = \frac{1}{\hbar\beta} \sum_{n=-\infty}^{\infty} \bar{q}_n \exp(\mathrm{i}\nu_n\tau)\,. \tag{5.5}$$

The Fourier representation of the imaginary time kernel $k(\tau)$ is given by eq. (4.20) and from eqs. (4.11) and (4.12) the expansion of the inhomogeneity (4.37) is found to read

$$f(\tau) = \frac{M}{\hbar\beta} \sum_{n=-\infty}^{\infty} \rho_n \exp(\mathrm{i}\nu_n\tau)\,, \tag{5.6}$$

where the Fourier coefficients

$$\rho_n = -\mathrm{i}\int_0^t \mathrm{d}s\,[f_n(s) + g_n(s)]x(s) \tag{5.7}$$

are functionals of the real time path $x(s)$.

The Fourier series expansion for $\bar{q}(\tau)$ periodically continues the path outside the interval $0 \le \tau \le \hbar\beta$. This leads to jump and cusp singularities at the endpoints. Hence, for the periodically continued path, the equation of motion (5.4) is satisfied only for $\tau \neq n\hbar\beta$, $n = 0, \pm1, \pm2, \ldots$ and there are δ- and δ'-function singularities at $\tau = n\hbar\beta$. These singularities must be accounted for in the equation of motion (5.4) which for the periodically continued path reads

$$M\ddot{\bar{q}} - \int_0^{\hbar\beta} \mathrm{d}\sigma\, k(\tau-\sigma)\bar{q}(\sigma) - M\omega_0^2\bar{q} = f(\tau) + Ma{:}\delta'(\tau){:} + Mb{:}\delta(\tau){:}\,, \tag{5.8}$$

where $:\delta(\tau):$ is the periodically continued δ-function defined in eq. (4.18), while $:\delta'(\tau):$ is its time derivative. The constants a and b in eq. (5.8) are related to the jumps of $\bar{q}(\tau)$ and $\dot{\bar{q}}(\tau)$ at the boundaries by

$$a = \bar{q}(0^+) - \bar{q}(0^-) = \bar{q}(0^+) - \bar{q}(\hbar\beta^-) = \bar{q}' - \bar{q} \tag{5.9}$$

and

$$b = \dot{\bar{q}}(0^+) - \dot{\bar{q}}(0^-) = \dot{\bar{q}}(0^+) - \dot{\bar{q}}(\hbar\beta^-)\,. \tag{5.10}$$

By virtue of eqs. (4.18), (4.20), and (5.6) the equation of motion (5.8) transforms into a relation among the Fourier coefficients

$$(-\nu_n^2 - \omega_0^2 - \zeta_n)\bar{q}_n - \rho_n = \mathrm{i}a\nu_n + b\,, \tag{5.11}$$

which gives

$$\bar{q}_n = -u_n(\mathrm{i}a\nu_n + b + \rho_n)\,, \tag{5.12}$$

where we introduced the abbreviation

$$u_n = (\omega_0^2 + \nu_n^2 + \zeta_n)^{-1}\,. \tag{5.13}$$

The coefficients a and b must now be determined so that the path $\bar{q}(\tau)$ satisfies the boundary conditions

$$\bar{q}(0^+) = \bar{q}'\,, \tag{5.14}$$

$$\bar{q}(\hbar\beta^-) = \bar{q}(0^-) = \bar{q}\,. \tag{5.15}$$

Because of the discontinuities of the periodically continued path at the endpoints, care must be taken in performing the limit $\tau \to 0$. From eqs. (5.12) and (5.13) we find

$$\bar{q}(\tau) = \frac{1}{\hbar\beta}\sum_{n=-\infty}^{\infty}{}' \frac{a}{\mathrm{i}\nu_n}\exp(\mathrm{i}\nu_n\tau) - \frac{1}{\hbar\beta}\sum_{n=-\infty}^{\infty}{}' \frac{a}{\mathrm{i}\nu_n}u_n(\omega_0^2+\zeta_n)\exp(\mathrm{i}\nu_n\tau)$$
$$-\frac{1}{\hbar\beta}\sum_{n=-\infty}^{\infty} u_n(b+\rho_n)\exp(\mathrm{i}\nu_n\tau)\,, \tag{5.16}$$

where the prime means the sum over all elements except $n = 0$. The second sum in eq. (5.16) is regular in the limit $\tau \to 0$ and gives a vanishing contribution. The third sum is also regular and gives for $\tau = 0$

$$\frac{1}{\hbar\beta}\sum_{n=-\infty}^{\infty} u_n(b+\rho_n) = b\Lambda + \frac{1}{\hbar\beta}\sum_{n=-\infty}^{\infty} u_n\rho_n\,, \tag{5.17}$$

where we introduced

$$\Lambda = \frac{1}{\hbar\beta}\sum_{n=-\infty}^{\infty} u_n = \frac{1}{\hbar\beta}\sum_{n=-\infty}^{\infty}\frac{1}{\omega_0^2+\nu_n^2+\zeta_n}\,. \tag{5.18}$$

The first sum in eq. (5.16), however, is discontinuous at the endpoints and describes a sawtooth-like behaviour with

$$\lim_{\tau\to 0^{\pm}}\frac{1}{\hbar\beta}\sum_{n=-\infty}^{\infty}{}' \frac{a}{\mathrm{i}\nu_n}\exp(\mathrm{i}\nu_n\tau) = \pm\frac{a}{2}\,. \tag{5.19}$$

By virtue of eqs. (5.17–5.19) we obtain from eq. (5.16)

$$\lim_{\tau\to 0^{\pm}} \bar{q}(\tau) = -b\Lambda - \frac{1}{\hbar\beta}\sum_{n=-\infty}^{\infty} u_n\rho_n \pm \frac{a}{2}\,, \tag{5.20}$$

which combines with eqs. (5.14) and (5.15) to yield

$$b = -\frac{1}{\Lambda}\left[\frac{1}{2}(\bar{q}+\bar{q}') + \frac{1}{\hbar\beta}\sum_{n=-\infty}^{\infty} u_n\rho_n\right]. \tag{5.21}$$

Using eqs. (5.9) and (5.21) we finally obtain for the Fourier coefficient $\bar{q}_n$ of the imaginary time trajectory

$$\bar{q}_n = u_n\left[\mathrm{i}\nu_n(\bar{q}-\bar{q}') + \frac{1}{2\Lambda}(\bar{q}+\bar{q}') + \frac{1}{\hbar\beta\Lambda}\sum_{m=-\infty}^{\infty} u_m\rho_m - \rho_n\right]. \tag{5.22}$$

This relation determines the minimal action path $\bar{q}(\tau)$ in imaginary time as a function of the endpoints $\bar{q}$ and $\bar{q}'$ and as a functional of the real time path $x(s)$. The dependence on $x(s)$ arises through the Fourier components ρ_n defined in eq. (5.7).

The Fourier representation (5.5) of $\bar{q}(\tau)$ and the definition (4.45) of the damping kernel $\gamma(s)$ may now be inserted into the expression (4.35) for the effective action $\Sigma[x, r, \bar{q}]$. Noting that $\dot{\bar{q}}(\tau)$ has a component proportional to $:\delta(\tau)$: which must be split off, we obtain for the harmonic potential (5.1)

$$\begin{aligned}\Sigma[x,r,\bar{q}] = {}& \mathrm{i}\frac{M}{2\hbar\beta}\sum_{n=-\infty}^{\infty}(\mathrm{i}\nu_n\bar{q}_n - \bar{q}' + \bar{q})(-\mathrm{i}\nu_n\bar{q}_{-n} - \bar{q}' + \bar{q}) + \mathrm{i}\frac{M}{2\hbar\beta}\sum_{n=-\infty}^{\infty}(\omega_0^2+\zeta_n)\bar{q}_n\bar{q}_{-n}\\ &+ \frac{\mathrm{i}M}{\hbar\beta}\sum_{n=-\infty}^{\infty}\rho_n\bar{q}_{-n} + \int_0^t \mathrm{d}s\, M\Big[\dot{x}\dot{r} - \omega_0^2 xr + \frac{1}{M}F(s)x(s) - r_{\mathrm{i}}\gamma(s)x(s)\\ &- \int_0^s \mathrm{d}u\,\gamma(s-u)x(s)\dot{r}(u) + \frac{\mathrm{i}}{2M}\int_0^t \mathrm{d}u\,K'(s-u)x(s)x(u)\Big],\end{aligned} \tag{5.23}$$

where we made use of eq. (4.37) and its Fourier representation (5.6). The first sum comes from the kinetic term of the imaginary time path. The singularities of the integrand at the endpoints of the corresponding integral in (4.35) are an artefact of the Fourier series representation and they do not contribute to the physical action. Now, the first three sums in eq. (5.23) may be evaluated explicitly by inserting eqs. (5.7) and (5.22) which yields

$$\begin{aligned}&\frac{\mathrm{i}M}{\hbar\beta}\sum_{n=-\infty}^{\infty}[\tfrac{1}{2}(\mathrm{i}\nu_n\bar{q}_n - \bar{q} + \bar{q}')(-\mathrm{i}\nu_n\bar{q}_{-n} - \bar{q} + \bar{q}') + \tfrac{1}{2}(\omega_0^2+\zeta_n)\bar{q}_n\bar{q}_{-n} + \rho_n\bar{q}_{-n}]\\ &= \mathrm{i}M\Big[\frac{1}{2\Lambda}\Big(\frac{\bar{q}+\bar{q}'}{2}\Big)^2 + \frac{\Omega}{2}(\bar{q}-\bar{q}')^2\Big]\\ &\quad + M\int_0^t \mathrm{d}s\,x(s)\Big[\frac{1}{2}(\bar{q}+\bar{q}')C_1(s) - \mathrm{i}(\bar{q}-\bar{q}')C_2(s) + \frac{\mathrm{i}}{2}\int_0^t \mathrm{d}u\,R'(s,u)x(u)\Big],\end{aligned} \tag{5.24}$$

where we introduced the frequency

$$\Omega = \frac{1}{\hbar\beta} \sum_{n=-\infty}^{\infty} u_n(\omega_0^2 + \zeta_n) = \frac{1}{\hbar\beta} \sum_{n=-\infty}^{\infty} \frac{\omega_0^2 + \zeta_n}{\omega_0^2 + \nu_n^2 + \zeta_n} \,. \tag{5.25}$$

The functions $C_1(s)$ and $C_2(s)$ are given by

$$C_1(s) = \frac{1}{\hbar\beta\Lambda} \sum_{n=-\infty}^{\infty} u_n g_n(s) \,, \tag{5.26}$$

$$C_2(s) = \frac{1}{\hbar\beta} \sum_{n=-\infty}^{\infty} u_n \nu_n f_n(s) \,, \tag{5.27}$$

and the kernel $R'(s, u)$ reads

$$R'(s, u) = -\Lambda C_1(s) C_1(u) + \frac{1}{\hbar\beta} \sum_{n=-\infty}^{\infty} u_n [g_n(s) g_n(u) - f_n(s) f_n(u)] \,. \tag{5.28}$$

Inserting eq. (5.24) into eq. (5.23), we obtain the effective action $\Sigma[x, r, \bar{q}]$ evaluated along the minimal action path $\bar{q}(\tau)$ as a function of its endpoints $\bar{q}$ and $\bar{q}'$ and as a functional of the real time paths $x(s)$ and $r(s)$. In terms of $\bar{r} = (\bar{q} + \bar{q}')/2$ and $\bar{x} = \bar{q} - \bar{q}'$ we have

$$\Sigma[x, r, \bar{q}] = \mathrm{i}\Sigma_\beta(\bar{x}, \bar{r}) + \Sigma_t[x, r] \,, \tag{5.29}$$

where

$$\Sigma_\beta(\bar{x}, \bar{r}) = M\left(\frac{1}{2\Lambda}\, \bar{r}^2 + \frac{\Omega}{2}\, \bar{x}^2\right) \tag{5.30}$$

and

$$\Sigma_t[x, r] = \int_0^t \mathrm{d}s\, M\left[\dot{x}\dot{r} - \omega_0^2 x r + \frac{1}{M}\, \bar{F}(s) x(s) - x(s)\, \frac{\mathrm{d}}{\mathrm{d}s} \int_0^s \mathrm{d}u\, \gamma(s-u) r(u)\right]$$
$$+ \frac{\mathrm{i}}{2}\, M \int_0^t \mathrm{d}s \int_0^t \mathrm{d}u\, R(s, u) x(s) x(u) \,. \tag{5.31}$$

Here we introduced the force

$$\bar{F}(s) = F(s) + M[\bar{r} C_1(s) - \mathrm{i}\bar{x} C_2(s)] \tag{5.32}$$

and the kernel

$$R(s, u) = R'(s, u) + K'(s-u)/M \,. \tag{5.33}$$

The action $\Sigma_\beta(\bar{x}, \bar{r})$ is the minimal action of the Euclidean functional integral (3.39) for harmonic potential. Accordingly, the reduced equilibrium density matrix $\rho_\beta(\bar{x}, \bar{r})$ may be written as

$$\rho_\beta(\bar{x}, \bar{r}) = \left(\frac{M}{2\pi\hbar\Lambda}\right)^{1/2} \exp\left[-\frac{1}{\hbar}\Sigma_\beta(\bar{x}, \bar{r})\right], \tag{5.34}$$

where the pre-exponential factor follows readily from the normalization of the state.

5.2. Extremal real time paths and minimal effective action

To proceed we have to determine the minimal action paths $x(s)$ and $r(s)$ in real time. For harmonic potential (5.1) but arbitrary damping kernel (4.45) the equations of motion (4.40, 4.41) for the real time paths $x(s)$ and $r(s)$ become

$$\ddot{r} + \frac{\mathrm{d}}{\mathrm{d}s}\int_0^s \mathrm{d}u\, \gamma(s-u)r(u) + \omega_0^2 r = \frac{1}{M}\bar{F}(s) + \mathrm{i}\int_0^t \mathrm{d}u\, R(s,u)x(u) \tag{5.35}$$

and

$$\ddot{x} - \frac{\mathrm{d}}{\mathrm{d}s}\int_s^t \mathrm{d}u\, \gamma(u-s)x(u) + \omega_0^2 x = 0\,. \tag{5.36}$$

Naturally, the equations of motion (5.35) and (5.36) are also readily obtained by variation of eq. (5.31) with respect to $x(s)$ and $r(s)$, respectively.

The value of the action $\Sigma_t[x, r]$ evaluated along the minimal action paths can now be determined in two different ways. Firstly, we can formally solve the equations of motion (5.35) and (5.36), and then insert the solutions in eq. (5.31) to obtain Σ_t as a function of the boundary values x_i, r_i, x_f, r_f, $\bar{x}$, and $\bar{r}$, where the dependence on the last two variables arises from the force $\bar{F}(s)$ given by eq. (5.32). After a partial integration of the first term in eq. (5.31) the action $\Sigma_t[x, r]$ takes the form

$$\Sigma_t[x,r] = M(x_\mathrm{f}\dot{r}_\mathrm{f} - x_\mathrm{i}\dot{r}_\mathrm{i}) - \int_0^t \mathrm{d}s\, Mx\left[\ddot{r} + \omega_0^2 r + \frac{\mathrm{d}}{\mathrm{d}s}\int_0^s \mathrm{d}u\, \gamma(s-u)r(u) - \frac{1}{M}\bar{F}\right]$$
$$+ \frac{\mathrm{i}}{2} M \int_0^t \mathrm{d}s \int_0^t \mathrm{d}u\, R(s,u)x(s)x(u)\,. \tag{5.37}$$

Due to the equation of motion (5.35), the last two terms cancel partly if the action is evaluated along the minimal action paths $x(s)$ and $r(s)$ and we obtain

$$\Sigma_t(x_\mathrm{f}, r_\mathrm{f}, x_\mathrm{i}, r_\mathrm{i}, \bar{x}, \bar{r}) = M(x_\mathrm{f}\dot{r}_\mathrm{f} - x_\mathrm{i}\dot{r}_\mathrm{i}) - \frac{\mathrm{i}}{2} M \int_0^t \mathrm{d}s \int_0^t \mathrm{d}u\, R(s,u)x(s)x(u)\,. \tag{5.38}$$

On the other hand, we can split the force (5.32) into its real and imaginary parts $\bar{F}(s) = \bar{F}'(s) + \mathrm{i}\bar{F}''(s)$. Accordingly, the minimal action path $r(s)$ splits into $r'(s) + \mathrm{i}r''(s)$ where $r''(s)$ satisfies the boundary conditions $r''(0) = r''(t) = 0$. Now, by disregarding the imaginary part $r''(s)$ and evaluating the action (5.37) along $x(s)$ and $r'(s)$ we find

$$\Sigma_t(x_\mathrm{f}, r_\mathrm{f}, x_\mathrm{i}, r_\mathrm{i}, \bar{x}, \bar{r}) = M(x_\mathrm{f}\dot{r}'_\mathrm{f} - x_\mathrm{i}\dot{r}'_\mathrm{i}) + \mathrm{i}\int_0^t \mathrm{d}s\, x(s)\Big[\bar{F}''(s) + \frac{M}{2}\int_0^t \mathrm{d}u\, R(s,u)x(u)\Big], \tag{5.39}$$

where we took advantage of the fact that $r'(s)$ satisfies the real part of eq. (5.35). However, we can easily show that eq. (5.39) is in fact the same as eq. (5.38). The imaginary part of eq. (5.35) gives

$$\int_0^t \mathrm{d}s\, x(s)\Big[\bar{F}''(s) + M\int_0^t \mathrm{d}u\, R(s,u)x(u)\Big] = \int_0^t \mathrm{d}s\, Mx\Big(\ddot{r}'' + \omega_0^2 r'' + \frac{\mathrm{d}}{\mathrm{d}s}\int_0^s \mathrm{d}u\, \gamma(s-u)r''(u)\Big). \tag{5.40}$$

Now, the last term of the rhs of eq. (5.40) may be integrated by parts to give

$$\int_0^t \mathrm{d}s\, x(s)\frac{\mathrm{d}}{\mathrm{d}s}\int_0^s \mathrm{d}u\, \gamma(s-u)r''(u) = -\int_0^t \mathrm{d}s\, r''(s)\frac{\mathrm{d}}{\mathrm{d}s}\int_s^t \mathrm{d}u\, \gamma(u-s)x(u)\,. \tag{5.41}$$

This and two partial integrations of the first term on the rhs of eq. (5.40) yields

$$\int_0^t \mathrm{d}s\, x(s)\Big[\bar{F}''(s) + M\int_0^t \mathrm{d}u\, R(s,u)x(u)\Big] = M(x_\mathrm{f}\dot{r}''_\mathrm{f} - x_\mathrm{i}\dot{r}''_\mathrm{i})\,, \tag{5.42}$$

where we made use of eq. (5.36) and the boundary conditions $r''(0) = r''(t) = 0$. Hence, the rhs of eq. (5.39) coincides indeed with the rhs of eq. (5.38). Consequently, it is sufficient to determine the real components of the minimal action paths and to evaluate the action with these solutions. A corresponding simplification of the calculation was also noted by Hakim and Ambegaokar [20] in their treatment of free Brownian motion with frequency-independent damping.

To proceed we have to solve the real part of eq. (5.35) with boundary conditions $r'(0) = r_\mathrm{i}$, $r'(t) = r_\mathrm{f}$ and eq. (5.36) with boundary conditions $x(0) = x_\mathrm{i}$ and $x(t) = x_\mathrm{f}$. The homogeneous parts of eqs. (5.35) and (5.36) look very similar. In fact we can easily show that eq. (5.36) is the backward equation of the homogeneous equation (5.35). Substituting $z(t-s)$ for $x(s)$, the lhs of eq. (5.36) becomes

$$\begin{aligned}
&\frac{\partial^2}{\partial s^2}z(t-s) - \frac{\mathrm{d}}{\mathrm{d}s}\int_s^t \mathrm{d}u\, \gamma(u-s)z(t-u) + \omega_0^2 z(t-s)\\
&\quad = \ddot{z}(t-s) - \frac{\mathrm{d}}{\mathrm{d}s}\int_0^{t-s} \mathrm{d}u\, \gamma(t-s-u)z(u) + \omega_0^2 z(t-s)\\
&\quad = \ddot{z}(t-s) + \frac{\mathrm{d}}{\mathrm{d}(t-s)}\int_0^{t-s} \mathrm{d}u\, \gamma(t-s-u)z(u) + \omega_0^2 z(t-s)\,,
\end{aligned} \tag{5.43}$$

where the dot denotes the derivative with respect to the argument as usual. This last expression has exactly the same structure as the homogeneous part of eq. (5.35) albeit at time $t - s$. Hence, solutions $r(s)$ of the homogeneous equation (5.35) are time-reversed solutions $r(t-s)$ of eq. (5.36), and vice versa.

The homogeneous part of eq. (5.35) can be Laplace transformed to give

$$z^2\hat{r}(z) - zr(0) - \dot{r}(0) + z\hat{\gamma}(z)\hat{r}(z) + \omega_0^2\hat{r}(z) = 0\,, \tag{5.44}$$

where the hat denotes the Laplace transform of a time-dependent quantity [cf. eq. (4.48)]. From eq. (5.44) we have

$$\hat{r}(z) = \frac{z}{z^2 + z\hat{\gamma}(z) + \omega_0^2}\, r(0) + \frac{1}{z^2 + z\hat{\gamma}(z) + \omega_0^2}\dot{r}(0)\,, \tag{5.45}$$

which enables us to write down two fundamental solutions of eq. (5.35). These solutions are distinguished by their initial conditions. The fundamental solution satisfying $\dot{r}(0) = 1$, $r(0) = 0$ will be denoted by $G_+(t)$ and its Laplace transform reads

$$\hat{G}_+(z) = (z^2 + z\hat{\gamma}(z) + \omega_0^2)^{-1}\,. \tag{5.46}$$

A second solution, $H_+(t)$, which satisfies the initial conditions $\dot{r}(0) = 0$, $r(0) = 1$ has the Laplace transform

$$\hat{H}_+(z) = \frac{z}{z^2 + z\hat{\gamma}(z) + \omega_0^2} = z\hat{G}_+(z)\,. \tag{5.47}$$

Since $G_+(0) = 0$, we have

$$H_+(s) = \dot{G}_+(s)\,. \tag{5.48}$$

Using eq. (5.48) the solution of the inhomogeneous equation (5.35) satisfying the boundary conditions $r(0) = r_i$ and $r(t) = r_f$ can be expressed entirely in terms of the function $G_+(s)$. The real part reads

$$\begin{aligned} r'(s) = {} & r_f \frac{G_+(s)}{G_+(t)} + r_i\left[\dot{G}_+(s) - \frac{G_+(s)}{G_+(t)}\,\dot{G}_+(t)\right] \\ & + \frac{1}{M}\int_0^s \mathrm{d}u\, G_+(s-u)\bar{F}'(u) - \frac{1}{M}\,\frac{G_+(s)}{G_+(t)}\int_0^t \mathrm{d}u\, G_+(t-u)\bar{F}'(u)\,, \end{aligned} \tag{5.49}$$

where $\bar{F}'(s)$ is the real part of the force (5.32).

Due to the relation (5.43) the solution of the equation of motion (5.36) for $x(s)$ can be built up using the fundamental solutions $G_+(t-s)$ and $\dot{G}_+(t-s)$. With the boundary conditions $x(0) = x_i$ and $x(t) = x_f$ we get

$$x(s) = x_i\,\frac{G_+(t-s)}{G_+(t)} + x_f\left[\dot{G}_+(t-s) - \frac{G_+(t-s)}{G_+(t)}\,\dot{G}_+(t)\right]. \tag{5.50}$$

To proceed, it is convenient to introduce also a fundamental solution of eq. (5.36) satisfying the initial conditions $x(0) = 0$ and $\dot{x}(0) = 1$. This solution will be denoted by $G_-(s)$. By virtue of eq. (5.43) the function $G_-(t-s)$ satisfies the homogeneous equation (5.35) with the final conditions $r(t) = 0$ and $\dot{r}(t) = 1$ and can thus be related to the fundamental solutions $G_+(s)$ and $H_+(s)$ through

$$G_-(s) = \frac{G_+(t-s)H_+(t) - G_+(t)H_+(t-s)}{G_+(t)\dot{H}_+(t) - \dot{G}_+(t)H_+(t)} \,. \tag{5.51}$$

It is readily seen that

$$\frac{G_-(s)}{G_-(t)} = \dot{G}_+(t-s) - \frac{G_+(t-s)}{G_+(t)}\,\dot{G}_+(t) \,. \tag{5.52}$$

Now, in terms of the Green's functions $G_\pm(s)$ the minimal action paths $r'(s)$ and $x(s)$ take the transparent form

$$r'(s) = r_\mathrm{i}\,\frac{G_-(t-s)}{G_-(t)} + r_\mathrm{f}\,\frac{G_+(s)}{G_+(t)} - \frac{1}{M}\,\frac{G_+(s)}{\cancel{G_+(t)}}\int_0^t \mathrm{d}u\, G_+(t-u)\bar{F}'(u) + \frac{1}{M}\int_0^s \mathrm{d}u\, G_+(s-u)\bar{F}'(u)\,, \tag{5.53}$$

$$x(s) = x_\mathrm{i}\,\frac{G_+(t-s)}{G_+(t)} + x_\mathrm{f}\,\frac{G_-(s)}{G_-(t)} \,. \tag{5.54}$$

These solutions may now be inserted into eq. (5.39). Using the specific form (5.32) of $\bar{F}(s)$, we obtain after some algebra

$$\begin{aligned}
\Sigma_t(x_\mathrm{f}, r_\mathrm{f}, x_\mathrm{i}, r_\mathrm{i}, \bar{x}, \bar{r}) = {} & M(x_\mathrm{f}r_\mathrm{f} + x_\mathrm{i}r_\mathrm{i})\,\frac{\dot{G}_+(t)}{G_+(t)} - M\Big(x_\mathrm{i}r_\mathrm{f}\,\frac{1}{G_+(t)} + x_\mathrm{f}r_\mathrm{i}\,\frac{1}{G_-(t)}\Big) \\
& + M\int_0^t \mathrm{d}s\left[x_\mathrm{i}\,\frac{G_+(t-s)}{G_+(t)} + x_\mathrm{f}\,\frac{G_-(s)}{\cancel{G_-(t)}}\right]\Big(\frac{1}{M}\,F(s) + \bar{r}C_1(s) - \mathrm{i}\bar{x}C_2(s)\Big) \\
& + \frac{\mathrm{i}}{2}\,Mx_\mathrm{i}^2\int_0^t \mathrm{d}s\int_0^t \mathrm{d}u\, R(s,u)\,\frac{G_+(t-s)}{G_+(t)}\,\frac{G_+(t-u)}{G_+(t)} \\
& + \mathrm{i}Mx_\mathrm{i}x_\mathrm{f}\int_0^t \mathrm{d}s\int_0^t \mathrm{d}u\, R(s,u)\,\frac{G_+(t-s)}{G_+(t)}\,\frac{G_-(u)}{G_-(t)} \\
& + \frac{\mathrm{i}}{2}\,Mx_\mathrm{f}^2\int_0^t \mathrm{d}s\int_0^t \mathrm{d}u\, R(s,u)\,\frac{G_-(s)}{\cancel{G_-(t)}}\,\frac{G_-(u)}{G_-(t)} \,.
\end{aligned} \tag{5.55}$$

Finally, inserting this result into eq. (5.29) the effective action evaluated along the minimal action paths emerges as an explicit function of the boundary values

$$\Sigma(x_f, r_f, t, x_i, r_i, \bar{x}, \bar{r}) = i\Sigma_\beta(\bar{x}, \bar{r}) + \Sigma_t(x_f, r_f, x_i, r_i, \bar{x}, \bar{r})$$

$$= iM\left(\frac{1}{2\Lambda}\,\bar{r}^2 + \frac{\Omega}{2}\,\bar{x}^2\right) + \int_0^t ds\left[x_i\,\frac{G_+(t-s)}{G_+(t)} + x_f\,\frac{G_-(s)}{G_-(t)}\right]F(s)$$

$$+ M(x_f r_f + x_i r_i)\,\frac{\dot{G}_+(t)}{G_+(t)} - M\left(x_i r_f\,\frac{1}{G_+(t)} + x_f r_i\,\frac{1}{G_-(t)}\right)$$

$$+ M\bar{r}(x_i C_1^+(t) + x_f C_1^-(t)) - iM\bar{x}(x_i C_2^+(t) + x_f C_2^-(t))$$

$$+ \frac{i}{2}\,M[x_i^2 R^{++}(t) + 2x_i x_f R^{+-}(t) + x_f^2 R^{--}(t)]\,, \tag{5.56}$$

where we used eq. (5.30) and introduced the functions

$$C_j^+(t) = \int_0^t ds\, C_j(s)\,\frac{G_+(t-s)}{G_+(t)}\,, \qquad j = 1, 2\,, \tag{5.57}$$

$$C_j^-(t) = \int_0^t ds\, C_j(s)\,\frac{G_-(s)}{G_-(t)}\,, \qquad j = 1, 2\,, \tag{5.58}$$

and

$$R^{+-}(t) = \int_0^t ds \int_0^t du\, R(s, u)\,\frac{G_+(t-s)}{G_+(t)}\,\frac{G_-(s)}{G_-(t)} \tag{5.59}$$

with $R^{++}(t)$ and $R^{--}(t)$ defined accordingly. In view of the relation (5.52) expressing $G_-(s)$ in terms of $G_+(t-s)$, these functions are not all independent. In fact it is readily seen that

$$C_j^-(t) = G_+(t)\,\frac{d}{dt}\,C_j^+(t)\,. \tag{5.60}$$

By the same token we can connect the functions $R^{++}(t)$, $R^{+-}(t)$, and $R^{--}(t)$. Introducing

$$\Psi(t, t') = \int_0^t ds \int_0^{t'} du\, R(s, u)\,\frac{G_+(t-s)}{G_+(t)}\,\frac{G_+(t'-u)}{G_+(t')}\,, \tag{5.61}$$

we have

$$R^{++}(t) = \Psi(t, t)\,, \tag{5.62}$$

$$R^{+-}(t) = R^{-+}(t) = G_+(t)[\partial\Psi(t, t')/\partial t]_{t=t'}\,, \tag{5.63}$$

$$R^{--}(t) = G_+^2(t)[\partial^2\Psi(t, t')/\partial t\partial t']_{t=t'}\,, \tag{5.64}$$

so that all functions defined in eqs. (5.57–5.59) can be expressed in terms of $C_1^+(t)$, $C_2^+(t)$, and $\Psi(t, t')$.

