

Effects of initial correlations on the dynamics of dissipative systems

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The time correlation functions for a Gaussian wave-packet preparation of the dissipative harmonic oscillator evolving from three initial conditions for the heat bath are calculated and compared with each other for Ohmic heat baths. The three initial distributions for the bath are the factorized, partially factorized, and unfactorized distributions. Explicit analytical formulas are derived and then used to study the effect of the three initial distributions on the subsequent dynamics. We find that the transient behavior does not depend sensitively on the initial condition as long as the initial Gaussian wave function of the system is centered at the equilibrium point. Differences become noticeable as the center of the wave packet is significantly shifted from the equilibrium point. These observations justify to some extent the prevalent use of factorized initial conditions for studying real time quantum dynamics in dissipative systems. The total energy in the system is also calculated for the three initial states and its relation to features in the decay is pointed out.

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I. INTRODUCTION

The challenge of numerical solution for the quantum dynamics of dissipative systems is slowly but surely being answered. The first numerical solutions for activated barrier crossing in a dissipative system [1] and for the spin boson problem [2,3] have been published over a decade ago. More recently, results have been reported for correlation functions of nonlinear systems coupled bilinearly to harmonic baths with hundreds of bath oscillators [4].

In most of these recent computations, the initial conditions of the bath are assumed to be factorized [5]. The factorization approximation is used since it simplifies the ensuing computation, which calls for averaging over the thermally distributed bath modes. When using the factorization approximation, this distribution is known analytically and is Gaussian.

The question of initial conditions is also of interest when deriving reduced equations of motion. Ankerhold [6] has recently derived reduced equations of motion which are more accurate than the Caldeira-Leggett high temperature reduced equation of motion [7] using unfactorized initial conditions. The factorization approximation has been used by Shao to derive reduced equations of motion [8] which are also more accurate than the Caldeira-Leggett high temperature equation of motion.

There have been several discussions on the effect of the initial conditions on the dynamics of dissipative systems [9–15]. For instance, Hakim and Ambegaokar [9] investigated the dynamics of a dissipative free particle evolving from factorized and nonfactorized initial states and observed different transient behaviors. As the bath is generally assumed to evolve from a displaced equilibrium state due to the couplings to the system, it is believed that the factorized initial state should be a good approximation only at weak dissipation. Recently, Ambegaokar derived an expression for the reduced density matrix of the dissipative harmonic oscil-

lator also by assuming a factorized initial condition [16]. He then discussed the issue of equilibration in Ref. [17]. Initial correlations have been also considered in the context of reduced equations of motion by Breuer and co-workers [18,19]. They employ projection operators and fourth order perturbation theory in the system bath coupling to, among others, study the effects of initial correlations on the dynamics.

The central question we consider in this paper is whether the use of the factorization approximation leads to serious errors, or whether it includes in it most of the relevant dynamics, so that further more sophisticated and entangled initial distributions are not needed for physically reasonable parameter ranges.

The paradigm of dissipative systems is the harmonic oscillator for which analytical results are known for almost twenty years [10]. Given the factorized initial condition, the master equation was first derived by Haake and Reibold [20] who also found anomalies in the case of strong damping and low temperature. The same master equation was later rederived by Hu, Paz, and Zhang [21] and by others [22]. Karrlein and Grabert [23] (see also Ref. [24]) analyzed the conditions for existence of an exact dissipative Liouville operator and also set up the master equation for thermal initial conditions. Without citing the result of Haake and Reibold, Ford and O'Connell [25] worked out the exact solution of such a master equation and pointed out the drawback inherent in the master equation. Recently, Pereverzev [26] studied the evolution of the damped harmonic oscillator for three classes of initial states for the bath modes, but assumed a factorized condition for the initial total density matrix. Van Kampen compared the reduced density matrix obtained from factorized and unfactorized initial conditions, claiming that the former is inappropriate [27]. His conclusion though is based on results derived from second order perturbation theory so it is not of general validity. Furthermore, the more recent results of Ref. [18] based on fourth order perturbation theory indicate that the differences are not so large.

Except for these works, however, we are not aware that even for the harmonic oscillator any other systematic study of the dynamics for different types of initial distributions have been undertaken. The aim of this paper is to understand what happens for the dissipative harmonic oscillator under differing conditions. We derive explicit expressions for the thermal correlation function using three different initial distributions. These correspond to factorized, partially factorized, and unfactorized initial conditions. The resulting analytical expressions are useful as benchmarks with which to compare other methods, whether approximate or numerically exact ones.

We conclude that as long as one is not in the strong friction regime, factorized initial conditions are sufficiently similar to the unfactorized case to justify their usage. Even when the friction is strong, there are cases where one may use partially factorized initial conditions to obtain very reasonable results. The detailed expressions derived in this paper may also be used as benchmarks for new methods of solving the dynamics of dissipative systems, such as the semiclassical initial value representation approach [28].

II. SETTING UP THE PROBLEM

We will study the dynamics of a dissipative system in which the system is initially prepared in the form of a Gaussian wave packet. The Hamiltonian of the system and the bath is

$$H = H_s + H_{s,B}. \quad (2.1)$$

The system and bath Hamiltonians are defined to be

$$H_s = \frac{1}{2}p_q^2 + V(q), \quad (2.2)$$

$$H_{s,B} = \frac{1}{2} \sum_{j=1}^N \left[p_{x_j}^2 + \omega_j^2 \left(x_j - \frac{c_j}{\omega_j^2} q \right)^2 \right] \equiv \sum_{j=1}^N h_j. \quad (2.3)$$

Initially the system wave function is chosen to be a Gaussian wave packet:

$$\langle q | \psi \rangle = \left(\frac{\Gamma}{\pi} \right)^{1/4} \exp \left(-\frac{\Gamma}{2} (q - q_a)^2 \right). \quad (2.4)$$

We will calculate the autocorrelation function of the projection operator $\hat{P}_\psi \equiv |\psi\rangle\langle\psi|$ and will distinguish between three choices for the initial conditions, namely

$$C_i(t) = \text{Tr} \{ \rho^{(i)}(0) \hat{P}_\psi \hat{P}_\psi(t) \} \quad i = 1, 2, 3, \quad (2.5)$$

where $\hat{P}_\psi(t) = e^{iHt/\hbar} \hat{P}_\psi e^{-iHt/\hbar}$ is the Heisenberg operator.

