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Low-Temperature and Long-Time Anomalies of a Damped Quantum Particle

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The time evolution of a damped quantum particle is discussed. Dissipation is modeled by the bilinear coupling to a set of harmonic oscillators. Using a functional integral technique that accounts for initial correlations between the particle and the reservoir, one can express the dynamics of the damped particle entirely in terms of equilibrium correlation functions. The long-time behavior of these correlations is determined for memory damping arising from the coupling to a reservoir with spectral density $I(\omega) \propto \omega^{\alpha}$ at low frequencies, where $\alpha > 0$. The time evolution of nonequilibrium initial states of the damped particle is discussed. At finite temperatures an initially localized state is found to spread subdiffusively or superdiffusively, depending on α. For $\alpha > 2$ the damping becomes ineffective for long times, and the width of a state grows kinematically. At zero temperature and for $\alpha < 1$, an initially localized state remains localized for all times. For $\alpha \geqslant 1$ the state spreads, but with a slower rate than at finite temperatures. Study of arbitrary initial states indicates that the process is ergodic at finite temperatures only for $\alpha \leqslant 2$ and at zero temperature for $1 \leqslant \alpha \leqslant 2$.

KEY WORDS: Dissipative quantum systems; Brownian motion; localization; anomalous diffusion; memory effects; functional integral techniques.

1. INTRODUCTION

In recent years considerable research has been directed concerning the influence of a dissipative environment on the dynamics of a quantum system. While most of the corresponding work in the 1960s and 1970s envisaged applications in quantum optics[1] and spin relaxation theory[2] and employed approximations suitable to those fields, recent interest has

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focused on the effect of strong damping and/or low temperatures, where the environmental coupling may not be treated perturbatively. In the low-temperature regime dissipation has been found to give rise to a number of novel quantum effects. Caldeira and Leggett[3] showed that the tunneling escape from a metastable state at $T=0$ is exponentially suppressed in the presence of damping. Subsequently, the effect of finite temperatures was discussed[4] and the predicted thermal enhancement of the tunneling rate of a damped system was observed experimentally.[5] Further, dissipation was found crucially to affect quantum mechanical coherence,[6] leading to dissipative phase transitions such as the localization in a periodic potential[7] and global phase coherence in granular superconductors.[8] Even in linear systems low-temperature anomalies such as algebraic long-time tails in correlation functions were found.[9]

Most of the recent theoretical work in the field has relied heavily on the functional integral representation of quantum mechanics introduced by Feynman.[10] If dissipation is modeled by a bilinear coupling of the system under consideration to a heat bath consisting of an infinite set of harmonic oscillators, the functional integral method allows for an exact elimination of the environmental degrees of freedom. For a study of nonequilibrium properties of a system, such as the relaxation of nonequilibrium initial states, the influence functional technique of Feynman and Vernon[11] is particularly useful. At present, however, the applicability of the method suffers from a somewhat unphysical factorization assumption for the initial state introduced in the original paper[11] and retained in most of the newer work.[6,12] A first effort toward a more realistic description was made by Hakim and Ambegaokar,[13] who treated a free Brownian particle in the presence of frequency-independent or Ohmic damping. However, for most situations of practical interest a more general approach is required.[14]

In the present paper, we study the dynamics of the simplest dissipative quantum system, namely a particle damped through the coupling to a heat bath enviroment, but not subject to any potential forces. This is the problem of free Brownian motion. We allow for arbitrary frequency dependence of the damping, and it turns out that it is just this frequency dependence that strongly influences the dynamics of the system. In Section 2 we present a generalization of the Feynman–Vernon theory which accounts for initial correlations between the particle and the environment. Within this approach the preparation and relaxation of a large class of initial states can be treated in a realistic way. Starting from a microscopic model, we determine the functional integral representation of the reduced density matrix of the Brownian particle valid for arbitrary temperatures and arbitrary damping strength.

The remaining threefold functional integral over the particle coordinates is solved exactly in Section 3. We show that the nonequilibrium dynamics can be expressed entirely in terms of equilibrium correlation functions of the Brownian particle. For arbitrary frequency dependence of the damping, these correlations are given in terms of their Laplace transforms.

In Section 4 we study the time evolution of correlation functions. First, we deal with the exactly soluble case of frequency-independent damping, where connections with the previous findings of Hakim and Ambegaokar[13] can be made. Subsequently, we discuss the general case of frequency-dependent friction. The long-time behavior of the correlations is found to depend only on the low-frequency properties of the damping, except for a mass renormalization, which occurs for small densities of low-frequency environmental modes. For a wide range of damping mechanisms, including those of interest in experiments, the asymptotic time dependence of the correlation functions is worked out explicitly.

In Section 5 we employ these results to discuss the relaxation of nonequilibrium initial states. As an example, we study the time evolution of an initially localized wave packet. The long-time behavior depends strongly on the dissipative mechanism. Diffusive spreading of the state is found only in the Ohmic case. For other forms of the damping, the behavior can be subdiffusive or superdiffusive, depending on whether the low-frequency friction is stronger or weaker than in the Ohmic case. Moreover, at zero temperature the damping can lead to a localization of the state even though the particle is not bounded by an external potential. Some of the results in this section were obtained in collaboration with G.-L. Ingold and published elsewhere in short form.[15] Finally, we discuss the long-time behavior of arbitrary initial states quite generally. We find that the process is not always ergodic. The conditions under which the effects of the preparation vanish asymptotically are given.

2. FUNCTIONAL INTEGRAL REPRESENTATION OF THE REDUCED DENSITY MATRIX

2.1. Microscopic Model

The model of a particle moving in a viscous medium that causes friction and exerts a fluctuating force upon the particle is used not only in its strict mechanical context, but has also led to an understanding of various other systems where fluctuations are important. Examples of phenomena where the analogy to Brownian motion is useful include macroscopic quantum tunneling in Josephson systems,[3-5] the diffusion of injected particles in solids,[16] or chemical reactions.[17] Here, we exclusively consider a mechanical particle of mass M, momentum p, and coordinate q, but the application to other phenomena may require an altogether different interpretation of these variables. The particle is free inasmuch as it is not subject to an external potential. Dissipation is introduced via a bilinear coupling to a set of N harmonic oscillators characterized by masses m_n, frequencies ω_n, momenta p_n, and coordinates q_n. Writing the interaction such that there is no coupling-induced renormalization of the potential,[3] we find for the corresponding Hamiltonian

$$H=\frac{p^2}{2M}+\sum_{n=1}^{N}\left[\frac{p_n^2}{2m_n}+\frac{1}{2}m_n\omega_n^2\left(x_n-\frac{c_n q}{m_n\omega_n^2}\right)^2\right] \tag{2.1}$$

An environmental coupling of this form has been widely used to model dissipation,[3,4,6–9,12,13][2] and allows for a description of many damping mechanisms of practical interest. However, the form (2.1) is not yet suitable for our purposes, since a spatial translation of the entire system would change its energy. Clearly, a Hamiltonian describing free Brownian motion must be translationally invariant. To avoid this problem, we make use of the fact that the environmental parameters do not separately affect the motion of the Brownian particle. Rather, only the combination $c_n^2/m_n\omega_n$ enters the description of the reduced dynamics. Hence, we may choose the coupling constants $c_n=m_n\omega_n^2$ without restricting the possible frequency dependence of the damping. The Hamiltonian then takes the translationally invariant form

$$H=\frac{p^2}{2M}+\sum_{n=1}^{N}\left[\frac{p_n^2}{2m_n}+\frac{1}{2}m_n\omega_n^2(x_n-q)^2\right] \tag{2.2}$$

In a mechanical model this system can be visualized as a particle that has many masses attached to it with springs (Fig. 1). The model described by the Hamiltonian (2.2) was also studied by Hakim and Ambegaokar.[13]

2.2. Preparation of the Initial State

In order to determine the time evolution of the system, the model Hamiltonian (2.2) has to be supplemented by information about the initial state of the system. In previous work,[6,11,12] it was frequently assumed that the initial density matrix factorizes into separate contributions from the Brownian particle and the environment. Then the coupling is switched on, and the relaxation toward the equilibrium state of the coupled system is

[2] See Ref. 18 for a review of earlier work.

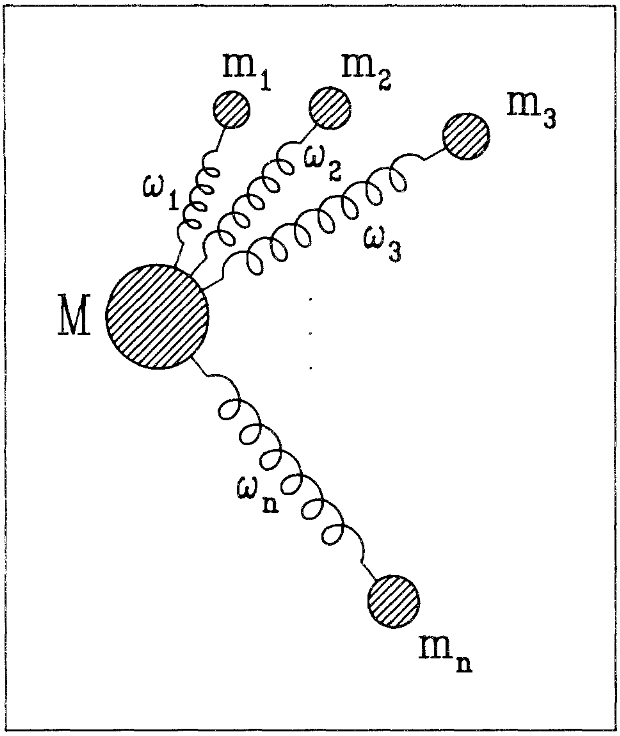

Fig. 1. A mechanical model of the Hamiltonian (2.2).

discussed. In real physical systems, however, such a switching on and off of the interaction is very rarely possible. Hence we use a more realistic prescription of how the initial state should be prepared. The starting point is the equilibrium state

$$W_\beta = Z_\beta^{-1} \exp(-\beta H) \tag{2.3}$$

of the entire system at inverse temperature $\beta = 1/k_B T$. Here,

$$Z_\beta = \mathrm{tr}[\exp(-\beta H)] \tag{2.4}$$

is the partition function of the system. An ensemble of systems described by the state (2.3) may generally be realized by waiting long enough. Since we are dealing with a free Brownian particle, there is a subtlety involved at this point. Clearly, the equilibrium density matrix of a particle that is not localized cannot be normalized on an infinite interval. Therefore, the partition function Z_β diverges for a free Brownian particle. However, it is only the trace over the particle coordinate that is divergent, whereas the trace over the reservoir degrees of freedom is well defined. Furthermore, the equilibrium density matrix of the Brownian particle will be distributed homogeneously in position space. Hence, it is natural to normalize the state on an interval of length L. Accordingly, for the system under consideration we replace (2.3) and (2.4) by

$$W_\beta^L = (N_\beta^L)^{-1} \exp(-\beta H) \tag{2.5}$$

where

$$N_\beta^L = \int_{q_0}^{q_0+L} dq \langle q| \operatorname{tr}_R[\exp(-\beta H)] |q\rangle \tag{2.6}$$

Because of the translational invariance of the Hamiltonian, q_0 is arbitrary and the normalization factor N_β^L is in fact proportional to L. It is now convenient to introduce a density matrix that is independent of the length of the normalization interval, namely

$$\bar{W}_\beta = \bar{N}_\beta^{-1} \exp(-\beta H) \tag{2.7}$$

where

$$\bar{N}_\beta = \langle q_0| \operatorname{tr}_R[\exp(-\beta H)] |q_0\rangle \tag{2.8}$$

is independent of q_0. The equilibrium state normalized on the interval L may then be written as

$$W_\beta^L = L^{-1} \bar{W}_\beta \tag{2.9}$$

Nonequilibrium initial states may now be prepared by means of a perturbation influencing the Brownian particle. The resulting initial density matrix W_0 may frequently be written as

$$W_0 = \sum_j O_j \bar{W}_\beta O_j' \tag{2.10}$$

Here, O_j and O_j' are operators acting on the Brownian particle, but not on the environmental degrees of freedom. This prescription of how an initial state should be prepared describes several situations of practical interest:

1. We can start out with the equilibrium system, add a time-dependent external force to the Hamiltonian, and study the response of the system to this force.

2. We may perform a measurement on the Brownian particle leading to a reduction of the state. In this case the operators O_j, O_j' project on the measured value or interval.

3. A correlation function $\langle A(t)B\rangle$ can formally by related to the expectation value of the observable A at time t with respect to the initial "ensemble" $B\bar{W}_\beta$. While $B\bar{W}_\beta$ is generally not a Hermitian operator, it still belongs to the class of initial states (2.10) and can be described within the theory developed below.