As we have already noted, the functional integral (4.34) is Gaussian for a harmonically bound particle. Thus the propagating function takes the form

$$J(x_f, r_f, t, x_i, r_i, \bar{x}, \bar{r}) = \frac{1}{N(t)} \exp\left[\frac{i}{\hbar} \Sigma(x_f, r_f, t, x_i, r_i, \bar{x}, \bar{r})\right], \tag{5.65}$$

where $N(t)$ is a normalization factor arising from the fluctuation modes about the minimal action paths. On the other hand, since the factor $N(t)$ is independent of the endpoints x_f, r_f, x_i, r_i, $\bar{x}$, and $\bar{r}$ it can more easily be determined from the conservation of normalization of the density matrix. This calculation and a number of further conclusions resulting in a simplification of $J(x_f, r_f, t, x_i, r_i, \bar{x}, \bar{r})$ will be presented in the following section.

6. Equilibrium correlation functions and response functions

In the preceding section we have calculated the minimal action $\Sigma(x_f, r_f, t, x_i, r_i, \bar{x}, \bar{r})$ of a damped harmonic oscillator which, apart from a time-dependent normalization factor, determines the function $J(x_f, r_f, t, x_i, r_i, \bar{x}, \bar{r})$ governing the time evolution of the density matrix. Although the result (5.56) manifestly displays the dependence of the minimal action on the boundary values, the time dependence of the action is still expressed in terms of auxiliary functions the physical meaning of which is unclear. In this section we shall apply the theory to calculate basic properties of the stationary equilibrium process of quantum Brownian motion. In turn, this will allow us to recast $J(x_f, r_f, t, x_i, r_i, \bar{x}, \bar{r})$ into a form particularly useful for further applications.

6.1. Linear response of the coordinate to an applied force

Let us first consider the response of a system initially in equilibrium to an external force $F(t)$ acting for $t \geq 0$. Then, we have $W_0 = W_\beta$ and, in terms of the sum and difference variables (4.30), the function $\lambda(q, \bar{q}, q', \bar{q}')$ characterizing the initial deviation from equilibrium [cf. (2.11)] simply becomes

$$\lambda_\beta(x_i, r_i, \bar{x}, \bar{r}) = \delta(x_i - \bar{x})\delta(r_i - \bar{r}) . \tag{6.1}$$

It is convenient to introduce the reduced function

$$\begin{aligned} J_\beta(x_f, r_f, t, x_i, r_i) &= \int d\bar{x}\, d\bar{r}\, J(x_f, r_f, t, x_i, r_i, \bar{x}, \bar{r})\lambda_\beta(x_i, r_i, \bar{x}, \bar{r}) \\ &= J(x_f, r_f, t, x_i, r_i, x_i, r_i) \end{aligned} \tag{6.2}$$

in terms of which the expectation value $\langle f(q)\rangle_t$ of a variable f which is a function of the particle coordinate q takes the form

$$\langle f(q)\rangle_t = \int dr_f\, f(r_f)\rho(r_f, x_f = 0, t) = \int dr_f\, dx_i\, dr_i\, f(r_f)\, J_\beta(0, r_f, t, x_i, r_i) . \tag{6.3}$$

Furthermore, we introduce the vector notation

$$\boldsymbol{a}_{\mathrm{i}} = \begin{pmatrix} x_{\mathrm{i}} \\ r_{\mathrm{i}} \end{pmatrix}; \qquad \boldsymbol{a}_{\mathrm{f}} = \begin{pmatrix} x_{\mathrm{f}} \\ r_{\mathrm{f}} \end{pmatrix}. \tag{6.4}$$

Now, inserting eqs. (5.65) and (5.56) into eq. (6.2) we obtain for $x_{\mathrm{f}} = 0$

$$J_\beta(0, r_{\mathrm{f}}, t, x_{\mathrm{i}}, r_{\mathrm{i}}) = \frac{1}{N(t)} \exp\left[-\frac{\mathrm{i}}{\hbar} \frac{M x_{\mathrm{i}}}{G_+(t)} \left(r_{\mathrm{f}} - \frac{1}{M} \int_0^t \mathrm{d}s\, G_+(t-s) F(s) \right) \right] \exp(-\tfrac{1}{2} \boldsymbol{a}_{\mathrm{i}} \boldsymbol{M}(t) \boldsymbol{a}_{\mathrm{i}}) , \tag{6.5}$$

where the time-dependent matrix $\boldsymbol{M}(t)$ is given by

$$\boldsymbol{M}(t) = \frac{M}{\hbar} \begin{pmatrix} \Omega - 2C_2^+(t) + R^{++}(t) & -\mathrm{i}(\dot{G}_+(t)/G_+(t) + C_1^+(t)) \\ -\mathrm{i}(\dot{G}_+(t)/G_+(t) + C_1^+(t)) & 1/\Lambda \end{pmatrix} \tag{6.6}$$

Using eqs. (6.3) and (6.5), we obtain for $f(q) = 1$ the normalization condition

$$\langle 1 \rangle_t = \int \mathrm{d}r_{\mathrm{f}}\, \mathrm{d}x_{\mathrm{i}}\, \mathrm{d}r_{\mathrm{i}}\, J_\beta(0, r_{\mathrm{f}}, t, x_{\mathrm{i}}, r_{\mathrm{i}}) = \frac{1}{N(t)} 2\pi\hbar \frac{1}{M} |G_+(t)| \left(2\pi\hbar \frac{1}{M} \Lambda \right)^{1/2} = 1 , \tag{6.7}$$

where we used

$$\int \mathrm{d}r_{\mathrm{f}} \exp\left(-\frac{\mathrm{i}}{\hbar} \frac{M}{G_+(t)} r_{\mathrm{f}} x_{\mathrm{i}} \right) = 2\pi\hbar \frac{1}{M} |G_+(t)| \delta(x_{\mathrm{i}}) . \tag{6.8}$$

The result (6.7) shows that the normalization factor $N(t)$ is given by

$$N(t) = 2\pi\hbar \frac{1}{M} |G_+(t)| \left(2\pi\hbar \frac{1}{M} \Lambda \right)^{1/2} . \tag{6.9}$$

The same result can be obtained by performing the functional integral over the fluctuations about the classical paths explicitly.

Now, the response of the coordinate q to the time-dependent force $F(s)$ follows from eq. (6.3) for $f(q) = q$. We find

$$\langle q \rangle_t = \int \mathrm{d}r_{\mathrm{f}}\, \mathrm{d}x_{\mathrm{i}}\, \mathrm{d}r_{\mathrm{i}}\, r_{\mathrm{f}} J_\beta(0, r_{\mathrm{f}}, t, x_{\mathrm{i}}, r_{\mathrm{i}}) = \int_0^t \mathrm{d}s\, G_+(t-s) \frac{1}{M} F(s) , \tag{6.10}$$

where we took advantage of the fact that

$$\int \mathrm{d}r_{\mathrm{f}}\, r_{\mathrm{f}} \exp\left(-\frac{\mathrm{i}}{\hbar} \frac{M}{G_+(t)} r_{\mathrm{f}} x_{\mathrm{i}} \right) = 2\pi\mathrm{i} \left(\frac{\hbar}{M} \right)^2 G_+(t) |G_+(t)| \delta'(x_{\mathrm{i}}) , \tag{6.11}$$

in which $\delta'(x)$ denotes the derivative of the δ-function. Hence, a partial integration and use of eq. (6.8) readily leads to the second equality in eq. (6.10). The response function $\chi(t)$ of the quantum oscillator defined through

$$\langle q \rangle_t = \int_0^t \mathrm{d}s\, \chi(t-s) F(s) \tag{6.12}$$

thus reads

$$\chi(t) = (1/M) G_+(t)\,, \tag{6.13}$$

for $t \geq 0$. In view of eq. (5.46), the Laplace transformed response function is given by

$$\hat{\chi}(z) = \frac{1}{M} \frac{1}{\omega_0^2 + z^2 + z\hat{\gamma}(z)}\,. \tag{6.14}$$

This result is in fact identical with the classical response function of a damped harmonic oscillator with frequency-dependent damping. For a strictly linear system as the one discussed here, the absence of quantum corrections to the response function is a consequence of Ehrenfest's theorem [35].

6.2. Coordinate autocorrelation function

Let us next consider the equilibrium coordinate autocorrelation function

$$C(t) = \langle q(t) q \rangle = \mathrm{tr}(q(t) q W_\beta)\,, \tag{6.15}$$

where tr denotes the trace over all coordinates of the entire system. Hence, $C(t)$ may formally be looked upon as the expectation value of the coordinate q at time t of a system with an initial "density matrix" $W_0 = qW_\beta$. As already mentioned in section 2 the initial state W_0 need not be a positive normalized density matrix for the present theory to hold. In view of eq. (2.11) the corresponding function $\lambda(q, \bar{q}, q', \bar{q}')$ then takes the form

$$\lambda_q(x_\mathrm{i}, r_\mathrm{i}, \bar{x}, \bar{r}) = (r_\mathrm{i} + \tfrac{1}{2} x_\mathrm{i}) \lambda_\beta(x_\mathrm{i}, r_\mathrm{i}, \bar{x}, \bar{r})\,. \tag{6.16}$$

Using eq. (6.2) the correlation function $C(t)$ may thus be written

$$C(t) = \int \mathrm{d}r_\mathrm{f}\, \mathrm{d}x_\mathrm{i}\, \mathrm{d}r_\mathrm{i}\, r_\mathrm{f}(r_\mathrm{i} + \tfrac{1}{2} x_\mathrm{i}) J_\beta(0, r_\mathrm{f}, t, x_\mathrm{i}, r_\mathrm{i})\,. \tag{6.17}$$

Now, we insert eq. (6.5) for vanishing external force $F(s)$. The integral over r_f may readily be performed by means of eq. (6.11). This gives a δ-function such that the integral over x_i becomes trivial leaving us with

$$C(t) = -\frac{2\pi \mathrm{i}}{N(t)} \left(\frac{\hbar}{M} G_+(t)\right)^2 \int \mathrm{d}r_\mathrm{i}\, (\tfrac{1}{2} - \tfrac{1}{2} M_{12}(t) r_\mathrm{i}^2) \exp\left(-\frac{M}{2\hbar\Lambda} r_\mathrm{i}^2\right). \tag{6.18}$$

Finally inserting $M_{12}(t)$ from eq. (6.6) and $N(t)$ from eq. (6.9) we gain

$$C(t) = S(t) + \mathrm{i} A(t)\,, \tag{6.19}$$

where the real part

$$S(t) = \frac{\hbar}{M} \Lambda(\dot{G}_+(t) + G_+(t)C_1^+(t)) \tag{6.20}$$

is the symmetrized correlation $(1/2)\langle q(t)q + qq(t)\rangle$ while the imaginary part

$$A(t) = -\frac{\hbar}{2M} G_+(t) = -\frac{\hbar}{2}\chi(t), \qquad \text{for } t \geq 0 \tag{6.21}$$

is the antisymmetrized correlation $(1/2\mathrm{i})\langle q(t)q - qq(t)\rangle$ which is related to the response function (6.13) in the usual way [45].

6.3. The fluctuation dissipation theorem

Because of the fluctuation dissipation theorem $S(t)$ and $\chi(t)$ are not independent. To recover this relation from our results we first note that eqs. (4.59), (5.13), and (5.46) combine to give

$$u_n = \hat{G}_+(|\nu_n|). \tag{6.22}$$

Hence, inserting eqs. (4.55) and (5.26) into eq. (5.57) we find

$$G_+(t)C_1^+(t) = \frac{1}{\hbar\beta\Lambda} \sum_{n=-\infty}^{\infty} \hat{G}_+(|\nu_n|) \int_0^t \mathrm{d}s\, G_+(t-s)[\gamma(s) - \zeta_n(s)]. \tag{6.23}$$

The Laplace transform $\hat{S}(z)$ of the symmetrized correlation function (6.20) thus takes the form

$$\hat{S}(z) = \frac{\hbar}{M} \Lambda z\hat{G}_+(z) + \frac{1}{\beta M} \sum_{n=-\infty}^{\infty} \hat{G}_+(|\nu_n|)\hat{G}_+(z)[\hat{\gamma}(z) - \hat{\zeta}_n(z)]. \tag{6.24}$$

Using eq. (4.58) we can relate the Laplace transform $\hat{\zeta}_n(z)$ to $\hat{\gamma}(z)$ through

$$\hat{\zeta}_n(z) = \frac{1}{z^2 - \nu_n^2}[z|\nu_n|\hat{\gamma}(|\nu_n|) - \nu_n^2\hat{\gamma}(z)]. \tag{6.25}$$

Furthermore, the frequency-dependent damping coefficient $\hat{\gamma}(z)$ may be eliminated in favour of $\hat{G}_+(z)$ by means of eq. (5.46). Finally, the Laplace transform $\hat{S}(z)$ emerges as

$$\hat{S}(z) = \frac{1}{\beta M} \sum_{n=-\infty}^{\infty} \frac{z}{\nu_n^2 - z^2}[\hat{G}_+(z) - \hat{G}_+(|\nu_n|)], \tag{6.26}$$

where we used eqs. (5.18) and (6.22). Due to the stationarity of the equilibrium process, $S(t)$ is an even function of t so that its Fourier transform

$$\tilde{S}(\omega) = \int_{-\infty}^{\infty} \mathrm{d}t\, S(t) \exp(\mathrm{i}\omega t) \tag{6.27}$$

is related to the Laplace transform $\hat{S}(z)$ by

$$\tilde{S}(\omega) = \hat{S}(\mathrm{i}\omega) + \hat{S}(-\mathrm{i}\omega)\,. \tag{6.28}$$

Hence, using eqs. (6.13) and (6.26), we obtain the fluctuation dissipation theorem

$$\tilde{S}(\omega) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} \frac{\mathrm{i}\omega}{\omega^2 + \nu_n^2} [\hat{\chi}(\mathrm{i}\omega) - \hat{\chi}(-\mathrm{i}\omega)]\,. \tag{6.29}$$

To cast this relation between the correlation and response functions into the usual form we introduce the dynamic susceptibility

$$\tilde{\chi}(\omega) = \int_{-\infty}^{\infty} \mathrm{d}t\, \chi(t) \exp(\mathrm{i}\omega t) = \hat{\chi}(-\mathrm{i}\omega)\,, \tag{6.30}$$

where the second equality holds since the response function vanishes for $t<0$. From eq. (6.29) and the series expansion (4.9) for $\tau = 0$, we easily see that the imaginary part

$$\tilde{\chi}''(\omega) = \tfrac{1}{2}\mathrm{i}[\hat{\chi}(\mathrm{i}\omega) - \hat{\chi}(-\mathrm{i}\omega)] \tag{6.31}$$

is related to $\tilde{S}(\omega)$ by

$$\tilde{S}(\omega) = \hbar \coth(\tfrac{1}{2}\omega\hbar\beta)\, \tilde{\chi}''(\omega) \tag{6.32}$$

which is a familiar form of the fluctuation dissipation theorem [45].

6.4. Linear response of the momentum to an applied force

So far we have considered the response and correlation functions for the coordinate q of the Brownian particle only. However, for a system initially in equilibrium which is subject to an external force $F(t)$ for $t>0$ we may also study the response of the momentum of the particle which is given by

$$\begin{aligned}\langle p \rangle_t &= \int \mathrm{d}x_\mathrm{f}\, \mathrm{d}r_\mathrm{f}\, \delta(x_\mathrm{f}) \left(\frac{\hbar}{\mathrm{i}} \frac{\partial}{\partial x_\mathrm{f}}\right) \rho(x_\mathrm{f}, r_\mathrm{f}, t) \\ &= \int \mathrm{d}r_\mathrm{f}\, \mathrm{d}x_\mathrm{i}\, \mathrm{d}r_\mathrm{i} \left[\frac{\hbar}{\mathrm{i}} \frac{\partial}{\partial x_\mathrm{f}} J_\beta(x_\mathrm{f}, r_\mathrm{f}, t, x_\mathrm{i}, r_\mathrm{i})\right]_{x_\mathrm{f}=0}\,.\end{aligned} \tag{6.33}$$

Inserting eqs. (5.56) and (5.65) in eq. (6.2) we obtain

$$\begin{aligned}\left[\frac{\hbar}{\mathrm{i}} \frac{\partial}{\partial x_\mathrm{f}} J_\beta(x_\mathrm{f}, r_\mathrm{f}, t, x_\mathrm{i}, r_\mathrm{i})\right]_{x_\mathrm{f}=0} &= M\Big[r_\mathrm{f} \frac{\dot{G}_+(t)}{G_+(t)} - \mathrm{i}x_\mathrm{i}(C_2^-(t) - R^{+-}(t)) \\ &+ r_\mathrm{i}\Big(C_1^-(t) - \frac{1}{G_-(t)}\Big) + \int_0^t \mathrm{d}s\, \frac{G_-(s)}{G_-(t)} \frac{F(s)}{M}\Big] J_\beta(0, r_\mathrm{f}, t, x_\mathrm{i}, r_\mathrm{i})\,.\end{aligned} \tag{6.34}$$

The integral over r_f in eq. (6.33) may now be performed using eqs. (6.8) and (6.11). The integral over x_i is then again trivial and we are left with

$$\langle p\rangle_t = \left(2\pi\,\frac{\hbar}{M}\,\Lambda\right)^{-1/2}\int \mathrm{d}r_i \int_0^t \mathrm{d}s\, F(s)\left(\frac{\dot G_+(t)}{G_+(t)}\,G_+(t-s)+\frac{G_-(s)}{G_-(t)}\right)\exp\left(-\frac{M}{2\hbar\Lambda}\,r_i^2\right), \tag{6.35}$$

where terms proportional to r_i in the integrand were dropped since they do not contribute to the integral. Now, by use of eqs. (5.52) and (6.13), the response of the momentum becomes

$$\langle p\rangle_t = M\int_0^t \mathrm{d}s\,\dot\chi(t-s)F(s)\,. \tag{6.36}$$

Indeed, this result is an immediate consequence of $p = M\dot q$.

6.5. Further correlation functions

We now turn to the momentum-coordinate correlation function

$$C_{pq}(t) = \langle p(t)q\rangle = \mathrm{tr}(p(t)qW_\beta)\,. \tag{6.37}$$

Following the reasoning leading to eq. (6.17) we easily see that $C_{pq}(t)$ may be written as

$$C_{pq}(t) = \int \mathrm{d}r_f\,\mathrm{d}x_i\,\mathrm{d}r_i\,(r_i+\tfrac{1}{2}x_i)\left[\frac{\hbar}{\mathrm{i}}\,\frac{\partial}{\partial x_f}\,J_\beta(x_f, r_f, t, x_i, r_i)\right]_{x_f=0} \tag{6.38}$$

Now, inserting eq. (6.34) for vanishing external force, and performing the integrations over r_f and x_i as above, the correlation (6.38) becomes

$$C_{pq}(t) = \frac{2\pi\hbar|G_+(t)|}{N(t)}\int \mathrm{d}r_i\left[-\frac{\mathrm{i}\hbar}{2M}\,\dot G_+(t)\right.$$
$$\left.+\,r_i^2\left(C_i^-(t)-\frac{1}{G_-(t)}+\mathrm{i}\,\frac{\hbar}{M}\,\dot G_+(t)M_{12}(t)\right)\right]\exp\left(-\frac{M}{2\hbar\Lambda}\,r_i^2\right). \tag{6.39}$$

The remaining Gaussian integral is easily done giving

$$C_{pq}(t) = \hbar\Lambda\left(C_1^-(t)-\frac{1}{G_-(t)}\right)+\hbar\Lambda\dot G_+(t)\left(C_1^+(t)+\frac{\dot G_+(t)}{G_+(t)}\right)-\mathrm{i}\,\frac{\hbar}{2}\,\dot G_+(t)\,. \tag{6.40}$$

Since the function $C_1^-(t)$ is connected with $C_1^+(t)$ by eq. (5.60) it can be expressed in terms of $G_+(t)$ and $S(t)$ by means of eq. (6.20). This yields

$$C_1^-(t) = -\ddot G_+(t)+\frac{\dot G_+^2(t)}{G_+(t)}+\frac{M}{\hbar\Lambda}\left[\dot S(t)-\frac{\dot G_+(t)}{G_+(t)}\,S(t)\right]. \tag{6.41}$$

Further, eq. (5.51) gives

$$\frac{1}{G_-(t)} = \frac{\dot{G}_+^2(t)}{G_+(t)} - \ddot{G}_+(t) . \tag{6.42}$$

Collecting the results, we find

$$C_{pq}(t) = M\dot{S}(t) - \mathrm{i}\frac{\hbar}{2}\dot{G}_+(t) = M\dot{C}(t) , \tag{6.43}$$

which is again an immediate consequence of $p = M\dot{q}$.

Let us now determine the coordinate-momentum correlation function

$$C_{qp}(t) = \langle q(t)p \rangle = \mathrm{tr}(q(t)pW_\beta) , \tag{6.44}$$

where the coordinate is measured after the momentum. To calculate this quantity directly from the functional integral we must consider an initial "density matrix" of the form $W_0 = pW_\beta$ which is associated with the preparation function

$$\lambda_p(q_\mathrm{i}, \bar{q}, q_\mathrm{i}', \bar{q}') = \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial q_\mathrm{i}}\lambda_\beta(q_\mathrm{i}, \bar{q}, q_\mathrm{i}', \bar{q}') = -\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial \bar{q}}\lambda_\beta(q_\mathrm{i}, \bar{q}, q_\mathrm{i}', \bar{q}') . \tag{6.45}$$

It is at this point that we first encounter an explicit example of an initial state which can be treated within our approach only because we have distinguished between the endpoints of the imaginary time path and the starting points of the real time paths. The time evolution of this state is described by the function

$$\begin{aligned} J_p(x_\mathrm{f}, r_\mathrm{f}, t, x_\mathrm{i}, r_\mathrm{i}) &= \int \mathrm{d}\bar{x}\,\mathrm{d}\bar{r}\,\lambda_p(x_\mathrm{i}, r_\mathrm{i}, \bar{x}, \bar{r}) J(x_\mathrm{f}, r_\mathrm{f}, t, x_\mathrm{i}, r_\mathrm{i}, \bar{x}, \bar{r}) \\ &= \frac{\hbar}{\mathrm{i}}\left[\frac{\partial}{\partial \bar{q}} J(x_\mathrm{f}, r_\mathrm{f}, t, x_\mathrm{i}, r_\mathrm{i}, \bar{q}, \bar{q}')\right]_{\bar{q}=q_\mathrm{i}, \bar{q}'=q_\mathrm{i}'} \\ &= M\left[x_\mathrm{i}(\tfrac{1}{2}C_1^+(t) + \mathrm{i}(\Omega - C_2^+(t))) + x_\mathrm{f}(\tfrac{1}{2}C_1^-(t) - \mathrm{i}C_2^-(t)) + \frac{\mathrm{i}}{2\Lambda} r_\mathrm{i}\right] \\ &\quad \times J_\beta(x_\mathrm{f}, r_\mathrm{f}, t, x_\mathrm{i}, r_\mathrm{i}) , \end{aligned} \tag{6.46}$$

where we used eqs. (5.56) and (5.65) to obtain the last line. The correlation function (6.44) may now be written as

$$C_{qp}(t) = \int \mathrm{d}r_\mathrm{f}\,\mathrm{d}x_\mathrm{i}\,\mathrm{d}r_\mathrm{i}\, r_\mathrm{f} J_p(0, r_\mathrm{f}, t, x_\mathrm{i}, r_\mathrm{i}) . \tag{6.47}$$

Inserting eq. (6.46) and performing the integrations over r_f and x_i by the method described above, we arrive at

$$C_{qp}(t) = -\frac{2\pi i M}{N(t)} (\hbar/M)^2 G_+(t)|G_+(t)|$$
$$\times \int dr_i \left[\tfrac{1}{2} C_1^+(t) - i C_2^+(t) + i\Omega - \frac{i}{2\Lambda} M_{12}(t) r_i^2 \right] \exp\left(-\frac{M}{2\hbar\Lambda} r_i^2 \right). \tag{6.48}$$

Now, inserting $M_{12}(t)$ from eq. (6.6) we see that $C_1^+(t)$ cancels. Further, combining eqs. (4.56), (5.27), and (6.22), the function $C_2^+(t)$ defined in eq. (5.57) takes the form

$$C_2^+(t) = -\frac{1}{\hbar\beta} \sum_{n=-\infty}^{\infty} \hat{G}_+(|\nu_n|) \int_0^t ds \, \frac{G_+(t-s)}{G_+(t)} \frac{d}{ds} \zeta_n(s). \tag{6.49}$$

The Laplace transform of $G_+(t)C_2^+(t)$ can now readily be expressed in terms of $\hat{G}_+(z)$ by means of eqs. (5.46) and (6.25). Comparing the result with eq. (6.26) we find

$$C_2^+(t) = \frac{M}{\hbar} \frac{\dot{S}(t)}{G_+(t)} + \Omega, \tag{6.50}$$

where Ω is defined in eq. (5.25). From eq. (6.48) the correlation $C_{qp}(t)$ now emerges as

$$C_{qp}(t) = -M\dot{S}(t) + i\frac{\hbar}{2} \dot{G}_+(t) = -M\dot{C}(t), \tag{6.51}$$

which is in accordance with the symmetry $C_{pq}(t) = -C_{qp}(t)$.

It is also straightforward to calculate the momentum autocorrelation function

$$C_{pp}(t) = \langle p(t)p \rangle = \mathrm{tr}(p(t)pW_\beta) \tag{6.52}$$

which in terms of $J_p(x_f, r_f, t, x_i, r_i)$ may be written as

$$C_{pp}(t) = \int dr_f \, dx_i \, dr_i \left[\frac{\hbar}{i} \frac{\partial}{\partial x_f} J_p(x_f, r_f, t, x_i, r_i) \right]_{x_f=0} \tag{6.53}$$

After the r_f and x_i integrations this gives

$$C_{pp}(t) = \left(\frac{M}{2\pi\hbar\Lambda} \right)^{1/2} \int dr_i \left(M\hbar \left[\dot{G}_+(t)(\Omega - C_2^+(t)) - C_2^-(t) - \frac{i}{2} C_1^-(t) - \frac{i}{2} \dot{G}_+(t) C_1^+(t) \right] \right.$$
$$\left. + i\frac{M^2}{2\Lambda} \left[\dot{G}_+(t) \left(\frac{\dot{G}_+(t)}{G_+(t)} + C_1^+(t) \right) + C_1^-(t) - \frac{1}{G_-(t)} \right] r_i^2 \right) \exp\left(-\frac{M}{2\hbar\Lambda} r_i^2 \right). \tag{6.54}$$

The remaining integration over r_i is readily performed and we obtain the expected result

$$C_{pp}(t) = -M^2\ddot{S}(t) + \frac{i}{2} M\hbar \ddot{G}_+(t) = -M^2\ddot{C}(t) \tag{6.55}$$

where the expressions (5.60) and (6.50) for the functions $C_j^{\pm}(t)$ were used.