The first choice for the initial conditions is

$$\rho^{(1)}(0) = \hat{P}_\psi e^{-\beta H_B} / Z_1, \quad (2.6)$$

where the bath Hamiltonian is defined as

$$H_B = \frac{1}{2} \sum_{j=1}^N [p_{x_j}^2 + \omega_j^2 x_j^2] \quad (2.7)$$

and the partition function of the bath is

$$Z_1 = \text{Tr}_B e^{-\beta H_B} = \prod_{j=1}^N \frac{1}{2 \sinh(\hbar\beta\omega_j/2)}. \quad (2.8)$$

This case is referred to as factorized initial conditions, i.e., the bath is initially *independent* of the system coordinate. The second (Hermitian) choice is

$$\rho^{(2)}(0) = \hat{P}_\psi e^{-\beta H_{s,B}} \hat{P}_\psi / Z_2, \quad (2.9)$$

where $Z_2 = \text{Tr} \{ \hat{P}_\psi e^{-\beta H_{s,B}} \} = Z_1$ due to the fact that the system wave function is normalized and that the Hamiltonian $H_{s,B}$ is diagonal in the system coordinate. We will refer to this case as partially factorized initial conditions.

The third (Hermitian) choice is using the full Hamiltonian, that is,

$$\rho^{(3)}(0) = \hat{P}_\psi e^{-\beta H} \hat{P}_\psi / Z_3, \quad (2.10)$$

where the ‘‘partition function’’ is defined as

$$Z_3 = \text{Tr} \{ \hat{P}_\psi e^{-\beta H} \} = \text{Tr}_B \langle \psi | e^{-\beta H} | \psi \rangle \quad (2.11)$$

and this case corresponds to nonfactorized initial conditions.

For all three correlation functions, by definition, $C_i(0) = 1$. In the absence of coupling to the bath, all three correlation functions are identical to the isolated system correlation function. In the infinite time limit, the dynamics is assumed to approach equilibrium [29]. The equilibrium reduced density operator is

$$\hat{\rho}_\beta = \frac{\text{Tr}_B \{ e^{-\beta H} \}}{Z}, \quad (2.12)$$

where $Z = \text{Tr} \{ e^{-\beta H} \}$ is the partition function of the full Hamiltonian. One then readily finds that for *any* choice of the initial thermal distribution, the equilibrium limit of the correlation functions is

$$C_i(t \rightarrow \infty) = \text{Tr}_s \{ \hat{\rho}_\beta \hat{P}_\psi \} = \frac{\text{Tr}_B \{ \langle \psi | e^{-\beta H} | \psi \rangle \}}{Z}, \quad (2.13)$$

such that the double brackets imply integration over the combined system and bath space.

Especially if the system potential is harmonic, it is useful to write down the correlation functions in the Wigner representation. Denoting the ‘‘densities’’ $\rho^{(i)}(0) \hat{P}_\psi$ in phase space as $\rho^{(i)}(p_q, q, \underline{p}_x, \underline{x})$, $i = 1, 2, 3$, and the phase space distribution of the projection operator \hat{P}_ψ of the system as

$$\psi(p_q, q) = \frac{1}{\pi \hbar} \exp \left(-\frac{1}{\hbar^2} p_q^2 - \Gamma (q - q_a)^2 \right) \quad (2.14)$$

one has that the correlation function for the dissipative harmonic oscillator is the phase space integral of the product of the density with the classically time evolved phase space density of \hat{P}_ψ :

$$C_i(t) = 2\pi \hbar \int \frac{dp_q dq d\underline{p}_x d\underline{x}}{(2\pi \hbar)^{N+1}} \rho^{(i)}(p_q, q, \underline{p}_x, \underline{x}) \psi[p_q(t), q(t)]. \quad (2.15)$$

One of the central purposes of this paper is to understand the differences in the behavior of the correlation function for the three different choices of thermal averaging. To obtain analytical expressions we review below briefly the normal mode transformation for a harmonic dissipative Hamiltonian [20,30].

III. THE NORMAL MODE TRANSFORMATION

The harmonic oscillator potential is

$$V(q) = \frac{1}{2} \omega^2 q^2. \quad (3.1)$$

Notice that we have allowed the origin of the potential to be at $q=0$. If the origin is at, say, q_0 one can always shift the definition of the system and bath modes so that one will finally remain with the nonshifted Hamiltonian. Since the full Hamiltonian is quadratic in the system and bath variables, it can be diagonalized and written down as

$$H = \frac{1}{2} \sum_{j=0}^N (p_{y_j}^2 + \lambda_j^2 y_j^2), \quad (3.2)$$

where the new coordinates and momenta are given by an orthogonal transformation matrix \mathbf{U} such that

$$q = \sum_{j=0}^N u_{j0} y_j, \quad x_k = \sum_{j=0}^N u_{jk} y_j. \quad (3.3)$$

The transformation matrix elements are given as [31]:

$$u_{j0}^2 = \left[1 + \sum_{k=1}^N \frac{c_k^2}{(\omega_k^2 - \lambda_j^2)^2} \right]^{-1}, \quad j = 0, 1, \dots, N \quad (3.4)$$

and

$$u_{jm} = \frac{c_m}{\lambda_j^2 - \omega_m^2} u_{j0}, \quad m = 1, \dots, N. \quad (3.5)$$

The normal mode frequencies λ_j are the $N+1$ solutions of the equation

$$\lambda^2 = \omega^2 \left[1 + \sum_{k=1}^N \frac{c_k^2}{\omega_k^2 (\omega_k^2 - \lambda^2)} \right]^{-1}. \quad (3.6)$$

Since now the Hamiltonian is a sum of separable harmonic oscillators it is easy to write down the time evolution of each of the normal modes:

$$y_j(t) = y_j \cos(\lambda_j t) + \frac{p_{y_j}}{\lambda_j} \sin(\lambda_j t) \quad (3.7)$$

and similarly for the momenta. It thus follows that

$$q(t) = \sum_{j=0}^N u_{j0} y_j(t). \quad (3.8)$$

From the definition of the normal mode transformation we have

$$y_j = u_{j0} q + \sum_{k=1}^N u_{jk} x_k \quad (3.9)$$

and a similar expression for the initial momentum p_{y_j} .