In particular, initial states of the form (2.10) include initial correlations between the Brownian particle and the environment that are neglected in a theory based on the factorization assumption. These correlations may strongly influence the subsequent time evolution.[13,19] In coordinate representation we write (2.10) as

$$W_0(q_i, x_{n,i}, q_i', x_{n,i}', 0)$$
$$= \int d\bar{q} \int d\bar{q}'\, \lambda_0(q_i, \bar{q}, q_i', \bar{q}')\, \bar{W}_\beta(\bar{q}, x_{n,i}, \bar{q}', x_{n,i}') \tag{2.11}$$

The function

$$\lambda_0(q_i, \bar{q}, q_i', \bar{q}') = \sum_j \langle q_i|\, O_j\, |\bar{q}\rangle \langle \bar{q}'|\, O_j'\, |q_i'\rangle \tag{2.12}$$

will be called *preparation function* from now on, since it contains complete information about the initial state. Tracing (2.11) over the reservoir, we obtain the initial reduced density matrix as

$$\rho(q_i, q_i', 0) = \langle q_i|\, \mathrm{tr}_R(W_0)\, |q_i'\rangle$$
$$= \int d\bar{q} \int d\bar{q}'\, \lambda_0(q_i, \bar{q}, q_i', \bar{q}')\, \bar{\rho}_\beta(\bar{q}, \bar{q}') \tag{2.13}$$

where

$$\bar{\rho}_\beta = \mathrm{tr}_R(\bar{W}_\beta) \tag{2.14}$$

is the reduced state of the Brownian particle associated with (2.7). Again, $\rho_\beta^L = \bar{\rho}_\beta/L$ is the reduced equilibrium state normalized on an interval of length L. In most cases of interest the initial state of the particle is localized, so that the initial density matrix W_0 can be normalized on the infinite interval. In this case it is convenient to include the proper normalization of the state in the preparation function, which then has the property

$$\int dq\, d\bar{q}\, d\bar{q}'\, \lambda_0(q, \bar{q}, q, \bar{q}')\, \bar{\rho}_\beta(\bar{q}, \bar{q}') = 1 \tag{2.15}$$

While the reduced equilibrium density matrix $\bar{\rho}_\beta(\bar{q}, \bar{q}')$ depends only on the relative coordinate $\bar{q} - \bar{q}'$, the preparation function will break the translational invariance in general. Finally, we note that the preparation function (2.12) gives a more detailed description of the initial state than the reduced density matrix (2.13). In addition to information about the Brownian particle, the preparation function also contains information about the initial correlations with the heat bath.

2.3. Functional Integral Representation of the Density Matrix

The density matrix at time t follows from the Liouville equation as

$$W(t) = \exp(-iHt/\hbar)\, W_0 \exp(iHt/\hbar) \tag{2.16}$$

Using (2.11) for the initial state, we can now write the coordinate representation of this relation in terms of functional integrals. The time evolution operator takes the form[10]

$$\langle q_f, x_{n,f} | \exp(-iHt/\hbar) | q_i, x_{n,i} \rangle = \int D[q]\, D[x_n] \exp\left(\frac{i}{\hbar} S[q, x_n]\right) \tag{2.17}$$

where we have to sum over all paths $q(s)$, $x_n(s)$ $(n = 1, ..., N)$ in real time $0 \leqslant s \leqslant t$ connecting $q(0) = q_i$, $x_n(0) = x_{n,i}$ with $q(t) = q_f$, $x_n(t) = x_{n,f}$. The path probability is weighted according to the action

$$S[q, x_n] = \int_0^t ds\, L(q, x_n) \tag{2.18}$$

where $L(q, x_n)$ is the Lagrangian associated with the Hamiltonian (2.2). A corresponding functional integral representation holds for the adjoint time evolution operator $\exp(iHt/\hbar)$, where both the paths and the endpoints will be distinguished by primes.

Further, the equilibrium density matrix (2.7) may be written as a Euclidean function integral according to[10]

$$\bar{W}_\beta(\bar{q}, x_{n,i}, \bar{q}', x'_{n,i}) = \bar{N}_\beta^{-1} \int D[\bar{q}]\, D[\bar{x}_n] \exp\left(-\frac{1}{\hbar} S^E[\bar{q}, \bar{x}_n]\right) \tag{2.19}$$

where the sum is over all paths $\bar{q}(\tau)$, $\bar{x}_n(\tau)$ $(n = 1, ..., N)$ in imaginary time $0 \leqslant \tau \leqslant \hbar\beta$ connecting $\bar{q}(0) = \bar{q}'$, $\bar{x}_n(0) = x'_{n,i}$ with $\bar{q}(\hbar\beta) = \bar{q}$, $\bar{x}_n(\hbar\beta) = x_{n,i}$. Here, the weight factor is determined by the Euclidean action

$$S^E[\bar{q}, \bar{x}_n] = \int_0^{\hbar\beta} d\tau\, L^E(\bar{q}, \bar{x}_n) \tag{2.20}$$

where $L^E(\bar{q}, \bar{x}_n)$ is the Euclidean Lagrangian, which follows from the ordinary Langrangian by a Wick rotation from real to imaginary time. In fact, for the present problem $L^E(\bar{q}, \bar{x}_n)$ is simply given by the Hamiltonian (2.2) if we express the momenta in terms of time derivatives of the conjugate coordinates.

Collecting these results, we obtain the density matrix (2.16) in the form

$$\begin{aligned} W(q_f, x_{n,f}, q'_f, x'_{n,f}, t) &= \int dq_i\, dq'_i\, d\bar{q}\, d\bar{q}'\, dx_{n,i}\, dx'_{n,i}\, \lambda_0(q_i, \bar{q}, q'_i, \bar{q}') \\ &\quad \times \bar{N}_\beta^{-1} \int D[q]\, D[x_n]\, D[q']\, D[x'_n]\, D[\bar{q}]\, D[\bar{x}_n] \\ &\quad \times \exp\left\{\frac{i}{\hbar}(S[q, x_n] - S[q', x'_n]) - \frac{1}{\hbar} S^E[\bar{q}, \bar{x}_n]\right\} \end{aligned} \tag{2.21}$$

which is a $(3N+3)$-fold functional integral over all paths $q(s)$, $x_n(s)$, $q'(s)$, $x'_n(s)$ $(n=1,..., N)$ in real time $0 \leqslant s \leqslant t$ connecting $q(0) = q_i$, $x_n(0) = x_{n,i}$, $q'(0) = q'_i$, $x'_n(0) = x'_{n,i}$ with $q(t) = q_f$, $x_n(t) = x_{n,f}$, $q'(t) = q'_f$, $x'_n(t) = x'_{n,f}$ and all paths $\bar{q}(\tau)$, $\bar{x}_n(\tau)$ $(n=1,..., N)$ in imaginary time $0 \leqslant \tau \leqslant \hbar\beta$ satisfying the boundary conditions $\bar{q}(0) = \bar{q}'$, $\bar{x}_n(0) = x'_{n,i}$ and $\bar{q}(\hbar\beta) = \bar{q}$, $\bar{x}_n(\hbar\beta) = x_{n,i}$.

2.4. Elimination of the Environment

Since the number of environmental modes is very large, the density matrix (2.21) contains much more information than we could hope to process or would be interested in. Rather, we want a closed description for the dynamics of the reduced density matrix. For the model under consideration the trace over the reservoir coordinates can indeed be performed, since the corresponding functional integrals are Gaussian and can be evaluated exactly.[10] The straightforward though slightly tedious calculation leads to an expression for the reduced density matrix at time t that is valid for arbitrary damping strength and arbitrary temperatures. We write it in the form

$$\begin{aligned} \rho(q_f, q'_f, t) &= \int dq_i\, dq'_i\, d\bar{q}\, d\bar{q}' \\ &\quad \times J(q_f, q'_f, t, q_i, q'_i, \bar{q}, \bar{q}')\, \lambda_0(q_i, \bar{q}, q'_i, \bar{q}') \end{aligned} \tag{2.22}$$

The newly introduced function

$$J(q_f, q_f', t, q_i, q_i', \bar{q}, \bar{q}')$$
$$= Z^{-1} \int D[q] D[q'] D[\bar{q}]$$
$$\times \exp\left\{\frac{iM}{2\hbar}(\dot{q}^2 - \dot{q}'^2) - \frac{M}{2\hbar}\dot{\bar{q}}^2\right\} F[q, q', \bar{q}] \qquad (2.23)$$

will be called the *propagating function*, since it contains the whole dynamical information about the Brownian particle. In this expression, $J(q_f, q_f', t, q_i, q_i', \bar{q}, \bar{q}')$ is defined as a triple functional integral over all real time paths $q(s)$, $q'(s)$, $0 \leqslant s \leqslant t$, and all imaginary time paths $\bar{q}(\tau)$, $0 \leqslant \tau \leqslant \hbar\beta$, satisfying the boundary conditions given above. The prefactor

$$Z = \bar{N}_\beta \prod_{n=1}^{N} 2 \sinh\left(\frac{1}{2}\omega_n \hbar\beta\right) \qquad (2.24)$$

normalizes the state, while

$$F[q, q', \bar{q}] = \exp\left(-\frac{1}{\hbar}\left\{-\int_0^{\hbar\beta} d\tau \int_0^{\tau} d\sigma\, K(-i\tau + i\sigma)\, \bar{q}(\tau)\, \bar{q}(\sigma)\right.\right.$$
$$+ \int_0^{\hbar\beta} d\tau \frac{1}{2}\mu\bar{q}^2(\tau)$$
$$- i \int_0^{\hbar\beta} d\tau \int_0^{t} ds\, K^*(s - i\tau)\, \bar{q}(\tau)[q(s) - q'(s)]$$
$$+ \int_0^{t} ds \int_0^{s} du\, [q(s) - q'(s)][K(s-u)\, q(u) - K^*(s-u)\, q'(u)]$$
$$\left.\left. + i \int_0^{t} ds \frac{1}{2}\mu[q^2(s) - q'^2(s)]\right\}\right) \qquad (2.25)$$

is the so-called influence functional describing the effects of the environment on the particle's motion. Here, we introduced the kernel

$$K(\theta) = \sum_{n=1}^{N} \frac{1}{2} m_n \omega_n^3 \frac{\cosh[\omega_n(\frac{1}{2}\hbar\beta - i\theta)]}{\sinh(\frac{1}{2}\omega_n \hbar\beta)} \qquad (2.26)$$

which is defined for complex times $\theta = s - i\tau$, $0 \leqslant \tau \leqslant \hbar\beta$. Finally, the terms with

$$\mu = \sum_{n=1}^{N} m_n \omega_n^2 \qquad (2.27)$$

compensate for the coupling-induced potential renormalization inherent in the local part of $K(\theta)$.

In (2.22) the two sources of information that we need to determine the time evolution of the density matrix are obvious. The initial state is characterized by the preparation function $\lambda_0(q_i, \bar{q}, q_i', \bar{q}')$, which describes the deviations from equilibrium. The dynamical information is contained in the propagating function $J(q_f, q_f', t, q_i, q_i', \bar{q}, p')$. Knowledge of the propagating function allows for an evaluation of the dynamics of arbitrary initial states in terms of quadratures.

3. EVALUATION OF THE PROPAGATING FUNCTION

In this section we evaluate the propagating function governing the time evolution of a free Brownian particle coupled to a heat bath with an arbitrary density of modes. Since dissipation always requires the coupling to a (quasi)continuum of environmental modes, we first introduce the spectral density

$$I(\omega) = \pi \sum_{n=1}^{N} \frac{1}{2} m_n \omega_n^3 \, \delta(\omega - \omega_n) \tag{3.1}$$

of the reservoir, which will be considered a continuous function of the frequency from now on. We see that despite our choosing the coupling constants c_n so that the Hamiltonian is translationally invariant, we can still model any desired frequency dependence of the spectral density by a suitable choice of the oscillator masses m_n. The kernel $K(\theta)$ and the constant μ occurring in the influence functional (2.25) can be written in terms of $I(\omega)$ as frequency integrals. Moreover, the constant μ can be eliminated altogether by partial integrations that split off the local parts in the double integrals in (2.25). Introducing the sum and difference coordinates

$$x = q - q'; \qquad r = (q + q')/2 \tag{3.2}$$

we can write the propagating function in the form

$$J(x_f, r_f, t, x_i, r_i, \bar{q}, \bar{q}') = Z^{-1} \int D[x]\, D[r] D[\bar{q}] \exp\left(\frac{i}{\hbar} \Sigma[x, r, \bar{q}]\right) \tag{3.3}$$

where the functional integral is over all real time paths $x(s)$, $r(s)$, $0 \leqslant s \leqslant t$, connecting $x(0) = x_i = q_i - q_i'$, $r(0) = r_i = (q_i + q_i')/2$ with $x(t) = x_f = q_f - q_f'$, $r(t) = r_f = (q_f + q_f')/2$ and all imaginary time paths $\bar{q}(\tau)$ specified above. The weight factor contains the effective action

$$\Sigma[x, r, \bar{q}] = i \int_0^{\hbar\beta} d\tau \frac{M}{2} \dot{\bar{q}}^2 + \frac{1}{2} \int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\sigma\, k(\tau - \sigma)\, \bar{q}(\tau)\, \bar{q}(\sigma)]$$
$$+ \int_0^{\hbar\beta} d\tau \int_0^t ds\, K^*(s - i\tau)\, \bar{q}(\tau)\, x(s)$$
$$+ \int_0^t ds\, M\dot{x}\dot{r} - \int_0^t ds\, Mx(s) \frac{d}{ds} \int_0^s du\, \gamma(s-u)\, r(u)$$
$$+ \frac{i}{2} \int_0^t ds \int_0^t du\, K'(s-u)\, x(s)\, x(u) \tag{3.4}$$

In this expression $K'(\theta)$ is the real part of the kernel (2.26), and

$$\gamma(t) = \frac{2}{M} \int_0^\infty \frac{d\omega}{\pi} \frac{I(\omega)}{\omega} \cos(\omega t) \tag{3.5}$$

is the damping kernel describing the frictional influence of the environment. The function $k(\tau)$ in (3.4) results from a partial integration of the influence kernel. It can be written in terms of the Laplace transform

$$\hat{\gamma}(z) = \int_0^\infty dt\, \gamma(t) \exp(-zt) = \frac{1}{M} \int_0^\infty \frac{d\omega}{\pi} \frac{I(\omega)}{\omega} \frac{2z}{\omega^2 + z^2} \tag{3.6}$$

of the damping kernel as

$$k(\tau) = \frac{M}{\hbar\beta} \sum_{n=-\infty}^{\infty} |\nu_n|\, \hat{\gamma}(|\nu_n|) \exp(i\nu_n \tau) \tag{3.7}$$

Here, $\nu_n = 2\pi n/\hbar\beta$ are the Matsubara frequencies.