6.6. Variances

So far we have not considered quantities which explicitly depend on the functions $R^{\pm\pm}(t)$ appearing in the action (5.56). However, the terms containing these functions are necessary in order that the equilibrium process be stationary. This is readily seen by studying the variances at time t of an equilibrium system. They are given by

$$\langle q^2\rangle_t = \int \mathrm{d}r_\mathrm{f}\,\mathrm{d}x_\mathrm{i}\,\mathrm{d}r_\mathrm{i}\, r_\mathrm{f}^2 J_\beta(0, r_\mathrm{f}, t, x_\mathrm{i}, r_\mathrm{i})\,, \tag{6.56}$$

$$\tfrac{1}{2}\langle pq + qp\rangle_t = \int \mathrm{d}r_\mathrm{f}\,\mathrm{d}x_\mathrm{i}\,\mathrm{d}r_\mathrm{i}\, r_\mathrm{f}\frac{\hbar}{\mathrm{i}}\left[\frac{\partial}{\partial x_\mathrm{f}} J_\beta(x_\mathrm{f}, r_\mathrm{f}, t, x_\mathrm{i}, r_\mathrm{i})\right]_{x_\mathrm{f}=0}, \tag{6.57}$$

$$\langle p^2\rangle_t = -\int \mathrm{d}r_\mathrm{f}\,\mathrm{d}x_\mathrm{i}\,\mathrm{d}r_\mathrm{i}\,\hbar^2\left[\frac{\partial^2}{\partial x_\mathrm{f}^2} J_\beta(x_\mathrm{f}, r_\mathrm{f}, t, x_\mathrm{i}, r_\mathrm{i})\right]_{x_\mathrm{f}=0}. \tag{6.58}$$

We may now insert the explicit expression for $J_\beta(x_\mathrm{f}, r_\mathrm{f}, t, x_\mathrm{i}, r_\mathrm{i})$ which is in fact the general expression (5.65) for $J(x_\mathrm{f}, r_\mathrm{f}, t, x_\mathrm{i}, r_\mathrm{i}, \bar{x}, \bar{r})$ with the effective action (5.56) taken at $\bar{r} = r_\mathrm{i}$ and $\bar{x} = x_\mathrm{i}$. Performing the Gaussian integrals in the usual order we obtain after some algebra

$$\langle q^2\rangle_t = \left(\frac{\hbar}{M} G_+(t)\right)^2\left[M_{11}(t) - \frac{\hbar}{M}\Lambda M_{12}^2(t)\right], \tag{6.59}$$

$$\begin{aligned}\tfrac{1}{2}\langle pq + qp\rangle_t &= M\langle q^2\rangle_t \frac{\dot{G}_+(t)}{G_+(t)} + \hbar G_+(t)\left(R^{+-}(t) - C_2^-(t)\right)\\ &\quad + \mathrm{i}\frac{\hbar^2\Lambda}{M} G_+(t)\left(C_1^-(t) - \frac{1}{G_-(t)}\right)M_{12}(t)\,,\end{aligned} \tag{6.60}$$

$$\begin{aligned}\langle p^2\rangle_t &= \hbar M R^{--}(t) + \hbar M\Lambda\left[C_1^-(t) - \frac{1}{G_-(t)}\right]^2 + M^2\frac{\dot{G}_+^2(t)}{G_+^2(t)}\left(\langle q^2\rangle_t - 2\frac{\hbar}{M}\Lambda\right)\\ &\quad + M\frac{\dot{G}_+(t)}{G_+(t)}\langle pq + qp\rangle_t\,,\end{aligned} \tag{6.61}$$

where the elements $M_{ij}(t)$ of the matrix $\boldsymbol{M}(t)$ were introduced in eq. (6.6). To proceed we now have to determine the functions $R^{\pm\pm}(t)$ more explicitly using the Laplace transform techniques which were employed above to transform the functions $C_j^{\pm}(t)$. The corresponding calculation is outlined in appendix B. The results for all auxiliary functions appearing in the action (5.56) are summarized in table 1. Using eq. (6.6) and table 1, the variances (6.59–6.61) become

$$\langle q^2\rangle_t = (\hbar/M)\Lambda\,, \tag{6.62}$$

$$\tfrac{1}{2}\langle pq + qp\rangle_t = 0\,, \tag{6.63}$$

$$\langle p^2\rangle_t = \hbar M\Omega\,, \tag{6.64}$$

Table 1
Relation between the functions $C_j^{\pm}(t)$, $R^{\pm\pm}(t)$ and the functions $G_+(t)$, $S(t)$

$$C_1^+(t) = \frac{1}{G_+(t)}\left[\frac{M}{\hbar\Lambda}\,S(t) - \dot{G}_+(t)\right]$$

$$C_1^-(t) = \frac{M}{\hbar\Lambda}\left[\dot{S}(t) - \frac{\dot{G}_+(t)}{G_+(t)}\,S(t)\right] - \ddot{G}_+(t) + \frac{\dot{G}_+^2(t)}{G_+(t)}$$

$$C_2^+(t) = \frac{M}{\hbar}\,\frac{\dot{S}(t)}{G_+(t)} + \Omega$$

$$C_2^-(t) = \frac{M}{\hbar}\left[\ddot{S}(t) - \frac{\dot{G}_+(t)}{G_+(t)}\,\dot{S}(t)\right]$$

$$R^{++}(t) = \Omega + 2\,\frac{M}{\hbar}\,\frac{\dot{S}(t)}{G_+(t)} + \frac{\Lambda}{G_+^2(t)}\left[1 - \left(\frac{M}{\hbar\Lambda}\,S(t)\right)^2\right]$$

$$R^{+-}(t) = \frac{M}{\hbar}\left[\ddot{S}(t) - \frac{\dot{G}_+(t)}{G_+(t)}\,\dot{S}(t)\right] - \frac{M^2}{\hbar^2\Lambda}\,\frac{1}{G_+^2(t)}\left[\left(\frac{\hbar}{M}\,\Lambda\right)^2\dot{G}_+(t) + G_+(t)S(t)\dot{S}(t) - \dot{G}_+(t)S^2(t)\right]$$

$$R^{--}(t) = \Omega - \frac{M^2}{\hbar^2\Lambda}\left[\dot{S}(t) - \frac{\dot{G}_+(t)}{G_+(t)}\,S(t)\right]^2 + \Lambda\,\frac{\dot{G}_+^2(t)}{G_+^2(t)}$$

Clearly, the variances are time independent as they should be for a system in thermal equilibrium. Furthermore, for eq. (6.26) we find

$$S(0) = \lim_{z\to\infty} z\hat{S}(z) = \frac{1}{\beta M}\sum_{n=-\infty}^{\infty}\hat{G}_+(|\nu_n|) = \frac{\hbar}{M}\Lambda\,, \tag{6.65}$$

$$\dot{S}(0) = \lim_{z\to\infty} z[z\hat{S}(z) - S(0)] = 0\,, \tag{6.66}$$

$$\ddot{S}(0) = \lim_{z\to\infty} z[z^2\hat{S}(z) - zS(0) - \dot{S}(0)] = \frac{1}{\beta M}\sum_{n=-\infty}^{\infty}[\nu_n^2\hat{G}_+(|\nu_n|) - 1] = -\frac{\hbar}{M}\,\Omega\,, \tag{6.67}$$

so that we recover the familiar relations

$$\langle q^2\rangle = S(0)\,, \tag{6.68}$$

$$\tfrac{1}{2}\langle pq + qp\rangle = M\dot{S}(0)\,, \tag{6.69}$$

$$\langle p^2\rangle = -M^2\ddot{S}(0)\,. \tag{6.70}$$

Table 2 collects the key formulas connecting variances, correlation functions and response functions of a damped harmonic oscillator with the model parameters M, ω_0, and $\hat{\gamma}(\omega)$.

6.7. Propagating function

Our previous result (5.56), (5.65) for the propagating function $J(x_f, r_f, t, x_i, r_i, \bar{x}, \bar{r})$ can now be rewritten entirely in terms of the correlation $C(t)$. Using table 1 we gain

$$J(x_f, r_f, t, x_i, r_i, \bar{x}, \bar{r}) = [4\pi|A(t)|]^{-1}(2\pi\langle q^2\rangle)^{-1/2}\exp\left(\frac{\mathrm{i}}{\hbar}\,\Sigma(x_f, r_f, t, x_i, r_i, \bar{x}, \bar{r})\right), \tag{6.71}$$

where

Table 2
The variances, correlation functions, and response functions of a damped harmonic oscillator in equilibrium in terms of the model parameters M, ω_0 and $\hat{\gamma}(\omega)$

Quantity	Laplace representation	Fourier representation
variance of position $\langle q^2 \rangle$	$\langle q^2 \rangle = \frac{1}{M\beta} \sum_{n=-\infty}^{\infty} \frac{1}{\omega_0^2 + \nu_n^2 + \lvert\nu_n\rvert \hat{\gamma}(\lvert\nu_n\rvert)}$	$\langle q^2 \rangle = \frac{\hbar}{M} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\omega \hat{\gamma}(-i\omega)}{(\omega_0^2 - \omega^2)^2 + \omega^2 \hat{\gamma}^2(-i\omega)} \coth(\frac{1}{2}\omega\hbar\beta)$
variance of momentum $\langle p^2 \rangle$	$\langle p^2 \rangle = \frac{M}{\beta} \sum_{n=-\infty}^{\infty} \frac{\omega_0^2 + \lvert\nu_n\rvert \hat{\gamma}(\lvert\nu_n\rvert)}{\omega_0^2 + \nu_n^2 + \lvert\nu_n\rvert \hat{\gamma}(\lvert\nu_n\rvert)}$	$\langle p^2 \rangle = M\hbar \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\omega^3 \hat{\gamma}(-i\omega)}{(\omega_0^2 - \omega^2)^2 + \omega^2 \hat{\gamma}^2(-i\omega)} \coth(\frac{1}{2}\omega\hbar\beta)$
antisymmetrized position autocorrelation function $A(t) = (1/2i)\langle [q(t), q] \rangle$	$\hat{A}(z) = -(\hbar/2M)[\omega_0^2 + z^2 + z\hat{\gamma}(z)]^{-1}$	$A(t) = -\frac{\hbar}{M} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\omega \hat{\gamma}(-i\omega)}{(\omega_0^2 - \omega^2)^2 + \omega^2 \hat{\gamma}^2(-i\omega)} \sin(\omega t)$
symmetrized position autocorrelation function $S(t) = (1/2)\langle q(t)q + qq(t) \rangle$	$\hat{S}(z) = \frac{2}{\hbar\beta} \sum_{n=-\infty}^{\infty} \frac{z}{z^2 - \nu_n^2} [\hat{A}(z) - \hat{A}(\lvert\nu_n\rvert)]$	$S(t) = \frac{\hbar}{M} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\omega \hat{\gamma}(-i\omega)}{(\omega_0^2 - \omega^2)^2 + \omega^2 \hat{\gamma}^2(-i\omega)} \coth(\frac{1}{2}\omega\hbar\beta) \cos(\omega t)$

additional formulae

position autocorrelation function	$C(t) = S(t) + iA(t)$;
response function	$\chi(t) = -(2/\hbar)A(t)\Theta(t)$;
Green's function	$G_+(t) = M\chi(t) = -(2/\hbar)MA(t)\Theta(t)$.

$$
\begin{aligned}
\Sigma(x_f, r_f, t, x_i, r_i, \bar{x}, \bar{r}) = {} & i\left(\frac{\hbar}{2\langle q^2 \rangle} \bar{r}^2 + \frac{\langle p^2 \rangle}{2\hbar} \bar{x}^2\right) \\
& + (x_i r_i + x_f r_f) M \frac{\dot{A}(t)}{A(t)} + x_i r_f \frac{\hbar}{2A(t)} - x_f r_i \frac{2}{\hbar} M^2 \left(\ddot{A}(t) - \frac{\dot{A}^2(t)}{A(t)}\right) \\
& + x_i \bar{r} \left[- M \frac{\dot{A}(t)}{A(t)} - \frac{\hbar S(t)}{2\langle q^2 \rangle A(t)} \right] + i x_i \bar{x} \left[- \frac{\langle p^2 \rangle}{\hbar} + \frac{M\dot{S}(t)}{2A(t)} \right] \\
& + x_f \bar{r} \left[\frac{2}{\hbar} M^2 \left(\ddot{A}(t) - \frac{\dot{A}^2(t)}{A(t)}\right) + \frac{M}{\langle q^2 \rangle} \left\{ \dot{S}(t) - \frac{\dot{A}(t)}{A(t)} S(t) \right\} \right] \\
& + i x_f \bar{x} \frac{M^2}{\hbar} \left\{ \dot{S}(t) \frac{\dot{A}(t)}{A(t)} - \ddot{S}(t) \right\} + i x_i^2 \left[\frac{\langle p^2 \rangle}{2\hbar} - \frac{M\dot{S}(t)}{2A(t)} + \frac{\hbar \langle q^2 \rangle}{8A^2(t)} \left(1 - \frac{S^2(t)}{\langle q^2 \rangle^2}\right) \right] \\
& + i x_i x_f \left[- \frac{M^2}{\hbar} \left\{ \dot{S}(t) \frac{\dot{A}(t)}{A(t)} - \ddot{S}(t) \right\} + \frac{M\langle q^2 \rangle}{2A^2(t)} \left\{ \dot{A}(t) \left(1 - \frac{S^2(t)}{\langle q^2 \rangle^2}\right) + A(t) \frac{S(t)\dot{S}(t)}{\langle q^2 \rangle^2} \right\} \right] \\
& + i x_f^2 \left[\frac{M^2 \dot{A}^2(t)}{2\hbar A^2(t)} \langle q^2 \rangle + \frac{\langle p^2 \rangle}{2\hbar} - \frac{M^2}{2\hbar \langle q^2 \rangle} \left\{ \frac{\dot{A}(t)}{A(t)} S(t) - \dot{S}(t) \right\}^2 \right] \\
& + x_i \int_0^t ds \frac{A(t-s)}{A(t)} F(s) - x_f \int_0^t ds \frac{2}{\hbar} M \left[\dot{A}(t-s) - A(t-s) \frac{\dot{A}(t)}{A(t)} \right] F(s) .
\end{aligned}
\tag{6.72}
$$

Clearly, the expression (6.71) is not defined for times t where $A(t) = 0$. Except for the special cases $t = 0$ and $t \to \infty$ treated below, there are additional zeros of $A(t)$ at intermediate times t_n in the case of an underdamped oscillator. For $t = t_n$ the function $J(x_f, r_f, t, x_i, r_i, \bar{x}, \bar{r})$ must be defined by a limiting procedure. The need for this regularization arises from the fact that for $A(t_n) = 0$ there is perfect focussing of all minimal action paths $x(t)$ starting from x_i. We obtain

$$J(x_f, r_f, t_n, x_i, r_i, \bar{x}, \bar{r}) = \lim_{t \to t_n} J(x_f, r_f, t, x_i, r_i, \bar{x}, \bar{r})$$

$$= \left[2\pi\langle q^2\rangle\left(1 - \frac{S^2(t_n)}{\langle q^2\rangle^2}\right)\right]^{-1/2} \delta\left(x_i + \frac{2}{\hbar} M\dot{A}(t_n)x_f\right) \exp\left[\frac{i}{\hbar} \Sigma'(x_f, r_f, t_n, x_i, r_i, \bar{x}, \bar{r})\right] \rho_\beta(\bar{x}, \bar{r}), \tag{6.73}$$

where

$$\Sigma'(x_f, r_f, t, x_i, r_i, \bar{x}, \bar{r}) = i\frac{\langle p^2\rangle}{2\hbar}(x_i^2 + x_f^2 - 2x_i\bar{x}) + i\frac{M^2}{\hbar}\ddot{S}(t)x_f(x_i - \bar{x})$$

$$-i\frac{M^2\dot{S}^2(t)}{2\hbar\langle q^2\rangle}x_f^2 + \frac{2}{\hbar}M^2\ddot{A}(t)x_f(\bar{r} - r_i) + M\frac{\dot{S}(t)}{\langle q^2\rangle}x_f\bar{r} - \int_0^t ds\,\frac{2}{\hbar}M\dot{A}(t-s)F(s)x_f$$

$$+i\frac{2}{\hbar}\left[\langle q^2\rangle - \frac{S^2(t)}{\langle q^2\rangle}\right]^{-1}\left[M\dot{A}(t)(\bar{r} - r_i) - \frac{\hbar}{2}\left(r_f - \frac{S(t)}{\langle q^2\rangle}\bar{r}\right)\right.$$

$$\left. + i\frac{M}{2}\dot{S}(t)\left(x_i - \bar{x} + \frac{S(t)}{\langle q^2\rangle}x_f\right) - \int_0^t ds\,A(t-s)F(s)\right]^2. \tag{6.74}$$

Here we made use of

$$\lim_{t \to t_n}(4\pi|A(t)|)^{-1}\exp\left[-\frac{\langle q^2\rangle}{8A^2(t)}\left(1 - \frac{S^2(t)}{\langle q^2\rangle^2}\right)x^2\right] = \left[2\pi\langle q^2\rangle\left(1 - \frac{S^2(t_n)}{\langle q^2\rangle^2}\right)\right]^{-1/2}\delta(x). \tag{6.75}$$

Hence, $J(x_f, r_f, t, x_i, r_i, \bar{x}, \bar{r})$ is well defined for all times $0 < t < \infty$. Special care must be taken for the zero of $A(t)$ at $t = 0$ since for $t \to 0$ the factor $(1 - S^2(t)/\langle q^2\rangle^2)$ approaches zero as well. However, for small times we can use the lowest order terms in the Taylor expansions of the correlation functions. From eqs. (6.66), (6.68), and (6.70) we get

$$S(t) = \langle q^2\rangle - \frac{\langle p^2\rangle}{2M^2}t^2 + O(t^4), \tag{6.76}$$

$$\dot{S}(t) = -\frac{\langle p^2\rangle}{M^2}t + O(t^3). \tag{6.77}$$

Further, eq. (6.21) readily gives

$$A(t) = -(\hbar/2M)t + O(t^3), \tag{6.78}$$

where we used $\dot{G}_+(0) = 1$. Now, inserting (6.76–6.78) in eqs. (6.71), (6.72) we find that for short times $J(x_f, r_f, t, x_i, r_i, \bar{x}, \bar{r})$ takes the form

$$J(x_f, r_f, t, x_i, r_i, \bar{x}, \bar{r}) = \frac{M}{2\pi\hbar t} \exp\left[\frac{iM}{\hbar t}(x_f - x_i)(r_f - r_i) + O(t)\right] \rho_\beta(\bar{x}, \bar{r}), \tag{6.79}$$

which in the limit $t \to 0$ becomes

$$J(x_f, r_f, 0, x_i, r_i, \bar{x}, \bar{r}) = \delta(x_f - x_i)\delta(r_f - r_i)\rho_\beta(\bar{x}, \bar{r}). \tag{6.80}$$

Hence, the density matrix properly reduces to the initial density matrix $\rho_0(x_i, r_i)$ for $t \to 0$.

The result (6.71, 6.72) is particularly convenient for further applications as will become clear below. The function $J(x_f, r_f, t, x_i, r_i, \bar{x}, \bar{r})$ determines the time evolution of a large class of initial states resulting from the preparation procedures discussed in section 2. As far as its practical value is concerned, $J(x_f, r_f, t, x_i, r_i, \bar{x}, \bar{r})$ can be compared with the conditional probability of a classical Gaussian process. However, due to its dependence on $\bar{x}$ and $\bar{r}$ it is in fact a more complicated quantity which fully takes into account the dependence of the process on the correlations between the particle and the reservoir in the initial state.

6.8. Effect of initial correlations

Initial correlations between the particle and the heat bath influence the stochastic process of Brownian motion already in the classical limit [41]. However, their influence on the stochastic process is more subtle in the quantum regime. By way of example, let us consider the initial state

$$W_1 = W_\beta + \langle p^2 \rangle^{-1/2} \tfrac{1}{2}(pW_\beta + W_\beta p), \tag{6.81}$$

which leads to the reduced density matrix

$$\rho_1 = \rho_\beta + \langle p^2 \rangle^{-1/2} \tfrac{1}{2}(p\rho_\beta + \rho_\beta p). \tag{6.82}$$

It is clear from eqs. (6.62–6.64) that in coordinate representation the reduced equilibrium density matrix ρ_β takes the form

$$\rho_\beta(x, r) = (2\pi\langle q^2 \rangle)^{-1/2} \exp\left[-\frac{1}{2}\left(\frac{r^2}{\langle q^2 \rangle} + \frac{\langle p^2 \rangle}{\hbar^2} x^2\right)\right]. \tag{6.83}$$

This result is also readily obtained from eq. (5.34). Inserting eq. (6.83) into eq. (6.82) we find

$$\rho_1(x, r) = \left(1 + \langle p^2 \rangle^{-1/2} \frac{\hbar\partial}{i\partial x}\right)\rho_\beta(x, r) = \left(1 + \langle p^2 \rangle^{1/2} \frac{i}{\hbar} x\right)\rho_\beta(x, r). \tag{6.84}$$

On the other hand, the same reduced density matrix is obtained, e.g. from the initial state

$$W_2 = W_\beta + \langle p^2 \rangle^{1/2} \frac{i}{\hbar} [q, W_\beta]. \tag{6.85}$$

The two density matrices W_1 and W_2 are associated with different preparation functions $\lambda(q, \bar{q}, q', \bar{q}')$ and, consequently, the Brownian particle will undergo a different stochastic process for each preparation despite the fact that the initial reduced density matrices are identical. However, the difference between the two preparations vanishes in the classical limit. Since the commutator $(i/\hbar)[\ ,\ ]$ reduces to the Poisson bracket we have

$$W_2^{\mathrm{cl}} = W_\beta^{\mathrm{cl}} - (k_{\mathrm{B}}TM)^{1/2} \frac{\partial}{\partial p} W_\beta^{\mathrm{cl}} = W_\beta^{\mathrm{cl}} + (k_{\mathrm{B}}TM)^{-1/2} p W_\beta^{\mathrm{cl}} = W_1^{\mathrm{cl}} , \tag{6.86}$$

where we used $\langle p^2 \rangle^{\mathrm{cl}} = k_{\mathrm{B}}TM$ and where W^{cl} denotes the classical probability distribution in phase space. It is in fact a general feature of the present theory that in the classical limit the function $\lambda(q, \bar{q}, q', \bar{q}')$ which depends on four variables reduces to a function determined uniquely in terms of the initial probability distribution in the two-dimensional phase space of the Brownian particle.

The explicit results obtained in this section clarify the physical meaning of some concepts introduced above. The quantum mechanical stochastic process is characterized by a "propagating function" $J(x_{\mathrm{f}}, r_{\mathrm{f}}, t, x_{\mathrm{i}}, r_{\mathrm{i}}, \bar{x}, \bar{r})$ and a "preparation function" $\lambda(x_{\mathrm{i}}, r_{\mathrm{i}}, \bar{x}, \bar{r})$. The function $J(x_{\mathrm{f}}, r_{\mathrm{f}}, t, x_{\mathrm{i}}, r_{\mathrm{i}}, \bar{x}, \bar{r})$ replaces the classical conditional probability. For the class of initial states introduced in section 2, the propagating function is determined entirely in terms of equilibrium properties of the process as it is the case for the classical stationary conditional probability. The preparation function $\lambda(x_{\mathrm{i}}, r_{\mathrm{i}}, \bar{x}, \bar{r})$ characterizes the particular initial state within the preparation class and replaces the classical initial phase space distribution. Apart from characterizing the initial state of the Brownian particle it also contains the additional information needed to specify a particular process out of those reducing to the same process in the classical limit.

7. Ohmic dissipation

In the preceding section we have shown that the time dependence of the propagating function $J(x_{\mathrm{f}}, r_{\mathrm{f}}, t, x_{\mathrm{i}}, r_{\mathrm{i}}, \bar{x}, \bar{r})$ can be expressed entirely in terms of the symmetrized part $S(t)$ and the antisymmetrized part $A(t)$ of the position autocorrelation function. However, for an arbitrary dissipative mechanism these quantities can only be determined in terms of their Laplace transforms. To gain explicit results we have to specify the frequency dependence of the damping coefficient. In this section we consider an Ohmic heat bath leading to frequency-independent damping. Ohmic reservoirs are of great theoretical and experimental relevance because they lead to Markovian damping terms in the classical equations of motion and they were successfully applied to explain recent experiments in the quantum regime [28]. Further, for Ohmic dissipation we can determine the time dependence of correlation functions explicitly and some of the calculations carried out so far simplify considerably. In fact, the bulk of previous work [14, 18–20] has dealt exclusively with Ohmic reservoirs. A Markovian or Ohmic damping kernel

$$\gamma(t) = 2\gamma\delta(t) \tag{7.1}$$

has a frequency-independent Laplace transform $\hat{\gamma}(\omega) = \gamma$ [cf. eq. (4.48)]. The classical equation of motion (4.46) then simply becomes

$$\ddot{q} + \gamma\dot{q} + \frac{1}{M} \frac{\partial}{\partial q} V(q, s) = 0 . \tag{7.2}$$

From eq. (4.50) we see that Ohmic damping emerges from the microscopic model only if the spectral density of the environment $I(\omega)$ takes the form [14]

$$I(\omega) = M\gamma\omega \,. \tag{7.3}$$

Clearly, the Markovian model can only be an approximation to the real world since a realistic spectral density vanishes in the limit $\omega \to \infty$. Nevertheless, a real heat bath with a high frequency cutoff ω_c but a linear spectral density of the form (7.3) for small frequencies $\omega \ll \omega_c$ can still behave like an Ohmic reservoir on the time scales relevant for an experiment provided they are large compared with ω_c^{-1}.

As is familiar from the theory of classical Markov processes, Ohmic damping leads to sum rule divergencies. Such a divergence arises here if we consider the equilibrium variances [35]. Using table 2 we have

$$\langle q^2 \rangle = \frac{1}{M\beta} \sum_{n=-\infty}^{\infty} \frac{1}{\omega_0^2 + \nu_n^2 + |\nu_n|\gamma} \tag{7.4}$$

and

$$\langle p^2 \rangle = \frac{M}{\beta} \sum_{n=-\infty}^{\infty} \frac{\omega_0^2 + |\nu_n|\gamma}{\omega_0^2 + \nu_n^2 + |\nu_n|\gamma} \,. \tag{7.5}$$

The last expression has an unphysical logarithmic divergence which points to its dependence on the environmental cutoff. The divergence is readily removed if we consider a realistic damping kernel with finite memory. For instance, a Drude model with $\gamma(t) = \gamma\omega_D \exp(-\omega_D t)$ leads to a finite value of $\langle p^2 \rangle$ given by

$$\langle p^2 \rangle = \frac{M}{\beta} \sum_{n=-\infty}^{\infty} \frac{\omega_0^2 + \gamma|\nu_n|\omega_D/(\omega_D + |\nu_n|)}{\omega_0^2 + \nu_n^2 + \gamma|\nu_n|\omega_D/(\omega_D + |\nu_n|)} \,. \tag{7.6}$$

Clearly, in the limit $\omega_D \gg \omega_0, \gamma$, the Drude model behaves like an Ohmic model except for very short times of order $1/\omega_D$. The temperature dependence of the variances $\langle q^2 \rangle$ and $\langle p^2 \rangle$ for a Drude model is depicted in fig. 3. We see that for high temperatures the variances are independent of γ and proportional to T as the equipartition law predicts. For low temperatures the variances approach a finite value. Note that the coordinate distribution of the damped oscillator is narrower than that of the undamped oscillator while the momentum distribution becomes broader due to dissipation.

It should also be noted that the constant μ given by eq. (4.4) is divergent for the Ohmic model. This does not affect the theory since μ cancels against the potential renormalization arising from the influence kernel $K(\theta)$. However, in a model without a counterterm in eq. (2.4) one has to take into account the potential renormalization and a proper treatment of the high frequency environmental modes is needed to keep μ finite.