To make further progress we define some auxiliary functions:

$$H(t) = \sum_{j=0}^N \frac{u_{j0}^2}{\lambda_j} \sin(\lambda_j t), \quad (3.10)$$

$$H_l(t) = \sum_{j=0}^N \frac{u_{j0} u_{jl}}{\lambda_j} \sin(\lambda_j t), \quad l = 1, \dots, N, \quad (3.11)$$

so that now we have

$$q(t) = q \dot{H}(t) + p_q H(t) + \sum_{l=1}^N [x_l \dot{H}_l(t) + p_{x_l} H_l(t)]. \quad (3.12)$$

The time dependence for the system momentum $p_q(t)$ is then given by the time derivative of the equation for $q(t)$.

We also note that the normal mode coordinate representation of the thermal operator is

$$\begin{aligned} \langle \underline{y} | e^{-\beta H} | \underline{y}' \rangle &= \prod_{j=0}^N \left(\frac{A_j}{2\pi} \right)^{1/2} \\ &\times \exp \left\{ -\frac{A_j}{2} [(y_j^2 + y_j'^2) \cosh(\gamma_j) - 2y_j y_j'] \right\} \end{aligned} \quad (3.13)$$

with

$$A_j = \frac{\lambda_j}{\hbar \sinh(\gamma_j)}, \quad \gamma_j = \hbar \beta \lambda_j \quad (3.14)$$

so that the Wigner representation of the thermal density $e^{-\beta H}$ is

$$\rho(p_y, \underline{y}) = \prod_{j=0}^N \frac{\tanh(\hbar \beta \lambda_j / 2)}{\pi \hbar} \exp \left[-\frac{\tanh(\hbar \beta \lambda_j / 2)}{\hbar \lambda_j} (p_{y_j}^2 + \lambda_j^2 y_j^2) \right]. \quad (3.15)$$

The continuum limit is obtained by defining spectral densities. The spectral density of the bath is defined as

$$J(\omega) = \frac{\pi}{2} \sum_{j=1}^N \frac{c_j^2}{\omega_j} [\delta(\omega - \omega_j) - \delta(\omega + \omega_j)] \quad (3.16)$$

and the associated friction function is the cosine Fourier transform of the spectral density:

$$\gamma(t) = \frac{2}{\pi} \int_0^\infty d\omega \frac{J(\omega)}{\omega} \cos(\omega t). \quad (3.17)$$

The spectral density of the normal modes is defined as [32]

$$I(\lambda) = \frac{\pi}{2} \sum_{j=1}^N \frac{u_{j0}^2}{\lambda_j} [\delta(\lambda - \lambda_j) - \delta(\lambda + \lambda_j)] \quad (3.18)$$

and one can show [33] that it is related to the spectral density of the bath modes $J(\omega)$ through the relationship

$$I(\lambda) = \frac{J(\lambda)}{[\omega^2 - \lambda^2 - \lambda \operatorname{Im}\{\hat{\gamma}(i\lambda)\}]^2 + J^2(\lambda)}. \quad (3.19)$$

The spectral densities are useful when considering the continuum limit of various functions that appear in the analytic expression in discrete form. For example, we consider the function $H(t)$ defined above in Eq. (3.10) and note that

$$H(t) = \sum_{j=0}^N \frac{u_{j0}^2}{\lambda_j} \sin(\lambda_j t) = \frac{2}{\pi} \int_0^\infty d\lambda I(\lambda) \sin(\lambda t). \quad (3.20)$$

IV. HARMONIC CORRELATION FUNCTIONS

A. Case 1: Factorized initial conditions

The definition of the Wigner distribution in phase space is

$$\begin{aligned} \rho^{(i)}(p_q, q, \underline{p}, \underline{x}) &= \left(\frac{1}{2\pi\hbar} \right)^{N+1} \int_{-\infty}^{\infty} d\xi_q e^{ip_q \xi_q / \hbar} \left\{ \prod_{j=1}^N d\xi_j e^{ip_{x_j} \xi_j / \hbar} \right\} \\ &\times \left\langle q + \frac{\xi_q}{2}, \underline{x} + \frac{\xi}{2} \left| \rho^{(i)}(0) \hat{P}_\psi \right| q - \frac{\xi_q}{2}, \underline{x} - \frac{\xi}{2} \right\rangle. \end{aligned} \quad (4.1)$$

When the initial conditions are factorized, one finds

$$\rho^{(1)}(p_q, q, \underline{p}, \underline{x}) = \left\{ \prod_{j=1}^N \rho_j(p_{x_j}, x_j) \right\} \psi(p_q, q) \quad (4.2)$$

with

$$\begin{aligned} \rho_j(p_{x_j}, x_j) &= \frac{\tanh(\hbar\beta\omega_j/2)}{\pi\hbar} \\ &\times \exp \left[-\tanh(\hbar\beta\omega_j/2) \left(\frac{1}{\hbar\omega_j} p_{x_j}^2 + \frac{\omega_j}{\hbar} x_j^2 \right) \right]. \end{aligned} \quad (4.3)$$

To obtain the correlation function we use Eq. (2.15) and the explicit time dependence of the system coordinate and momentum as obtained from Eq. (3.12). This leaves us with the necessity of performing Gaussian integrals over the initial conditions to obtain an explicit formula for the correlation function.