3.1. The Minimal Action

Since the system under consideration is linear, the dependence of the propagating function on the boundary values $\bar{q}$, $\bar{q}'$, x_i, r_i, x_f, and r_f can be determined completely by considering those paths that minimize the effective action (3.4). The equations of motion for these minimal action paths are readily found to read

$$M\ddot{\bar{q}} - \int_0^{\hbar\beta} d\sigma\, k(\tau - \sigma)\, \bar{q}(\sigma) = -i \int_0^t ds\, K^*(s - i\tau)\, x(s) \tag{3.8}$$

for the imaginary time path $\bar{q}(\tau)$, and

$$M\ddot{r} + M\frac{d}{ds}\int_0^s du\, \gamma(s-u)\; r(u) = i\int_0^t du\, K'(s-u)\, x(u) + \int_0^{\hbar\beta} d\tau\, K^*(s-i\tau)\, \bar{q}(\tau) \tag{3.9}$$

$$M\ddot{x} - M\frac{d}{ds}\int_s^t du\, \gamma(u-s)\, x(u) = 0 \tag{3.10}$$

for the real time paths $r(s)$ and $x(s)$. In view of the evolution equation (3.9), it becomes obvious why $\gamma(t)$ is called the damping kernel.

Let us first consider the dynamics in imaginary time. Since we need a solution of (3.8) only in the interval $0 \leqslant \tau \leqslant \hbar\beta$, it is convenient to expand $\bar{q}(\tau)$ in a Fourier series according to

$$\bar{q}(\tau) = \frac{1}{\hbar\beta}\sum_{n=-\infty}^{\infty} \bar{q}_n \exp(i\nu_n\tau) \tag{3.11}$$

The Fourier coefficients $\bar{q}_n$ are determined in Appendix A as functions of the endpoints $\bar{q}$ and $\bar{q}'$ and as functionals of the real time path $x(s)$, which appears as an inhomogeneity in (3.8). The result of this calculation is

$$\bar{q}_0 = \frac{\hbar}{2}(\bar{q}+\bar{q}') + i\int_0^t ds\, x(s) \sum_{n=-\infty}^{\infty}{}' \zeta_n(s)[\nu_n^2 + |\nu_n|\, \hat{\gamma}(|\nu_n|)]^{-1} \tag{3.12}$$

$$\bar{q}_n = [\nu_n^2 + |\nu_n|\, \hat{\gamma}(|\nu_n|)]^{-1}\left\{ i\nu_n(\bar{q}-\bar{q}') - i\int_0^t ds\, x(s)\left[\zeta_n(s) + \nu_n^{-1}\frac{d}{ds}\zeta_n(s)\right]\right\} \quad \text{for} \quad n \neq 0 \tag{3.13}$$

where the prime denotes the omission of the $n=0$ element in the sum. Here, we have introduced the functions

$$\zeta_n(s) = \frac{1}{2}|\nu_n| \int_0^\infty du\, \gamma(u)\, \{\exp[-|\nu_n(s+u)|] + \exp[-|\nu_n(s-u)|]\} \tag{3.14}$$

When the result is inserted in (3.4) the effective action emerges as

$$\begin{aligned}\Sigma[x,r] = {} & iM\frac{\Omega}{2}(\bar{q}-\bar{q}')^2 + \frac{i}{2}M\int_0^t ds\int_0^t du\, R(s,u)\, x(s)\, x(u) \\ & + \int_0^t ds\, M\left\{\dot{x}\dot{r} - x(s)\frac{d}{ds}\int_0^s du\, \gamma(s-u)\, r(u) \right. \\ & \left. + x(s)\left[\frac{1}{2}(\bar{q}+\bar{q}')\, \gamma(s) - i(\bar{q}-\bar{q}')\, C(s)\right]\right\}\end{aligned} \tag{3.15}$$

where we introduced the frequency

$$\Omega = \frac{1}{\hbar\beta}\left[1 + \sum_{n=-\infty}^{\infty}{}' \; [|\nu_n| + \hat{\gamma}(|\nu_n|)]^{-1}\,\hat{\gamma}(|\nu_n|)\right] \tag{3.16}$$

and the functions

$$C(s) = -\frac{d}{ds}\frac{1}{\hbar\beta}\sum_{n=-\infty}^{\infty}{}' \; [\nu_n^2 + |\nu_n|\,\hat{\gamma}(|\nu_n|)]^{-1}\,\zeta_n(s) \tag{3.17}$$

$$\begin{aligned} R(s,u) = {} & \frac{1}{M}K'(s-u) + \frac{1}{\hbar\beta}\sum_{n=-\infty}^{\infty}{}' \; [\nu_n^2 + |\nu_n|\,\hat{\gamma}(|\nu_n|)]^{-1}\,\zeta_n(s)\,\zeta_n(u) \\ & - \frac{1}{\hbar\beta}\frac{\partial^2}{\partial s\,\partial u}\sum_{n=-\infty}^{\infty}{}' \; [\nu_n^2 + |\nu_n|\,\hat{\gamma}(|\nu_n|)]^{-1}\,\nu_n^{-2}\zeta_n(s)\,\zeta_n(u)] \end{aligned} \tag{3.18}$$

The real time equations of motion (3.9) and (3.10) are also readily solved. The Green's function of (3.9), denoted by $G_+(s)$, satisfies the homogeneous equation with the initial conditions $G_+(0) = 0$ and $\dot{G}_+(0) = 1$ and has the Laplace transform

$$\hat{G}_+(z) = [z^2 + z\hat{\gamma}(z)]^{-1} \tag{3.19}$$

The equation of motion (3.10) for $x(s)$ can be viewed as the backward equation to the homogeneous part of (3.9), which means that it has time-reversed solutions. The backward Green's function $G_-(s)$ is connected with the forward propagator $G_+(s)$ by

$$G_-(s) = \frac{G_+(t-s)\,\dot{G}_+(t) - G_+(t)\,\dot{G}_+(t-s)}{G_+(t)\,\ddot{G}_+(t) - \dot{G}_+^2(t)} \tag{3.20}$$

The solutions of (3.9) and (3.10) satisfying the boundary conditions $x(0) = x_i$, $r(0) = r_i$, $x(t) = x_f$, and $r(t) = r_f$ are now readily determined. Inserting these solutions into the action (3.4), we obtain after some algebra

$$\begin{aligned} &\Sigma(x_f, r_f, t, x_i, r_i, \bar{x}, \bar{r}) \\ &\quad = iM\frac{\Omega}{2}\bar{x}^2 - iM\bar{x}[x_i C^+(t) + x_f C^-(t)] \\ &\qquad + M[x_f(r_f - \bar{r}) + x_i(r_i - \bar{r})]\frac{\dot{G}_+(t)}{G_+(t)} \\ &\qquad - M\left[x_i(r_f - \bar{r})\frac{1}{G_+(t)} + x_f(r_i - \bar{r})\frac{1}{G_-(t)}\right] \\ &\qquad + \frac{i}{2}M[x_i^2 R^{++}(t) + 2x_i x_f R^{+-}(t) + x_f^2 R^{--}(t)] \end{aligned} \tag{3.21}$$

where we introduced the functions

$$C^{+}(t)=\int_0^t ds\, C(s)\frac{G_+(t-s)}{G_-(t)};\qquad C^{-}(t)=\int_0^t ds\, C(s)\frac{G_-(s)}{G_-(t)} \tag{3.22}$$

$$R^{+-}(t)=\int_0^t ds\int_0^t du\, R(s,u)\frac{G_+(t-s)}{G_+(t)}\frac{G_-(s)}{G_-(t)} \tag{3.23}$$

while $R^{++}(t)$ and $R^{--}(t)$ are defined analogously. The result (3.21) makes obvious that the minimal action depends only on relative coordinates. With (3.21) the dependence of the propagating function on the endpoints is completely determined according to

$$J(x_f, r_f, t, x_i, r_i, \bar{x}, \bar{r})=\frac{1}{N(t)}\exp\left[\frac{i}{\hbar}\Sigma(x_f, r_f, t, x_i, r_i, \bar{x}, \bar{r})\right] \tag{3.24}$$

Here, $N(t)$ is a time-dependent normalization factor, which can be evaluated by performing the functional integration over the fluctuations about the minimal action paths. On the other hand, this factor may be obtained more conveniently from the fact that the trace of a state is conserved. The reduced density matrix at time t may now be written [cf. (2.22)]

$$\rho(x_f, r_f, t)=\int dx_i\, dy\, d\bar{x}\, d\bar{y}\, J(x_f, y, t, x_i, \bar{x}, \bar{y})\,\lambda(r_f-y, x_i, \bar{y}, \bar{x}) \tag{3.25}$$

where, apart from (3.2), we introduced the relative coordinates

$$y=r_f-r_i;\qquad \bar{y}=r_i-\bar{r} \tag{3.26}$$

The propagating function $J(x_f, y, t, x_i, \bar{x}, \bar{y})$ is obtained from (3.24) when the action (3.21) is expressed in terms of relative coordinates, and the preparation function $\lambda(r, x_i, \bar{y}, \bar{x})$ is related to the function $\lambda_0(q_i, \bar{q}, q_i', \bar{q}')$ [cf. (2.12)] by

$$\lambda(r, x_i, \bar{y}, \bar{x})=\lambda_0(r+x_i/2, r-\bar{y}+\bar{x}/2, r-x_i/2, r-\bar{y}-\bar{x}/2) \tag{3.27}$$

3.2. Relation of the Propagating Function to the Displacement Correlation Function

Although the time evolution of an initial state is determined in principle via the propagating function (3.24), the interpretation of this result is hindered by the occurrence of integrals such as (3.22), and (3.23), the physical meaning of which is unclear. In order to get more insight, it is useful to connect the result (3.24) with physical properties of the Brownian particle.

Let us first evaluate the unknown normalization factor $N(t)$ in (3.24). To that aim we study the time evolution of the equilibrium state W_β^L normalized on an interval of length L. The preparation function then follows from (2.12) and (3.27) as

$$\lambda_\beta^L(r, x_i, \bar{y}, \bar{x}) = L^{-1}\delta(x_i - \bar{x})\,\delta(\bar{y}) \tag{3.28}$$

Now, the equilibrium average $\langle A\rangle$ of an observable may be defined as

$$\langle A\rangle = \lim_{L\to\infty} \int_{-L/2}^{L/2} dq\, \langle q|\, \mathrm{tr}_R(A W_\beta^L)\, |q\rangle \tag{3.29}$$

Clearly, the expectation value of the unity operator should remain 1 for all times. Using (3.25), we have

$$\begin{aligned}\langle 1\rangle_t &= \lim_{L\to\infty} \int_{-L/2}^{L/2} dr_f \int dx_i\, dy\, d\bar{x}\, d\bar{r} \\ &\quad\times J(0, y, t, x_i, \bar{x}, \bar{y})\, \lambda_\beta^L(r_f - y, x_i, \bar{y}, \bar{x}) \\ &= \int dx_i\, dy\, J(0, y, t, x_i, x_i, 0)\end{aligned} \tag{3.30}$$

Inserting the minimal action (3.21), we obtain from the integral over y a δ-function in x_i. Hence, we find

$$N(t) = 2\pi(\hbar/M)\,|G_+(t)| \tag{3.31}$$

This result can also be obtained by evaluating the functional integral over the fluctuations about the minimal action paths explicitly.