Let us now consider the explicit form of some of our previous results in the Ohmic case. From eq. (4.51) we see that Ohmic damping arises from an influence kernel $K(\theta)$, $\theta = t - i\tau$, of the form

$$K(\theta) = -\frac{\pi M\gamma}{(\hbar\beta)^2} \sinh^{-2}(\tfrac{1}{2}\nu\theta) \,, \tag{7.7}$$

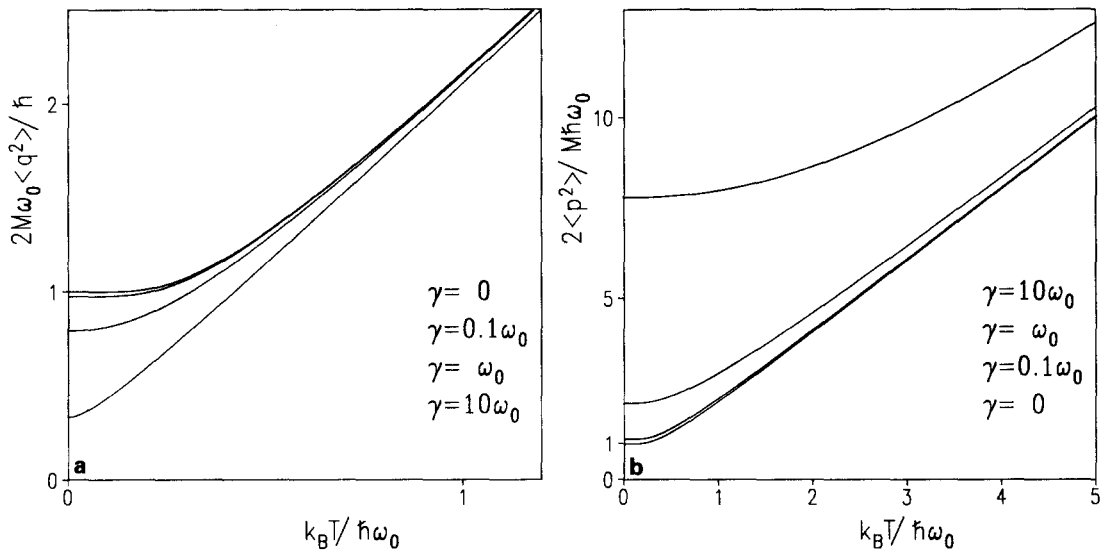

Fig. 3. The temperature dependence of the equilibrium variances (a) $\langle q^2\rangle$ and (b) $\langle p^2\rangle$ of a damped harmonic oscillator is shown for a Drude model where $\hat{\gamma}(\omega) = \gamma\omega_D/(\omega + \omega_D)$. Results are depicted for $\omega_D = 10\omega_0$ and for various values of γ.

where $\nu = \nu_1 = 2\pi/\hbar\beta$. For real times ($\tau \to 0^+$) this gives

$$K(t) = -\frac{\pi M\gamma}{(\hbar\beta)^2}\sinh^{-2}(\tfrac{1}{2}\nu t) + iM\gamma\delta'(t)\,, \tag{7.8}$$

while the imaginary time kernel is given by

$$K(-i\tau) = \frac{\pi M\gamma}{(\hbar\beta)^2}\sin^{-2}(\tfrac{1}{2}\nu\tau)\,. \tag{7.9}$$

The Fourier coefficients (4.55), (4.56) of the influence kernel are determined through

$$\zeta_n(s) = \gamma|\nu_n|\exp(-|\nu_n|s)\,, \tag{7.10}$$

which follows from eq. (4.58) by virtue of eq. (7.1). Using table 2, the Laplace transform of the Green's function $G_+(t)$ emerges as

$$\hat{G}_+(z) = (z^2 + \omega_0^2 + z\gamma)^{-1} = \frac{1}{2i\zeta}\left(\frac{1}{z+\lambda_2} - \frac{1}{z+\lambda_1}\right), \tag{7.11}$$

where $\lambda_{1,2}$ are the eigenvalues of a harmonic oscillator with Ohmic damping given by

$$\lambda_{1,2} = \tfrac{1}{2}\gamma \pm i\zeta \tag{7.12}$$

with the frequency of damped oscillations

$$\zeta = (\omega_0^2 - \tfrac{1}{4}\gamma^2)^{1/2}\,, \tag{7.13}$$

which becomes imaginary in the overdamped case $\gamma > 2\omega_0$. The inverse Laplace transform of eq. (7.11) is easily determined to read

$$G_+(t) = \frac{1}{2\mathrm{i}\zeta}\,[\exp(-\lambda_2 t) - \exp(-\lambda_1 t)] = \frac{1}{\zeta}\sin(\zeta t)\exp(-\tfrac{1}{2}\gamma t)\,. \tag{7.14}$$

Accordingly, the backward Green's function $G_-(t)$ follows from eqs. (5.48) and (5.51) as

$$G_-(t) = \frac{1}{\zeta}\sin(\zeta t)\exp(\tfrac{1}{2}\gamma t)\,. \tag{7.15}$$

Our result (5.56) may now be compared with the findings of Caldeira and Leggett [19] who studied quantum Brownian motion in a harmonic potential with Ohmic damping using the factorization assumption for the initial state. As mentioned in section 4, in our approach the correlations between the particle and the environment in the initial state are described in terms of the imaginary time path $\bar{q}(\tau)$, and we recover the conventional Feynman–Vernon theory by dropping all contributions arising from $\bar{q}(\tau)$. Accordingly, the action describing the time evolution of factorizing initial states is the $\bar{q}$-independent part of eq. (5.55) which for vanishing external force $F(s)$ is given by

$$\begin{aligned}\Sigma^{\mathrm{FV}}(x_\mathrm{f}, r_\mathrm{f}, t, x_\mathrm{i}, r_\mathrm{i}) &= M(x_\mathrm{f} r_\mathrm{f} + x_\mathrm{i} r_\mathrm{i})\,\frac{\dot{G}_+(t)}{G_+(t)} - M\Big(x_\mathrm{i} r_\mathrm{f}\,\frac{1}{G_+(t)} + x_\mathrm{f} r_\mathrm{i}\,\frac{1}{G_-(t)}\Big)\\
&+ \frac{\mathrm{i}}{2}\,x_\mathrm{i}^2 \int_0^t \mathrm{d}s \int_0^t \mathrm{d}u\, K'(s-u)\,\frac{G_+(t-s)}{\cancel{G_+(t)}}\,\frac{G_+(t-u)}{G_+(t)} + \mathrm{i}x_\mathrm{i}x_\mathrm{f}\int_0^t \mathrm{d}s \int_0^t \mathrm{d}u\, K'(s-u)\,\frac{G_+(t-s)}{\cancel{G_+(t)}}\,\frac{G_-(u)}{G_-(t)}\\
&+ \frac{\mathrm{i}}{2}\,x_\mathrm{f}^2 \int_0^t \mathrm{d}s \int_0^t \mathrm{d}u\, K'(s-u)\,\frac{G_-(s)}{\cancel{G_-(t)}}\,\frac{G_-(u)}{G_-(t)}\end{aligned} \tag{7.16}$$

where we noted that terms proportional to the functions $C_1(s)$, $C_2(s)$, and $R'(s, u)$ arise from $\bar{q}(\tau)$ as is explicitly seen from eq. (5.24). Hence, in the last three terms of eq. (5.55) only the part $(1/M)K'(s-u)$ of $R(s, u)$ [cf. eq. (5.33)] gives a contribution to Σ^{FV}. Noting that in the Ohmic case the formula (4.23) for the real part of the real time kernel $K(s)$ becomes

$$K'(s) = M\gamma \int_0^\infty \frac{\mathrm{d}\omega}{\pi}\,\omega\coth(\tfrac{1}{2}\omega\hbar\beta)\cos(\omega s)\,, \tag{7.17}$$

the action (7.16) with (7.14) and (7.15) can now be compared with the result obtained by Caldeira and Leggett [19]. Their eq. (6.26) agrees with our result (7.16) except for a difference in the first term which springs from the fact that they disregarded the last term in eq. (4.29).

Let us now consider the explicit time dependence of the correlation functions $S(t)$ and $A(t)$ which determine the time evolution of the propagating function $J(x_\mathrm{f}, r_\mathrm{f}, t, x_\mathrm{i}, r_\mathrm{i}, \bar{x}, \bar{r})$. The antisymmetrized correlation function (6.21) follows readily from eq. (7.14) as

$$A(t) = -\frac{\hbar}{2M\zeta}\sin(\zeta t)\exp(-\tfrac{1}{2}\gamma t)\,. \tag{7.18}$$

The Laplace transform (6.26) of the symmetrized correlation function $S(t)$ becomes in the Ohmic case

$$\hat{S}(z) = \frac{1}{\beta M}\sum_{n=-\infty}^{\infty}\frac{z}{\nu_n^2 - z^2}\left[(\omega_0^2 + z^2 + \gamma z)^{-1} - (\omega_0^2 + \nu_n^2 + \gamma|\nu_n|)^{-1}\right], \tag{7.19}$$

where we inserted eq. (7.11). Rewriting this expression in the form

$$\begin{aligned}\hat{S}(z) = \frac{1}{4i\zeta\beta M}\sum_{n=-\infty}^{\infty}\Bigg[&\frac{1}{z+|\nu_n|}\left(\frac{1}{|\nu_n|+\lambda_2} + \frac{1}{|\nu_n|-\lambda_2} - \frac{1}{|\nu_n|+\lambda_1} - \frac{1}{|\nu_n|-\lambda_1}\right)\\ &+\frac{1}{z+\lambda_1}\left(\frac{1}{|\nu_n|-\lambda_1} - \frac{1}{|\nu_n|+\lambda_1}\right) + \frac{1}{z+\lambda_2}\left(\frac{1}{|\nu_n|+\lambda_2} - \frac{1}{|\nu_n|-\lambda_2}\right)\Bigg],\end{aligned} \tag{7.20}$$

we obtain the correlation function $S(t)$ as a sum of exponentials. We find

$$S(t) = \frac{\hbar}{4M\zeta}\left[\exp(-\lambda_2 t)\coth(\tfrac{1}{2}i\hbar\beta\lambda_2) - \exp(-\lambda_1 t)\coth(\tfrac{1}{2}i\hbar\beta\lambda_1)\right] - \Gamma(t)\,, \tag{7.21}$$

where we made use of eq. (4.9) and introduced

$$\Gamma(t) = \frac{\gamma}{M\beta}\sum_{n=-\infty}^{\infty}\frac{|\nu_n|\exp(-|\nu_n|t)}{(\omega_0^2 + \nu_n^2)^2 - \gamma^2\nu_n^2}\,. \tag{7.22}$$

Hence, we recover from the functional integral approach the standard result [35]. The expression (7.22) for $\Gamma(t)$ may be written as

$$\begin{aligned}\Gamma(t) = \frac{1}{2i\beta\zeta M}\Bigg(&\frac{1}{\lambda_1}\left[F(1, \frac{\lambda_1}{\nu}; 1+\frac{\lambda_1}{\nu}; e^{-\nu t}) - F(1, -\frac{\lambda_1}{\nu}; 1-\frac{\lambda_1}{\nu}; e^{-\nu t})\right]\\ &-\frac{1}{\lambda_2}\left[F(1, \frac{\lambda_2}{\nu}; 1+\frac{\lambda_2}{\nu}; e^{-\nu t}) - F(1, -\frac{\lambda_2}{\nu}; 1-\frac{\lambda_2}{\nu}; e^{-\nu t})\right]\Bigg)\end{aligned} \tag{7.23}$$

where $F(a, b; c; z)$ is a hypergeometric function.

For later reference let us briefly discuss the long-time behaviour of $S(t)$ in the underdamped case where $\gamma < 2\omega_0$. For high temperatures $k_B T \gg \hbar\gamma/4\pi$ the function $\Gamma(t)$ decays very rapidly and the long-time behaviour of the correlation function is governed entirely by the $\exp(-\frac{1}{2}\gamma t)$ decay of the first two terms in eq. (7.21). For lower temperatures the $n = \pm 1$ terms in eq. (7.22) become increasingly important and in the regime $0 < k_B T < \hbar\gamma/4\pi$ we asymptotically have $S(t) \propto \exp(-\nu t)$. For $T = 0$ all elements of the sum (7.22) add up to a long-time tail and we find $S(t) \propto t^{-2}$ for long times $t \gg 2/\gamma$ [35, 37]. These findings directly extend to the overdamped case if γ is replaced by $\gamma - (\gamma^2 - 4\omega_0^2)^{1/2}$.

With eqs. (7.18) and (7.21) we know the explicit time dependence of the propagating function in the Ohmic case. Naturally, explicit results may also be obtained for more complicated forms of the spectral density. Once $\hat{\gamma}(z)$ is a rational function of z we can always determine the time dependence of the

correlation functions $S(t)$ and $A(t)$ in terms of the eigenvalues of the associated classical equation of motion. For the special case of a Drude model where $\hat{G}_+(z)$ has three poles most of the algebra necessary is provided in recent work [35, 44].

8. Relaxation of nonequilibrium initial states

In sections 5.1–6.7 we computed the exact propagating function $J(x_f, r_f, t, x_i, r_i, \bar{x}, \bar{r})$ of a quantum mechanical oscillator which is damped by a linear dissipative mechanism of arbitrary strength and arbitrary frequency dependence. This result allows for a study of the time evolution of a large class of initial states. In the following we treat various situations of interest. The general discussion will be independent of the form of the dissipative mechanism but more specific results will be given for the Ohmic case. We will make no use of the external force $F(t)$ in this section.

8.1. Approach to equilibrium

Let us consider the density matrix

$$\rho(x_f, r_f, t) = \int \mathrm{d}x_i\, \mathrm{d}r_i\, \mathrm{d}\bar{x}\, \mathrm{d}\bar{r}\, J(x_f, r_f, t, x_i, r_i, \bar{x}, \bar{r})\lambda(x_i, r_i, \bar{x}, \bar{r}) \tag{8.1}$$

in the limit $t \to \infty$. We shall assume that we approach ∞ through a sequence of times which avoids the exceptional points t_n with $A(t_n) = 0$ occurring in the underdamped case. Then we can explicitly use the form (6.71), (6.72) of the propagating function. The extension to arbitrary sequences of timepoints is straightforward using the regularized form (6.73), (6.74) whenever necessary.

Here, we consider the case that $G_+(t)$ and consequently $A(t)$ and $S(t)$ as well as their time derivatives vanish for $t \to \infty$. Further, since we excluded the zeros of $A(t)$ the ratio $\dot{A}(t)/A(t)$ is bounded so that terms like $S(t)\dot{A}(t)/A(t)$ also vanish in the limit considered. It should be noted, however, that although the correlations do decay for most dissipative mechanisms of interest it is not the most general case. If the spectrum of environmental oscillators has a sharp cutoff (i.e. $I(\omega) = 0$ for $\omega > \omega_D$) and the cutoff frequency is smaller or of the order of ω_0, or if $I(\omega)$ has a band structure with finite gaps where $I(\omega) = 0$, it can happen that the correlations do not decay for long times.

To proceed it is convenient to introduce a scaled variable $k_i = x_i/A(t)$ in terms of which eq. (8.1) takes the form

$$\rho(x_f, r_f, t) = \frac{1}{4\pi} \int \mathrm{d}k_i\, \mathrm{d}r_i\, \mathrm{d}\bar{x}\, \mathrm{d}\bar{r}\, \lambda(A(t)k_i, r_i, \bar{x}, \bar{r})\rho_\beta(\bar{x}, \bar{r})$$
$$\times \exp\left[\frac{\mathrm{i}}{\hbar}\, \Sigma(x_f, r_f, t, A(t)k_i, r_i, \bar{x}, \bar{r})\right] \tag{8.2}$$

For large times the exponent becomes

$$\Sigma(x_f, r_f, t, A(t)k_i, r_i, \bar{x}, \bar{r}) = \mathrm{i}\frac{\hbar}{8}\langle q^2\rangle k_i^2 + \mathrm{i}\left(\frac{M}{2}\langle q^2\rangle \frac{\dot{A}(t)}{A(t)} x_f - \mathrm{i}\frac{\hbar}{2} r_f\right)k_i$$
$$+ \mathrm{i}\left(\frac{\langle p^2\rangle}{2\hbar} + \frac{M^2}{2\hbar}\langle q^2\rangle \frac{\dot{A}^2(t)}{A(t)}\right)x_f^2 + M\frac{\dot{A}(t)}{A(t)} x_f r_f + \Delta\Sigma_t\,, \tag{8.3}$$

where $\Delta\Sigma_t$ contains terms vanishing in the limit $t\to\infty$. Since the first argument of the function $\lambda(A(t)k_i, r_i, \bar{x}, \bar{r})$ approaches zero for $t\to\infty$, the integral over k_i can be performed essentially by completing the square in the exponent. We are left with

$$\lim_{t\to\infty} \rho(x_f, r_f, t) = \rho_\beta(x_f, r_f) \int dr_i\, d\bar{x}\, d\bar{r}\, \lambda(0, r_i, \bar{x}, \bar{r})\rho_\beta(\bar{x}, \bar{r})\,. \tag{8.4}$$

Now, because of eq. (3.36) we have

$$\int dr_i\, d\bar{x}\, d\bar{r}\, \lambda(0, r_i, \bar{x}, \bar{r})\rho_\beta(\bar{x}, \bar{r}) = \int dr_i\, \rho_0(0, r_i) = \mathrm{tr}(\rho_0)\,. \tag{8.5}$$

Hence, if we start out with a normalized initial state, the system approaches for $t\to\infty$ the equilibrium state ρ_β independent of the particular form of the function $\lambda(x_i, r_i, \bar{x}, r)$. This result remains valid at $T = 0$ but the approach to equilibrium may be extremely slow due to the long time tails discussed in the previous section.

8.2. Relaxation of expectation values

The decay of nonequilibrium initial states is easily monitored by studying the time evolution of expectation values. Let us first consider the average coordinate which may be written as

$$\langle q\rangle_t = \int dr_f\, dx_i\, dr_i\, d\bar{x}\, d\bar{r}\, r_f J(0, r_f, t, x_i, r_i, \bar{x}, \bar{r})\lambda(x_i, r_i, \bar{x}, \bar{r})\,. \tag{8.6}$$

Inserting the explicit form (6.71), (6.72) of the propagating function we obtain after some algebra

$$\langle q\rangle_t = \dot{G}_+(t)\langle q\rangle_0 + \frac{1}{M} G_+(t)\langle p\rangle_0 + \left[\frac{S(t)}{\langle q^2\rangle} - \dot{G}_+(t)\right]\langle \bar{r}\rangle_0 - \left[\frac{M}{\hbar}\dot{S}(t) + \frac{\langle p^2\rangle}{M\hbar} G_+(t)\right] i\langle \bar{x}\rangle_0\,, \tag{8.7}$$

where $\langle q\rangle_0$ and $\langle p\rangle_0$ denote the initial nonequilibrium values of the coordinate and momentum while

$$\langle \bar{r}\rangle_0 = \int dr_i\, d\bar{x}\, d\bar{r}\, \lambda(0, r_i, \bar{x}, \bar{r})\bar{r}\rho_\beta(\bar{x}, \bar{r})\,, \tag{8.8}$$

$$\langle \bar{x}\rangle_0 = \int dr_i\, d\bar{x}\, d\bar{r}\, \lambda(0, r_i, \bar{x}, \bar{r})\bar{x}\rho_\beta(\bar{x}, \bar{r}) \tag{8.9}$$

are additional terms arising from the correlations between the Brownian particle and the environmental oscillators in the initial state. Using table 1 and eq. (5.57) we see that the time dependence of the last two terms in eq. (8.7) may be related to the functions $C_j(s)$ introduced in eqs. (5.26), (5.27) by

$$\frac{S(t)}{\langle q^2\rangle} - \dot{G}_+(t) = \int_0^t ds\, G_+(t-s)C_1(s)\,, \tag{8.10}$$

$$\frac{M}{\hbar}\dot{S}(t) + \frac{\langle p^2\rangle}{M\hbar} G_+(t) = \int_0^t ds\, G_+(t-s)C_2(s)\,, \tag{8.11}$$

so that eq. (8.7) may be rewritten in the form

$$\langle q\rangle_t = \dot{G}_+(t)\langle q\rangle_0 + \frac{1}{M}\,G_+(t)\langle p\rangle_0 + \frac{1}{M}\int_0^t \mathrm{d}s\; G_+(t-s)\langle \bar{F}(s)\rangle_0\,, \tag{8.12}$$

where

$$\bar{F}(s) = MC_1(s)\bar{r} - \mathrm{i}MC_2(s)\bar{x} \tag{8.13}$$

is the force introduced in eq. (5.32). Clearly, the average coordinate is a solution of

$$M\langle \ddot{q}\rangle_t + \frac{\mathrm{d}}{\mathrm{d}t}\int_0^t \mathrm{d}s\; M\gamma(t-s)\langle q\rangle_s + M\omega_0^2\langle q\rangle_t = \langle \bar{F}(t)\rangle_0\,, \tag{8.14}$$

which is the classical equation of motion (4.43) with an inhomogeneity $\langle \bar{F}(t)\rangle_0 - M\gamma(t)\langle q\rangle_0$. In view of Ehrenfest's theorem the average force $\langle \bar{F}(t)\rangle_0$ should be related to the initial values of the coordinates and momenta of the environmental oscillators. This is shown in appendix *C*.

For later convenience we introduce the time-dependent coordinates

$$q_1(t) = \dot{G}_+(t)q\,, \tag{8.15}$$

$$q_2(t) = G_+(t)\;p/M\,, \tag{8.16}$$

$$q_3(t) = [S(t)/\langle q^2\rangle - \dot{G}_+(t)]\bar{r}\,, \tag{8.17}$$

$$q_4(t) = -\frac{\mathrm{i}}{\hbar}\left[M\dot{S}(t) + \frac{1}{M}\langle p^2\rangle G_+(t)\right]\bar{x}\,, \tag{8.18}$$

in terms of which the result (8.7) may be written in the compact form

$$\langle q\rangle_t = \sum_{\alpha=1}^{4}\langle q_\alpha(t)\rangle_0\,. \tag{8.19}$$

The functions $q_1(t)$ and $q_2(t)$ describe the dependence of the expectation value on the initial coordinate and the initial velocity of the Brownian particle, while the functions $q_3(t)$ and $q_4(t)$ describe the influence of the initial values of the environmental oscillators. Clearly, the average momentum of the Brownian particle at time t takes the form

$$\langle p\rangle_t = M\sum_{\alpha=1}^{4}\langle \dot{q}_\alpha(t)\rangle_0 \tag{8.20}$$

and thus contains no additional information about the relaxation process.

Next, let us study the time evolution of the second moments $\langle q^2\rangle_t$, $\frac{1}{2}\langle pq + qp\rangle_t$, and $\langle p^2\rangle_t$ given by

$$\langle q^2\rangle_t = \int \mathrm{d}r_\mathrm{f}\,\mathrm{d}x_\mathrm{i}\,\mathrm{d}r_\mathrm{i}\,\mathrm{d}\bar{x}\,\mathrm{d}\bar{r}\,r_\mathrm{f}^2 J(0, r_\mathrm{f}, t, x_\mathrm{i}, r_\mathrm{i}, \bar{x}, \bar{r})\lambda(x_\mathrm{i}, r_\mathrm{i}, \bar{x}, \bar{r})\,, \tag{8.21}$$

$$\tfrac{1}{2}\langle pq + qp\rangle_t = \int \mathrm{d}x_\mathrm{f}\,\mathrm{d}r_\mathrm{f}\,\mathrm{d}x_\mathrm{i}\mathrm{d}r_\mathrm{i}\,\mathrm{d}\bar{x}\,\mathrm{d}\bar{r}\,\delta(x_\mathrm{f})r_\mathrm{f}\left(\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x_\mathrm{f}}\right)J(x_\mathrm{f}, r_\mathrm{f}, t, x_\mathrm{i}, r_\mathrm{i}, \bar{x}, \bar{r})\lambda(x_\mathrm{i}, r_\mathrm{i}, \bar{x}, \bar{r})\,, \tag{8.22}$$

$$\langle p^2\rangle_t = \int \mathrm{d}x_\mathrm{f}\,\mathrm{d}r_\mathrm{f}\,\mathrm{d}x_\mathrm{i}\,\mathrm{d}r_\mathrm{i}\,\mathrm{d}\bar{x}\,\mathrm{d}\bar{r}\,\delta(x_\mathrm{f})(-\hbar^2)\frac{\partial^2}{\partial x_\mathrm{f}^2} J(x_\mathrm{f}, r_\mathrm{f}, t, x_\mathrm{i}, r_\mathrm{i}, \bar{x}, \bar{r})\lambda(x_\mathrm{i}, r_\mathrm{i}, \bar{x}, \bar{r})\,. \tag{8.23}$$

Again inserting the explicit form (6.71), (6.72) of the propagating function a straightforward calculation leads us to

$$\langle q^2\rangle_t = \langle q^2\rangle\left[1 - \frac{S^2(t)}{\langle q^2\rangle^2}\right] + \frac{\langle p^2\rangle}{M^2}\,G_+^2(t) + 2G_+(t)\dot{S}(t) + \sum_{\nu,\,\mu=1}^{4}\langle q_\nu(t)q_\mu(t)\rangle_0\,, \tag{8.24}$$

$$\begin{aligned}\tfrac{1}{2}\langle pq + qp\rangle_t &= \tfrac{1}{2}\,M\,\frac{\mathrm{d}}{\mathrm{d}t}\langle q^2\rangle_t \\ &= \frac{\langle p^2\rangle}{M}\,G_+(t)\dot{G}_+(t) + M\dot{G}_+(t)\dot{S}(t) + MG_+(t)\ddot{S}(t) - M\,\frac{S(t)\dot{S}(t)}{\langle q^2\rangle} \\ &\quad + M\sum_{\nu,\mu=1}^{4}\tfrac{1}{2}\langle \dot{q}_\nu(t)q_\mu(t) + q_\nu(t)\dot{q}_\mu(t)\rangle_0\end{aligned} \tag{8.25}$$

$$\langle p^2\rangle_t = \langle p^2\rangle[\dot{G}_+^2(t) + 1] - M^2\,\frac{\dot{S}^2(t)}{\langle q^2\rangle} + 2M^2\dot{G}_+(t)\ddot{S}(t) + M^2\sum_{\nu,\mu=1}^{4}\langle \dot{q}_\nu(t)\dot{q}_\mu(t)\rangle_0\,. \tag{8.26}$$

These formulas give the second moments in terms of their initial values $\langle q^2\rangle_0$, $\frac{1}{2}\langle pq + qp\rangle_0$, $\langle p^2\rangle_0$ and their final equilibrium values $\langle q^2\rangle$, $\langle p^2\rangle$. There are also additional terms proportional to $\langle q\bar{r}\rangle_0$, $\langle q\bar{x}\rangle_0$, $\langle p\bar{r}\rangle_0$, $\langle p\bar{x}\rangle_0$, $\langle \bar{r}^2\rangle_0$, $\langle \bar{r}\bar{x}\rangle_0$, and $\langle \bar{x}^2\rangle_0$ which arise from correlations between the Brownian particle and the reservoir in the initial state. Clearly, we may determine the time evolution of the higher moments by the same method. These contain new information only if the initial density matrix is non-Gaussian. A more detailed discussion of the relaxation of expectation values for specific initial states will be given in sections 8.3 and 8.4.

8.3. Relaxation of factorizing initial states

In this section we briefly consider the time evolution of expectation values for a Brownian particle starting from a factorizing initial state. This case is obtained from the results in section 8.2 by setting all terms containing $\bar{x}$ and $\bar{r}$ equal to zero. The first moments then read

$$\langle q\rangle_t^{\mathrm{FV}} = \dot{G}_+(t)\langle q\rangle_0 + \frac{1}{M}\,G_+(t)\langle p\rangle_0 \tag{8.27}$$

and

$$\langle p\rangle_t^{\mathrm{FV}} = M\ddot{G}_+(t)\langle q\rangle_0 + \dot{G}_+(t)\langle p\rangle_0\,. \tag{8.28}$$

For an Ohmic heat bath the evolution of the second equation is discontinuous at $t=0$ since $\lim_{t\to 0}\langle p\rangle_t^{\mathrm{FV}} = \langle p\rangle_0 - M\gamma\langle q\rangle_0$ is generally not equal to $\langle p\rangle_0$ [cf. eq. (7.14)]. This is due to the fact that $\ddot{G}_+(0)\neq 0$ for a strictly Ohmic reservoir. Once we introduce an environmental cutoff ω_{D}, we have $\ddot{G}_+(0)=0$ and the jump of $\langle p\rangle_t$ no longer happens instantaneously but takes place on the time scale ω_{D}^{-1}. On the other hand, for a nonfactorizing initial state we have $\lim_{t\to 0}\langle p\rangle_t^{\mathrm{FV}} = \langle p\rangle_0 - M\gamma(\langle q\rangle_0 - \langle \bar{r}\rangle_0)$ so that even for Ohmic damping an initial discontinuity occurs only for preparations where $\langle q\rangle_0 \neq \langle \bar{r}\rangle_0$.

The time evolution of the second moments for factorizing initial states are obtained accordingly. The mean square of the coordinate is given by

$$\langle q^2\rangle_t^{\mathrm{FV}} = \dot{G}_+^2(t)\langle q^2\rangle_0 + \frac{1}{M^2}\,G_+^2(t)\langle p^2\rangle_0 + \frac{1}{M}\,G_+(t)\dot{G}_+(t)\langle pq+qp\rangle_0$$
$$+\left[1-\frac{S^2(t)}{\langle q^2\rangle^2}\right]\langle q^2\rangle + 2G_+(t)\dot{S}(t) + \frac{1}{M^2}\,G_+^2(t)\langle p^2\rangle\,. \tag{8.29}$$

Caldeira and Leggett [19] have studied this quantity for an initial wavepacket with $\langle p^2\rangle_0 = p_0^2 + \hbar^2/(4\langle q^2\rangle_0)$ and $\langle pq+qp\rangle_0 = 0$. In this case eq. (8.29) is equivalent to their eq. (6.34) if the term neglected by these authors is restored. Clearly, the correct approach of the equilibrium variance $\langle q^2\rangle$ for $t\to\infty$ is evident from both the result (8.29) for factorizing initial states and the more general expression (8.24).

8.4. Coherent and squeezed states

We now turn to a class of initial states, namely coherent and squeezed states, which are of interest in various fields including quantum optics, optical communications, and high precision measurements near the quantum limit. Coherent states have been widely used to describe the radiation field of lasers [9, 46], and the question of how a dissipative environment affects their time evolution was recently discussed by several authors [47, 48] mainly on the basis of master equation methods. The weak coupling master equation, though being a very good approximation for many problems, cannot be used for temperatures close to zero and/or moderate to strong damping [13, 49]. The following analysis [23] is not subject to those limitations and describes systems for arbitrarily low temperatures and arbitrarily strong damping.