To do this, we introduce into Eq. (2.15) the identity through two delta functions,

$$\begin{aligned} 1 &= \int_{-\infty}^{\infty} dz \delta[z - q(t)], \\ &= \int_{-\infty}^{\infty} dp_z \delta[p_z - p_q(t)], \end{aligned} \quad (4.4)$$

and their Fourier representations, so that

$$\begin{aligned} C_1(t) &= \frac{\hbar}{2\pi} \int_{-\infty}^{\infty} dz dp_z dk d\xi e^{ikz} e^{i\xi p_z} [\psi(p_z, z)] \int_{-\infty}^{\infty} dp_q dq \prod_{j=1}^N dp_{x_j} dx_j \psi(p_q, q) \prod_{j=1}^N \rho_j(p_{x_j}, x_j) \\ &\times e^{-ik\{q\dot{H}(t) + p_q H(t) + \sum_{l=1}^N [x_l \dot{H}_l(t) + p_{x_l} H_l(t)]\}} e^{-i\xi\{q\ddot{H}(t) + p_q \dot{H}(t) + \sum_{l=1}^N [x_l \ddot{H}_l(t) + p_{x_l} \dot{H}_l(t)]\}}. \end{aligned} \quad (4.5)$$

One can now perform the Gaussian integrations over all the variables except (k, ξ) to find the intermediate result:

$$\begin{aligned} C_1(t) &= \frac{\hbar}{2\pi} \int_{-\infty}^{\infty} dk d\xi \exp \left(-\frac{k^2 + [k\dot{H}(t) + \xi\ddot{H}(t)]^2}{4\Gamma} - \{\xi^2 + [kH(t) + \xi\dot{H}(t)]^2\} \frac{\hbar^2 \Gamma}{4} \right) \\ &\times \prod_{j=1}^N \exp \left[-\frac{\hbar}{\tanh(\hbar\beta\omega_j/2)} \left(\frac{[k\dot{H}_j(t) + \xi\ddot{H}_j(t)]^2}{4\omega_j} + \frac{\omega_j [kH_j(t) + \xi\dot{H}_j(t)]^2}{4} \right) \right] \\ &\times \exp(-iq_a \{k[\dot{H}(t) - 1] + \xi\ddot{H}(t)\}). \end{aligned} \quad (4.6)$$

Using the notation

$$Q_1(t) = \frac{1 + \dot{H}(t)^2}{\hbar\Gamma} + \hbar\Gamma H(t)^2 + \sum_{j=1}^N \frac{1}{\tanh(\hbar\beta\omega_j/2)} \left(\frac{\dot{H}_j(t)^2}{\omega_j} + \omega_j H_j(t)^2 \right), \quad (4.7)$$

$$Q_2(t) = \frac{\ddot{H}(t)^2}{\hbar\Gamma} + \hbar\Gamma[1 + \dot{H}(t)^2] + \sum_{j=1}^N \frac{1}{\tanh(\hbar\beta\omega_j/2)} \times \left(\frac{\ddot{H}_j(t)^2}{\omega_j} + \omega_j \dot{H}_j(t)^2 \right) \quad (4.8)$$

carrying out the remaining two Gaussian integrations one finally finds that the correlation function is

$$C_1(t) = \frac{2}{\sqrt{D_1(t)}} e^{[-q_a^2 \hbar D_1(t)] [\dot{H}(t) - 1]^2 Q_2(t) - [\dot{H}(t) - 1] \ddot{H}(t) \dot{Q}_1(t) + \ddot{H}(t)^2 Q_1(t)}, \quad (4.9)$$

where

$$D_1(t) = Q_1(t)Q_2(t) - \frac{1}{4}\dot{Q}_1(t)^2. \quad (4.10)$$

Note that indeed at time $t=0$ the correlation function $C_1(0) = 1$, as it should be.

B. Case 2: Partially factorized initial conditions

In this case the Wigner representation of the initial density takes the form

$$\rho^{(2)}(p_q, q, \underline{p}, \underline{x}) = \left\{ \prod_{j=1}^N \rho_j(p_{x_j}, x_j) \right\} \psi(p_q, q) \Phi(q, \underline{x}), \quad (4.11)$$

where $\Phi(q, \underline{x})$ represents the initial correlation of the system and the bath, and is found to be

$$\Phi(q, \underline{x}) = \left(\frac{\Gamma}{G + \Gamma} \right)^{1/2} \exp\left(\frac{Q(\underline{x})^2 + 2Q(\underline{x})\Gamma q_a - \Gamma G q_a^2}{G + \Gamma} \right) \quad (4.12)$$

with

$$G \equiv \frac{1}{\hbar} \sum_{j=1}^N \frac{c_j^2}{\omega_j^3} \tanh\left(\frac{\hbar\beta\omega_j}{2} \right) \quad (4.13)$$

and

$$Q(\underline{x}) = \frac{1}{\hbar} \sum_{j=1}^N \frac{c_j}{\omega_j} x_j \tanh\left(\frac{\hbar\beta\omega_j}{2} \right). \quad (4.14)$$

Note that the function G is readily available in the continuum limit via the spectral density $J(\omega)$.