Next, we consider the propagating function for short times. Clearly, the functions (3.22), (3.23) in the action (3.21) vanish for $t\to 0$. Further, the initial condition $G_+(0)=0$ and $\dot{G}_+(0)=1$ yield $G_+(t)\simeq G_-(t)\simeq t$ for small times. The propagating function thus becomes

$$\begin{aligned}&J(x_f, y, t, x_i, \bar{x}, \bar{y}) \\ &\quad= \frac{M}{2\pi\hbar t}\exp\left[\frac{iM}{\hbar t}(x_f - x_i)\,y + O(t)\right]\exp\left(-\frac{M\Omega}{2\hbar}\bar{x}^2\right)\end{aligned} \tag{3.32}$$

In the limit $t\to 0$ the first exponential combines with the prefactor to give two δ-functions and we obtain

$$J(x_f, y, 0, x_i, \bar{x}, \bar{y}) = \delta(x_f - x_i)\,\delta(y)\exp\left(-\frac{M\Omega}{2\hbar}\bar{x}^2\right) \tag{3.33}$$

Combining this result with (3.25) and (3.28), we find the coordinate representation of the unnormalized equilibrium density matrix (2.14) to read

$$\bar{\rho}_\beta(\bar{x}) = \exp\left(-\frac{M\Omega}{2\hbar}\bar{x}^2\right) = \exp\left(-\frac{\langle p^2\rangle}{2\hbar^2}\bar{x}^2\right) \tag{3.34}$$

Here, the second equality introduces the equilibrium variance of the momentum of the Brownian particle, which follows from (3.16) as

$$\langle p^2\rangle = M\hbar\Omega = \frac{M}{\beta}\left[1 - 2\sum_{n=1}^{\infty}\frac{\hat{\gamma}(\nu_n)}{\nu_n + \hat{\gamma}(\nu_n)}\right] \tag{3.35}$$

Since the equilibrium state does not depend on $\bar{r}$, the variance of the coordinate diverges, as was to be expected for a free Brownian particle.

Let us now study the time-dependent autocorrelation of the position of the Brownian particle. Due to the divergence of the equilibrium variance $\langle q^2\rangle$ in the limit $L\to\infty$, the autocorrelation function of the coordinate $\langle q(t)q\rangle$ will also diverge. Instead, we consider the correlation of the displacement $q(t)-q(0)$ with the initial coordinate $q(0)$. The displacement correlation function

$$Q(t) = S(t) + iA(t) = \langle [q(t)-q(0)]\, q(0)\rangle \tag{3.36}$$

is regular for all times. Using the stationarity of the equilibrium expectation value, we see that its real part

$$S(t) = \tfrac{1}{2}\langle [q(t)-q(0)]\, q(0) + q(0)[q(t)-q(0)]\rangle$$

is connected with the mean square displacement $s(t)$ by

$$s(t) = \langle [q(t)-q(0)]^2\rangle = -2S(t) \tag{3.37}$$

and its imaginary part $A(t) = (1/2i)\langle [q(t), q(0)]\rangle$ is the antisymmetrized correlation. The correlation function (3.36) can now be determined from the propagating function (3.24). By virtue of (3.29), we find

$$Q(t) = \lim_{L\to\infty}\int_{-L/2}^{L/2} dr_f \int dx_i\, dy\, d\bar{x}\, d\bar{y} \times (y - x_i/2)(r_f - y + x_i/2)\, J(0, y, t, x_i, \bar{x}, \bar{y})\, \lambda_\beta^L(r_f - y, x_i, \bar{y}, \bar{x}) \tag{3.38}$$

Inserting (3.24) with the minimal action (3.21) and (3.28), we obtain for the real part of the displacement correlation

$$S(t) = \frac{\hbar}{2M} G_+^2(t)[2C^+(t) - R^{++}(t) - \Omega] \tag{3.39}$$

while the imaginary part reads

$$A(t) = -\frac{\hbar}{2M} G_+(t) \qquad \text{for} \quad t \geqslant 0 \tag{3.40}$$

We now have to determine the auxiliary functions (3.22), (3.23) occurring in the minimal action. We first note that these functions are not all independent. Rather, using (3.20), we find

$$C^-(t) = G_+(t) \frac{d}{dt} C^+(t) \tag{3.41}$$

while the functions $R^{\pm\pm}(t)$ can be derived from

$$\Psi(t, t') = \int_0^t ds \int_0^{t'} du\, R(s, u) \frac{G_+(t-s)}{G_+(t)} \frac{G_+(t'-u)}{G_+(t')} \tag{3.42}$$

according to

$$R^{++}(t) = \Psi(t, t) \tag{3.43}$$

$$R^{+-}(t) = R^{-+}(t) = G_+(t) \left[\frac{\partial}{\partial t} \Psi(t, t') \right]_{t=t'} \tag{3.44}$$

$$R^{--}(t) = G_+^2(t) \left[\frac{\partial^2}{\partial t\, \partial t'} \Psi(t, t') \right]_{t=t'} \tag{3.45}$$

A method of how these functions may be evaluated is outlined in Appendix B. It is found that they can all be expressed in terms of the Green's function $G_+(t)$ and the real part of the displacement correlation function, which has the Laplace transform

$$\hat{S}(z) = \frac{1}{M\beta} \left\{ -\frac{1}{z^2} \frac{1}{z + \hat{\gamma}(z)} + 2 \sum_{n=1}^{\infty} \frac{1}{\nu_n^2 - z^2} \left[\frac{1}{z + \hat{\gamma}(z)} - \frac{\nu_n}{z} \frac{1}{\nu_n + \hat{\gamma}(\nu_n)} \right] \right\} \tag{3.46}$$

Collecting the results and using (3.40), we find for the propagating function the form

$$J(x_f, y, t, x_i, \bar{x}, \bar{y}) = \frac{1}{4\pi |A(t)|} \exp\left[\frac{i}{\hbar} \Sigma(x_f, y, t, x_i, \bar{x}, \bar{y}) \right] \tag{3.47}$$

with

$$
\begin{aligned}
&\Sigma(x_f, y, t, x_i, \bar{x}, \bar{y}) \\
&\quad = i\frac{\langle p^2\rangle}{2\hbar}\bar{x}^2 + ix_i^2\left[\frac{\langle p^2\rangle}{2\hbar} - \frac{M\dot{S}(t)}{2A(t)} - \frac{\hbar S(t)}{4A^2(t)}\right] \\
&\quad + (x_i\bar{y} + x_f y)M\frac{\dot{A}(t)}{A(t)} + x_i y\frac{\hbar}{2A(t)} - x_f\bar{y}\frac{2}{\hbar}M^2\left[\ddot{A}(t) - \frac{\dot{A}^2(t)}{A(t)}\right] \\
&\quad + ix_i\bar{x}\left[-\frac{\langle p^2\rangle}{\hbar} + \frac{M\dot{S}(t)}{2A(t)}\right] + ix_f\bar{x}\frac{M^2}{\hbar}\left[\dot{S}(t)\frac{\dot{A}(t)}{A(t)} - \ddot{S}(t)\right] \\
&\quad + ix_i x_f\left\{-\frac{M^2}{\hbar}\left[\dot{S}(t)\frac{\dot{A}(t)}{A(t)} - \ddot{S}(t)\right]\right. \\
&\quad \left. + \frac{M}{2A^2(t)}[A(t)\dot{S}(t) - 2\dot{A}(t)S(t)]\right\} \\
&\quad + ix_f^2\left\{\frac{\langle p^2\rangle}{2\hbar} + \frac{M^2\dot{A}(t)}{\hbar A(t)}\left[\dot{S}(t) - \frac{\dot{A}(t)}{A(t)}S(t)\right]\right\}
\end{aligned} \tag{3.48}
$$

Hence, the entire dynamics of the system for arbitrary initial states can be expressed in terms of the symmetrized part $S(t)$ and the antisymmetrized part $A(t)$ of the displacement correlation function (3.36). This correlation is an equilibrium property, but together with the (time-independent) preparation function it also determines the nonequilibrium dynamics of the Brownian particle. The propagating function may be viewed as a quantum analog of the classical two-point probability, which is the conditional probability multiplied by the equilibrium distribution. Like this classical probability, the propagating function can be expressed in terms of equilibrium correlations. However, the quantum propagator is a more complicated quantity because of the dependence on two additional variables $\bar{x}$ and $\bar{y}$ associated with initial correlations between particle and heat bath. In the following section we discuss the time dependence of the displacement correlation for different damping mechanisms of interest.

4. TIME DEPENDENCE OF THE CORRELATION FUNCTIONS

In the preceding section we saw that the displacement correlation function $Q(t)$ completely determines the time dependence of the propagating function $J(x_f, r_f, t, x_i, r_i, \bar{x}, \bar{r})$. However, for an arbitrary dissipative mechanism the correlation is known only in terms of the Laplace transforms of its real part $S(t)$ and its imaginary part $A(t)$, respectively. To gain explicit results in the time domain, we have to specify the frequency dependence of the damping coefficient. In this section we first consider the important case of Ohmic damping, where exact results can be obtained. Subsequently, we discuss the asymptotic long-time dependence in the general case of a damping mechanism of arbitrary frequency dependence.

4.1. Ohmic Damping

Let us first consider a heat bath leading to frequency-independent or Ohmic 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.[5] Further, for Ohmic dissipation we can determine the time dependence of correlation functions explicitly. A Markovian or Ohmic damping kernel

$$\gamma(t) = 2\gamma\delta(t) \tag{4.1}$$

has a frequency-independent Laplace transform $\hat{\gamma}(\omega) = \gamma$ [cf. (3.6)]. In the microscopic model, Ohmic damping is realized if the spectral density of the environment $I(\omega)$ takes the form[3]

$$I(\omega) = M\gamma\omega \tag{4.2}$$

As is familiar from the theory of classical Markov processes, Ohmic damping leads to sum rule divergences. Such a divergence arises here if we consider the equilibrium variance of the momentum. From (3.35) we have

$$\langle p^2 \rangle = \frac{M}{\beta} \sum_{n=-\infty}^{\infty} \frac{\gamma}{\gamma + |\nu_n|} \tag{4.3}$$

which is logarithmically divergent. Clearly, this divergence is an artefact of the unphysical high-frequency behavior of the spectral density (4.2). If we consider a realistic damping kernel with finite memory, the divergence is readily removed. For instance, a Drude model with $\gamma(t) = \gamma\omega_{\mathrm{D}} \exp(-\omega_{\mathrm{D}} t)$ leads to a finite value of $\langle p^2 \rangle$ given by

$$\langle p^2 \rangle = \frac{M}{\beta} \sum_{n=-\infty}^{\infty} \frac{\gamma\omega_{\mathrm{D}} |\nu_n|}{(\omega_{\mathrm{D}} + |\nu_n|)\nu_n^2 + \gamma\omega_{\mathrm{D}} |\nu_n|} \tag{4.4}$$

In the limit $\omega_{\mathrm{D}} \gg \gamma$ the Drude model behaves like an Ohmic model except for very short times of order $1/\omega_{\mathrm{D}}$. For high temperatures the variance (4.4) gives $\langle p^2 \rangle = Mk_{\mathrm{B}}T$ as the equipartition law predicts. For $T \to 0$ the damping leads to a nonvanishing finite value of $\langle p^2 \rangle$. Without dissipation the momentum of a free particle can be sharp variable.

Let us now consider the correlations. Using (3.40) and inserting $\hat{\gamma}(z) = \gamma$ in (3.19), we have for the antisymmetrized correlation function

$$A(t) = -\frac{\hbar}{2M} G_+(t) = -\frac{\hbar}{2M\gamma}[1 - \exp(-\gamma t)] \qquad \text{for} \quad t \geqslant 0 \tag{4.5}$$

The Green's function $G_+(t)$ determines the response of a Brownian particle initially in equilibrium to an external force $F(t)$ according to

$$\langle q \rangle_t = M^{-1} \int_0^t ds\, G_+(t-s)\, F(s) \tag{4.6}$$

For a time-independent force this yields the average momentum

$$\langle p \rangle_t = G_+(t) F = \frac{1}{\gamma}[1 - \exp(-\gamma t)] F \tag{4.7}$$

so that the particle is accelerated at first but after a time of order γ^{-1} a finite asymptotic velocity is reached, which increases with decreasing friction. Ohmic damping thus provides a good description for the familiar motion in viscous media, where the behavior (4.7) is usually realized.