Coherent states are eigenstates of the annihilation operator $a = (M\omega_0/2\hbar)^{1/2}q + \mathrm{i}(2\hbar M\omega_0)^{-1/2}p$ of the harmonic oscillator defined by [46]

$$a|\alpha\rangle = \alpha|\alpha\rangle\,, \tag{8.30}$$

where α is the complex eigenvalue. A coherent state is obtained by letting the displacement operator

$$D(\alpha) = \exp(\alpha a^+ - \alpha^* a) \tag{8.31}$$

act on the groundstate, i.e.

$$|\alpha\rangle = D(\alpha)|0\rangle\,. \tag{8.32}$$

A generalization of these states is obtained by considering the eigenstates of the operator

$$b = \cosh(|z|)\, a + \exp(-\mathrm{i}\phi_z) \sinh(|z|)\, a^+ , \tag{8.33}$$

which is again an annihilation operator satisfying $[b, b^+] = 1$. Here, z is a complex parameter $z = |z| \exp(\mathrm{i}\phi_z)$. These so-called squeezed states or two-photon coherent states [50] are generated by letting the squeeze operator

$$S(z) = \exp\left[\frac{z}{2}\, a^2 - \frac{z^*}{2}\, a^{+2}\right] \tag{8.34}$$

and subsequently the displacement operator $D(\alpha)$ act on the ground state, i.e.

$$|S(\alpha, z)\rangle = D(\alpha) S(z) |0\rangle . \tag{8.35}$$

Hence, by putting $z = 0$ we recover a coherent state as a special case of a squeezed state.

While in a coherent state the variances of potential and kinetic energy are equal and fulfill the minimum uncertainty relation $\sigma_p \sigma_q = \hbar^2/4$, these variances differ from each other in a squeezed state. For example the spatial width σ_q of a state is "squeezed" at the cost of a wider momentum distribution. This squeezing could improve the attainable signal to noise ratio which is important in many practical problems in fibre optics, optical waveguides, or gravitational wave detection [51].

The general mechanism to generate squeezed states is to act on the system by a perturbation of the Hamiltonian which contains components proportional to $ca + c^* a^+$ for displacing the state and proportional to $(d/2)a^2 + (d^*/2)a^{+2}$ for squeezing the state. Note, that the time evolution operator associated with H then has terms of the form of the displacement operator $D(\alpha)$ and the squeeze operator $S(z)$, respectively. Then after a while the perturbation is expected to cause a nonequilibrium part of the density matrix which is close to a coherent or squeezed state. Let us assume that the effect of this perturbation on a system initially in equilibrium generates a nonequilibrium initial state of the form

$$W_s = O_s W_\beta O_s^+ , \tag{8.36}$$

where

$$O_s = D(\alpha) S(z) \tag{8.37}$$

is an operator acting on the coordinates of the Brownian particle only. Hence, the density matrix (8.36) belongs to the class of initial states discussed in section 2. Clearly, if we trace (8.36) over the reservoir the resulting density matrix is not the density matrix of an ideal squeezed state (8.35). However, by including the full environmental coupling, eq. (8.36) is much closer to the experimental situation and we shall call

$$\rho_s = \mathrm{tr}_R(W_s) = O_s \rho_\beta O_s^+ \tag{8.38}$$

the density matrix of a "real" squeezed state. In the limit of zero damping and zero temperature we have

$$\lim_{T\to 0}\lim_{\dot{\gamma}(\omega)\to 0}\rho_s = |S(\alpha, z)\rangle\langle S(\alpha, z)|\,, \tag{8.39}$$

so that the density matrix reduces to the projection on an ideal squeezed state.

Let us now consider the coordinate representation of the operator O_s. Here, we choose the squeezing parameter z to be real which means that the nondiagonal variance σ_{pq} vanishes initially. Then the state is squeezed such that the principal axes of the uncertainty ellipse are coordinate and momentum. This is the case of interest, generally. For complex z the ellipse gets rotated in the p,q-plane. Now, the matrix element of the squeeze operator can be written

$$\langle q|S(z)|q'\rangle = \langle q|\exp\left(\frac{z}{2}\right)\exp\left(\frac{\mathrm{i}}{\hbar}\,zpq\right)|q'\rangle\,. \tag{8.40}$$

Taking the derivative with respect to z and using the coordinate representation of the operators p and q we obtain the differential equation

$$\left[\frac{\partial}{\partial z} - q\,\frac{\partial}{\partial q} - \frac{1}{2}\right]\langle q|S(z)|q'\rangle = 0\,. \tag{8.41}$$

With the boundary condition $\langle q|S(0)|q'\rangle = \delta(q-q')$ the solution is found to read

$$\langle q|S(z)|q'\rangle = \zeta^{1/2}\delta(\zeta q - q')\,, \tag{8.42}$$

where

$$\zeta = \exp(z)\,. \tag{8.43}$$

The same method readily yields the coordinate representation of the displacement operator. Writing eq. (8.31) as

$$D(p_0, q_0) = \exp\left(-\frac{\mathrm{i}}{\hbar}\,q_0 p\right)\exp\left(\frac{\mathrm{i}}{\hbar}\,p_0 q\right)\exp\left(\frac{\mathrm{i}}{2\hbar}\,p_0 q_0\right), \tag{8.44}$$

where we defined

$$q_0 = (2\hbar/M\omega_0)^{1/2}\,\mathrm{Re}(\alpha)\,, \tag{8.45}$$

$$p_0 = (2\hbar M\omega_0)^{1/2}\,\mathrm{Im}(\alpha)\,, \tag{8.46}$$

we obtain

$$\langle q|D(p_0, q_0)|q'\rangle = \exp\left(\frac{\mathrm{i}}{\hbar}\,p_0 q\right)\exp\left(\frac{\mathrm{i}}{2\hbar}\,p_0 q_0\right)\delta(q - q_0 - q')\,. \tag{8.47}$$

From eq. (2.12) we have that the preparation function $\lambda_s(q, \bar{q}, q', \bar{q}')$ is connected with the operator O_s by

$$\lambda_s(q, \bar{q}, q', \bar{q}') = \langle q|O_s|\bar{q}\rangle\langle\bar{q}'|O_s^+|q'\rangle\,. \tag{8.48}$$

Using the results (8.42) and (8.47), its representation in sum and difference coordinates becomes

$$\lambda_s(x, r, \bar{x}, \bar{r}) = \zeta \exp\left(\frac{\mathrm{i}}{\hbar}\, p_0 x\right) \delta(\zeta x - \bar{x})\, \delta(\zeta(r - q_0) - \bar{r})\,, \tag{8.49}$$

which gives for the initial reduced density matrix

$$\rho_s(x, r) = (2\pi\zeta^{-2}\langle q^2\rangle)^{-1/2} \exp\left[-\frac{\zeta^2}{2\langle q^2\rangle}(r - q_0)^2 - \frac{\zeta^2\langle p^2\rangle}{2\hbar^2}\, x^2 + \frac{\mathrm{i}}{\hbar}\, p_0 x\right]. \tag{8.50}$$

We can now use the results of the previous section to determine the time evolution of the expectation values of the dynamical variables. Since the initial state described by eq. (8.50) is Gaussian it is characterized by its first and second moments. From (8.50) we easily obtain

$$\langle q\rangle_0 = q_0\,; \qquad \langle p\rangle_0 = p_0\,, \tag{8.51}$$

as well as

$$\langle q^2\rangle_0 = q_0^2 + \zeta^{-2}\langle q^2\rangle\,; \qquad \tfrac{1}{2}\langle pq + qp\rangle_0 = p_0 q_0\,; \qquad \langle p^2\rangle_0 = p_0^2 + \zeta^2\langle p^2\rangle\,. \tag{8.52}$$

Hence, the parameter α occurring in the displacement operator (8.31) is related to the initial position and momentum by

$$\alpha = \left(\frac{M\omega_0}{2\hbar}\right)^{1/2}\langle q\rangle_0 + \mathrm{i}(2\hbar M\omega_0)^{-1/2}\langle p\rangle_0\,, \tag{8.53}$$

while the constant z in the squeeze operator (8.34) determines the squeezing of the width of the distribution in coordinate and momentum space according to

$$\frac{\sigma_q(0)}{\langle q^2\rangle} = \frac{\langle p^2\rangle}{\sigma_p(0)} = \exp(-2z)\,. \tag{8.54}$$

Here, we introduced the variances of position

$$\sigma_q(t) = \langle q^2\rangle_t - \langle q\rangle_t^2 \tag{8.55}$$

and momentum

$$\sigma_p(t) = \langle p^2\rangle_t - \langle p\rangle_t^2\,, \tag{8.56}$$

which for the squeezed state (8.50) are related by

$$\sigma_q(0)\sigma_p(0) = \langle q^2\rangle\langle p^2\rangle\,. \tag{8.57}$$

We note that for complex parameter z this relation generalizes to read

$$\sigma_{pq}^2(0) = \sigma_q(0)\sigma_p(0) - \langle q^2\rangle\langle p^2\rangle\,, \tag{8.58}$$

where

$$\sigma_{pq}(t) = \tfrac{1}{2}\langle pq + qp\rangle_t - \langle p\rangle_t\langle q\rangle_t \tag{8.59}$$

is the cross variance. Besides eqs. (8.51) and (8.52) we also have to determine the initial expectation values containing $\bar{x}$ and $\bar{r}$ [cf. eqs. (8.8), (8.9)]. Using the form (8.49) of the preparation function we find

$$\langle\bar{x}\rangle_0 = 0\,; \qquad \langle\bar{r}\rangle_0 = 0\,, \tag{8.60}$$

$$\langle\bar{x}^2\rangle_0 = 0\,; \qquad \langle\bar{r}\bar{x}\rangle_0 = 0\,; \qquad \langle\bar{r}^2\rangle_0 = \langle q^2\rangle\,, \tag{8.61}$$

$$\langle q\bar{x}\rangle_0 = 0\,; \qquad \langle q\bar{r}\rangle_0 = \zeta^{-1}\langle q^2\rangle\,, \tag{8.62}$$

$$\langle p\bar{x}\rangle_0 = (\hbar/\mathrm{i})\zeta\,; \qquad \langle p\bar{r}\rangle_0 = 0\,. \tag{8.63}$$

From eqs. (8.19), (8.51), and (8.60) the time evolution of the coordinate expectation value follows as

$$\langle q\rangle_t = q_0\dot{G}_+(t) + (1/M)p_0G_+(t)\,, \tag{8.64}$$

while eq. (8.20) gives for the average momentum

$$\langle p\rangle_t = q_0M\ddot{G}_+(t) + p_0\dot{G}_+(t)\,. \tag{8.65}$$

Hence, the mean values of coordinate and momentum of a squeezed state follow the well-known classical trajectories and are temperature independent.

The relaxation of the initial displacement and momentum is conveniently visualized by defining, in analogy to eq. (8.53), a complex time-dependent displacement parameter

$$\alpha(t) = (M\omega_0/2\hbar)^{1/2}\langle q\rangle_t + \mathrm{i}(2\hbar M\omega_0)^{-1/2}\langle p\rangle_t\,. \tag{8.66}$$

Inserting eqs. (8.64, 8.65) we have

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}|\alpha(t)|^2 = \frac{M}{\hbar\omega_0}\, & q_0^2\ddot{G}_+(t)[\dddot{G}_+(t) + \omega_0^2\dot{G}_+(t)] + (M\hbar\omega_0)^{-1}p_0^2\dot{G}_+(t)[\ddot{G}_+(t) + \omega_0^2G_+(t)] \\ & + (\hbar\omega_0)^{-1}p_0q_0(\dddot{G}_+(t)[\ddot{G}_+(t) + \omega_0^2G_+(t)] + \dot{G}_+(t)[\dddot{G}_+(t) + \omega_0^2\dot{G}_+(t)])\,.\end{aligned} \tag{8.67}$$

In the case of Ohmic dissipation we can use the equation of motion for the Green's function

$$\ddot{G}_+(t) + \gamma\dot{G}_+(t) + \omega_0^2G_+(t) = 0 \tag{8.68}$$

to obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}|\alpha(t)|^2 = -\frac{M\gamma}{\hbar\omega_0}\left[\ddot{G}_+(t)q_0 + \frac{1}{M}\dot{G}_+(t)p_0\right]^2 \tag{8.69}$$

which is clearly negative. Hence, the absolute value of the displacement parameter decreases monotonously towards zero. The resulting trajectory in the p, q-plane is a spiral approaching the origin.

The time evolution of the second moments is obtained by inserting the initial values (8.52) and (8.61–8.63) in the general expressions (8.24–8.26). Further, inserting (8.64, 8.65) for $\langle q\rangle_t$ and $\langle p\rangle_t$ we find

$$\sigma_q(t) = 2G_+(t)\dot{S}(t)(1-\zeta) - 2\dot{G}_+(t)S(t)(1-\zeta^{-1}) + \langle q^2\rangle[1+\dot{G}_+^2(t)(1-\zeta^{-1})^2] + \frac{\langle p^2\rangle}{M^2}G_+^2(t)(1-\zeta)^2, \tag{8.70}$$

$$\sigma_{pq}(t) = \tfrac{1}{2}M\frac{\mathrm{d}}{\mathrm{d}t}\sigma_q(t), \tag{8.71}$$

$$\sigma_p(t) = 2M^2\dot{G}_+(t)\ddot{S}(t)(1-\zeta) - 2M^2\ddot{G}_+(t)\dot{S}(t)(1-\zeta^{-1}) + \langle q^2\rangle M^2\ddot{G}_+^2(t)(1-\zeta^{-1})^2 + \langle p^2\rangle[1+\dot{G}_+^2(t)(1-\zeta)^2]. \tag{8.72}$$

Since the initial state (8.50) is Gaussian and the Hamiltonian for $t>0$ is quadratic, the reduced density matrix will remain Gaussian for all times. Therefore it is determined uniquely by its first and second moments derived above. In fact, it is easily shown that the density matrix at time t is given by

$$\rho(x,r,t) = (2\pi\sigma_q(t))^{-1/2}\exp\Big[-\frac{1}{2\sigma_q(t)}(r-\langle q\rangle_t)^2 - \frac{1}{2\hbar^2}\Big(\sigma_p(t)-\frac{\sigma_{pq}^2(t)}{\sigma_q(t)}\Big)x^2 + \frac{\mathrm{i}}{\hbar}\Big\{\langle p\rangle_t + \frac{\sigma_{pq}(t)}{\sigma_q(t)}(r-\langle q\rangle_t)\Big\}x\Big], \tag{8.73}$$

which reduces to $\rho_s(x,r)$ for $t=0$ and goes to $\rho_\beta(x,r)$ for $t\to\infty$. In order to discuss the decay of the squeezed fluctuations in more detail it is convenient to introduce the Wigner representation [52]

$$W(p,q,t) = \frac{1}{2\pi\hbar}\int \mathrm{d}x\,\rho(x,q,t)\exp\Big(-\frac{\mathrm{i}}{\hbar}px\Big) \tag{8.74}$$

of the density matrix (8.73). The Wigner function which is the quantum analogue of a classical probability distribution emerges as [23]

$$W(p,q,t) = \frac{1}{2\pi}[\sigma_q(t)\sigma_p(t)k(t)]^{-1/2}\exp\Big[-\frac{1}{2}\Big\{\frac{(q-\langle q\rangle_t)^2}{\sigma_q(t)k(t)} + \frac{(p-\langle p\rangle_t)^2}{\sigma_p(t)k(t)} - \frac{2\sigma_{pq}(t)}{\sigma_q(t)\sigma_p(t)k(t)}(q-\langle q\rangle_t)(p-\langle p\rangle_t)\Big\}\Big], \tag{8.75}$$

where $k(t) = 1-\sigma_{pq}^2(t)/(\sigma_p(t)\sigma_q(t))$. Let us further introduce the dimensionless variables $\tilde{q} = (2M\omega_0/\hbar)^{1/2}q$ and $\tilde{p} = (2/\hbar M\omega_0)^{1/2}p$ and the variances $\tilde{\sigma}_q(t)$, $\tilde{\sigma}_p(t)$, and $\tilde{\sigma}_{pq}(t)$ scaled accordingly. Setting the expression in braces in eq. (8.75) equal to 1 defines an uncertainty ellipse in the $\tilde{p}$, $\tilde{q}$-plane which is centred at $\tilde{p} = \langle\tilde{p}\rangle_t$ and $\tilde{q} = \langle\tilde{q}\rangle_t$ and characterizes the width of the fluctuations. At $t=0$ the principal axes of this ellipse point in the $\tilde{p}$- and $\tilde{q}$-direction and they have the lengths $\tilde{\sigma}_p^{1/2}(0)$ and $\tilde{\sigma}_q^{1/2}(0)$. For $t>0$ the ellipse gets rotated and the lengths of the axes oscillate. Note that we have scaled

the variables such that the ground state of the undamped oscillator is described by a unit circle while the equilibrium state is ellipsoidal due to the dissipation.

Although the relation (8.58) characterizing the initial "real" squeezed state is not valid for $t > 0$ due to the dissipation, we may say that the system is in a squeezed state as long as the fluctuations in one variable are smaller than the fluctuations of the ground state. In terms of the scaled variables this means that the minor axis of the uncertainty ellipse is shorter than 1. Now, the principal axes of the rotated ellipse are given by [23]

$$x_{\pm}(t) = [\tfrac{1}{2}(\tilde{\sigma}_q(t) + \tilde{\sigma}_p(t) \pm \sqrt{(\tilde{\sigma}_q(t) - \tilde{\sigma}_p(t))^2 + 4\tilde{\sigma}_{pq}^2(t)})]^{1/2}\,, \tag{8.76}$$

where the plus and minus sign hold for the major and minor axis, respectively. Figure 4 shows the time evolution of these axes for a Drude model with $\hat{\gamma}(\omega) = \gamma\omega_D/(\omega + \omega_D)$ for two temperatures. For those times t_n when $\tilde{\sigma}_{pq}(t_n) = 0$ the axes $x_{\pm}(t_n)$ point in the $\tilde{p}$- and $\tilde{q}$-direction. If the state is initially squeezed such that $\tilde{\sigma}_q(t_0 = 0) < 1$ the minor axis will again point in the $\tilde{q}$-direction for even values of the index n labelling the timepoints t_n. For a sequence of these timepoints the time evolution of the uncertainty ellipse in the $\tilde{p}$, $\tilde{q}$-plane is shown in fig. 5.

Dissipation influences the squeezing in two ways. It leads to a decay of the squeezed fluctuations and changes their absolute values. Let us first discuss the lifetime of the squeezing. It is seen from fig. 4 that the decay rate is roughly temperature independent. This can be understood by using the explicit time dependence of the Green's function and correlation function for frequency-independent damping [eqs. (7.14) and (7.21)]. For high temperatures $T > \hbar\gamma/4\pi k_B$ all terms in eqs. (8.70–8.72) for the variances decay as $\exp(-\gamma t)$ or faster so that the damping constant is the only relevant parameter for the lifetime of the squeezing. For lower temperatures we still have terms proportional to $\exp(-\gamma t)$ but some of the additional terms proportional to $\exp[-(\frac{1}{2}\gamma + \nu_n)t]$ decay slower. For moderate to strong damping these

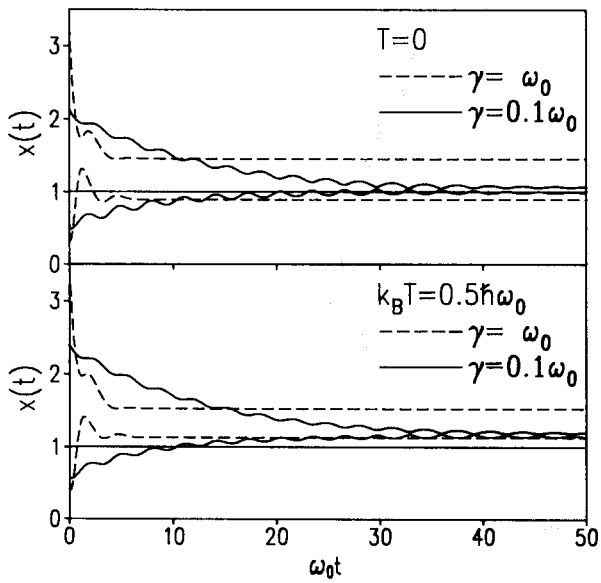

Fig. 4. Time evolution of the principal axes $x_{\pm}(t)$ of the uncertainty ellipse of a squeezed state for a Drude model with $\omega_D = 10\omega_0$ and for an initial squeezing parameter $\zeta = 2$. The horizontal line marks the size of the vacuum fluctuations.

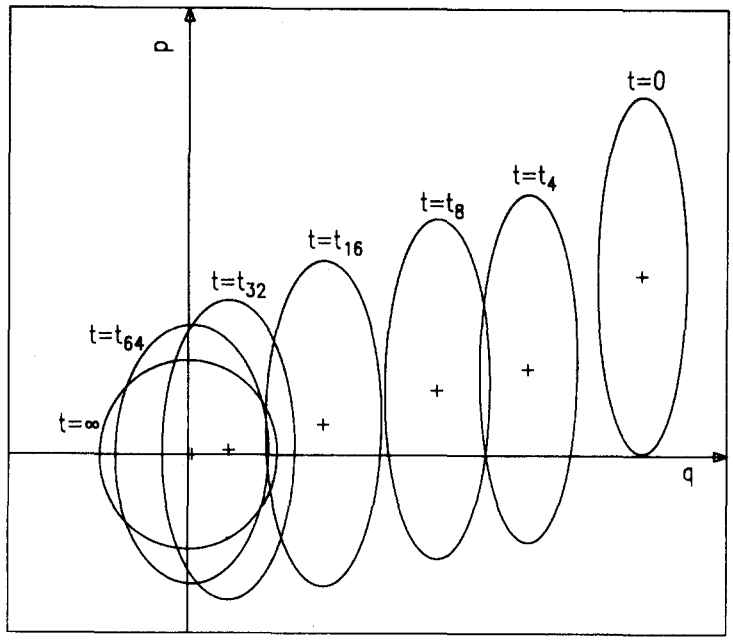

Fig. 5. Time evolution of the uncertainty ellipse of a squeezed state in the $\tilde{p}$, $\tilde{q}$-plane for some of the timepoints t_n where $\tilde{\sigma}_{pq}(t_n)$ vanishes. The centre of the ellipse gives the oscillation amplitudes $\langle q\rangle_{t_n}$ and $\langle p\rangle_{t_n}$ while the axes are $x_+(t_n)=\tilde{\sigma}_p^{1/2}(t_n)$ and $x_-(t_n)=\tilde{\sigma}_q^{1/2}(t_n)$. Depicted are the results for a Drude model with $\omega_D=10\omega_0$, $\gamma=0.01\omega_0$, $\zeta=2$, $T=0$, $\tilde{q}_0=5$ and $\tilde{p}_0=2$.

latter terms determine the lifetime of the squeezed fluctuations which is of the order of $2\gamma^{-1}$. For weak damping ($\gamma \ll \omega_0$) one has to note that all terms which decay slower than $\exp(-\gamma t)$ are by a factor of γ/ω_0 smaller so that they become important only after a period of time when most of the squeezing has already died out. Hence, for weakly damped systems the lifetime of the squeezing is of order γ^{-1} for all temperatures [23] and the result of the weak coupling theory [48] is valid even at $T=0$.

Figure 4 also shows that the initial squeezing below the vacuum fluctuations is increased by dissipation. While stronger damping leads to a faster decay of the "dynamical" squeezing (i.e. the squeezing produced by the generation mechanism), the "static" squeezing of the equilibrium variance below the vacuum level is increased by the damping. This second effect of dissipation is not described by a weak coupling theory and it is more pronounced for stronger damping. However, even for the weakly damped system shown in fig. 4 it has the consequence that the $T=0$ curve for the minor axis takes about twice as long to reach the vacuum line than the finite-temperature curve. The condition of low temperatures is not very stringent in the optical regime where even at room temperature $k_B T<0.1\hbar\omega_0$ but it requires millikelvin temperatures if one works with microwaves.

PART III. FREE BROWNIAN MOTION

9. Time evolution of a damped free particle

In this section we continue our discussion of linear dissipative systems by considering a Brownian particle which is not subject to an external potential. The Hamiltonian

$$H = \frac{p^2}{2M} + \sum_{n=1}^{N} \left[\frac{p_n^2}{2m_n} + \frac{1}{2} m_n \omega_n^2 \left(x_n - \frac{c_n q}{m_n \omega_n^2} \right)^2 \right] \tag{9.1}$$

upon which we base this study follows from (2.1–2.4) by putting $V(q, t) = 0$. This is the simplest microscopic model for a dissipative system. In contrast to the harmonic case treated above the coordinate of the Brownian particle is not bounded. Without loss of generality we can assume that $c_n = m_n \omega_n^2$ because in this case the spectral density (4.1) takes the form

$$I(\omega) = \frac{1}{2} \sum_{n=1}^{N} m_n \omega_n^3 \delta(\omega - \omega_n)$$

which can still model any desired frequency dependence provided we choose the spectrum of environmental oscillators accordingly. With this choice of parameters the model described by the Hamiltonian (9.1) can be visualized as a particle of mass M with many harmonic oscillators attached to it as depicted in fig. 6. In this form the model is explicitly translationally invariant [20].

9.1. The displacement correlation function

To obtain the propagating function for free Brownian motion we have to take the limit $\omega_0 \to 0$ of our previous results for the damped harmonic oscillator. For simplicity we also assume that $F(t) = 0$. The coupling to an external force bears no new features as compared with the harmonic case and it can easily be restored at a later stage. In the limit $\omega_0 \to 0$ the variance $\langle q^2 \rangle$ becomes (cf. table 2)

$$\langle q^2 \rangle^{\mathrm{F}} = \lim_{\omega_0 \to 0} \langle q^2 \rangle = \frac{2}{M\beta} \sum_{n=1}^{\infty} \frac{1}{\nu_n^2 + \nu_n \hat{\gamma}(\nu_n)} + \lim_{\omega_0 \to 0} \frac{1}{M\beta\omega_0^2}, \tag{9.2}$$

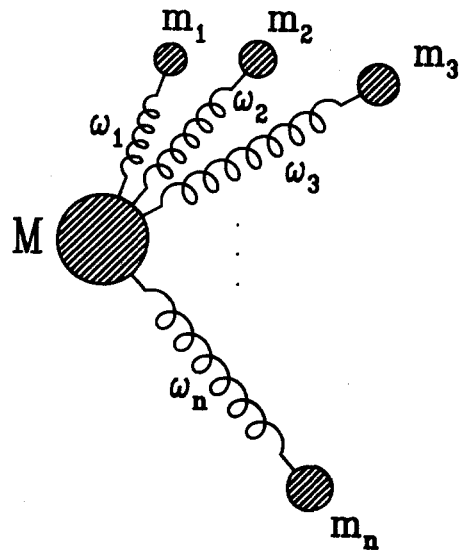

Fig. 6. A mechanical model of the Hamiltonian (9.1) for $c_n = m_n \omega_n^2$.

where the superscript F denotes quantities for free Brownian motion, henceforth. Clearly, the expression (9.2) diverges due to the last term. This is a consequence of the fact that the particle is not bound. The same type of divergence is met when we consider the symmetrized coordinate autocorrelation function. Using table 2 the Laplace transform $\hat{S}^{\mathrm{F}}(z)$ is found to read

$$\hat{S}^{\mathrm{F}}(z) = \frac{2}{M\beta} \sum_{n=1}^{\infty} \frac{z}{\nu_n^2 - z^2} \left[\frac{1}{z^2 + z\hat{\gamma}(z)} - \frac{1}{\nu_n^2 + \nu_n \hat{\gamma}(\nu_n)} \right] - \frac{1}{M\beta} \frac{1}{z^2} \frac{1}{z + \hat{\gamma}(z)} + \lim_{\omega_0 \to 0} \frac{1}{M\beta z \omega_0} \tag{9.3}$$

which is again divergent. However, the quantity of interest in the theory of free Brownian motion is not the autocorrelation function of the coordinate but the correlation of the displacement $q(t) - q(0)$ with the initial coordinate $q(0)$. This displacement correlation is defined by

$$Q^{\mathrm{F}}(t) = \tfrac{1}{2}\{\langle [q(t) - q(0)]q(0)\rangle + \langle q(0)[q(t) - q(0)]\rangle\} = S^{\mathrm{F}}(t) - \langle q^2 \rangle^{\mathrm{F}} . \tag{9.4}$$

By virtue of eqs. (9.2) and (9.3), the Laplace transform $\hat{Q}^{\mathrm{F}}(z)$ of the displacement correlation becomes

$$\begin{aligned} \hat{Q}^{\mathrm{F}}(z) &= \hat{S}^{\mathrm{F}}(z) - (1/z)\langle q^2 \rangle^{\mathrm{F}} \\ &= \frac{1}{M\beta} \left\{ -\frac{1}{z^2} \frac{1}{z + \hat{\gamma}(z)} + 2 \sum_{n=1}^{\infty} \frac{1}{\nu_n^2 - z^2} \left[\frac{1}{z + \hat{\gamma}(z)} - \frac{\nu_n}{z} \frac{1}{\nu_n + \hat{\gamma}(\nu_n)} \right] \right\} . \end{aligned} \tag{9.5}$$

This expression is regular so that we can employ the displacement correlation $Q^{\mathrm{F}}(t)$ instead of $S^{\mathrm{F}}(t)$ to formulate the theory. Using the stationarity of the equilibrium process it is readily established that $Q^{\mathrm{F}}(t)$ determines the mean square displacement of the Brownian particle according to

$$s(t) = \langle (q(t) - q(0))^2 \rangle = -2Q^{\mathrm{F}}(t) \tag{9.6}$$

which is the quantity investigated usually in the theory of Brownian movement.