The correlation function is then found as in the case of factorized initial conditions; the Gaussian integrals are carried out by introducing the Fourier decomposition of three delta functions for the variables $p_q(t)$, $q(t)$, $Q(\underline{x})$ to find

$$C_2(t) = \frac{2}{\sqrt{D_2(t)}} \exp\left\{ -\frac{q_a^2}{\hbar D_2(t)} E_2(t) \right\} \quad (4.15)$$

and we have used the notation

$$D_2(t) = Q_1(t)Q_2(t) - \frac{1}{4}\dot{Q}_1(t)^2 - \dot{Q}_1(t) \frac{[\ddot{M}(t) - \ddot{H}(t)][\dot{M}(t) - \dot{H}(t)]}{\hbar\Gamma} + Q_1(t) \times \left[\frac{\ddot{M}(t) - \ddot{H}(t)}{\hbar\Gamma} \right] + Q_2(t) \left[\frac{\dot{M}(t) - \dot{H}(t)}{\hbar\Gamma} \right], \quad (4.16)$$

$$E_2(t) = \frac{([\ddot{M}(t) - \ddot{H}(t)][1 - \dot{M}(t)] - \ddot{M}(t)[\dot{M}(t) - \dot{H}(t)])^2}{\hbar\Gamma} + Q_2(t)[1 - \dot{M}(t)]^2 - [1 - \dot{M}(t)]\ddot{M}(t)\dot{Q}_1(t) + \ddot{M}(t)^2 Q_1(t), \quad (4.17)$$

and

$$\dot{M}(t) = \dot{H}(t) + \sum_{j=1}^N \frac{c_j}{\omega_j} \dot{H}_j(t) \quad (4.18)$$

with $Q_1(t)$ and $Q_2(t)$ defined as in Eqs. (4.7) and (4.8).

C. Case 3: Unfactorized initial conditions

Although involving only Gaussian integrals, the algebra becomes even more tedious in this case. First we present the Wigner representation of the normalized initial distribution. For this purpose we note that the normalization integral is

$$Z_3 = \text{Tr}\{\langle \psi | e^{-\beta H} | \psi \rangle\} = Z \frac{2}{\sqrt{(\Gamma + \sum_{j=0}^N u_{j0}^2 r_j) [1/\Gamma + \sum_{j=0}^N (u_{j0}^2/s_j)]}} \times e^{-q_a^2 [1/\Gamma + \sum_{j=0}^N (u_{j0}^2/s_j)]} \quad (4.19)$$

and we have used the notation:

$$s_j = \frac{\lambda_j}{\hbar} \tanh\left(\frac{\hbar\beta\lambda_j}{2} \right), \quad r_j = \frac{\lambda_j^2}{\hbar^2 s_j}, \quad j = 0, \dots, N. \quad (4.20)$$

Note that Z_3/Z is also the equilibrium limit of the correlation functions [see also Eq. (2.13)]. It may be readily evaluated in the continuum limit, using the spectral density of the normal modes [Eq. (3.18)]. The equilibrium limit is a function of the damping parameters.

After some algebra one then finds that the phase space distribution of the initial conditions is

$$\rho^{(3)}(\underline{p}_y, \underline{y}) = \rho(\underline{p}_y, \underline{y}) \psi(p_q, q)^2 (\pi \hbar)^2 \left(\frac{(\Gamma + \sum_{j=0}^N u_{j0}^2 r_j) \left[1 + \Gamma \sum_{j=0}^N (u_{j0}^2 / s_j) \right]}{(\Gamma + \sum_{j=0}^N u_{j0}^2 s_j) \left[1 + \Gamma \sum_{j=0}^N (u_{j0}^2 / r_j) \right]} \right)^{1/2} \times \exp \left(\frac{P^2}{\hbar^2 (\Gamma + \sum_{j=0}^N u_{j0}^2 s_j)} + \frac{\Gamma Q^2}{\left[1 + \Gamma \sum_{j=0}^N (u_{j0}^2 / r_j) \right]} + \frac{\Gamma q_a^2}{1 + \Gamma \sum_{j=0}^N (u_{j0}^2 / s_j)} \right), \quad (4.21)$$

where we have used the notation

$$q = \sum_{j=0}^N u_{j0} y_j, \quad p_q = \sum_{j=0}^N u_{j0} p_{y_j}, \quad Q = \sum_{j=0}^N \frac{u_{j0} p_{y_j}}{\hbar r_j} + \frac{p_q}{\hbar \Gamma},$$

$$P = \hbar \left(\sum_{j=0}^N u_{j0} s_j y_j + \Gamma (q - q_a) \right). \quad (4.22)$$

To obtain the correlation function one introduces the Fourier representation of six delta functions, corresponding to the variables $q, p_q, q(t), p_q(t), Q, P$. One then finally finds that the correlation function is

$$C_3(t) = \frac{2\hbar}{\sqrt{D_3(t)}} \exp \left(- \frac{\Gamma_s^2 q_a^2}{\Gamma^2 D_3(t)} E_3(t) \right). \quad (4.23)$$

The determinant $D_3(t)$ takes the form

$$D_3(t) = D_{qq}(t) D_{pp}(t) - D_{pq}(t)^2 \quad (4.24)$$

with

$$D_{qq}(t) = \frac{1}{\Gamma_s} - \frac{\Gamma_s}{\Gamma^2} M_3(t)^2 - \frac{\hbar^2 \Gamma^2}{\Gamma_c} L_3(t)^2 + 2 \frac{\dot{H}(t)^2}{\Gamma} + 2 \hbar^2 \Gamma H(t)^2, \quad (4.25)$$

$$D_{pp}(t) = \hbar^2 \Gamma_c - \frac{\Gamma_s}{\Gamma^2} \dot{M}_3(t)^2 - \frac{\hbar^2 \Gamma^2}{\Gamma_c} \dot{L}_3(t)^2 + 2 \frac{\ddot{H}(t)^2}{\Gamma} + 2 \hbar^2 \Gamma \dot{H}(t)^2, \quad (4.26)$$

$$D_{pq}(t) = \frac{\Gamma_s}{\Gamma^2} M_3(t) \dot{M}_3(t) + \frac{\hbar^2 \Gamma^2}{\Gamma_c} L_3(t) \dot{L}_3(t) - 2 \frac{\dot{H}(t) \ddot{H}(t)}{\Gamma} - 2 \hbar^2 \Gamma H(t) \dot{H}(t), \quad (4.27)$$