Using (3.46), one can also readily establish the time dependence of the symmetrized displacement correlation $S(t)$. We find

$$\begin{aligned} S(t) = &-\frac{1}{M\beta\gamma} t + \frac{1}{M\beta\gamma^2} - \frac{2}{M\beta} \sum_{n=1}^{\infty} \frac{1}{\nu_n^2 + \nu_n \gamma} \\ &- \frac{\hbar}{2M\gamma} \cot\left(\frac{\hbar\beta\gamma}{2}\right) \exp(-\gamma t) + \frac{2\gamma}{M\beta} \sum_{n=1}^{\infty} \frac{\exp(-\nu_n t)}{\nu_n(\gamma^2 - \nu_n^2)} \end{aligned} \tag{4.8}$$

In the classical limit $\hbar \to 0$ this yields the familiar result

$$S_{\mathrm{cl}}(t) = -\frac{1}{M\beta\gamma} t + \frac{1}{M\beta\gamma^2}[1 - \exp(-\gamma t)] \tag{4.9}$$

For long times and finite temperatures, the displacement correlation is proportional to t, since all the remaining terms in (4.8) are either constant or vanish for $t \to \infty$. Hence, we can define the diffusion coefficient

$$D = \frac{1}{2} \lim_{t \to \infty} \frac{1}{t} s(t) = -\lim_{t \to \infty} \frac{1}{t} S(t) \tag{4.10}$$

which depends on the temperature and the strength of the damping according to the Einstein relation

$$D = 1/M\beta\gamma = k_{\mathrm{B}} T/M\gamma \tag{4.11}$$

For finite temperatures the Brownian particle undergoes a diffusion process in the presence of an Ohmic reservoir. At $T=0$, however, the diffusion coefficient vanishes, and the displacement correlation is no longer $\propto t$ in the long-time limit. Since the Matsubara frequencies ν_n become continuous at $T=0$, the sums in (4.8) have to be replaced by integrals. For the time derivative of $S(t)$ we obtain

$$\dot{S}_0(t) = \frac{\hbar\gamma}{\pi M} \int_0^\infty d\nu \, \frac{\exp(-\nu t)}{\nu^2 - \gamma^2} \tag{4.12}$$

which can be expressed in terms of the exponential integral

$$Ei(x) = \int_{-\infty}^{x} dy \, \frac{\exp(y)}{y} \tag{4.13}$$

For real $x > 0$ this definition is analytically continued by

$$\overline{Ei}(x) = \lim_{\varepsilon \to 0} \frac{1}{2} \left[Ei(x + i\varepsilon) + Ei(x - i\varepsilon) \right] \tag{4.14}$$

Using $S(0) = 0$, we have from (4.12)

$$S_0(t) = \frac{\hbar}{2\pi M} \int_0^t ds \, \left[Ei(-\gamma s) \exp(\gamma s) - \overline{Ei}(\gamma s) \exp(-\gamma s) \right] \tag{4.15}$$

For long times, this integral grows logarithmically according to

$$S_0(t) \simeq -\frac{\hbar}{\pi M \gamma} \ln(\gamma t) \qquad \text{for} \quad t \to \infty \tag{4.16}$$

Hence, at zero temperature, the growth of the displacement correlation [and because of (3.37) also of the mean square displacement] is no longer diffusive $\propto t$, but only $\propto \ln(t)$. The reason for this slower rate of growth is the lack of thermal fluctuations in the reservoir that could kick the particle.

4.2. Frequency-Dependent Damping

For a frequency-dependent damping mechanism we can in general no longer obtain exact results for the correlation functions the way we did in the Ohmic case. We can, however, examine the asymptotic behavior for arbitrary frequency dependence of the damping. 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 α is a real, positive number. Negative values of α cannot occur because the definition (3.1) 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, we can describe the reservoir by

$$I(\omega) = M g_\alpha \omega^\alpha \Theta(\omega_c - \omega); \qquad \alpha > 0 \tag{4.17}$$

We note that most of the following results do not depend on this special choice of a 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 behavior of the correlations only if the exponent $\alpha \geqslant 2$, 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 (4.17) 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 (4.17). Reservoirs of the form (4.17) were discussed in various contexts. For instance, the coupling of a charged defect to electrons can be modeled 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.[3]

Inserting the spectral density in (3.6), the frequency-dependent damping coefficient is found to read

$$\hat{\gamma}(\omega) = \frac{2g_\alpha}{\alpha\pi}\frac{\omega_c^\alpha}{\omega} F\left(1, \frac{\alpha}{2}; 1 + \frac{\alpha}{2}; -\frac{\omega_c^2}{\omega^2}\right) \tag{4.18}$$

where $F(a, b; c; z)$ is the hypergeometric function. For small frequencies we can use the asymptotic expansion of the hypergeometric function, yielding[15]

$$\hat{\gamma}(\omega) = \begin{cases} [g_\alpha/\sin(\frac{1}{2}\pi\alpha)]\,\omega^{\alpha-1}[1 + O(\omega/\omega_c, (\omega/\omega_c)^{2-\alpha})] & \text{for} \quad 0 < \alpha < 2 \\ (g_2/\pi)\,\omega \ln(1 + \omega_c^2/\omega^2) & \text{for} \quad \alpha = 2 \\ [2g_\alpha \omega_c^{\alpha-2}/\pi(\alpha-2)]\,\omega(1 - \{\pi(\alpha-2)/2\sin[\frac{1}{2}\pi(\alpha-2)]\} & \\ \qquad \times (\omega/\omega_c)^{\alpha-2} + O(\omega^2/\omega_c^2)) & \text{for} \quad 2 < \alpha < 4 \\ [2g_\alpha \omega_c^{\alpha-2}/\pi(\alpha-2)]\,\omega[1 + O(\omega^2/\omega_c^2)] & \text{for} \quad \alpha \geqslant 4 \end{cases} \tag{4.19}$$

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

[3] Relevant articles can be traced through Ref. 20.

integer values of α. Otherwise, derivatives of order n of $\hat{\gamma}(\omega)$ diverge when $n \geqslant \alpha - 1$.

4.2.1. The Antisymmetrized Displacement Correlation Function

The antisymmetrized displacement correlation follows from (3.19) and (3.40) as

$$A(t) = \frac{i\hbar}{4\pi M} \int_{-i\infty+\varepsilon}^{i\infty+\varepsilon} dz \, \frac{\exp(zt)}{z^2 + z\hat{\gamma}(z)} \tag{4.20}$$

Let us first consider the case $\alpha < 2$. Inserting (4.19), we obtain

$$A(t) \simeq \frac{i\hbar}{4\pi M} \frac{\sin(\pi\,\alpha/2)}{g_\alpha} t^{\alpha-1} \int_{-i\infty+\varepsilon}^{i\infty+\varepsilon} dx \times \frac{\exp(x)}{x^\alpha[1 + O(x/\omega_c t, (x/\omega_c t)^{2-\alpha})]} \quad \text{for} \quad t \to \infty, \ \alpha < 2 \tag{4.21}$$

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

$$A(t) \simeq -\frac{\hbar \sin(\pi\,\alpha/2)}{2Mg_\alpha \Gamma(\alpha)} t^{\alpha-1}[1 + O((\omega_c t)^{-1}, (\omega_c t)^{\alpha-2})] \quad \text{for} \quad t \to \infty, \quad \alpha < 2 \tag{4.22}$$

This long-time expansion includes the corresponding limit of the exact Ohmic result (4.5), since the corrections vanish for $\omega_c \to \infty$.

For $\alpha = 2$ an analogous analysis of (4.20) yields

$$A(t) \simeq -\frac{\pi\hbar}{4g_2 M} \frac{t}{\ln(t)} \{1 + O[\ln^{-1}(t)]\} \qquad \text{for} \quad t \to \infty, \quad \alpha = 2 \tag{4.23}$$

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

$$A(t) \simeq -\frac{\hbar}{2M_r} t \left\{ 1 + \frac{M}{M_r} \left[g_\alpha / \sin\left(\pi \frac{\alpha - 2}{2}\right) \Gamma(4-\alpha) \right] t^{2-\alpha} + O(\omega_c^{-2} t^{-2}, \omega_c^{-\alpha} t^{-\alpha}) \right\} \quad \text{for} \quad t \to \infty, \quad \alpha > 2 \tag{4.24}$$

where we introduced the renormalized mass

$$M_r = M[1 + 2g_\alpha \omega_c^{\alpha-2}/\pi(\alpha - 2)] \qquad \text{for} \quad \alpha > 2 \tag{4.25}$$

For later use we have included in (4.24) 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 $\langle p \rangle_t = G_+(t) F = -(2M/\hbar) A(t) F$. 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 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.[15] 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 (4.25) of M_r in terms of the microscopic model. Using (4.17) and (3.1), we have

$$M_r = M + 2 \int_0^\infty \frac{d\omega}{\pi} \frac{I(\omega)}{\omega^3} = M + \sum_{n=1}^{N} m_n \tag{4.26}$$

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 $\alpha \leqslant 2$ 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 center of mass of the environment.

4.2.2. The Symmetrized Displacement Correlation Function at Finite Temperatures

Let us now consider the long-time behavior of the real part $S(t)$ of the displacement correlation. While the imaginary part $A(t)$ and the Green's function $G_+(t)$ discussed before are temperature-independent quantities, the asymptotic time dependence of $S(t)$ at finite temperatures differs strongly from the zero-temperature case. At finite temperatures, all terms in the sum in (3.46) giving the Laplace transform of $S(t)$ lead to exponentially decaying or constant terms in the time domain. Thus, the leading long-time dependence stems from the first term in (3.46). This term, however, is connected with the antisymmetrized correlation by

$$\hat{S}(z) \simeq \frac{2}{\hbar\beta} \frac{\hat{A}(z)}{z} \qquad \text{for} \quad z \to 0, \quad T > 0 \tag{4.27}$$

Accordingly, we have, for long times,

$$S(t) \simeq \frac{2}{\hbar\beta} \int_0^t ds\, A(s) \qquad \text{for} \quad t \to \infty, \quad T > 0 \tag{4.28}$$

so that in the long-time limit the symmetrized displacement correlation is but a time integral of the antisymmetrized correlation. Using (4.22)–(4.24), we have

$$S(t) \simeq \begin{cases} -[\sin(\pi\,\alpha/2)/M\beta g_\alpha \Gamma(\alpha+1)]\; t^\alpha[1 + O(t^{-1}, t^{\alpha-2})] & \text{for } \alpha < 2 \\ -(\pi/4M\beta g_2)\,(t^2/\ln(t))\{1 + O[\ln^{-1}(t)]\} & \text{for } \alpha = 2 \\ -(t^2/2M_r\beta)[1 + O(t^{-2}, t^{2-\alpha})] & \text{for } \alpha > 2 \end{cases}$$
$$t \to \infty, \quad T > 0 \tag{4.29}$$

Because of (3.37), 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 behavior $\propto t$ 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 behavior, 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 (cf. next section).

4.2.3. The Symmetrized Displacement Correlation at Zero Temperature

Let us now consider the correlation $S(t)$ for $T = 0$. Then the frequencies ν_n are continuous and the sum in (3.46) has to be replaced by an integral. We have

$$\hat{S}_0(z) = \frac{2}{\pi} \frac{1}{z} \int_0^\infty d\nu\, \frac{1}{\nu^2 - z^2} [\hat{f}(\nu) - \hat{f}(z)] = \frac{2}{\pi} \frac{1}{z} \int_0^\infty d\nu\, \frac{1}{\nu^2 - z^2} \hat{f}(\nu) \tag{4.30}$$

where

$$\hat{f}(z) = z^2 \hat{A}(z) \tag{4.31}$$

Inserting in (4.30) for $\hat{f}(v)$ the definition of the Laplace transform, one may transform the expression to read

$$z^2\hat{S}_0(z)=\frac{2}{\pi}\int_0^\infty dt\,\exp(-zt)\int_0^\infty dx\,\frac{1}{x^2-1}\,\frac{1}{x}\,f\left(\frac{t}{x}\right) \tag{4.32}$$

Now, because of $S_0(0)=\dot{S}_0(0)=0$, the lhs of this relation is just the Laplace transform of $\ddot{S}_0(t)$. Since the rhs also has the structure of a Laplace transform, we can write

$$\ddot{S}_0(t)=\frac{2}{\pi}\int_0^\infty dx\,\frac{1}{x^2-1}\,\frac{1}{x}\,f\left(\frac{t}{x}\right)=\frac{2}{\pi}\int_0^\infty dx\,\frac{1}{x^2-1}\,\frac{1}{x}\,\ddot{A}\left(\frac{t}{x}\right) \tag{4.33}$$

where the second equality holds, since $A(0)=0$. Integrating this equation twice, we obtain

$$S_0(t)=\frac{2}{\pi}\int_0^\infty dx\,\frac{x}{x^2-1}\,A\left(\frac{t}{x}\right) \tag{4.34}$$

since all boundary terms do not contribute to the integral.

We can now insert the asymptotic laws (4.22)–(4.24) for the antisymmetrized correlation $A(t)$ and obtain the long-time dependence of $S_0(t)$. For $0<\alpha<1$, $A(t)$ vanishes asymptotically. Substituting $u=t/x$, we can perform the limit $t\to\infty$ in the integrand, yielding

$$\lim_{t\to\infty} S_0(t)=\frac{2}{\pi}\int_0^\infty du\,\frac{1}{u}\,A(u)=\frac{2}{\pi}\int_0^\infty dz\,\hat{A}(z) \qquad \text{for} \quad \alpha<1 \tag{4.35}$$

Using (4.19) and (4.20), we find

$$\lim_{t\to\infty} S_0(t)=-\left[\hbar/M(2-\alpha)\sin\left(\frac{\pi}{2-\alpha}\right)\right]\left[\sin\left(\pi\frac{\alpha}{2}\right)\Big/g_\alpha\right]^{1/(2-\alpha)}$$
$$\times\left[1+O(t^{-1})\right] \qquad \text{for} \quad \alpha<1 \tag{4.36}$$

Hence, for a sub-Ohmic reservoir at zero temperature the symmetrized displacement correlation remains finite in the limit $t\to\infty$. We will see in the next section that this has profound consequences for the time evolution of nonequilibrium initial states.