Since the antisymmetrized correlation function $A(t)$ vanishes initially, no subtraction such as in eq. (9.4) is necessary. We have

$$A^{\mathrm{F}}(t) = \frac{1}{2\mathrm{i}} \langle [q(t) - q(0), q(0)] \rangle = \frac{1}{2\mathrm{i}} \langle [q(t), q(0)] \rangle , \tag{9.7}$$

so that the time-ordered displacement correlation function reads

$$C^{\mathrm{F}}(t) = \langle [q(t) - q(0)]q(0) \rangle = Q^{\mathrm{F}}(t) + \mathrm{i}A^{\mathrm{F}}(t) . \tag{9.8}$$

Using table 2 and taking the limit $\omega_0 \to 0$ we obtain for the Laplace transform of $A^{\mathrm{F}}(t)$

$$\hat{A}^{\mathrm{F}}(z) = -\frac{\hbar}{2M} \hat{G}_+^{\mathrm{F}}(z) = -\frac{\hbar}{2M} (z^2 + z\hat{\gamma}(z))^{-1} . \tag{9.9}$$

More explicit results for the time dependence of the correlation functions can only be obtained if we specify the frequency dependence of the damping coefficient $\hat{\gamma}(\omega)$.

9.2. The propagating function

Let us first consider the equilibrium density matrix of a free Brownian particle. By simply taking the limit $\langle q^2\rangle \to \infty$ in eq. (6.83) the prefactor would go to zero as a consequence of the fact that the density matrix of a nonlocalized particle cannot be normalized on the interval $(-\infty, +\infty)$. Hence, we define an equilibrium density matrix $\rho_\beta^{\mathrm{F}}(q, q')$ which is normalized on an interval of length L according to

$$\rho_\beta^{\mathrm{F}}(q, q') = L^{-1} \exp\left[-\frac{\langle p^2\rangle^{\mathrm{F}}}{2\hbar^2} (q - q')^2 \right]. \tag{9.10}$$

In contrast to the equilibrium state, most initial states of interest can be normalized on the entire interval. It is then convenient to introduce the density matrix

$$\bar{\rho}_\beta^{\mathrm{F}}(q, q') = L\rho_\beta^{\mathrm{F}}(q, q') = \exp\left[-\frac{\langle p^2\rangle^{\mathrm{F}}}{2\hbar^2} (q - q')^2 \right] \tag{9.11}$$

which is normalized on an interval of length 1 and to redefine the preparation function $\lambda_0^{\mathrm{F}}(q, \bar{q}, q', \bar{q}')$ for free Brownian motion such that all normalization factors are included in $\lambda_0^{\mathrm{F}}(q, \bar{q}, q', \bar{q}')$. The initial reduced density matrix is then written as [cf. eq. (3.36)]

$$\rho_0(q, q') = \int \mathrm{d}\bar{q}\, \mathrm{d}\bar{q}'\, \lambda_0^{\mathrm{F}}(q, \bar{q}, q', \bar{q}')\bar{\rho}_\beta^{\mathrm{F}}(\bar{q}, \bar{q}') . \tag{9.12}$$

Using the definition (9.4) of the displacement correlation function we can now determine the propagating function (6.71), (6.72) in the free Brownian motion limit. Then terms proportional to $(\langle q^2\rangle^{\mathrm{F}})^{-1}$ vanish, and the propagating function for free Brownian motion depends only on the relative coordinates

$$y = r_{\mathrm{f}} - r_{\mathrm{i}} ; \qquad \bar{y} = r_{\mathrm{i}} - \bar{r} . \tag{9.13}$$

This fact is of course a natural consequence of the translational invariance of the model. The propagating function reads

$$J^{\mathrm{F}}(x_{\mathrm{f}}, y, t, x_{\mathrm{i}}, \bar{x}, \bar{y}) = \frac{1}{4\pi|A^{\mathrm{F}}(t)|} \exp\left[\frac{\mathrm{i}}{\hbar} \Sigma^{\mathrm{F}}(x_{\mathrm{f}}, y, t, x_{\mathrm{i}}, \bar{x}, \bar{y}) \right], \tag{9.14}$$

where

$$\begin{aligned}
\Sigma^{\mathrm{F}}(x_{\mathrm{f}}, y, t, x_{\mathrm{i}}, \bar{x}, \bar{y}) &= \mathrm{i} \frac{\langle p^2\rangle^{\mathrm{F}}}{2\hbar} \bar{x}^2 \\
&+ (x_{\mathrm{i}}\bar{y} + x_{\mathrm{f}}y) M \frac{\dot{A}^{\mathrm{F}}(t)}{A^{\mathrm{F}}(t)} + x_{\mathrm{i}}y \frac{\hbar}{2A^{\mathrm{F}}(t)} - x_{\mathrm{f}}\bar{y} \frac{2}{\hbar} M^2 \left[\ddot{A}^{\mathrm{F}}(t) - \frac{\dot{A}^{\mathrm{F}}(t)^2}{A^{\mathrm{F}}(t)} \right] \\
&+ \mathrm{i}x_{\mathrm{i}}\bar{x} \left[-\frac{\langle p^2\rangle^{\mathrm{F}}}{\hbar} + \frac{M\dot{Q}^{\mathrm{F}}(t)}{2A^{\mathrm{F}}(t)} \right] + \mathrm{i}x_{\mathrm{f}}\bar{x} \frac{M^2}{\hbar} \left[\dot{Q}^{\mathrm{F}}(t) \frac{\dot{A}^{\mathrm{F}}(t)}{A^{\mathrm{F}}(t)} - \ddot{Q}^{\mathrm{F}}(t) \right]
\end{aligned}$$

$$+\mathrm{i}x_\mathrm{i}^2\left[\frac{\langle p^2\rangle^\mathrm{F}}{2\hbar}-\frac{M\dot{Q}^\mathrm{F}(t)}{2A^\mathrm{F}(t)}-\frac{\hbar Q^\mathrm{F}(t)}{4A^\mathrm{F}(t)^2}\right]$$

$$+\mathrm{i}x_\mathrm{i}x_\mathrm{f}\left[-\frac{M^2}{\hbar}\left\{\dot{Q}^\mathrm{F}(t)\frac{\dot{A}^\mathrm{F}(t)}{A^\mathrm{F}(t)}-\ddot{Q}^\mathrm{F}(t)\right\}+\frac{M}{2A^\mathrm{F}(t)^2}\{A^\mathrm{F}(t)\dot{Q}^\mathrm{F}(t)-2\dot{A}^\mathrm{F}(t)Q^\mathrm{F}(t)\}\right]$$

$$+\mathrm{i}x_\mathrm{f}^2\left[\frac{\langle p^2\rangle^\mathrm{F}}{2\hbar}+\frac{M^2\dot{A}^\mathrm{F}(t)}{\hbar A^\mathrm{F}(t)}\left\{\dot{Q}^\mathrm{F}(t)-\frac{\dot{A}^\mathrm{F}(t)}{A^\mathrm{F}(t)}\,Q^\mathrm{F}(t)\right\}\right]. \tag{9.15}$$

Here $J^\mathrm{F}(x_\mathrm{f}, y, t, x_\mathrm{i}, \bar{x}, \bar{y})$ is normalized in accordance with eq. (9.11) and determines the density matrix at time t according to

$$\rho(x_\mathrm{f}, r_\mathrm{f}, t)=\int \mathrm{d}x_\mathrm{i}\,\mathrm{d}y\,\mathrm{d}\bar{x}\,\mathrm{d}\bar{y}\,J^\mathrm{F}(x_\mathrm{f}, y, t, x_\mathrm{i}, \bar{x}, \bar{y})\lambda^\mathrm{F}(r_\mathrm{f}-y, x_\mathrm{i}, \bar{y}, \bar{x})\,. \tag{9.16}$$

The preparation function $\lambda^\mathrm{F}(r, x_\mathrm{i}, \bar{y}, \bar{x})$ is related to the function $\lambda_0^\mathrm{F}(q, \bar{q}, q', \bar{q}')$ defined above by

$$\lambda^\mathrm{F}(r, x_\mathrm{i}, \bar{y}, \bar{x})=\lambda_0^\mathrm{F}(r+x_\mathrm{i}/2, r-\bar{y}+\bar{x}/2, r-x_\mathrm{i}/2, r-\bar{y}-\bar{x}/2)\,. \tag{9.17}$$

As in the harmonic case the time dependence of the propagating function is determined completely by the correlation functions $A^\mathrm{F}(t)$ and $Q^\mathrm{F}(t)$. Again, the propagating function (9.14, 9.15) is not defined for times where $A^\mathrm{F}(t)=0$. There is always a zero of $A^\mathrm{F}(t)$ at $t=0$ where the previous result (6.80) for the harmonic oscillator remains valid. We have

$$J^\mathrm{F}(x_\mathrm{f}, y, 0, x_\mathrm{i}, \bar{x}, \bar{y})=\bar{\rho}_\beta^\mathrm{F}(\bar{x})\delta(x_\mathrm{f}-x_\mathrm{i})\delta(y)\,. \tag{9.18}$$

Other zeros of $A^\mathrm{F}(t)$ are usually not expected for free Brownian motion. However, for particular forms of $\hat{\gamma}(z)$ leading to such zeros, the same regularization of the propagating function as in the harmonic case may be applied.

10. Ohmic dissipation

In this section we consider specifically the Ohmic model introduced in section 7. There $\hat{\gamma}(\omega)=\gamma$, and we obtain from eq. (9.9)

$$A^\mathrm{F}(t)=-(\hbar/2M\gamma)\{1-\exp(-\gamma t)\} \tag{10.1}$$

which gives the well-known expression

$$\chi^\mathrm{F}(t)=(1/M\gamma)\{1-\exp(-\gamma t)\} \tag{10.2}$$

for the response function of a free Brownian particle. The time dependence of the symmetrized displacement correlation function $Q^\mathrm{F}(t)$ can also readily be evaluated for an Ohmic heat bath. Inserting $\hat{\gamma}(\omega)=\gamma$ in eq. (9.5) the expression can be rewritten in the form

$$\hat{Q}^{\mathrm{F}}(z) = \frac{1}{M\beta}\left\{\frac{1}{\gamma^2 z} - \frac{1}{\gamma z^2} + \sum_{n=-\infty}^{\infty} \frac{1}{\nu_n^2 - \gamma^2}\,\frac{1}{z+\gamma} - \sum_{n=1}^{\infty} \frac{2}{\nu_n^2 + \nu_n\gamma}\,\frac{1}{z} + \sum_{n=1}^{\infty} \frac{2\gamma}{\nu_n(\gamma^2 - \nu_n^2)}\,\frac{1}{z+\nu_n}\right\}. \tag{10.3}$$

The inverse Laplace transform of this expression is easily obtained as

$$Q^{\mathrm{F}}(t) = -\frac{1}{M\beta\gamma}\,t + \frac{1}{M\beta\gamma^2} - \frac{2}{M\beta}\sum_{n=1}^{\infty}\frac{1}{\nu_n^2 + \nu_n\gamma} - \frac{\hbar}{2M\gamma}\cot\left(\frac{\hbar\beta\gamma}{2}\right)\exp(-\gamma t) + \frac{2\gamma}{M\beta}\sum_{n=1}^{\infty}\frac{\exp(-\nu_n t)}{\nu_n(\gamma^2 - \nu_n^2)}\,, \tag{10.4}$$

where we used the representation of $\cot(x)$ as an infinite sum, i.e.

$$\cot(x) = \sum_{n=-\infty}^{\infty}\frac{x}{x^2 - \pi^2 n^2}\,. \tag{10.5}$$

In the classical limit $\hbar \to 0$ the expression (10.4) for the displacement correlation function simplifies to give the familiar result

$$Q_{\mathrm{cl}}^{\mathrm{F}}(t) = -\frac{1}{M\beta\gamma}\,t + \frac{1}{M\beta\gamma^2}\,(1 - \exp(-\gamma t)) \tag{10.6}$$

which is proportional to t for long times. For lower but finite temperatures the long time behaviour of the quantum mechanical correlation $Q^{\mathrm{F}}(t)$ is also governed by the term $-t/(M\beta\gamma)$, since the remaining terms in eq. (10.4) are either constant or vanish for large t. The diffusion coefficient can now be defined in the usual way through

$$D = \tfrac{1}{2}\lim_{t\to\infty}\frac{1}{t}\,s(t) = -\lim_{t\to\infty}\frac{1}{t}\,Q^{\mathrm{F}}(t) \tag{10.7}$$

which for $T > 0$ gives the familiar Einstein relation

$$D = 1/M\beta\gamma = k_{\mathrm{B}}T/M\gamma\,. \tag{10.8}$$

Note that the long-time behaviour of the Brownian particle characterized by D is not affected by quantum fluctuations.

The case $T = 0$ needs special care. Then the diffusion coefficient vanishes and the displacement correlation grows at a slower rate. Since the frequencies ν_n become continuous the sums have to be replaced by integrals according to

$$\lim_{T\to 0}\frac{1}{\beta}\sum_{n=1}^{\infty} f(\nu_n) = \frac{\hbar}{2\pi}\int_0^{\infty} \mathrm{d}\nu\, f(\nu)\,. \tag{10.9}$$

For the time derivative of the displacement correlation we obtain from eq. (10.4) in the limit $T \to 0$

$$\dot{Q}_0^{\mathrm{F}}(t) = \frac{\hbar\gamma}{\pi M} \int_0^\infty \mathrm{d}\nu \, \frac{\exp(-\nu t)}{\nu^2 - \gamma^2} \,. \tag{10.10}$$

This integral can be evaluated in terms of the exponential integral function $\mathrm{Ei}(x)$ which for all x not on the positive real axis is defined by

$$\mathrm{Ei}(x) = \int_{-\infty}^{x} \mathrm{d}y \, \frac{\exp(y)}{y} \tag{10.11}$$

and which for $x > 0$ is continued by

$$\overline{\mathrm{Ei}}(x) = \lim_{\varepsilon \to 0} \tfrac{1}{2}[\mathrm{Ei}(x + \mathrm{i}\varepsilon) + \mathrm{Ei}(x - \mathrm{i}\varepsilon)] \,. \tag{10.12}$$

Since $Q^{\mathrm{F}}(0) = 0$ (cf. eq. (9.4)), we find from eq. (10.10)

$$Q_0^{\mathrm{F}}(t) = \frac{\hbar}{2\pi M} \int_0^t \mathrm{d}s \, [\mathrm{Ei}(-\gamma s)\exp(\gamma s) - \overline{\mathrm{Ei}}(\gamma s)\exp(-\gamma s)] \,. \tag{10.13}$$

For long times this integral grows like the logarithm [20]

$$Q_0^{\mathrm{F}}(t) \simeq -\frac{\hbar}{\pi M \gamma} \log(\gamma t) \,, \qquad \text{for} \quad t \to \infty \,, \tag{10.14}$$

which shows that in the absence of thermal fluctuations the mean square displacement of a Brownian particle grows slower than in a diffusion process.

In the Ohmic case the momentum dispersion is again logarithmically divergent like the expression (7.5) for the harmonic oscillator. From table 2 we obtain in the limit $\omega_0 \to 0$

$$\langle p^2 \rangle^{\mathrm{F}} = \frac{M}{\beta} \sum_{n=-\infty}^{\infty} \frac{\gamma}{\gamma + |\nu_n|} \,. \tag{10.15}$$

However, this ultraviolet divergence has nothing to do with the infrared divergence of the correlation function (9.3). Rather, it is a consequence of the unphysical high-frequency behaviour of an ideal Ohmic reservoir. The divergence of $\langle p^2 \rangle^{\mathrm{F}}$ is readily removed if we introduce an environmental cutoff, e.g. by the Drude regularization described in section 7.

The asymptotic behaviour of the propagating function (9.14, 9.15) for $t \to \infty$ cannot be studied in parallel to the harmonic case because the correlation functions do not go to zero in the free Brownian motion limit. Rather, we insert the asymptotic laws $Q^{\mathrm{F}}(t) = -Dt$ and $A^{\mathrm{F}}(t) = -a$ into (9.14, 9.15). Since the mean square displacement grows diffusively, we have to retain terms of order $y/t^{1/2}$ while all other terms $\propto t^{\nu}$ $(\nu < 0)$ vanish. The propagating function then becomes

$$J(x_{\mathrm{f}}, y, t, x_{\mathrm{i}}, \bar{x}, \bar{y}) \simeq \bar{\rho}_\beta^{\mathrm{F}}(x_{\mathrm{f}}) \bar{\rho}_\beta^{\mathrm{F}}(\bar{x}) \, \frac{1}{4\pi a} \exp\Big[-\Big(\frac{D}{4a^2} t + \frac{\langle p^2 \rangle^{\mathrm{F}}}{2\hbar^2} - \frac{MD}{\hbar a} \Big) x_{\mathrm{i}}^2$$
$$+ \Big\{ \frac{\mathrm{i}}{2a} (y + \bar{y}) + \Big(\frac{\langle p^2 \rangle^{\mathrm{F}}}{\hbar^2} - \frac{MD}{\hbar a} \Big) \bar{x} - \frac{MD}{\hbar a} x_{\mathrm{f}} \Big\} x_{\mathrm{i}} \Big] \,, \qquad \text{for} \quad t \to \infty, \; T > 0 \,. \tag{10.16}$$

Completing the square in the exponent we have in the limit $t\to\infty$, $T>0$

$$J(x_f, y, t, x_i, \bar{x}, \bar{y}) \simeq \bar{\rho}^F_\beta(x_f)\bar{\rho}^F_\beta(\bar{x})\,\frac{1}{4\pi a}\exp\Big[-\frac{D}{4a^2}\,t\Big(x_i+\frac{ia}{Dt}\,y\Big)^2\Big]\exp\Big(-\frac{1}{4Dt}\,y^2\Big)$$

$$=\bar{\rho}^F_\beta(x_f)\bar{\rho}^F_\beta(\bar{x})\delta(x_i)(4\pi Dt)^{-1/2}\exp\Big(-\frac{1}{4Dt}\,y^2\Big)\,. \tag{10.17}$$

To obtain the second equality we noted that the first exponential approaches a δ-function as $t\to\infty$. An initial state characterized by $\lambda^F(r_f - y, x_i, \bar{y}, \bar{x})$ thus asymptotically becomes

$$\rho(x_f, r_f, t) \simeq (4\pi Dt)^{-1/2}\exp\Big(-\frac{1}{4Dt}\,r_f^2\Big)\bar{\rho}^F_\beta(x_f)\int \mathrm{d}r_i\,\mathrm{d}\bar{x}\,\mathrm{d}\bar{y}\,\lambda^F(r_i, 0, \bar{y}, \bar{x})\bar{\rho}^F_\beta(\bar{x})\,, \tag{10.18}$$

for $t\to\infty$, $T>0$. Here, we put $y = r_f - r_i$ in eq. (10.17) and noted that the terms $\propto r_i$ vanish in the limit $t\to\infty$ since for a state initially localized around the origin it is the final coordinate which is responsible for the growth of y. Now, the integral in the last line is just the trace of the initial state. Hence, for a normalized initial state localized in a finite region the asymptotic time-evolution of the density matrix becomes

$$\rho(x_r, r_f, t) \simeq (8\pi Dt)^{-1/2}\exp\Big(-\frac{1}{8Dt}\,r_f^2\Big)\exp\Big(-\frac{\langle p^2\rangle^F}{2\hbar^2}\,x_f^2\Big)\,, \tag{10.19}$$

for $t\to\infty$, $T>0$, where the first exponential together with the prefactor describes the diffusive spreading of the state while the last term represents the equilibrium distribution of the momentum. A corresponding analysis shows that at zero temperature the approach to equilibrium happens at a slower rate according to the logarithmic law (10.14).

11. Frequency-dependent damping

11.1. Spectral density and damping coefficient

For a frequency-dependent damping mechanism we can in general no longer obtain exact results for the correlation functions like we did in the Ohmic case. We can, however, examine the asymptotic behaviour for arbitrary frequency dependence of the damping [24]. The long-time dependence of a function is determined by its Laplace transform for arguments with a small positive real part. Hence, the results will depend mainly on the low-frequency properties of the damping. Let us consider a class of reservoirs where the spectral density $I(\omega)$ at low frequencies is $\propto\omega^\alpha$ where the spectral exponent α is a real positive number. Negative values of α cannot occur because the definition (4.1) of the spectral density implies $I(0) = 0$. In order to describe a realistic heat bath, we have to cut off the spectral density at high frequencies. Choosing a sharp cutoff at ω_c, the reservoir is described by

$$I(\omega) = Mg_\alpha\omega^\alpha\Theta(\omega_c - \omega)\,; \qquad \alpha>0\,. \tag{11.1}$$

We note that most of the following results do not depend on this special choice of the cutoff but are also met if we consider a soft cutoff, where $I(\omega)$ vanishes continuously as $\omega\to\infty$. In fact, the high-frequency

properties of the heat bath affect the long time behaviour of the correlations only if the spectral exponent $\alpha \geq 2$ where the damping leads to a renormalization of the mass of the Brownian particle (see below). For times $t \gg \omega_c^{-1}$ a real reservoir can therefore be described by a spectral density of the form (11.1) coinciding with the true spectral density at low frequencies plus a modified bare mass of the particle which compensates for the high frequency deviations from eq. (11.1). Reservoirs of the form (11.1) were discussed in various contexts. For instance, the coupling of a charged defect to electrons can be modelled by Ohmic dissipation, i.e. $\alpha = 1$. In the case of a phonon bath in d dimensions one gets $\alpha = d$ or $\alpha = d + 2$ depending on the symmetry of the coupling.

Inserting the spectral density in eq. (4.49), the frequency-dependent damping coefficient is found to read

$$\hat{\gamma}(\omega) = \frac{2g_\alpha}{\alpha\pi} \frac{\omega_c^\alpha}{\omega} F\left(1, \frac{\alpha}{2}; 1 + \frac{\alpha}{2}; -\frac{\omega_c^2}{\omega^2}\right), \tag{11.2}$$

where $F(a, b; c; z)$ is the hypergeometric function. For small frequencies we can use the asymptotic expansion of the hypergeometric function yielding [24]

$$\hat{\gamma}(\omega) = \begin{cases} \{g_\alpha / \sin(\frac{1}{2}\pi\alpha)\}\omega^{\alpha-1}[1 + O(\omega/\omega_c, (\omega/\omega_c)^{2-\alpha})], & \text{for } 0 < \alpha < 2, \\ (g_2/\pi)\omega \ln(1 + \omega_c^2/\omega^2), & \text{for } \alpha = 2, \\ (2g_\alpha \omega_c^{\alpha-2}/\pi(\alpha-2))\omega[1 - \{\pi(\alpha-2)/2\sin(\frac{1}{2}\pi(\alpha-2))\} \\ \quad \times (\omega/\omega_c)^{\alpha-2} + O(\omega^2/\omega_c^2)], & \text{for } 2 < \alpha < 4, \\ (2g_\alpha \omega_c^{\alpha-2}/\pi(\alpha-2))\omega[1 + O(\omega^2/\omega_c^2)], & \text{for } \alpha \geq 4, \end{cases} \tag{11.3}$$

where we included the next to leading order term in the case $2 < \alpha < 4$ for later purposes. For $\omega = 0$ the damping coefficient is only analytical for odd integer values of α. Otherwise, derivatives of order n of $\hat{\gamma}(\omega)$ diverge when $n \geq \alpha - 1$.

11.2. The antisymmetrized displacement correlation function

Now, the antisymmetrized displacement correlation follows from (9.9) as

$$A^F(t) = \frac{i\hbar}{4\pi M} \int_{-i\infty+\varepsilon}^{i\infty+\varepsilon} dz \, \frac{\exp(zt)}{z^2 + z\hat{\gamma}(z)} . \tag{11.4}$$

Let us first consider the case $\alpha < 2$. Inserting eq. (11.3) we obtain

$$A^F(t) \simeq \frac{i\hbar}{4\pi M} \frac{\sin(\pi\alpha/2)}{g_\alpha} t^{\alpha-1} \int_{-i\infty+\varepsilon}^{i\infty+\varepsilon} dx \, \frac{\exp(x)}{x^\alpha[1 + O(x/\omega_c t, (x/\omega_c t)^{2-\alpha})]} , \tag{11.5}$$

for $t \to \infty$. For long times we can expand the integrand in a power series in $x/\omega_c t$. The leading term yields a representation of Euler's gamma function, so that

$$A^F(t) \simeq -\frac{\hbar \sin(\pi\alpha/2)}{2Mg_\alpha \Gamma(\alpha)} t^{\alpha-1}[1 + O((\omega_c t)^{-1}, (\omega_c t)^{\alpha-2})], \tag{11.6}$$

for $t \to \infty$. This long time expansion includes the corresponding limit of the exact Ohmic result (10.1) since the corrections vanish for $\omega_c \to \infty$.

For $\alpha = 2$ an analogous analysis of eq. (11.4) yields

$$A^F(t) \simeq -\frac{\pi\hbar}{4g_2 M} \frac{t}{\ln(t)} [1 + O(\ln^{-1}(t))], \tag{11.7}$$

for $t \to \infty$, where we omitted the constant which renders the argument of the logarithm dimensionless. The value of this constant depends on the corrections to the leading order time dependence.

In the case $\alpha > 2$ we obtain

$$A^F(t) \simeq -\frac{\hbar}{2M_r} t\left[1 + \frac{M}{M_r} \frac{g_\alpha}{\sin(\pi(\alpha-2)/2)\Gamma(4-\alpha)} t^{2-\alpha} + O(\omega_c^{-2}t^{-2}, \omega_c^{-\alpha}t^{-\alpha})\right], \tag{11.8}$$

for $t \to \infty$, where we introduced the renormalized mass

$$M_r = M[1 + 2g_\alpha \omega_c^{\alpha-2}/\pi(\alpha-2)], \tag{11.9}$$

for $\alpha > 2$. For later use we have included in eq. (11.8) the leading correction for $2 < \alpha < 4$.

We can now discuss the effect of a constant driving force on the Brownian particle in the different regimes. The response of the momentum to an applied force is $\langle p \rangle_t^F = G_+^F(t)F = -(2M/\hbar)A^F(t)F$. For $\alpha < 1$ (sub-Ohmic damping) the force drags the particle away but the velocity becomes arbitrarily small for large times where the strong damping at low frequencies is important. In the Ohmic case ($\alpha = 1$) we obtain a constant velocity as has been argued before. For $\alpha > 1$ (super-Ohmic damping) the velocity of the particle grows as time increases. As the spectral exponent α exceeds 2, the damping effectively vanishes for long times, and we obtain a constant acceleration F/M_r of the particle. Hence, the Brownian particle behaves as a free particle for $\alpha > 2$, albeit with a renormalized mass M_r [24]. This mass renormalization is the only effect of the environmental coupling that survives for long times. This is easily understood if we consider the definition (11.9) of M_r in terms of the microscopic model. Using eqs. (11.1) and (4.1) we have

$$M_r = M + 2\int_0^\infty \frac{d\omega}{\pi} \frac{I(\omega)}{\omega^3} = M + \sum_{n=1}^{N} m_n \tag{11.10}$$

so that the renormalized mass is just the sum of the masses of the Brownian particle and all environmental oscillators. For $\alpha > 2$ these oscillators are dragged along by the Brownian particle in the long-time limit. For $\alpha \leq 2$ the sum of the masses of the environmental oscillators is infinite. Then M_r does not appear in the theory and the Brownian particle is damped when it moves relative to the motionless centre of mass of the environment.

11.3. The symmetrized displacement correlation function

Let us now consider the long-time behaviour of the real part $Q^F(t)$ of the displacement correlation. While the imaginary part $A^F(t)$ and the Green's function $G_+^F(t)$ which we discussed before are

temperature-independent quantities, the asymptotic time dependence of $Q^{\mathrm{F}}(t)$ at finite temperatures differs strongly from the zero temperature case. At finite temperatures, all terms in the sum in eq. (9.5) giving the Laplace transform of $Q^{\mathrm{F}}(t)$ lead to exponentially decaying or constant terms in the time domain. Thus, the leading long-time dependence stems from the first term in eq. (9.5). This term, however, is connected with the antisymmetrized correlation by

$$\hat{Q}^{\mathrm{F}}(z) \simeq \frac{2}{\hbar\beta} \frac{\hat{A}^{\mathrm{F}}(z)}{z}, \qquad \text{for} \quad z \to 0,\ T > 0. \tag{11.11}$$

Accordingly, we have for long times

$$Q^{\mathrm{F}}(t) \simeq \frac{2}{\hbar\beta} \int_0^t \mathrm{d}s\, A^{\mathrm{F}}(s), \qquad \text{for} \quad t \to \infty,\ T > 0, \tag{11.12}$$

so that in the long-time limit the symmetrized displacement correlation is but a time integral of the antisymmetrized correlation. Using (11.6–11.8) we have in the limit $t \to \infty$, $T > 0$

$$Q^{\mathrm{F}}(t) \simeq \begin{cases} -\dfrac{\sin(\pi\alpha/2)}{M\beta g_\alpha \Gamma(\alpha+1)}\, t^\alpha [1 + \mathrm{O}(t^{-1}, t^{\alpha-2})], & \text{for} \quad \alpha < 2, \\ -(\pi/4M\beta g_2)(t^2/\ln(t))[1 + \mathrm{O}(\ln^{-1}(t))], & \text{for} \quad \alpha = 2, \\ -(t^2/2M_{\mathrm{t}}\beta)[1 + \mathrm{O}(t^{-2}, t^{2-\alpha})], & \text{for} \quad \alpha > 2. \end{cases} \tag{11.13}$$

Because of eq. (9.6) these asymptotic laws also determine the long-time dependence of the mean square displacement in equilibrium. For $\alpha < 2$ the mean square displacement grows $\propto t^\alpha$ which includes diffusive behaviour $\propto t$ in the Ohmic case. Sub-Ohmic damping ($\alpha < 1$) results in subdiffusive growth of the mean square displacement while super-Ohmic damping ($\alpha > 1$) yields a faster, superdiffusive time dependence. In the borderline case $\alpha = 2$ we get no simple power law behaviour, while for $\alpha > 2$ we again observe the asymptotic vanishing of the friction. The particle behaves as if it had started with a certain velocity which is then conserved. The damping is effective only on an intermediate time scale needed to establish this velocity.