$$M_3(t) = \dot{H}(t) + \hbar \Gamma \sum_{j=0}^N \frac{u_{j0}^2}{\lambda_j \tanh(\hbar \beta \lambda_j / 2)} \cos(\lambda_j t), \quad (4.28)$$

$$L_3(t) = H(t) + \frac{1}{\hbar \Gamma} \sum_{j=0}^N \frac{u_{j0}^2}{\tanh(\hbar \beta \lambda_j / 2)} \sin(\lambda_j t), \quad (4.29)$$

$$\Gamma_s = \Gamma + \sum_{j=0}^N u_{j0}^2 s_j, \quad \Gamma_r = \left(\frac{1}{\Gamma} + \sum_{j=0}^N \frac{u_{j0}^2}{r_j} \right)^{-1}, \quad (4.30)$$

and the exponent is

$$E_3(t) = \left(M_3(t) - \frac{\Gamma}{\Gamma_s} \right)^2 D_{pp}(t) - 2 \left(M_3(t) - \frac{\Gamma}{\Gamma_s} \right) \dot{M}_3(t) D_{pq}(t) + \dot{M}_3(t)^2 D_{qq}(t). \quad (4.31)$$

It is noteworthy that these results may be readily expressed in the continuum limit through the spectral density function for the normal modes.

D. Additional properties

Some insight into the relaxation dynamics may be obtained by considering the initial average energy of the combined system and bath for the three choices of the initial conditions. In case 1, that is, for factorized initial conditions, the initial average energy of the system and the bath is

$$\begin{aligned} \langle E \rangle_1 &= \int_{-\infty}^{\infty} dp_q dq \psi(p_q, q) \int_{-\infty}^{\infty} \prod_{j=1}^N [dp_{x_j} dx_j \phi_j(p_{x_j}, x_j)] H \\ &= \frac{\omega^2 + \sum_{j=1}^N (c_j^2 / \omega_j^2) + \hbar^2 \Gamma^2}{4\Gamma} + \frac{1}{2} \left(\omega^2 + \sum_{j=1}^N \frac{c_j^2}{\omega_j^2} \right) q_a^2 \\ &\quad + \frac{1}{2} \sum_{j=1}^N \frac{\hbar \omega_j}{\tanh(\hbar \beta \omega_j / 2)}. \end{aligned} \quad (4.32)$$

For partially factorized initial conditions, case 2, the initial average energy of the system and the bath is

$$\begin{aligned} \langle E \rangle_2 &= \int_{-\infty}^{\infty} dp_q dq \psi(p_q, q) \int_{-\infty}^{\infty} \prod_{j=1}^N \\ &\quad \times [dp_{x_j} dx_j \phi_j(p_{x_j}, x_j, q) \Phi(p_q, q, \underline{x})] \end{aligned} \quad (4.33)$$

$$H = \frac{\omega^2 + \hbar^2 \Gamma^2}{4\Gamma} + \frac{1}{2} \left(\omega^2 q_a^2 + \frac{1}{\Gamma} \sum_{j=1}^N \frac{c_j^2}{\omega_j^2} \right) + \frac{1}{2} \sum_{j=1}^N \frac{\hbar \omega_j}{\tanh(\hbar \beta \omega_j / 2)}.$$

One notes that when considered as a function of the location of the center of the initial wave packet (q_a), the average energy difference $\langle E \rangle_2 - \langle E \rangle_1$ is positive for small q_a but becomes negative as q_a increases. In other words, one of the

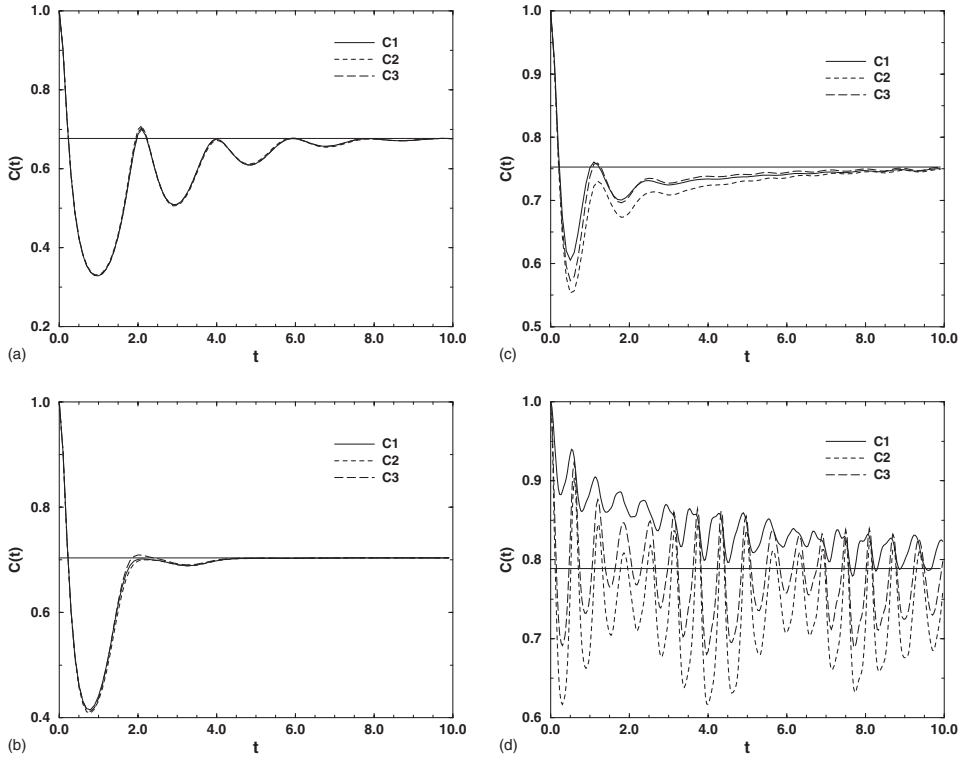


FIG. 1. The dependence of the unshifted Gaussian wave packet correlation function on the friction strength at low temperature. Panels (a)–(d) show results for the damping parameter $\gamma = 1, 3, 10, 50$, respectively. The solid, small dashed, and large dashed lines correspond to the respective choices of factorized, partially factorized, and nonfactorized initial conditions. The center of the initial Gaussian wave packet is located at the minimum of the harmonic oscillator potential ($q_a=0$). The horizontal solid line denotes the equilibrium limit. For further details, see the text.

differences between the factorized and partially factorized cases is in the total energy deposited in the system.