For $\alpha=1$ the antisymmetrized correlation approaches a constant in the long-time limit, leading to a logarithmic divergence of the integral (4.34). Splitting the integral into an integral form 0 to t and a correction, we obtain

$$S_0(t)\simeq-\frac{\hbar}{\pi M g_1}\ln(t)\,\{1+O[\ln^{-1}(t)\}\qquad \text{for} \quad t\to\infty, \quad \alpha=1 \tag{4.37}$$

which is the long-time expansion of the exact Ohmic correlation (4.15).

In the interval $1<\alpha<2$ the result (4.22) for $A(t)$ leads to the zero-temperature displacement correlation

$$S_0(t) \simeq -\frac{\hbar}{2Mg_\alpha \Gamma(\alpha)}\left[\sin^2\left(\pi\frac{2-\alpha}{2}\right)\Big/\cos\left(\pi\frac{2-\alpha}{2}\right)\right] t^{\alpha-1} \times [1+O(t^{\alpha-2})] \qquad \text{for} \quad t\to\infty, \quad 1<\alpha<2 \tag{4.38}$$

The case $\alpha=2$ is again not described by a simple power law behavior. Inserting (4.23) in (4.34), we get

$$\begin{aligned} S_0(t) &\simeq -\frac{\hbar}{2Mg_2}\frac{t}{\ln(t)}\int_0^\infty dy \frac{1}{y^2-1}\frac{1}{1-\ln(y)/\ln(t)} \\ &\simeq -\frac{\hbar\pi^2}{8Mg_2}\frac{t}{\ln^2(t)}[1+O(\ln^{-1}(t)] \qquad \text{for} \quad t\to\infty, \quad \alpha=2 \end{aligned} \tag{4.39}$$

where we have expanded the second term in the integrand to obtain the second equality.

For $\alpha>2$ the leading term $\propto t$ in the long-time expansion (4.24) of $A(t)$ gives no contribution to (4.34). Hence, the corrections to the linear growth of $A(t)$ that are explicitly given in (4.24) are important. We find

$$S_0(t) \simeq -\frac{\hbar g_\alpha}{2\Gamma(4-\alpha)}\frac{M}{M_r^2}\left[\cos\left(\pi\frac{\alpha-2}{2}\right)\right]^{-1} t^{3-\alpha} \times [1+O(t^{2-\alpha})] \qquad \text{for} \quad t\to\infty, \quad 2<\alpha<3 \tag{4.40}$$

where M_r is the renormalized mass (4.25). The case $\alpha=3$, corresponding to the coupling to a three-dimensional phonon bath, is similar to the Ohmic case ($\alpha=1$). The displacement correlation again grows logarithmically according to

$$S_0(t) \simeq -\frac{\hbar g_3}{\pi}\frac{M}{M_r^2}\ln(t)\,\{1+O[\ln^{-1}(t)]\} \qquad \text{for} \quad t\to\infty, \quad \alpha=3 \tag{4.41}$$

Similarly, the situation for $\alpha>3$ resembles sub-Ohmic damping. Since the leading term $\propto t$ in $A(t)$ gives no contribution, we obtain from (4.34)

$$\begin{aligned} \lim_{t\to\infty} S_0(t) &= \frac{2}{\pi}\int_0^\infty du\left[\frac{1}{u}A(u) - \dot{A}(t\to\infty)\right] \\ &= \frac{2}{\pi}\int_0^\infty dz\left[\hat{A}(z)+\frac{\hbar}{2M_r}\frac{1}{z^2}\right] \qquad \text{for} \quad \alpha>3 \end{aligned} \tag{4.42}$$

so that $S_0(t)$ approaches a constant 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 $S_0(t \to \infty)$ for $\alpha > 3$ is the only result where the high-frequency properties of the damping enter the long-time behavior 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

$$q_\infty = \left[\hbar/M(2-\alpha) \sin\left(\frac{\pi}{2-\alpha}\right) \right] \left[\sin\left(\pi \frac{\alpha}{2}\right) \Big/ g_\alpha \right]^{1/(2-\alpha)} \qquad \text{for} \quad \alpha < 1 \tag{4.43}$$

and the constants

$$d_\alpha = \begin{cases} \hbar/\pi M g_1 & \text{for} \quad \alpha = 1 \\ [\hbar/2Mg_\alpha \Gamma(\alpha)] \sin^2\left(\pi \frac{2-\alpha}{2}\right) \Big/ \cos\left(\pi \frac{2-\alpha}{2}\right) & \text{for} \quad 1 < \alpha < 2 \\ \pi^2 \hbar/8Mg_2 & \text{for} \quad \alpha = 2 \\ \hbar M g_\alpha \Big/ \left[2M_r^2 \Gamma(4-\alpha) \cos\left(\pi \frac{\alpha-2}{2}\right) \right] & \text{for} \quad 2 < \alpha < 3 \\ \hbar M g_3/\pi M_r^2 & \text{for} \quad \alpha = 3 \end{cases} \tag{4.44}$$

Further, for $\alpha \leqslant 2$

$$\mu_\alpha = \begin{cases} Mg_\alpha \Gamma(\alpha+1)/\sin(\pi\, \alpha/2) & \text{for} \quad \alpha < 2 \\ 4Mg_2/\pi & \text{for} \quad \alpha = 2 \end{cases} \tag{4.45}$$

is a generalized mobility, which is connected to the generalized diffusion coefficient D_α by

$$D_\alpha = 1/\beta\mu_\alpha = k_B T/\mu_\alpha \qquad \text{for} \quad \alpha \leqslant 2 \tag{4.46}$$

Finally, for $\alpha > 2$

$$v_\beta = (M_r \beta)^{-1/2} = (k_B T/M_r)^{1/2} \tag{4.47}$$

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 I. Comparing the behavior of the mean square displacement $s(t)$ at finite temperatures with the $T=0$ result, we see a remarkable difference. Whereas the rate of growth at finite temperatures gets faster with increasing α and

Table I. 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 $A(t)$ of the Displacement Correlation Function in Terms of the Exponent α and the Quantities Defined in (4.43)–(4.47)[a]

α	$s_0(t)\ [T=0]$	$A(t)$	$s(t)\ [T>0]$
$0<\alpha<1$	$2q_\infty$		
$\alpha=1$	$2d_1 \ln(t)\{1+O[\ln^{-1}(t)]\}$	$-(\alpha\hbar/2\mu_\alpha)t^{\alpha-1}[1+O(t^{-1}, t^{\alpha-2})]$	$2D_\alpha t^\alpha[1+O(t^{-1}, t^{\alpha-2})]$
$1<\alpha<2$	$2d_\alpha t^{\alpha-1}[1+O(t^{\alpha-2})]$		
$\alpha=2$	$[2d_2 t/\ln^2(t)]\{1+O[\ln^{-1}(t)]\}$	$[-(\hbar/\mu_2)t/\ln(t)]\{1+O[\ln^{-1}(t)]\}$	$[2D_2 t^2/\ln(t)]\{1+O[\ln^{-1}(t)]\}$
$2<\alpha<3$	$2d_\alpha t^{3-\alpha}[1+O(t^{2-\alpha})]$		
$\alpha=3$	$2d_3 \ln(t)\{1+O[\ln^{-1}(t)]\}$	$-(\hbar/2M_r)t[1+O(t^{-2}, t^{2-\alpha})]$	$v_\beta^2 t^2[1+O(t^{-2}, t^{2-\alpha})]$
$3<\alpha$	const		

[a] The symmetrized part $S(t)$ of the displacement correlation function is given by $S(t) = -s(t)/2$.

then saturates for $\alpha > 2$, there is a maximum for $\alpha = 2$ in the zero-temperature case. A faster growth of $s(t)$ for larger α seems natural because with growing α there are fewer environmental oscillators at low frequencies and the damping is less effective for long times. The contrary result at $T = 0$ for $\alpha > 2$ is connected with the fact that the limit $\alpha \to \infty$ corresponds to a free particle. The latter, however, has vanishing momentum at $T = 0$. Hence, the zero-temperature mean square displacement $s_0(t)$ vanishes, too.

5. 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. In Section 3 we saw that the dynamics of such a state can be expressed entirely in terms of the displacement correlation function $Q(t)$. Since in the preceding section we obtained analytic results for the long-time behavior 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.

5.1. Broadening of an Initially Localized Wave Packet

5.1.1. Time Evolution of a Gaussian Density Matrix

Let us first consider a Brownian particle that is initially localized. Such a state may be prepared, e.g., using a device that lets particles pass at position q with probability $w(q, 0)$. This position measurement is described by the projection operator

$$P_q = \int dq\, w^{1/2}(q, 0)\, |q\rangle\langle q| \tag{5.1}$$

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

$$w(q, 0) = (2\pi\sigma_0)^{-1/2} \exp(-q^2/2\sigma^0) \tag{5.2}$$

The normalized initial density matrix is simply $W_0 = P_q \bar{W}_\beta P_\beta$, so that the preparation function follows from (2.12) and (3.27) as

$$\lambda(r, x, \bar{y}, \bar{x}) = (2\pi\sigma_0)^{-1/2} \exp\left(-\frac{r^2}{2\sigma_0} - \frac{x^2}{8\sigma_0}\right) \delta(x - \bar{x})\, \delta(\bar{y}) \tag{5.3}$$

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

$$\rho_0(x, r) = (2\pi\sigma_0)^{-1/2} \exp\left[-\frac{r^2}{2\sigma_0} - \left(\frac{\langle p^2\rangle}{2\hbar^2} + \frac{1}{8\sigma_0}\right) x^2\right] \tag{5.4}$$

Inserting the preparation function (5.3) and the propagating function (3.47), (3.48), in (3.25), we obtain the density matrix at time t as

$$\begin{aligned}\rho(x, r, t) = {} & [2\pi\sigma(t)]^{-1/2} \exp\left(-\frac{\langle p^2\rangle}{2\hbar^2} x^2\right) \\ & \times \exp\left(-\frac{1}{2\sigma(t)} \left\{ r^2 + 2\frac{i}{\hbar} Mxr \left[\dot{S}(t) - \frac{A(t)\,\dot{A}(t)}{\sigma_0}\right] \right.\right. \\ & \left.\left. - \frac{M^2}{\hbar^2} x^2 \left[\dot{S}^2(t) - \dot{A}(t)^2 \left(1 + 2\frac{S(t)}{\sigma_0}\right) - \frac{2}{\sigma_0} A(t)\,\dot{A}(t)\,\dot{S}(t)\right]\right\}\right)\end{aligned} \tag{5.5}$$

Since the particle had no average velocity in the initial state, the wave packet remains centered at the origin. The width $\sigma^{1/2}(t)$ can be expressed through the correlations $S(t)$ and $A(t)$ via

$$\sigma(t) = \sigma_0 - 2S(t) + A^2(t)/\sigma_0 \tag{5.6}$$

Since the symmetrized displacement correlation $S(t) = -s(t)/2$ is always negative, the wave packet can only become broader with increasing time.

5.1.2. Asymptotic Spreading of the State

Let us now discuss how the long-time behavior of the variance (5.6) depends on the dissipative mechanism. To that aim we can use the asymptotic laws for the correlation functions, which are summarized in Table I. At finite temperatures we obtain[15]

$$\sigma(t) \simeq \begin{cases} 2D_\alpha t^\alpha & \text{for} \quad \alpha<2 \\ 2D_2 t^2/\ln(t) & \text{for} \quad \alpha=2 \\ (v_\beta^2+\hbar^2/4\sigma_0 M_r^2)\,t^2 & \text{for} \quad \alpha>2 \end{cases}$$

$$t\to\infty, \quad T>0 \tag{5.7}$$

Hence, the state spreads diffusively in the Ohmic case ($\alpha=1$), while for sub-/super-Ohmic damping we have a sub-/superdiffusive rate of growth of the variance, respectively. For all $\alpha\leqslant 2$ the asymptotic behavior of $\sigma(t)$ is completely determined by the symmetric part $S(t)$ of the displacement correlation. The antisymmetrized part contributes only for $\alpha>2$, where we have a kinematic spreading with a velocity v_∞ given by

$$v_\infty^2 = v_\beta^2+\hbar^2/4\sigma_0 M_r^2 \tag{5.8}$$

In the classical limit only the first term in this expression survices. 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 (5.8) 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 $S(t)$ results in a slower spreading of the state for $\alpha\leqslant 2$, while for $\alpha>2$ the asymptotic behavior is qualitatively unchanged. Using Table I, we have[15]

$$\sigma_0(t) \simeq \begin{cases} 2q_\infty+\sigma_0 & \text{for} \quad \alpha<1 \\ 2d_1\ln(t) & \text{for} \quad \alpha=1 \\ (\alpha^2\hbar^2/4\mu_\alpha^2\sigma_0)\,t^{2\alpha-2} & \text{for} \quad 1<\alpha<2 \\ (2\hbar^2/\mu_\alpha^2\sigma_0)\,t^2/\ln^2(t) & \text{for} \quad \alpha=2 \\ (\hbar^2/4\sigma_0 M_r^2)\,t^2 & \text{for} \quad \alpha>2 \end{cases}$$

$$t\to\infty, \quad T=0 \tag{5.9}$$

Here it is the antisymmetric correlation $A(t)$ that dominates the asymptotic behavior for all $\alpha>1$. For $\alpha>2$, Eq. (5.8) 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 behavior for $\alpha=3/2$. For Ohmic damping we now have a logarithmic growth. Most remarkable, however, is the behavior 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[15]

$$\xi = \sigma_0^{1/2}(t \to \infty) = (2q_\infty + \sigma_0)^{1/2} \tag{5.10}$$

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.[7] 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 (5.7), 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 (5.7) as $T \to 0$.