Let us now consider the correlation $Q^{\mathrm{F}}(t)$ for $T = 0$. Then the frequencies ν_n are continuous and the sum in eq. (9.5) has to be replaced by an integral. We have

$$\hat{Q}_0^{\mathrm{F}}(z) = \frac{2}{\pi} \frac{1}{z} \int_0^\infty \mathrm{d}\nu\, \frac{1}{\nu^2 - z^2} [\hat{f}(\nu) - \hat{f}(z)] = \frac{2}{\pi} \frac{1}{z} \int_0^\infty \mathrm{d}\nu\, \frac{1}{\nu^2 - z^2}\, \hat{f}(\nu), \tag{11.14}$$

where

$$\hat{f}(z) = z^2 \hat{A}^{\mathrm{F}}(z). \tag{11.15}$$

In the time domain this gives a relation between $Q_0^{\mathrm{F}}(t)$ and $A^{\mathrm{F}}(t)$

$$Q_0^{\mathrm{F}}(t) = \frac{2}{\pi} \int_0^\infty \mathrm{d}x\, \frac{x}{x^2 - 1}\, A^{\mathrm{F}}(t/x). \tag{11.16}$$

We can now insert the asymptotic laws (11.6–11.8) for the antisymmetrized correlation $A^{\mathrm{F}}(t)$ and obtain the long-time dependence of $Q_0^{\mathrm{F}}(t)$. Evaluating the integral (11.16) for $t\to\infty$ one finds [24]

$$Q_0^{\mathrm{F}}(t)\simeq\begin{cases}-\left[\hbar/M(2-\alpha)\sin\left(\frac{\pi}{2-\alpha}\right)\right]\left[\sin\left(\pi\frac{\alpha}{2}\right)\Big/g_\alpha\right]^{1/(2-\alpha)} & \\ \quad\times[1+\mathrm{O}(t^{-1})]\,, & \text{for}\quad \alpha<1\,,\\ -\frac{\hbar}{\pi M g_1}\ln(t)\,[1+\mathrm{O}(\ln^{-1}(t))]\,, & \text{for}\quad \alpha=1\,,\\ -\frac{\hbar}{2Mg_\alpha\Gamma(\alpha)}\left[\sin^2\left(\pi\frac{2-\alpha}{2}\right)\Big/\cos\left(\pi\frac{2-\alpha}{2}\right)\right]t^{\alpha-1} & \\ \quad\times[1+\mathrm{O}(t^{\alpha-2})]\,, & \text{for}\quad 1<\alpha<2\,,\\ -\frac{\hbar\pi^2}{8Mg_2}\frac{t}{\ln^2(t)}[1+\mathrm{O}(\ln^{-1}(t))]\,, & \text{for}\quad \alpha=2\,,\\ -\frac{\hbar g_\alpha}{2\Gamma(4-\alpha)}\frac{M}{M_{\mathrm{r}}^2}\left[\cos\left(\pi\frac{\alpha-2}{2}\right)\right]^{-1}t^{3-\alpha}[1+\mathrm{O}(t^{2-\alpha})]\,, & \text{for}\quad 2<\alpha<3\,,\\ -\frac{\hbar g_3}{\pi}\frac{M}{M_{\mathrm{r}}^2}\ln(t)\,[1+\mathrm{O}(\ln^{-1}(t))]\,, & \text{for}\quad \alpha=3\,,\\ \text{constant}\,, & \text{for}\quad \alpha>3\,.\end{cases}\tag{11.17}$$

For a sub-Ohmic reservoir ($\alpha<1$) at zero temperature the symmetrized displacement correlation remains finite in the limit $t\to\infty$. We will see in section 12 that this has profound consequences for the time evolution of nonequilibrium initial states. For $\alpha=1$, we have the long-time expansion of the exact Ohmic correlation (10.13). For $1<\alpha<2$, the zero temperature displacement correlation grows by a power law. The case $\alpha=2$, however, is not described by a simple power law behaviour. For $2<\alpha<3$, we again have a power law growth. The case $\alpha=3$ corresponding to the coupling to a 3-dimensional phonon bath is similar to the Ohmic case ($\alpha=1$) and the displacement correlation again grows logarithmically. Likewise, the situation for $\alpha>3$ resembles sub-Ohmic damping. Then $Q_0^{\mathrm{F}}(t)$ approaches a constant

$$Q_0^{\mathrm{F}}(\infty)=\frac{2}{\pi}\int_0^\infty \mathrm{d}z\left[\hat{A}^{\mathrm{F}}(z)+\frac{\hbar}{2M_{\mathrm{r}}}\frac{1}{z^2}\right],\tag{11.18}$$

for $\alpha>3$ in the long-time limit. This last expression, however, cannot be evaluated using the low-frequency expansion of the damping coefficient. Apart from the mass renormalization, the value of $Q_0^{\mathrm{F}}(t\to\infty)$ for $\alpha>3$ is the only result where the high-frequency properties of the damping enter the long-time behaviour of the correlations.

For later use it is worthwhile to recollect the asymptotic results for all correlation functions. To simplify the notation, we introduce the length

$$q_\infty=\left[\hbar/M(2-\alpha)\sin\left(\frac{\pi}{2-\alpha}\right)\right]\left[\sin\left(\pi\frac{\alpha}{2}\right)\Big/g_\alpha\right]^{1/(2-\alpha)}\,,\tag{11.19}$$

for $\alpha < 1$ and the constants

$$d_\alpha = \begin{cases} \hbar/(\pi M g_1)\,, & \text{for } \alpha = 1\,, \\ (\hbar/2Mg_\alpha \Gamma(\alpha))\sin^2(\pi(2-\alpha)/2)/\cos(\pi(2-\alpha)/2)\,, & \text{for } 1<\alpha<2\,, \\ \pi^2\hbar/(8Mg_2)\,, & \text{for } a = 2\,, \\ [\hbar M g_\alpha/2M_r^2\Gamma(4-\alpha)\cos(\pi(\alpha-2)/2)]\,, & \text{for } 2<\alpha<3\,, \\ \hbar M g_3/(\pi M_r^2)\,, & \text{for } \alpha = 3\,. \end{cases} \tag{11.20}$$

Further, for $\alpha \leq 2$

$$\mu_\alpha = \begin{cases} Mg_\alpha \Gamma(\alpha+1)/\sin(\pi\alpha/2)\,, & \text{for } \alpha<2\,, \\ 4Mg_2/\pi\,, & \text{for } \alpha = 2\,, \end{cases} \tag{11.21}$$

is a generalized mobility which is connected with the generalized diffusion coefficient D_α by

$$D_\alpha = 1/\beta\mu_\alpha = k_B T/\mu_\alpha\,. \tag{11.22}$$

Finally, for $\alpha > 2$

$$v_\beta = (M_r\beta)^{-1/2} = (k_B T/M_r)^{1/2} \tag{11.23}$$

is the mean thermal velocity of a particle with mass M_r. In terms of these definitions, the asymptotic time laws are summarized in table 3. The exponent of the asymptotic time dependence of the response function and the mean square displacement is shown in fig. 7 as a function of the spectral exponent α

Table 3
Asymptotic long-time dependence of the mean square displacement [$s_0(t)$ for $T=0$ and $s(t)$ for $T>0$] and the antisymmetrized part $A^F(t)$ of the displacement correlation function in terms of the exponent α and the quantities defined in eqs. (11.19–11.23). The symmetrized part $Q^F(t)$ of the displacement correlation function is given by $Q^F(t) = -s(t)/2$

α	$s_0(t)$ [$T=0$]	$A^F(t)$	$s(t)$ [$T>0$]
$0<\alpha<1$	$2q_\infty$	$-(\alpha\hbar/2\mu_\alpha)t^{\alpha-1}$ $\times[1+O(t^{-1}, t^{\alpha-2})]$	$2D_\alpha t^\alpha$ $\times[1+O(t^{-1}, t^{\alpha-2})]$
$\alpha=1$	$2d_1\ln(t)$ $\times[1+O(\ln^{-1}(t))]$		
$1<\alpha<2$	$2d_\alpha t^{\alpha-1}$ $\times[1+O(t^{\alpha-2})]$		
$\alpha=2$	$2d_2 t/\ln^2(t)$ $\times[1+O(\ln^{-1}(t))]$	$-(\hbar/\mu_2)t/\ln(t)$ $\times[1+O(\ln^{-1}(t))]$	$2D_2 t^2/\ln(t)$ $\times[1+O(\ln^{-1}(t))]$
$2<\alpha<3$	$2d_\alpha t^{3-\alpha}$ $\times[1+O(t^{2-\alpha})]$	$-(\hbar/2M_r)t$ $\times[1+O(t^{-2}, t^{2-\alpha})]$	$2(v_\beta^2/2)t^2$ $\times[1+O(t^{-2}, t^{2-\alpha})]$
$\alpha=3$	$2d_3\ln(t)$ $\times[1+O(\ln^{-1}(t))]$		
$3<\alpha$	constant		

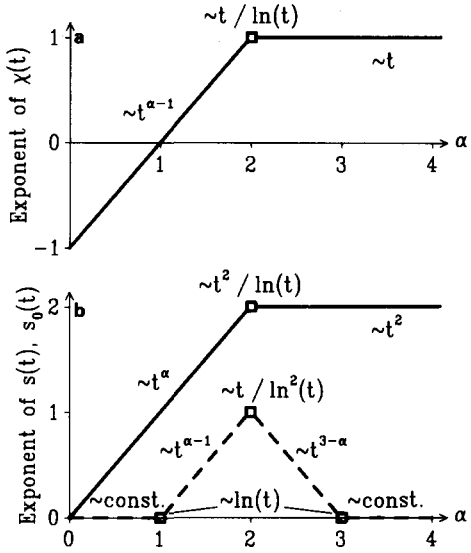

Fig. 7. (a) The exponent of the asymptotic time dependence of the response function $\chi(t)$ is shown as a function of the spectral exponent α. (b) The solid (dashed) line shows the exponent of the asymptotic time dependence of the mean square displacement $s(t)(s_0(t))$ for finite (zero) temperature as a function of the spectral exponent α.

characterizing the spectral density of the low frequency environmental modes. These results can also be derived by a more standard approach in which damping is described through a memory kernel [53].

12. Relaxation of nonequilibrium initial states

Let us now discuss the time evolution of a free Brownian particle starting from a nonequilibrium state generated by a preparation mechanism of the form described in section 2. We have seen that the dynamics of such a state can be expressed entirely in terms of the displacement correlation function $C^{F}(t)$. Since in the preceding section we have obtained analytic results for the long time behaviour of this correlation for practically all linear dissipative mechanisms of interest, we are now in the position to study how (or whether) a nonequilibrium initial state approaches equilibrium.

12.1. Time evolution of a Gaussian density matrix

Let us first consider a Brownian particle which is initially localized. Such a state may be prepared, e.g., using a device which lets pass particles at position q with probability $w(q,0)$. This position measurement is described by the projection operator

$$P_q = \int \mathrm{d}q\, w^{1/2}(q,0)|q\rangle\langle q|\,. \tag{12.1}$$

If we especially want to prepare a Gaussian wave packet, the measuring device can be visualized as a Gaussian slit against which an ensemble of particles propagates. We are then interested only in the

dynamics in the plane of the slit and not in the direction of this propagation. Choosing a state localized around the origin with width $\sigma_0^{1/2}$, the initial probability distribution $w(q,0)$ is given by

$$w(q,0) = (2\pi\sigma_0)^{-1/2} \exp(-q^2/2\sigma_0) . \tag{12.2}$$

The normalized initial density matrix is simply $W_0 = P_q \bar{W}_\beta P_q$, so that the preparation function follows from eqs. (2.12) and (9.17) as

$$\lambda^{\mathrm{F}}(r, x, \bar{y}, \bar{x}) = (2\pi\sigma_0)^{-1/2} \exp\left(-\frac{r^2}{2\sigma_0} - \frac{x^2}{8\sigma_0}\right) \delta(x-\bar{x})\delta(\bar{y}) . \tag{12.3}$$

Note that the position measurement also influences the nondiagonal coordinate of the density matrix and therefore affects the momentum distribution. As the uncertainty relation requires, a localization in position space yields a broader distribution in the conjugate variable. At time $t = 0$ the reduced density matrix is given by

$$\rho_0(x, r) = (2\pi\sigma_0)^{-1/2} \exp\left[-\frac{r^2}{2\sigma_0} - \left(\frac{\langle p^2\rangle^{\mathrm{F}}}{2\hbar^2} + \frac{1}{8\sigma_0}\right)x^2\right] . \tag{12.4}$$

Inserting the preparation function (12.3) and the propagating function (9.14, 9.15) in eq. (9.16) we obtain the density matrix at time t as

$$\begin{aligned}\rho(x, r, t) = {} & [2\pi\sigma(t)]^{-1/2} \exp\left(-\frac{\langle p^2\rangle^{\mathrm{F}}}{2\hbar^2} x^2\right) \\ & \times \exp\left[-\frac{1}{2\sigma(t)}\left\{r^2 + 2\frac{\mathrm{i}}{\hbar} Mxr\left(\dot{Q}^{\mathrm{F}}(t) - \frac{A^{\mathrm{F}}(t)\dot{A}^{\mathrm{F}}(t)}{\sigma_0}\right)\right.\right. \\ & \left.\left. - \frac{M^2}{\hbar^2} x^2\left[\dot{Q}^{\mathrm{F}}(t)^2 - \dot{A}^{\mathrm{F}}(t)^2\left\{1 + 2\frac{Q^{\mathrm{F}}(t)}{\sigma_0}\right\} - \frac{2}{\sigma_0} A^{\mathrm{F}}(t)\dot{A}^{\mathrm{F}}(t)\dot{Q}^{\mathrm{F}}(t)\right]\right\}\right] .\end{aligned} \tag{12.5}$$

Since the particle had no average velocity in the initial state, the wave packet remains centred at the origin. The width $\sigma^{1/2}(t)$ can be expressed through the correlations $Q^{\mathrm{F}}(t)$ and $A^{\mathrm{F}}(t)$ via

$$\sigma(t) = \sigma_0 - 2Q^{\mathrm{F}}(t) + A^{\mathrm{F}}(t)^2/\sigma_0 . \tag{12.6}$$

Since the symmetrized displacement correlation $Q^{\mathrm{F}}(t) = -s(t)/2$ is always negative, the wave packet can only become broader with increasing time.

12.2. Asymptotic spreading of the state

Let us now discuss how the long time behaviour of the variance (12.6) depends on the dissipative mechanism. To that aim we can use the asymptotic laws for the correlation functions which are summarized in table 3. At finite temperatures we obtain [24] for $t \to \infty$,

$$\sigma(t) \simeq \begin{cases} 2D_\alpha t^\alpha , & \text{for } \alpha < 2 , \\ 2D_2 t^2/\ln(t) , & \text{for } \alpha = 2 , \\ (v_\beta^2 + \hbar^2/4\sigma_0 M_r^2)t^2 , & \text{for } \alpha > 2 . \end{cases} \tag{12.7}$$

Hence, the state spreads diffusively in the Ohmic case ($\alpha = 1$) while for sub/super-Ohmic damping we have a sub/super-diffusive rate of growth of the variance, respectively. For all $\alpha \leq 2$ the asymptotic behaviour of $\sigma(t)$ is completely determined by the symmetric part $Q^F(t)$ of the displacement correlation. The antisymmetrized part contributes only for $\alpha > 2$ where we have a kinematic spreading with a velocity v_∞ given by

$$v_\infty^2 = v_\beta^2 + \hbar^2/4\sigma_0 M_r^2 . \tag{12.8}$$

In the classical limit only the first term in this expression survives. It stems from the symmetrized correlation and gives simply the thermal velocity of a particle with the renormalized mass M_r. The second term in eq. (12.8) is a quantum correction originating in the antisymmetric correlation. It becomes increasingly important at lower temperatures. This contribution to the asymptotic velocity may be viewed upon as a consequence of the uncertainty relation since it gives the minimal velocity fluctuations of a particle of mass M_r initially localized with variance σ_0.

At zero temperature the slower rate of increase of $Q^F(t)$ results in a slower spreading of the state for $\alpha \leq 2$ while for $\alpha > 2$ the asymptotic behaviour is qualitatively unchanged. Using table 3 we have for $t \to \infty$, $T = 0$

$$\sigma_0(t) \simeq \begin{cases} 2q_\infty + \sigma_0 , & \text{for } \alpha < 1 , \\ 2d_1 \ln(t) , & \text{for } \alpha = 1 , \\ (\alpha^2\hbar^2/4\mu_\alpha^2\sigma_0)t^{2\alpha-2} , & \text{for } 1 < \alpha < 2 , \\ (2\hbar^2/\mu_\alpha^2\sigma_0)t^2/\ln^2(t) , & \text{for } \alpha = 2 , \\ (\hbar^2/4\sigma_0 M_r^2)t^2 , & \text{for } \alpha > 2 . \end{cases} \tag{12.9}$$

Here it is the antisymmetric correlation $A^F(t)$ which dominates the asymptotic behaviour for all $\alpha > 1$. For $\alpha > 2$ eq. (12.8) for the asymptotic velocity is still correct since the thermal contribution v_β vanishes as $T \to 0$. Between $\alpha = 1$ and $\alpha = 2$ we cover the sub- and superdiffusive regimes including diffusive behaviour for $\alpha = 3/2$. For Ohmic damping we now have a logarithmic growth. Most remarkable, however, is the behaviour for sub-Ohmic dissipation ($\alpha < 1$). The initially localized state remains localized for all times although there is no external potential hindering the particle from drifting away. The localization length [24]

$$\xi = \sigma_0^{1/2}(t \to \infty) = (2q_\infty + \sigma_0)^{1/2} \tag{12.10}$$

consists of a dynamical part springing from the asymptotic value $2q_\infty$ of the mean square displacement $s_0(t)$ plus the initial width of the state. For $\alpha \to 0$ the localization length approaches the initial width whereas it diverges as the Ohmic case is approached. This corresponds to the crossover from the localized region to the logarithmic spreading of the state.

A localization of a particle by the dissipative influence of a heat bath was also found for Ohmic damping in the presence of a periodic potential [54]. In this case, however, the Ohmic coupling constant has to exceed a critical value in order to obtain a confined state while in our problem all nonvanishing values of the coupling lead to the localization of the particle as long as the exponent of the spectral density is less than 1. We add that for very low temperatures where the state does spread asymptotically according to eq. (12.7) the particle is still localized for times of order $\hbar/k_B T$ which may become very long due to the continuous vanishing of the leading time dependence in (12.7) as $T \to 0$.

12.3. Long time behaviour for arbitrary initial states at finite temperatures

Let us now consider the general behaviour of the propagating function (9.14, 9.15) for the different types of damping. Using the asymptotic correlations summarized in table 3, we can determine how initial states described by an arbitrary preparation function of the form discussed in section 2 behave for long times. This analysis is carried out in detail in ref. [24]. For an arbitrary state initially localized around 0 one finds for the density matrix in the limit of long times for $\alpha < 2$, $t \to \infty$, $T > 0$

$$\rho(x_f, r_f, t) \simeq (4\pi D_\alpha t^\alpha)^{-1/2} \exp\left(-\frac{1}{4D_\alpha} t^{-\alpha} r_f^2\right) \exp\left(-\frac{\langle p^2\rangle^F}{2\hbar^2} x_f^2\right), \tag{12.11}$$

where the first two terms describe the spreading of the state in position space while the last term shows that the momentum distribution of arbitrary initial states approaches the correct equilibrium distribution. For $\alpha = 2$, $t \to \infty$, $T > 0$ the analysis yields

$$\rho(x_f, r_f, t) \simeq \left[\frac{\ln(t)}{4\pi D_2 t^2}\right]^{1/2} \exp\left(-\frac{\ln(t)}{4D_2 t^2} r_f^2\right) \exp\left(-\frac{\langle p^2\rangle^F}{2\hbar^2} x_f^2\right), \tag{12.12}$$

where the spreading in position space occurs according to the faster law $t^2/\ln(t)$. In summary, for $\alpha \leq 2$ the state of the Brownian particle always approaches the equilibrium state as $t \to \infty$.

For $\alpha > 2$, however, the evolution of the density matrix of an initially localized state for long times is given by

$$\begin{aligned}\rho(x_f, r_f, t) &\simeq \frac{M_r}{2\pi\hbar t} \exp\left(-\frac{\phi}{2\hbar^2} x_f^2\right) \int dx_i\, \lambda^\infty(x_i) \exp\left[-i \frac{M_r}{\hbar t} r_f\left(x_i - \frac{M}{M_r} x_f\right)\right] \\ &= (M_r/\hbar t)\tilde{\lambda}^\infty(M_r r_f/\hbar t) \exp\left(\frac{iM}{\hbar t} r_f x_f\right) \exp\left(-\frac{\phi}{2\hbar^2} x_f^2\right)\end{aligned} \tag{12.13}$$

for $t \to \infty$, $T > 0$, $\alpha > 2$, with

$$\phi = \langle p^2\rangle^F - M^2 v_\beta^2 . \tag{12.14}$$

The reduced preparation function λ^∞ is defined by

$$\begin{aligned}\lambda^\infty(x_i) = &\int dr_i\, d\bar{x}\, d\bar{y}\, \lambda^F(r_i, x_i, \bar{y}, \bar{x}) \\ &\times \exp\left[-\frac{1}{2\hbar^2}\{\langle p^2\rangle^F(\bar{x} - x_i)^2 + 2MM_r v_\beta^2 x_i(\bar{x} - x_i) + M_r^2 v_\beta^2 x_i^2\}\right]\end{aligned} \tag{12.15}$$

with Fourier transform

$$\tilde{\lambda}^{\infty}(k_i) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}x_i \, \lambda^{\infty}(x_i) \exp(-\mathrm{i}k_i x_i) \,. \tag{12.16}$$

From eq. (12.13) it becomes clear that the asymptotic form of the density matrix still depends on the initial state for $\alpha > 2$. This is due to the fact that for $\alpha > 2$ the centre of mass velocity of the entire system is a conserved quantity the statistics of which is time independent.

Let us examine the distributions in coordinate and momentum space in more detail. The Wigner function corresponding to eq. (12.13) is given by

$$W(p, q, t) \simeq \left(\frac{M_r}{\hbar t}\right)(2\pi\phi)^{-1/2} \tilde{\lambda}^{\infty}\left(\frac{M_r q}{\hbar t}\right) \exp\left[-\frac{1}{2\phi}\left(p - M\frac{q}{t}\right)^2\right] \tag{12.17}$$

for $t \to \infty$, $T > 0$, $\alpha > 2$. Accordingly, the probability distribution in position space

$$\begin{aligned} w(q, t) &= \int \mathrm{d}p \, W(p, q, t) = \rho(0, q, t) \\ &\simeq (M_r/\hbar t)\tilde{\lambda}^{\infty}(M_r q/\hbar t) \,, \qquad \text{for} \quad t \to \infty, \; T > 0, \; \alpha > 2 \end{aligned} \tag{12.18}$$

depends only on the scaled variable $v = q/t$. Defining the probability distribution

$$\Omega(v) = \lim_{t \to \infty} t w(vt, t) = (M_r/\hbar)\tilde{\lambda}^{\infty}(M_r v/\hbar) \tag{12.19}$$

of this variable we have

$$w(q, t) = t^{-1} \, \Omega(q/t) \tag{12.20}$$

for $t \to \infty$, $T > 0$, $\alpha > 2$. Hence, the probability distribution in coordinate space behaves asymptotically as if the state had initially been localized at the origin with velocity distribution $\Omega(v)$. Then the spreading of the state is kinematical according to $q = vt$. The dissipation is effective only during intermediate times where momentum is transferred from the particle to the reservoir. Afterwards, the particle behaves as if it were free. The asymptotic velocity distribution $\Omega(v)$ is the distribution of the centre of mass velocity which depends on both the coupling to the heat bath and on those properties of the initial state entering its reduced preparation function.

The velocity distribution $\Omega(v)$ differs from the asymptotic momentum distribution of the Brownian particle which is given by

$$\begin{aligned} w_{\infty}(p) &= \lim_{t \to \infty} \int \mathrm{d}q \, W(p, q, t) \\ &= (2\pi\phi)^{-1/2} \int \mathrm{d}v \, \Omega(v) \exp\left[-\frac{1}{2\phi}(p - Mv)^2\right], \qquad \text{for} \quad T > 0, \; \alpha > 2 \,. \end{aligned} \tag{12.21}$$

Hence, apart from the momentum corresponding to the value given by $\Omega(v)$ there are dynamical fluctuations of magnitude ϕ in the momentum distribution. These fluctuations result from the environmental coupling [24].

12.4. Long time behaviour for arbitrary initial states at zero temperature

As we have already seen in the example of an initially localized wave packet, the long time behaviour at zero temperature differs from the finite T results. Let us start our discussion of the zero temperature asymptotics with the region $0 < \alpha < 1$. Using table 3 we obtain for the propagating function

$$J^{\mathrm{F}}(x_{\mathrm{f}}, y, t, x_{\mathrm{i}}, \bar{x}, \bar{y}) \simeq \bar{\rho}^{\mathrm{F}}_{\beta}(x_{\mathrm{f}})\bar{\rho}^{\mathrm{F}}_{\beta}(\bar{x})\,\frac{\mu_\alpha t^{1-\alpha}}{2\pi\alpha\hbar}$$
$$\times \exp\left[-\frac{\mu_\alpha^2 q_\infty}{\alpha^2\hbar^2}\, t^{2-2\alpha}\{x_{\mathrm{i}} + \mathrm{i}(\alpha\hbar/2\mu_\alpha q_\infty t^{1-\alpha})(y+\bar{y})\}^2\right] \exp\left[-\frac{1}{4q_\infty}(y+\bar{y})^2\right]$$
$$\simeq \bar{\rho}^{\mathrm{F}}_{\beta}(x_{\mathrm{f}})\bar{\rho}^{\mathrm{F}}_{\beta}(\bar{x})\delta(x_{\mathrm{i}})(4\pi q_\infty)^{-1/2} \exp\left[-\frac{1}{4q_\infty}(y+\bar{y})^2\right] \tag{12.22}$$

for $t \to \infty$, $T = 0$, $\alpha < 1$. Hence, for $\alpha < 1$ every localized initial state keeps a finite width for all times. This extends our finding for the Gaussian initial state considered in section 12.1 to the general case. We may again define a reduced preparation function by

$$\lambda^{\infty}_{\ell}(\bar{r}) = \int \mathrm{d}r_{\mathrm{i}}\,\mathrm{d}\bar{x}\;\lambda^{\mathrm{F}}(r_{\mathrm{i}}, 0, r_{\mathrm{i}} - \bar{r}, \bar{x})\bar{\rho}^{\mathrm{F}}_{\beta}(\bar{x})\,. \tag{12.23}$$

Then the asymptotic Wigner function can be written as

$$\lim_{t\to\infty} W(p, q, t) \simeq w^{\mathrm{F}}_{\beta}(p) w_\infty(q) \tag{12.24}$$

for $T = 0$, $\alpha < 1$ with the equilibrium momentum distribution

$$w^{\mathrm{F}}_{\beta}(p) = (2\pi\langle p^2\rangle^{\mathrm{F}})^{-1/2} \exp\left(-\frac{p^2}{2\langle p^2\rangle^{\mathrm{F}}}\right) \tag{12.25}$$

and the coordinate distribution

$$w_\infty(q) = (4\pi q_\infty)^{-1/2} \int \mathrm{d}\bar{r} \exp\left[-\frac{1}{4q_\infty}(q-\bar{r})^2\right] \lambda^{\infty}_{\ell}(\bar{r}) \tag{12.26}$$

for $T = 0$, $\alpha < 1$, which shows that the localization length is roughly the sum of the asymptotic contribution $2q_\infty$ plus an effective width of the initial state which is inherent in the reduced preparation function $\lambda^{\infty}_{\ell}(\bar{r})$. Since the effects of the reduced preparation function die out at finite temperatures, our model with $\alpha < 1$ provides a simple example for a dissipative phase transition at $T = 0$.