Finally, for unfactorized initial conditions, case 3, one finds

$$\begin{aligned} \langle E \rangle_3 = & \frac{1}{2} \sum_{j=0}^N \frac{\hbar \lambda_j}{\tanh(\hbar \beta \lambda_j / 2)} + \frac{\Gamma q_a^2 \sum_{j=0}^N u_{j0}^2 \lambda_j^2 (1/\Gamma + 1/s_j)^2}{2(1 + \Gamma/S)} \\ & - \frac{\hbar^2 (R_2 - \Gamma^2)}{4(R + \Gamma)} - \frac{2}{\Gamma} \sum_{j=0}^N u_{j0}^2 \lambda_j^2 \\ & + \frac{\Gamma \sum_{j=0}^N u_{j0}^2 \lambda_j^2 (1/\Gamma + 1/s_j)^2}{1 + \Gamma/S}, \end{aligned} \quad (4.34)$$

where we used the notation

$$\frac{1}{S} = \sum_{j=0}^N \frac{u_{j0}^2}{s_j}, \quad (4.35)$$

$$R = \sum_{j=0}^N u_{j0}^2 r_j, \quad (4.36)$$

and

$$R_2 = \sum_{j=0}^N u_{j0}^2 r_j^2. \quad (4.37)$$

We shall see in the numerical examples below that the average energy for the unfactorized case lies usually in between the factorized and partially factorized initial distributions.

V. NUMERICAL RESULTS

The harmonic bath is discretized using the methodology of Ref. [34]. The frequencies and coupling coefficients of the harmonic bath are chosen so as to mimic an Ohmic bath with a cutoff frequency ω_c and friction coefficient γ so that the spectral density is

$$J(\omega) = \gamma \omega \exp^{-\omega/\omega_c}. \quad (5.1)$$

The discretization for a finite number of oscillators as suggested by Wang *et al.* implies that

$$\omega_j = -\omega_c \ln \left\{ 1 - \frac{j}{N_b} \left[1 - \exp\left(-\frac{\omega_m}{\omega_c}\right) \right] \right\}, \quad (5.2)$$

$$c_j = \omega_j \sqrt{\frac{2}{\pi} \frac{\eta \omega_c}{N_b} \left[1 - \exp\left(-\frac{\omega_m}{\omega_c}\right) \right]}, \quad (5.3)$$

where ω_m is the maximal bath frequency (chosen in this paper as $4\omega_c$) and N_b is the number of bath oscillators used. In the computations below we verified that for the time span studied, the continuum limit is reached for the correlation functions when using 40 bath degrees of freedom. The parameters chosen in the numerical computations are $\omega_c=2\omega$, $\Gamma=10$, $\omega=\sqrt{2}$, $\hbar=1$, and $\beta=10$. In Fig. 1, for the case that $q_a=0$, we plot the correlation function for overdamped ($\gamma=50$), strong ($\gamma=10$), moderate ($\gamma=3$), and weak ($\gamma=1$) friction, respectively, and for the three choices of initial conditions as described above. Given these parameters, one creates the discretized bath of harmonic oscillators and then diagonalizes the Hamiltonian to obtain the normal mode form. The resulting normal mode frequencies and orthogonalization

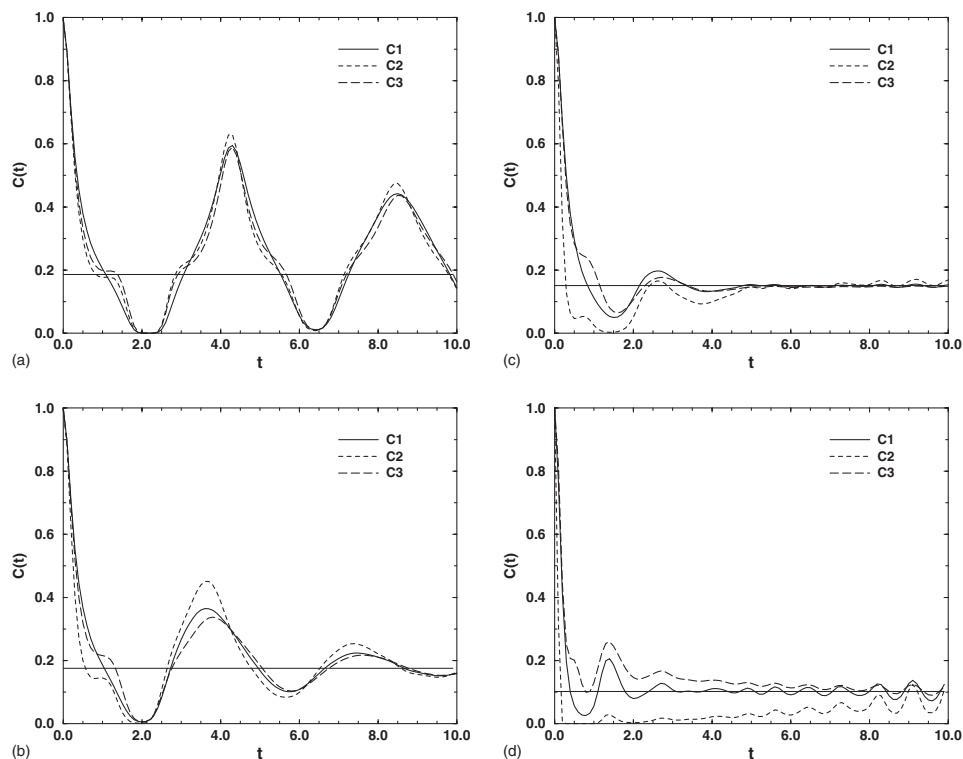


FIG. 2. The dependence of the shifted Gaussian wave-packet correlation function on the friction strength at low temperature. Panels (a)–(d) show results for the damping parameter $\gamma = 0.3, 1, 3, 10$, respectively. Other notation is as in Fig. 1. The center of the initial Gaussian wave packet is located at $q_a = 1$. For further details, see the text.

matrix are used to obtain the relevant dissipation functions needed to compute the correlation functions.