5.2. Long-Time Behavior for Arbitrary Initial States

Let us now consider the general behavior of the propagating function (3.47), (3.48) for the different types of damping. Using the asymptotic correlations summarized in Table I, we can determine how initial states described by an arbitrary preparation function of the form discussed in Section 2 behave for long times. Because of the different asymptotic behavior of the displacement correlation in various regions of the parameter space, this analysis is divided into several subsections.

5.2.1. Finite Temperatures and $\alpha \leqslant 2$

In the limit of long times we can drop all contributions in the exponent of the propagating function that vanish as $t \to \infty$ except for those terms of order $y/s^{1/2}(t)$, where $s(t)$ is the mean square displacement. These latter terms have to be retained, since they describe the spreading of the state.

For $\alpha < 2$ we thus find

$$
\begin{aligned}
&J(x_f, y, t, x_i, \bar{x}, \bar{y}) \\
&\quad \simeq \bar{\rho}_\beta(x_f)\,\bar{\rho}_\beta(\bar{x})(\mu_\alpha/2\pi\alpha\hbar t^{\alpha-1}) \\
&\quad\quad \exp\left\{-x_i^2\left(\frac{\mu_\alpha}{\beta\alpha^2\hbar^2}\,t^{2-\alpha}+\frac{\langle p^2\rangle}{2\hbar^2}-\frac{M}{\hbar^2\beta}\right)\right. \\
&\quad\quad -x_i\left[\left(\frac{i\mu_\alpha}{\alpha\hbar}\right)t^{1-\alpha}(y+\bar{y})\right. \\
&\quad\quad \left.\left.+\frac{M}{\alpha\hbar^2\beta}(2-\alpha)x_f+\left(\frac{M}{\hbar^2\beta}-\frac{\langle p^2\rangle}{\hbar^2}\right)\bar{x}\right]\right\} \quad \text{for } t\to\infty,\ T>0,\ \alpha<2
\end{aligned} \tag{5.11}
$$

Completing the square in the exponent and omitting terms negligible for $t \to \infty$, we obtain

$$
\begin{aligned}
&J(x_f, y, t, x_i, \bar{x}, \bar{y}) \\
&\quad \simeq \bar{\rho}_\beta(x_f)\,\bar{\rho}_\beta(\bar{x})\,\frac{\mu_\alpha}{2\pi\alpha\hbar t^{\alpha-1}} \\
&\quad\quad \times\exp\left[-\frac{\mu_\alpha}{\beta\alpha^2\hbar^2}\,t^{2-\alpha}\left(x_i+i\frac{\alpha\hbar\beta}{2t}\,y\right)^2\right] \\
&\quad\quad \times\exp\left(-\frac{1}{4D_\alpha}\,t^{-\alpha}y^2\right) \qquad \text{for} \quad t\to\infty,\ T>0,\ \alpha<2 \\
&\quad = \bar{\rho}_\beta(x_f)\,\bar{\rho}_\beta(\bar{x})\,\delta(x_i)(4\pi D_\alpha t^\alpha)^{-1/2}\exp\left(-\frac{1}{4D_\alpha}\,t^{-\alpha}y^2\right)
\end{aligned} \tag{5.12}
$$

To obtain the second equality, we noted that the first exponential approaches a δ-function as $t \to \infty$. The reduced density matrix evolving from an initial state characterized by the preparation function $\lambda(r_f - y, x_i, \bar{y}, \bar{x})$ is then given by

$$
\begin{aligned}
\rho(x_f, r_f, t) &\simeq (4\pi D_\alpha t^\alpha)^{-1/2}\exp\left(-\frac{1}{4D_\alpha}\,t^{-\alpha}r_f^2\right)\bar{\rho}_\beta(x_f) \\
&\quad \times\int dr_i\,d\bar{x}\,d\bar{y}\,\lambda(r_i, 0, \bar{y}, \bar{x})\,\bar{\rho}_\beta(\bar{x}) \\
&\qquad \text{for} \quad t\to\infty, \quad T>0, \quad \alpha<2
\end{aligned} \tag{5.13a}
$$

Here, we put $y = r_f - r_i$ in (5.12) and noted that terms in the exponent proportional to r_i give no contribution in the limit $t \to \infty$, since for a state initially localized around 0 it is the final coordinate r_f that is responsible for the growth of y. Because of (2.15) the last integral is simply the trace over the initial state, which we assume to be normalized. Hence, we have

$$\rho(x_f, r_f, t) \simeq (4\pi D_\alpha t^\alpha)^{-1/2} \exp\left(-\frac{1}{4D_\alpha} t^{-\alpha} r_f^2\right)$$
$$\times \exp\left(-\frac{\langle p^2\rangle}{2\hbar^2} x_f^2\right) \quad \text{for} \quad t \to \infty, \quad T>0, \quad \alpha<2 \tag{5.13b}$$

where the first two terms describe the spreading of the state in position state, while the last term shows that the momentum distribution of arbitrary initial states approaches the correct equilibrium distribution.

For $\alpha = 2$ the same analysis yields

$$\rho(x_f, r_f, t) \simeq \left(\frac{\ln(t)}{4\pi D_2 t^2}\right)^{1/2} \exp\left(-\frac{\ln(t)}{4D_2 t^2} r_f^2\right)$$
$$\times \exp\left(-\frac{\langle p^2\rangle}{2\hbar^2} x_f^2\right) \quad \text{for} \quad t \to \infty, \quad T>0, \quad \alpha=2 \tag{5.14}$$

where the spreading in position space occurs according to the faster law $t^2/\ln(t)$. In summary, for $\alpha \leqslant 2$ the state of the Brownian particle always approaches the equilibrium state as $t \to \infty$.

5.2.2. Finite Temperatures and $\alpha > 2$

We again proceed as above and determine the long-time behavior of the propagating function retaining terms of order $y/s^{1/2}(t)$. Using Table I, we find

$$J(x_f, y, t, x_i, \bar{x}, \bar{y})$$
$$\simeq \frac{M_r}{2\pi\hbar t} \exp\left(-\frac{\phi}{2\hbar^2} x_f^2\right) \exp\left[-i\frac{M_r}{\hbar t} y \left(x_i - \frac{M}{M_r} x_f\right)\right]$$
$$\times \exp\left\{-\frac{1}{2\hbar^2}\left[\langle p^2\rangle(\bar{x}-x_i)^2 + 2MM_r v_\beta^2 x_i(\bar{x}-x_i) + M_r^2 v_\beta^2 x_i^2\right]\right\}$$
$$\text{for} \quad t \to \infty, \quad T>0, \quad \alpha>2 \tag{5.15}$$

where we introduced

$$\phi = \langle p^2\rangle - M^2 v_\beta^2 \tag{5.16}$$

Now, there appears no δ-function in x_i for $t \to \infty$. Hence, we do not obtain the structure of a trace over the initial state, and we expect some effects of the preparation to survive in the long-time limit. As above, for a state initially localized near the origin, the growth of the variable $y = r_f - r_i$ in the asymptotic propagating function is due to the growth of r_f, since r_i becomes negligible against r_f for long times. Further, the asymptotic propagating function no longer depends on $\bar{y}$ and its dependence on $\bar{x}$ is not coupled to the final coordinates. We therefore define the reduced preparation function

$$\lambda^{\infty}(x_i) = \int dr_i\, d\bar{x}\, d\bar{y}\, \lambda(r_i, x_i, \bar{y}, \bar{x}) \times \exp\left\{ -\frac{1}{2\hbar^2} [\langle p^2 \rangle (\bar{x} - x_i)^2 + 2MM_r v_\beta^2 x_i(\bar{x} - x_i) + M_r^2 v_\beta^2 x_i^2] \right\} \tag{5.17}$$

which determines the evolution of the density matrix of an initially localized state for long times according to

$$\begin{aligned} \rho(x_f, r_f, t) &\simeq \frac{M_r}{2\pi\hbar t} \exp\left(-\frac{\phi}{2\hbar^2} x_f^2 \right) \times \int dx_i\, \lambda^{\infty}(x_i) \exp\left[-i \frac{M_r}{\hbar t} r_f \left(x_i - \frac{M}{M_r} x_f \right) \right] \\ &= (M_r/\hbar t) \tilde{\lambda}^{\infty}\left(\frac{M_r r_f}{\hbar t} \right) \exp\left(\frac{iM}{\hbar t} r_f x_f \right) \\ &\quad \times \exp\left(-\frac{\phi}{2\hbar^2} x_f^2 \right) \qquad \text{for} \quad t \to \infty, \quad T > 0, \quad \alpha > 2 \end{aligned} \tag{5.18}$$

Here, the second equality introduces the Fourier transform

$$\tilde{\lambda}^{\infty}(k_i) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dx_i\, \lambda^{\infty}(x_i) \exp(-ik_i x_i) \tag{5.19}$$

of the reduced preparation function. The asymptotic form of the density matrix still depends on the inital state for $\alpha > 2$. This is due to the fact that for $\alpha > 2$ the center-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 (5.18) is given by

$$W(p, q, t) \simeq (M_r/\hbar t)(2\pi\phi)^{-1/2} \tilde{\lambda}^{\infty}(M_r q/\hbar t) \times \exp[-(1/2\phi)(p - M\, q/t)^2] \qquad \text{for} \quad t \to \infty, \quad T > 0, \quad \alpha > 2 \tag{5.20}$$

Accordingly, the probability distribution in position space

$$w(q, t) = \int dp\, W(p, q, t) = \rho(0, q, t)$$
$$\simeq (M_r/\hbar t)\, \tilde{\lambda}^{\infty}(M_r q/\hbar t) \qquad \text{for} \quad t \to \infty, \quad T > 0, \quad \alpha > 2 \tag{5.21}$$

depends only on the scaled variable $v = q/t$. Defining the probability distribution

$$\Omega(v) = \lim_{t \to \infty} t w(vt, t) = (M_r/\hbar)\, \tilde{\lambda}^{\infty}(M_r v/\hbar) \tag{5.22}$$

of this variable, we have

$$w(q, t) = (1/t)\, \Omega(q/t) \qquad \text{for} \quad t \to \infty, \quad T > 0, \quad \alpha > 2 \tag{5.23}$$

Hence, the probability distribution in coordinate space behaves asymptotically as if the state had initially been localized at the origin with a 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. Afterward, the particle behaves as if it were free. This behavior is related to the vanishing of the integral $\int_0^\infty dt\, \gamma(t)$, so that for long times the classical equation of motion allows for a solution with constant velocity. The asymptotic velocity distribution $\Omega(v)$ is the distribution of the center-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 $\Omega(v)$ completely determines the spreading of the state in position space. However, it differs from the asymptotic momentum distribution of the Brownian particle, which is given by

$$w_\infty(p) = \lim_{t \to \infty} \int dq\, W(p, q, t)$$
$$= (2\pi\phi)^{-1/2} \int dv\, \Omega(v) \exp\left[-\frac{1}{2\phi} (p - Mv)^2 \right] \qquad \text{for} \quad T > 0, \quad \alpha > 2 \tag{5.24}$$

Hence, apart from the momentum corresponding to the value given by $\Omega(v)$, there are dynamial fluctuations of magnitude ϕ in the momentum distribution. These fluctuations result from the environmental coupling and they cannot be observed in the broad coordinate distribution. For vanishing coupling we have $M_r = M$ and $\langle p^2 \rangle = Mk_B T$, so that the momentum distribution indeed reduces to

$$w_\infty(p) = (1/M)\, \Omega(p/M) \qquad \text{for} \quad \hat{\gamma}(\omega) = 0, \quad T > 0, \quad \alpha > 2 \tag{5.25}$$

On the other hand, the additional momentum fluctuations survive in the classical limit, where $\phi = (1 - M/M_r)\, Mk_B T$.