For Ohmic damping the asymptotic density matrix is found to read

$$\rho(x_f, r_f, t) \simeq [4\pi d_1 \ln(t)]^{-1/2} \exp\left[-\frac{r_f^2}{4d_1 \ln(t)}\right] \exp\left(-\frac{\langle p^2\rangle^F}{2\hbar^2} x_f^2\right) \tag{12.27}$$

for $t\to\infty$, $T=0$, $\alpha=1$, where the prefactor together with the first exponential describes the logarithmic spreading in position space while the momentum distribution reaches equilibrium as described by the last term. Hence, the effects of the initial preparation die out completely and the system is ergodic inasmuch as every initial state reaches a unique equilibrium state in the limit $t\to\infty$.

Finally, we consider the super-Ohmic case $\alpha>1$. The finite temperature definition (12.15) of the reduced preparation function simplifies at $T=0$ to read

$$\lambda_0^\infty(x_i) = \int \mathrm{d}r_i\, \mathrm{d}\bar{x}\, \mathrm{d}\bar{y}\, \lambda^F(r_i, x_i, \bar{y}, \bar{x}) \bar{\rho}_\beta^F(\bar{x} - x_i) \tag{12.28}$$

and the density matrix for long times now takes the form

$$\rho(x_f, r_\tau, t) \simeq [2|A^F(t)|]^{-1} \exp\left(\frac{iM}{\hbar t} c_\alpha r_f x_f\right) \bar{\rho}_\beta^F(x_f) \tilde{\lambda}_0^\infty(r_f/2|A^F(t)|) \tag{12.29}$$

for $t\to\infty$, $T=0$, $\alpha>1$, where $c_\alpha=\alpha-1$ for $1<\alpha<2$ and $c_\alpha=1$ for $\alpha\geq 2$. The probability distribution of the coordinate is given by

$$w(q,t) = [2|A^F(t)|]^{-1} \tilde{\lambda}_0^\infty(q/2|A^F(t)|) \tag{12.30}$$

for $t\to\infty$, $T=0$, $\alpha>1$, and the asymptotic momentum distribution follows from eq. (12.29) as

$$w_\infty(p) = \lim_{t\to\infty} (2\pi\langle p^2\rangle^F)^{-1/2} \int \mathrm{d}k\, \tilde{\lambda}_0^\infty(k) \exp\left[-\frac{1}{2\langle p^2\rangle^F}\left\{p - 2Mc_\alpha \frac{|A^F(t)|}{t} k\right\}^2\right] \tag{12.31}$$

for $t\to\infty$, $T=0$, $\alpha>1$. For $1<\alpha\leq 2$ the antisymmetric correlation $A^F(t)$ grows slower than $\propto t$. Hence, the initial state is not coupled to the final variables and the momentum distribution approaches its equilibrium form, eq. (12.25). Again we find that the system is ergodic. For $\alpha>2$ the correlation $A^F(t)$ grows $\propto t$ and the situation is basically the same as in the finite temperature case. Again the spreading in position space resembles an ensemble of free particles that started near the origin with a velocity distribution given by eq. (12.19). The momentum distribution (12.31) may be transformed to read

$$w_\infty(p) = (2\pi\langle p^2\rangle^F)^{-1/2} \int \mathrm{d}v\, \Omega(v) \exp\left[-\frac{1}{2\langle p^2\rangle^F}(p - Mv)^2\right] \tag{12.32}$$

for $t\to\infty$, $T=0$, $\alpha>2$, which is the zero temperature limit of eq. (12.21). Again the system is not ergodic since the final momentum distribution depends on the preparation via the centre of mass velocity distribution $\Omega(v)$. The dependence of the asymptotic states for $t\to\infty$ of free Brownian motion on α and T is illustrated in fig. 8.

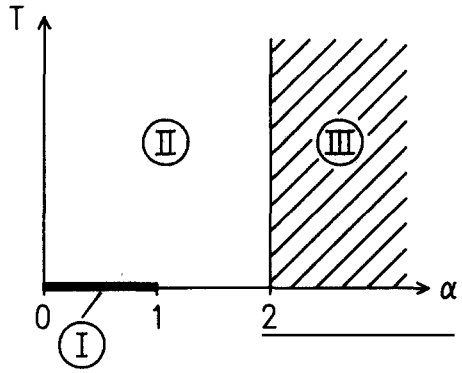

Fig. 8. The regions in the α–T-plane with different properties of the asymptotic states for $t \to \infty$ are shown in a phase diagram. Region I: unique asymptotic momentum distribution but localization in position space. Region II: unique asymptotic state independent of initial conditions. Region III: asymptotic momentum distribution depends on initial conditions.

Appendix A. Elimination of an environmental oscillator

We want to compute the integral (3.21)

$$F_n[q, x_{n_f}, x_{n_i}] = \int \mathcal{D}x_n \exp\left[\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}s \left(\tfrac{1}{2}m_n(\dot{x}_n^2 - \omega_n^2 x_n^2) + qc_n x_n - q^2 \frac{c_n^2}{2m_n\omega_n^2}\right)\right], \tag{A.1}$$

where we have to sum over all paths $x_n(s)$ of the nth environmental oscillator with $x_n(0) = x_{n_i}$ and $x_n(t) = x_{n_f}$. Since the functional integral is Gaussian, its dependence on the boundary values x_{n_i}, x_{n_f} may be obtained by expanding about the path $\tilde{x}_n(s)$ minimizing the action in the exponent of eq. (A.1) [17]. Decomposing

$$x_n(s) = \tilde{x}_n(s) + \xi_n(s) \tag{A.2}$$

where $\tilde{x}_n(0) = x_{n_i}$ and $\tilde{x}_n(t) = x_{n_f}$, we have

$$F_n[q, x_{n_f}, x_{n_i}] = \exp\left[\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}s \left(\tfrac{1}{2}m_n(\dot{\tilde{x}}_n^2 - \omega_n^2\tilde{x}_n^2) + qc_n\tilde{x}_n - q^2\frac{c_n^2}{2m_n\omega_n^2}\right)\right]$$

$$\times \int \mathcal{D}\xi_n \exp\left[\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}s \left(\tfrac{1}{2}m_n(\dot{\xi}_n^2 - \omega_n^2\xi_n^2)\right)\right]. \tag{A.3}$$

The functional integral over ξ_n sums over all paths $\xi(s)$ with $\xi_n(0) = \xi_n(t) = 0$ so that the dependence on x_{n_i} and x_{n_f} is completely included in the first exponential. To obtain eq. (A.3) we made use of the fact that $\tilde{x}_n(s)$ is a trajectory that minimizes the action, i.e. that terms linear in $\xi_n(s)$ are absent.

Let us first consider the first term in eq. (A.3). The Lagrangian equation of motion reads

$$m_n\ddot{\tilde{x}}_n(s) + m_n\omega_n^2\tilde{x}_n(s) = c_n q(s), \tag{A.4}$$

where the term on the rhs is a time-dependent force acting on the environmental oscillator due to its coupling to the Brownian particle. The solution of eq. (A.4) satisfying the boundary conditions is

$$\tilde{x}_n(s) = \frac{\chi_n(s)}{\chi_n(t)}\, x_{n_f} + \frac{\chi_n(t-s)}{\chi_n(t)}\, x_{n_i} - c_n\Big[\frac{\chi_n(s)}{\chi_n(t)} \int_0^t \mathrm{d}u\, \chi_n(t-u)q(u) - \int_0^s \mathrm{d}u\, \chi_n(s-u)q(u)\Big], \tag{A.5}$$

where

$$\chi_n(t) = (m_n\omega_n)^{-1} \sin(\omega_n t) \tag{A.6}$$

is the response function of the nth environmental oscillator. To compute the action of the trajectory $\tilde{x}_n(s)$ we perform an integration by parts and use the equation of motion (A.4). This yields

$$\int_0^t \mathrm{d}s \left[\frac{1}{2}\, m_n(\dot{\tilde{x}}_n^2 - \omega_n^2\tilde{x}_n^2) + qc_n\tilde{x}_n - q^2\, \frac{c_n^2}{2m_n\omega_n^2}\right]$$

$$= \tfrac{1}{2}m_n(\tilde{x}_n(t)\dot{\tilde{x}}_n(t) - \tilde{x}_n(0)\dot{\tilde{x}}_n(0)) - \tfrac{1}{2}c_n \int_0^t \mathrm{d}s\, q(s)\tilde{x}_n(s) - \frac{c_n^2}{2m_n\omega_n^2} \int_0^t \mathrm{d}s\, q^2(s)\,. \tag{A.7}$$

Inserting the solution (A.5) into this expression we get the result (3.23).

We still have to evaluate the path integral over the fluctuations $\xi_n(s)$ around the classical path $\tilde{x}_n(s)$. Even though this integral depends neither on the boundary values x_{n_i}, x_{n_f} nor on the path $q(s)$ of the Brownian particle it may still contribute a time-dependent factor to the normalization of $F_n[q, x_{n_f}, x_{n_i}]$. This factor can be determined by expanding the integrand into a Fourier series according to

$$\xi_n(s) = \sum_{\alpha=1}^{\infty} \xi_n^\alpha \sin(\nu_\alpha s); \qquad \nu_\alpha = \pi\alpha/t\,, \tag{A.8}$$

where we already made use of the fact that only paths with $\xi_n(0) = \xi_n(t) = 0$ have to be summed over. Due to the orthogonality of the sine functions, the integrand in the second term of eq. (A.3) becomes

$$\exp\Big[\frac{\mathrm{i}}{\hbar} \int_0^t \mathrm{d}s\, (\tfrac{1}{2}m_n(\dot{\xi}_n^2 - \omega_n^2\xi_n^2))\Big] = \exp\Big[\mathrm{i}\,\frac{m_n t}{4\hbar} \sum_{\alpha=1}^{\infty} (\xi_n^{\alpha^2}(\nu_\alpha^2 - \omega_n^2))\Big] \tag{A.9}$$

while the integration measure is

$$\int \mathscr{D}\xi_n \cdots = \prod_{\alpha=1}^{\infty} \Big(N^{-1} \int_{-\infty}^{\infty} \mathrm{d}\xi_n^\alpha \cdots\Big), \tag{A.10}$$

where N is a constant independent of ω_n which arises from the Jacobian of the transformation (A.8). By virtue of eqs. (A.9) and (A.10) the functional integral factorizes into regular Gaussian integrals over the Fourier components ξ_n^α which can be done separately. One finds

$$f_n(t) = \int \mathcal{D}\xi_n \exp\left[\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}s(\tfrac{1}{2}m_n(\dot{\xi}_n^2 - \omega_n^2\xi_n^2))\right] = C\prod_{\alpha=1}^{\infty}(1-\omega_n^2/\nu_\alpha^2)^{-1/2} \tag{A.11}$$

where the constant C collects all factors independent of ω_n. Noting that

$$\prod_{\alpha=1}^{\infty}\left(1-\frac{\omega_n^2 t^2}{\pi^2\alpha^2}\right) = \frac{\sin(\omega_n t)}{\omega_n t}\,, \tag{A.12}$$

we have

$$f_n(t) = C\left[\frac{\omega_n t}{\sin(\omega_n t)}\right]^{1/2}. \tag{A.13}$$

The constant C can be determined by evaluating the Jacobian of the transformation (A.8). On the other hand, it can easily be obtained by comparing eq. (A.11) with the well-known result for a free particle. In the limit $\omega_n \to 0$ we have [17]

$$f_n(t, \omega = 0) = C = (m_n/2\pi\mathrm{i}\hbar t)^{1/2}. \tag{A.14}$$

Collecting the results, we obtain eqs. (3.22) and (3.23).

Appendix B. Determination of the auxiliary function $\Psi(t, t')$

Let us consider the function

$$\Phi(t, t') = G_+(t)G_+(t')\Psi(t, t')\,. \tag{B.1}$$

Using eq. (5.61) we find for the double Laplace transform

$$\hat{\Phi}(z, z') = \hat{G}_+(z)\hat{G}_+(z')\tilde{R}(z, z')\,, \tag{B.2}$$

where by virtue of eq. (5.33)

$$\hat{R}(z, z') = \hat{R}'(z, z') + \frac{1}{M}\frac{1}{z+z'}\left[\hat{K}'(z) + \hat{K}'(z')\right]. \tag{B.3}$$

From eq. (4.11) we obtain for $\tau = 0$

$$K'(s) = \frac{M}{\hbar\beta}\sum_{n=-\infty}^{\infty} g_n(s) \tag{B.4}$$

so that the Laplace transform $\hat{K}'(z)$ becomes

$$\hat{K}'(z) = \frac{M}{\hbar\beta}\sum_{n=-\infty}^{\infty}(\hat{\gamma}(z) - \hat{\zeta}_n(z))\,, \tag{B.5}$$

where we used eq. (4.55). By virtue of eq. (6.25) this yields

$$\hat{K}'(z) = \frac{M}{\hbar\beta} \sum_{n=-\infty}^{\infty} \frac{z}{z^2 - \nu_n^2} (z\hat{\gamma}(z) - |\nu_n|\hat{\gamma}(|\nu_n|)) . \tag{B.6}$$

Further, the double Laplace transform of $R'(s, u)$ follows readily from eq. (5.28) using eqs. (4.55), (4.56), and (6.22). We obtain

$$\hat{R}'(z, z') = -\Lambda \hat{C}_1(z)\hat{C}_1(z') + \frac{1}{\hbar\beta} \sum_{n=-\infty}^{\infty} \hat{G}_+(|\nu_n|)$$
$$\times \left[(\hat{\gamma}(z) - \hat{\zeta}_n(z))(\hat{\gamma}(z') - \hat{\zeta}_n(z')) - \frac{1}{\nu_n^2} (z\hat{\zeta}_n(z) - \zeta_n)(z'\hat{\zeta}_n(z') - \zeta_n) \right] . \tag{B.7}$$

Inserting eq. (6.25) for $\hat{\zeta}_n(z)$ and eq. (4.59) for ζ_n we find

$$\hat{R}'(z, z') = -\Lambda \hat{C}_1(z)\hat{C}_1(z') + \frac{1}{\hbar\beta} \sum_{n=-\infty}^{\infty} \hat{G}_+(|\nu_n|) \frac{zz' - \nu_n^2}{(z^2 - \nu_n^2)(z'^2 - \nu_n^2)}$$
$$\times [z\hat{\gamma}(z) - |\nu_n|\hat{\gamma}(|\nu_n|)][z'\hat{\gamma}(z') - |\nu_n|\hat{\gamma}(|\nu_n|)] . \tag{B.8}$$

The results (B.6) and (B.8) may now be inserted in eq. (B.3) to yield the double Laplace transform $\hat{R}(z, z')$. Eliminating the damping coefficient $\hat{\gamma}(z)$ in favour of $\hat{G}_+(z)$ by means of eq. (5.46) we get after some rearranging

$$\hat{R}(z, z') = -\Lambda \hat{C}_1(z)\hat{C}_1(z') + \sum_{\alpha=1}^{4} \hat{R}_\alpha(z, z') , \tag{B.9}$$

where

$$\hat{R}_1(z, z') = \frac{1}{\hbar\beta} \left[zz' \sum_{n=-\infty}^{\infty} \hat{G}_+(|\nu_n|) + \sum_{n=-\infty}^{\infty} \hat{G}_+(|\nu_n|)(\omega_0^2 + |\nu_n|\hat{\gamma}(|\nu_n|) \right] , \tag{B.10}$$

$$\hat{R}_2(z, z') = \frac{1}{\hbar\beta} [\hat{G}_+(z)\hat{G}_+(z')]^{-1} \sum_{n=-\infty}^{\infty} \left[z\hat{G}_+(z) \frac{z'}{\nu_n^2 - z'^2} (\hat{G}_+(|\nu_n|) - \hat{G}_+(z')) \right.$$
$$+ z'\hat{G}_+(z') \frac{z}{\nu_n^2 - z^2} (\hat{G}_+(|\nu_n|) - \hat{G}_+(z)) + \hat{G}_+(z) \frac{1}{\nu_n^2 - z'^2} (z'^2\hat{G}_+(z') - \nu_n^2\hat{G}_+(|\nu_n|))$$
$$\left. + \hat{G}_+(z') \frac{1}{\nu_n^2 - z^2} (z^2\hat{G}_+(z) - \nu_n^2\hat{G}_+(|\nu_n|)) \right] , \tag{B.11}$$

$$\hat{R}_3(z, z') = \frac{1}{\hbar\beta} [\hat{G}_+(z)\hat{G}_+(z')]^{-1} \sum_{n=-\infty}^{\infty} \frac{\hat{G}_+(|\nu_n|)(zz' - \nu_n^2)}{(\nu_n^2 - z^2)(\nu_n^2 - z'^2)} , \tag{B.12}$$

$$\hat{R}_4(z, z') = \frac{1}{\hbar\beta} [\hat{G}_+(z)\hat{G}_+(z')]^{-1} \frac{1}{z + z'} \sum_{n=-\infty}^{\infty} \left[z \frac{\hat{G}_+(z)}{\nu_n^2 - z^2} + z' \frac{\hat{G}_+(z')}{\nu_n^2 - z'^2} \right] . \tag{B.13}$$

In view of eq. (B.9) we can rewrite (B.2) as

$$\hat{\Phi}(z, z') = \sum_{\alpha=0}^{4} \hat{\Phi}_\alpha(z, z') , \tag{B.14}$$

where

$$\hat{\Phi}_0 = -\Lambda \hat{G}_+(z)\hat{C}_1(z)\hat{G}_+(z')\hat{C}_1(z') \tag{B.15}$$

and

$$\hat{\Phi}_\alpha(z, z') = \hat{G}_+(z)\hat{G}_+(z')\hat{R}_\alpha(z, z') ; \qquad \alpha = 1, 2, 3, 4 . \tag{B.16}$$

Now, we can determine the inverse Laplace transform of the terms in eq. (B.14). Since $\hat{G}_+(z)\hat{C}_1(z)$ is the Laplace transform of $G_+(t)C_1^+(t)$ which is connected with the correlation function by eq. (6.20), we have

$$\Phi_0(t, t') = -\Lambda\left[\frac{M}{\hbar\Lambda} S(t) - \dot{G}_+(t)\right]\left[\frac{M}{\hbar\Lambda} S(t') - \dot{G}_+(t')\right] . \tag{B.17}$$

Next, using eqs. (5.18) and (5.25) we can write the inverse Laplace transform of $\hat{\Phi}_1(z, z')$ as

$$\Phi_1(t, t') = \Lambda \dot{G}_+(t)\dot{G}_+(t') + \Omega G_+(t)G_+(t') , \tag{B.18}$$

where we took advantage of the fact that $G_+(0) = 0$. In order to identify $\Phi_2(t, t')$ let us first note that the Laplace transform of the derivative of the correlation function $S(t)$ is given by

$$\hat{\dot{S}}(z) = z\hat{S}(z) - S(0) = \frac{1}{M\beta} \sum_{n=-\infty}^{\infty} \frac{1}{\nu_n^2 - z^2} [z^2 \hat{G}_+(z) - \nu_n^2 \hat{G}_+(|\nu_n|)] . \tag{B.19}$$

Now, using eqs. (6.26) and (B.19) we readily see that

$$\Phi_2(t, t') = \frac{M}{\hbar} [G_+(t)\dot{S}(t') + G_+(t')\dot{S}(t) - \dot{G}_+(t)S(t') - \dot{G}_+(t')S(t)] . \tag{B.20}$$

The inverse Laplace transform of $\hat{\Phi}_3(z, z')$ can be written in terms of hyperbolic functions as

$$\begin{aligned} \Phi_3(t, t') &= \frac{1}{\hbar\beta} \sum_{n=-\infty}^{\infty} \hat{G}_+(|\nu_n|)[\cosh(\nu_n t)\cosh(\nu_n t') - \sinh(\nu_n t)\sinh(\nu_n t')] \\ &= \frac{1}{\hbar\beta} \sum_{n=-\infty}^{\infty} \hat{G}_+(|\nu_n|)\cosh[\nu_n(t - t')] . \end{aligned} \tag{B.21}$$

Finally, the last term in eq. (B.14) takes the form

$$\hat{\Phi}_4(z, z') = \frac{1}{z + z'} [\hat{\phi}(z) + \hat{\phi}(z')] , \tag{B.22}$$

where

$$\hat{\phi}(z) = \frac{1}{\hbar\beta} \sum_{n=-\infty}^{\infty} \frac{z}{\nu_n^2 - z^2} \hat{G}_+(z) . \tag{B.23}$$

Clearly, the inverse of $\hat{\phi}(z)$ is the convolution

$$\phi(t) = -\frac{1}{\hbar\beta} \sum_{n=-\infty}^{\infty} \int_0^t \mathrm{d}s \, G_+(t-s) \cosh(\nu_n s) . \tag{B.24}$$

Now, since eq. (B.22) is equivalent to

$$\Phi_4(t, t') = \frac{1}{2} [\phi(t-t') + \phi(t'-t)] , \tag{B.25}$$

we obtain by inserting eq. (B.24)

$$\Phi_4(t, t') = -\frac{1}{2\hbar\beta} \sum_{n=-\infty}^{\infty} \int_0^{t-t'} \mathrm{d}s \, [G_+(t-t'-s) - G_+(t'-t+s)] \cosh(\nu_n s) . \tag{B.26}$$

Collecting the results we get from eq. (B.1)

$$\begin{aligned} \Psi(t, t') = \Omega &+ \frac{M}{\hbar} \left[\frac{\dot{S}(t)}{G_+(t)} + \frac{\dot{S}(t')}{G_+(t')} \right] - \frac{M^2}{\hbar^2 \Lambda} \frac{S(t)}{G_+(t)} \frac{S(t')}{G_+(t')} \\ &+ \frac{1}{\hbar\beta} [G_+(t) G_+(t')]^{-1} \sum_{n=-\infty}^{\infty} \hat{G}_+(|\nu_n|) \cosh[\nu_n (t-t')] \\ &- \frac{1}{2\hbar\beta} [G_+(t) G_+(t')]^{-1} \sum_{n=-\infty}^{\infty} \int_0^{t-t'} \mathrm{d}s \, [G_+(t-t'-s) - G_+(t'-t+s)] \cosh(\nu_n s) . \end{aligned} \tag{B.27}$$

With (5.62–5.64) this result readily leads to the functions $R^{\pm\pm}(t)$ given in table 1.

Appendix C. Microscopic origin of the inhomogeneity in the equation of motion for $\langle q \rangle_t$

In this appendix we relate the inhomogeneity of eq. (8.14) to the initial condition of the bath. At $t = 0$, the mean value of the coordinate x_n of the nth oscillator may be written

$$\langle x_n \rangle_0 = \int \mathrm{d}r_\mathrm{i} \, \mathrm{d}\bar{q} \, \mathrm{d}\bar{q}' \, \lambda(0, r_\mathrm{i}, \bar{q}, \bar{q}') \langle \bar{q} | \mathrm{tr}_\mathrm{R}(x_n W_\beta) | \bar{q}' \rangle . \tag{C.1}$$

The quantity $\langle \bar{q} | \mathrm{tr}_\mathrm{R}(x_n W_\beta) | \bar{q}' \rangle$ differs from the reduced equilibrium density matrix $\rho_\beta(\bar{q}, \bar{q}')$ only inasmuch as the trace over the nth environmental oscillator contains an additional factor x_n. From eqs. (3.25), (3.26) it is easily seen that this gives rise to a factor $\int_0^{\hbar\beta} \mathrm{d}\tau \, \phi_n(\tau) \bar{q}(\tau)$ in the functional integral

representation of $\langle \bar{q}|\mathrm{tr}_R(x_n W_\beta)|\bar{q}'\rangle$, where

$$\phi_n(\tau) = \frac{c_n}{2m_n\omega_n} \frac{\sinh[\omega_n(\hbar\beta - \tau)] + \sinh(\omega_n\tau)}{\cosh(\omega_n\hbar\beta) - 1} = \frac{c_n}{2m_n\omega_n} \frac{\cosh[\omega_n(\frac{1}{2}\hbar\beta - \tau)]}{\sinh(\frac{1}{2}\omega_n\hbar\beta)} . \tag{C.2}$$

We find

$$\langle \bar{q}|\mathrm{tr}_R(x_n W_\beta)|\bar{q}'\rangle = \frac{1}{Z}\int \mathcal{D}\bar{q} \int_0^{\hbar\beta} \mathrm{d}\tau\, \phi_n(\tau)\bar{q}(\tau)$$
$$\times \exp\left[-\frac{1}{\hbar}\left\{S_0^E[\bar{q}] + \frac{1}{2}\int_0^{\hbar\beta}\mathrm{d}\tau \int_0^{\hbar\beta}\mathrm{d}\sigma\, k(\tau-\sigma)\bar{q}(\tau)\bar{q}(\sigma)\right\}\right], \tag{C.3}$$

where the functional integral runs over all paths connecting $\bar{q}(0) = \bar{q}'$ with $\bar{q}(\hbar\beta) = \bar{q}$. Here we took advantage of the fact that in the absence of x_n we obtain the functional integral representation (3.39) of $\rho_\beta(\bar{q}, \bar{q}')$. The formula (C.3) is still valid for arbitrary potential. In the harmonic case it can readily be evaluated since only the minimal action path gives a contribution to the additional factor. The minimal action path is a solution of the equation of motion (5.4) for vanishing inhomogeneity. Hence, inserting eq. (5.22) for $\rho_n = 0$ we readily obtain

$$\langle \bar{q}|\mathrm{tr}_R(x_n W_\beta)|\bar{q}'\rangle = \tfrac{1}{2}(\bar{q} + \bar{q}')\rho_\beta(\bar{q}, \bar{q}') \frac{1}{\hbar\beta\Lambda} \sum_{j=-\infty}^{\infty} \frac{c_n u_j}{m_n(\omega_n^2 + \nu_j^2)} . \tag{C.4}$$

A similar calculation shows that

$$\langle \bar{q}|\mathrm{tr}_R(p_n W_\beta)|\bar{q}'\rangle = \frac{1}{Z}\int \mathcal{D}\bar{q} \int_0^{\hbar\beta} \mathrm{d}\tau\, \psi_n(\tau)\bar{q}(\tau)$$
$$\times \exp\left[-\frac{1}{\hbar}\left\{S_0^E[\bar{q}] + \frac{1}{2}\int_0^{\hbar\beta}\mathrm{d}\tau \int_0^{\hbar\beta}\mathrm{d}\sigma\, k(\tau-\sigma)\bar{q}(\tau)\bar{q}(\sigma)\right\}\right], \tag{C.5}$$

where

$$\psi_n(\tau) = \frac{\mathrm{i}}{2} c_n \frac{\sinh[\omega_n(\frac{1}{2}\hbar\beta - \tau)]}{\sinh(\frac{1}{2}\omega_n\hbar\beta)} , \tag{C.6}$$

which in the harmonic case gives

$$\langle \bar{q}|\mathrm{tr}_R(p_n W_\beta)|\bar{q}'\rangle = \mathrm{i}(\bar{q} - \bar{q}')\rho_\beta(\bar{q}, \bar{q}') \frac{1}{\hbar\beta} \sum_{j=-\infty}^{\infty} \frac{c_n \nu_j^2 u_j}{\omega_n^2 + \nu_j^2} . \tag{C.7}$$

By virtue of eqs. (C.4) and (C.7) the initial mean values of the environmental oscillators may be written

$$\langle x_n \rangle_0 = \frac{1}{\hbar\beta\Lambda} \sum_{j=-\infty}^{\infty} \frac{c_n u_j}{m_n(\omega_n^2 + \nu_j^2)} \langle \bar{r} \rangle_0 , \tag{C.8}$$

$$\langle p_n \rangle_0 = \frac{1}{\hbar\beta} \sum_{j=-\infty}^{\infty} \frac{c_n \nu_j^2 u_j}{\omega_n^2 + \nu_j^2} \mathrm{i} \langle \bar{x} \rangle_0 . \tag{C.9}$$

These relations hold for all initial states of the form discussed in section 2. Next, we note that as a consequence of eqs. (4.1), (4.13), and (4.14) the functions (5.26), (5.27) may be transformed to read

$$C_1(s) = \frac{1}{M\hbar\beta\Lambda} \sum_{n=1}^{N} \sum_{j=-\infty}^{\infty} \frac{c_n^2 u_j}{m_n(\omega_n^2 + \nu_j^2)} \cos(\omega_n s) , \tag{C.10}$$

$$C_2(s) = \frac{1}{M\hbar\beta} \sum_{n=1}^{N} \sum_{j=-\infty}^{\infty} \frac{1}{m_n\omega_n} \frac{c_n^2 \nu_j^2 u_j}{\omega_n^2 + \nu_j^2} \sin(\omega_n s) . \tag{C.11}$$

Combining (C.8–C.11) the average force (8.13) can be cast into the form

$$\langle \bar{F}(s) \rangle_0 = \sum_{n=1}^{N} c_n \left[\langle x_n \rangle_0 \cos(\omega_n s) + \frac{\langle p_n \rangle_0}{m_n\omega_n} \sin(\omega_n s) \right] . \tag{C.12}$$

It is now easily checked that eq. (8.14) with (C.12) is indeed identical to the equation of motion following from the averaged Heisenberg equations of motion.

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