From Fig. 1, one notes that only in the overdamped friction limit is there a noticeable difference between the three choices, and even here the differences between unfactorized and partially factorized initial conditions are only quantitative in nature. However, if the initial wave packet is significantly shifted, that is, for the case that $q_a = 1$, one finds, as shown in Fig. 2, that the differences between the three distributions are much larger. Here, the four panels correspond to the friction values $\gamma = 0.3, 1.0, 3.0$, and 10.0 . All other parameters are the same as in Fig. 1. In this case, we find that the choice of factorized initial conditions is closer to the unfactorized case than the partially factorized choice.

As already noted in the previous section, when the shift q_a becomes sufficiently large, the total energy in the system is smaller when comparing the partially factorized case to the unfactorized case. This is shown in Fig. 3, where we plot the average energy per mode for the three initial distributions as a function of q_a . Interestingly, the unfactorized average energy lies in between the two other cases. It is thus not surprising that when considering the correlation functions shown in Fig. 2, one finds that initially the decay is fastest for the partially factorized initial conditions and slowest for the factorized case. The differences increase with increasing shift in the initial location of the Gaussian wave packet. This is another indication why all three initial conditions are so similar when the shift $q_a = 0$.

VI. DISCUSSION

In this paper we presented analytical formulas for the correlation function of a dissipative harmonic oscillator, pre-

pared initially as a Gaussian wave packet, using three different initial distributions for the thermal bath. The study has been limited to an Ohmic heat bath with a cutoff frequency, as this is the usual model employed in the study of dissipative systems. From the computations presented, it would seem that for most “reasonable” parameter ranges, the use of factorized initial conditions does not lead to qualitative changes in the relaxation dynamics. This observation justifies to some extent the prevalent use of factorized initial conditions in various exact quantum and approximate semiclassical simulations of dynamics in dissipative systems.

We have also seen that the use of partially factorized initial conditions does not lead to any dramatic improvement in the agreement with nonfactorized initial conditions. Since the partially factorized case is somewhat more difficult to implement numerically than the fully factorized choice, these results would imply that the extra effort involved is not justified. However, the difference between factorized and partially factorized dynamics is indicative also of the difference between these two choices and the nonfactorized initial distribution. So in case of doubt, one should carry out the computation for the factorized and partially factorized cases and, only if the difference between them is significant, resort to the nonfactorized initial distribution.

Shifting the mean location of the initial Gaussian wave packet away from the equilibrium point magnifies the differences between the three distributions. The magnification comes from the fact that the shift appears exponentially in the correlation function. However, the rapid decay may also be considered as a rapid dephasing of the original wave packet, which is caused by the dissipative bath; this dephasing is faster the further the initial wave packet is from the thermal distribution. However, as already noted, qualita-

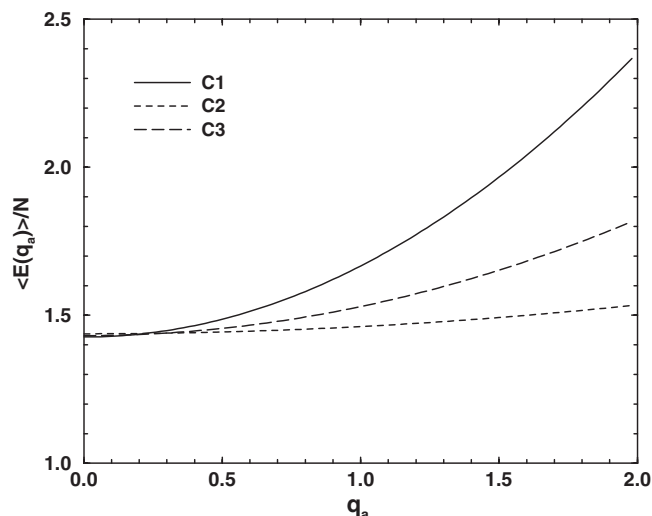


FIG. 3. The dependence of the total energy per mode on the initial shift of the Gaussian wave packet at low temperature. The three lines correspond to the three choices of factorized, partially factorized, and nonfactorized initial conditions for the bath. For further details, see the text.

tively, the rate of this initial fast decay does not change drastically as one changes the initial conditions of the heat bath.

We have also seen that the different choices of initial conditions lead to a different total energy for the combined system and bath. However, here too the differences are quantitative, and for all three choices the correlation function

relaxes to its equilibrium value even though the total energy is different.

The results presented in this paper were for very low temperature. As one increases the temperature of the bath, the initial correlations become even less important as has also been noted by Breuer *et al.* [18]. The partially factorized distribution becomes identical to the unfactorized distribution in the classical high temperature limit.

The results for the dissipative harmonic oscillator do not guarantee that correlations remain moderate also for anharmonic systems. Given present day technology, one can repeat the tests presented in this paper for anharmonic systems but with a limited number of bath oscillators if the temperature is sufficiently low. The present study has been limited to Ohmic heat baths. It could very well be that spectral densities that lead to subdiffusive motion would further accentuate the differences between the various initial densities. We have also limited ourselves to the study of the evolution of a Gaussian wave packet. Other observables might be more sensitive, as, for example, in the study of decoherence. One should keep in mind that the sensitivity to initial correlations does depend on the observable. For each case considered, one should perhaps repeat the kind of study presented in this paper, before undertaking an expensive numerical computation based on factorized initial conditions.

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