5.2.3. Zero Temperature

As we have already seen in the example of an initially localized wave packet, the long-time behavior 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 I, we obtain for the propagating function

$$\begin{aligned}
&J(x_f, y, t, x_i, \bar{x}, \bar{y}) \\
&\quad \simeq \bar{\rho}_\beta(x_f)\, \bar{\rho}_\beta(\bar{x})\, \frac{\mu_\alpha t^{1-\alpha}}{2\pi\alpha\hbar} \\
&\qquad \times \exp\left\{ -\frac{\mu_\alpha^2 q_\infty}{\alpha^2 \hbar^2}\, t^{2-2\alpha} \left[x_i + i\, \frac{\alpha\hbar}{2\mu_\alpha q_\infty t^{1-\alpha}}\, (y + \bar{y}) \right]^2 \right\} \\
&\qquad \times \exp\left[-\frac{1}{4q_\infty}\, (y + \bar{y})^2 \right] \\
&\quad \simeq \bar{\rho}_\beta(x_f)\, \bar{\rho}_\beta(\bar{x})\, \delta(x_i)(4\pi q_\infty)^{-1/2} \exp\left[-\frac{1}{4q_\infty}\, (y + \bar{y})^2 \right] \\
&\qquad \text{for} \quad t \to \infty, \quad T = 0, \quad \alpha < 1
\end{aligned} \tag{5.26}$$

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 5.1 to the general case. Since the asymptotic propagating function depends only on $r_f - \bar{r}$ [cf. (3.26)], we may again define a reduced preparation function by

$$\lambda_i^\infty(\bar{r}) = \int dr_i\, d\bar{x}\, \lambda(r_i, 0, r_i - \bar{r}, \bar{x})\, \bar{\rho}_\beta(\bar{x}) \tag{5.27}$$

Then the asymptotic Wigner function can be written as

$$\lim_{t \to \infty} W(p, q, t) \simeq w_\beta(p)\, w_\infty(q) \qquad \text{for} \quad T = 0, \quad \alpha < 1 \tag{5.28}$$

with the equilibrium momentum distribution

$$w_\beta(p) = (2\pi \langle p^2 \rangle)^{-1/2} \exp(-p^2/2\langle p^2 \rangle) \tag{5.29}$$

and the coordinate distribution

$$w_\infty(q) = (4\pi q_\infty)^{-1/2} \int d\bar{r} \exp\left[-\frac{1}{4q_\infty}(q-\bar{r})^2\right] \lambda_l^\infty(\bar{r}) \qquad \text{for} \quad T=0, \ \alpha<1 \tag{5.30}$$

which gives the localization length as a sum of the asymptotic contribution $2q_\infty$ plus an effective width of the initial state, which is inherent in the reduced preparation function $\lambda_l^\infty(\bar{r})$. 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 $T=0$.

Next, we consider Ohmic damping. Then the asymptotic density matrix is readily found to read

$$\rho(x_f, r_f, t) \simeq [4\pi d_1 \ln(t)]^{-1/2} \exp\left[-\frac{r_f^2}{4d_1 \ln(t)}\right] \times \exp\left(-\frac{\langle p^2\rangle}{2\hbar^2} x_f^2\right) \qquad \text{for} \quad t\to\infty, \quad T=0, \quad \alpha=1 \tag{5.31}$$

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 the equilibrium state in the limit $t\to\infty$.

Finally, we consider the super-Ohmic case, $\alpha>1$. Now we obtain no δ-function in x_i in the asymptotic propagating function for $t\to\infty$. Since the thermal velocity v_β vanishes, the finite-temperature definition (5.17) of the reduced preparation function simplifies at $T=0$ to read

$$\lambda_0^\infty(x_i) = \int dr_i \, d\bar{x} \, d\bar{y} \, \lambda(r_i, x_i, \bar{y}, \bar{x}) \, \bar{\rho}_\beta(\bar{x}-x_i) \tag{5.32}$$

The density matrix for long times then takes the form

$$\begin{aligned}\rho(x_f, r_f, t) &\simeq [4\pi |A(t)|]^{-1} \bar{\rho}_\beta(x_f) \int dx_i \, \lambda_0^\infty(x_i) \exp\left(\frac{-ir_f x_i}{2|A(t)|} + \frac{iMc_\alpha r_f x_f}{\hbar t}\right) \\ &= [2|A(t)|]^{-1} \exp\left(\frac{iM}{\hbar t} c_\alpha r_f x_f\right) \bar{\rho}_\beta(x_f) \, \tilde{\lambda}_0^\infty\left(\frac{r_f}{2|A(t)|}\right) \\ &\qquad \text{for} \quad t\to\infty, \quad T=0, \quad \alpha>1\end{aligned} \tag{5.33}$$

where $c_\alpha = \alpha-1$ for $1<\alpha<2$ and $c_\alpha=1$ for $\alpha\geqslant 2$. The probability distribution of the coordinate is given by

$$w(q,t) = [2|A(t)|]^{-1} \tilde{\lambda}_0^\infty(q/2|A(t)|) \qquad \text{for} \quad t\to\infty, \quad T=0, \quad \alpha>1 \tag{5.34}$$

and the asymptotic momentum distribution follows from (5.33) as

$$w_\infty(p) = \lim_{t\to\infty} (2\pi\langle p^2\rangle)^{-1/2} \int dk \tilde{\lambda}_0^\infty(k) \times \exp\left\{-\frac{1}{2\langle p^2\rangle}\left[p - \frac{2Mc_\alpha |A(t)|}{t} k\right]^2\right\}$$
$$\text{for} \quad t\to\infty, \quad T=0, \quad \alpha>1 \tag{5.35}$$

For $1<\alpha\leqslant 2$ the antisymmetric correlation $A(t)$ grows more slowly than $\propto t$. Hence, the initial state is not coupled to the final variables and the momentum distribution approaches its equilibrium form (5.29). Again we find that the system is ergodic. For $\alpha>2$ the correlation $A(t)$ 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 (5.22). The momentum distribution (5.35) may be transformed to read

$$w_\infty(p) = (2\pi\langle p^2\rangle)^{-1/2} \int dv\, \Omega(v) \exp\left[-\frac{1}{2\langle p^2\rangle}(p-Mv)^2\right]$$
$$\text{for} \quad t\to\infty, \quad T=0, \quad \alpha>2 \tag{5.36}$$

which is the zero-temperature limit of (5.24). Again the system is not ergodic, since the final momentum distribution depends on the preparation via the center-of-mass velocity distribution $\Omega(v)$. Finally, we mention that these results for $T=0$ are not purely academic, since the zero-temperature behavior is also found for low finite temperatures for intermediate times $\omega_c^{-1} \ll t \ll \hbar/k_B T$.

APPENDIX A. EVALUATION OF THE FOURIER COEFFICIENTS FOR THE IMAGINARY TIME PATH

We want to find a solution of the equation of motion (3.8) in imaginary time $0\leqslant\tau\leqslant\hbar\beta$ in terms of the Fourier series (3.11). Now, a Fourier series representation periodically continues the path $\bar{q}(\tau)$ outside the interval $[0, \hbar\beta]$. This leads to jump and cusp singularities at the endpoints, which must be accounted for by additional terms in the equation of motion. Hence, (3.8) is replaced by

$$M\ddot{\bar{q}} - \int_0^{\hbar\beta} d\sigma\, k(\tau-\sigma)\, \bar{q}(\sigma)$$
$$= -i\int_0^t ds\, K^*(s-i\tau)\, x(s) + Ma :\delta'(\tau): + Mb :\delta(\tau): \tag{A.1}$$

Here, $:\delta(\tau):$ and $:\delta'(\tau):$ are the δ-function and its time derivative periodically continued for $\tau = n\hbar\beta$ ($n = 0, \pm 1,...$) and the coefficients a and b have to be determined such that the solution of (A.1) satisfies the boundary conditions

$$\bar{q}(0^+) = \bar{q}'; \qquad \bar{q}(\hbar\beta^-) = \bar{q}(0^-) = \bar{q} \tag{A.2}$$

The Fourier expansion of $k(\tau)$ is given in (3.7), while the kernel $K^*(s - i\tau)$ can be written as

$$K^*(s - i\tau) = \frac{M}{\hbar\beta} \sum_{n=-\infty}^{\infty} \left[\gamma(s) - \zeta_n(s) - \frac{1}{\nu_n} \frac{d}{ds} \zeta_n(s) \right] \exp(i\nu_n \tau) \tag{A.3}$$

where $\zeta_n(s)$ is defined in (3.14). Inserting the Fourier expansions (3.7), (3.11), and (A.3) into the equation of motion (A.1), we obtain

$$[-\nu_n^2 - |\nu_n|\, \hat{\gamma}(|\nu_n|)]\, \bar{q}_n = ia\nu_n + b - i \int_0^t ds\, x(s) \left[\gamma(s) - \zeta_n(s) - \frac{1}{\nu_n} \frac{d}{ds} \zeta_n(s) \right] \tag{A.4}$$

For $n = 0$ this equation leaves the Fourier coefficient $\bar{q}_0$ undetermined, but fixes the constant b according to

$$b = i \int_0^t ds\, x(s)\, \gamma(s) \tag{A.5}$$

For $n \neq 0$ we obtain from (A.4) the Fourier coefficients (3.13). In reinserting these results in (3.11), one must take care in performing the limit $\tau \to 0$, $\hbar\beta$ because of the discontinuities at the endpoints. We therefore decompose

$$\begin{aligned} &\sum_{n=-\infty}^{\infty}{}' (-i\nu_n u_n) \exp(i\nu_n \tau) \\ &\quad = \sum_{n=-\infty}^{\infty}{}' \frac{1}{i\nu_n} \exp(i\nu_n \tau) - \sum_{n=-\infty}^{\infty}{}' \frac{1}{i\nu_n} u_n\, |\nu_n|\, \hat{\gamma}(|\nu_n|) \exp(i\nu_n \tau) \end{aligned} \tag{A.6}$$

where $u_n = [\nu_n^2 + |\nu_n|\, \hat{\gamma}(|\nu_n|)]^{-1}$ and where the prime denotes the omission of the $n = 0$ element in the sum. Here, the second sum on the rhs is regular and vanishes for $\tau \to 0$, whereas the first sum describes a sawtooth-like behavior with

$$\lim_{\tau \to 0^\pm} \frac{1}{\hbar\beta} \sum_{n=-\infty}^{\infty}{}' \frac{1}{i\nu_n} \exp(i\nu_n \tau) = \pm \frac{1}{2} \tag{A.7}$$

Using (A.2), we can now determine the remaining constants a and $\bar{q}_0$. We obtain

$$a = \bar{q}' - \bar{q} \tag{A.8}$$

as well as (3.12).

APPENDIX B. EVALUATION OF THE AUXILIARY FUNCTIONS $C^+(t)$ AND $\Psi(t, t')$

Let us first consider the Laplace transform of the function $\xi(t) = G_+(t)\, C^+(t)$. Using (3.17) and (3.22), we find

$$\hat{\xi}(z) = -\frac{1}{\hbar\beta} \hat{G}_+(z) \sum_{n=-\infty}^{\infty} \hat{G}_+(|\nu_n|)[z\hat{\zeta}_n(z) + |\nu_n|\, \hat{\gamma}(|\nu_n|)] \qquad \text{(B.1)}$$

From (3.14) we obtain

$$\hat{\zeta}_n(z) = \frac{1}{z^2 - \nu_n^2} [z\, |\nu_n|\, \hat{\gamma}(|\nu_n|) - \nu_n^2 \hat{\gamma}(z)] \qquad \text{(B.2)}$$

We can now eliminate $\hat{\gamma}(z)$ in favor of $\hat{G}_+(z)$ by virtue of (3.19). In terms of the Laplace transform (3.46) of the symmetrized displacement correlation function and the momentum variance (3.35), $\hat{\xi}(z)$ takes the form

$$\hat{\xi}(z) = z\hat{S}(z) + \frac{\langle p^2 \rangle}{M\hbar} \hat{G}_+(z) \qquad \text{(B.3)}$$

Since $S(0) = 0$, this transfers to the time domain to read

$$C^+(t) = \frac{\dot{S}(t)}{G_+(t)} + \frac{\langle p^2 \rangle}{M\hbar} \qquad \text{(B.4)}$$

The function $\Psi(t, t')$, which determines the time dependence of $R^{\pm\pm}(t)$ via (3.43)–(3.45), can now be evaluated analogously by considering the double Laplace transform of $G_+(t)\, G_+(t')\, \Psi(t, t')$. Again the result can be conveniently expressed in terms of the Green's function $G_+(t)$ and the symmetrized correlation $S(t)$. After some algebra we find

$$\begin{aligned}
\Psi(t, t') = {} & \frac{\langle p^2 \rangle}{M\hbar} + \frac{M}{\hbar} \left[\frac{\dot{S}(t)}{G_+(t)} + \frac{\dot{S}(t')}{G_+(t')} \right] \\
& - \frac{M}{\hbar} [G_+(t)\, G_+(t')]^{-1} [S(t) + S(t')] \\
& + \frac{1}{\hbar\beta} [G_+(t)\, G_+(t')]^{-1} \sum_{n=-\infty}^{\infty} \hat{G}_+(|\nu_n|)[\cosh\{\nu_n(t - t')\} - 1] \\
& - \frac{1}{2\hbar\beta} [G_+(t)\, G_+(t')]^{-1} \\
& \times \sum_{n=-\infty}^{\infty} \int_0^{t - t'} ds\, [G_+(t - t' - s) - G_+(t' - t + s)] \cosh(\nu_n s)
\end{aligned} \qquad \text{(B.5)}$$

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