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Quantum Brownian motion in a general environment: Exact master equation with nonlocal dissipation and colored noise

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We use the influence functional path-integral method to derive an exact master equation for the quantum Brownian motion of a particle linearly coupled to a general environment (ohmic, subohmic, or supraohmic) at arbitrary temperature and apply it to study certain aspects of the loss of quantum coherence.

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I. INTRODUCTION AND SUMMARY

Recent revival of interest in quantum Brownian motion (QBM) as a paradigm of quantum open systems was motivated by possible observation of macroscopic effects in quantum systems (such as dissipation in tunneling [1–4]) and problems of quantum measurement theory (such as the loss of quantum coherence due to a system's interaction with its environment [5–8]). We are led to this very old problem because of our interest in the issue of quantum-to-classical transition in quantum cosmology [9,10], which involves quantum decoherence [11,12], dissipation [13], and correlation problems [14]. This issue also enters in the foundations of semiclassical gravity [15] which involves back reaction, particle creation, and dissipation problems as well [16,17]. How noise and fluctuations can act as germs of galaxies in inflationary and other evolutionary cosmologies [18,19] is also an important issue which statistical-mechanics studies can help to clarify.

These problems all point to the necessity of a better understanding of the nature and structure of quantum open systems, especially for quantum fields. The interplay of statistical and quantum effects in processes involving noise and fluctuation such as dissipation, decoherence, correlation, particle creation, and back reaction could have left indelible marks on the state of the early Universe, which in its evolution could have strongly influenced the outcome of our present observable classical Universe [20]. The complexity of these problems requires the extension of previous analysis of the QBM problem to nonlinear couplings and more general environments giving rise to nonlocal dissipations, and colored noise, and eventually for stochastic quantum fields. This paper is a first step in this direction.

The effect of nonlocal dissipation and colored noise in Brownian motion has been thoroughly studied for classical systems using semiphenomenological (e.g., Langevin) equations [21], but only to a limited extent for quantum systems with the master equation (the evolution equation for the reduced density matrix). The master equation has been derived before with different methods, but all previous works have been restricted to the particular class of ohmic environment, for which the dissipation is always local (but the noise is colored in the low-temperature regime). For this kind of environment the most complete work to date is that of Unruh and Zurek [7], who derived a master equation using canonical methods. The reader can find in that paper references to earlier work.

In this series of papers we treat this problem for the most general environment which produces a colored noise and induces nonlocal dissipation in the system. We opt for the influence functional (IF) path-integral method of Feynman and Vernon [22] which was previously used by Caldeira and Leggett [3], who derived a master equation for the ohmic environment at high temperature. One of its many advantages is that it can be easily extended to field theory. In fact, it is largely equivalent to the Schwinger-Keldysh closed-time-path integral formalism [23] which we have earlier used for treating cosmological back-reaction problems [16] and for constructing a quantum kinetic field theory in flat and curved spacetimes [24]. The influence functional method was originally designed to be used in problems where the initial conditions were factorizable but it has since been extended to more general cases by Hakim and Ambegaokar [25] and more recently by Grabert *et al.* [4], and by Caldeira and collaborators [26]. (By a factorizable initial condition it is meant that the initial density matrix is a product of a function of the environment variables and a function of the system variables.)

Our contribution in this paper (paper I) is the derivation of an exact master equation, Eq. (1.4) for the reduced density matrix of a system coupled linearly to a general environment (with a general spectral density—ohmic, supra- or subohmic) at arbitrary temperature. This derivation, presented in Sec. II, is done from first principles using path-integral methods. The master equation

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can accommodate all possible forms of the nonlocal dissipation kernel and nonlocal noise kernel, the non-Markovian character residing only in the time-dependent coefficients of this equation [27]. Our derivation assumes a factorizable initial condition but does not assume any particular relation among the different time scales in the problem.

In Sec. III we give approximate analytic results for some special cases and present numerical solutions for the time-dependent coefficients in our master equation for both ohmic and nonohmic environments (Figs. 1–6). We discuss the behavior of the diffusion and dissipation coefficients, examine the validity of some methods used before and comment on the conclusions previously drawn in relation to the decoherence problem [7]. As a simple example of decoherence, we consider the decay of interference between two Gaussian wave packets [8] in a general environment. We derive an analytic expression for the decay function $D(t)$ [Eq. (3.22)] and present numerically its behavior for ohmic and nonohmic cases at high and low temperatures (Fig. 7).

In a following paper (paper II [28]), we shall discuss the same problem with nonlinear coupling, arriving at the master equation perturbatively. We also demonstrate with these more general cases the existence of a general fluctuation-dissipation relation. Paper III extends this problem to field theory, both in flat and curved spacetimes [29].

In what follows we explain the nature and circumstances of our problem and summarize our results.

A. System and environment, fluctuation and dissipation

Our system is a Brownian particle with mass M and natural (bare) frequency Ω. The environment is modeled by a set of harmonic oscillators with mass m_n and natural frequency ω_n. The particle is coupled linearly to each oscillator with strength C_n. The action of the combined system + environment is

$$
\begin{aligned}
S[x,q] &= S[x]+S_E[q]+S_{\text{int}}[x,q] \\
&= \int_0^t ds\left[\frac{1}{2}M(\dot{x}^2-\Omega^2 x^2)+\sum_n\left[\tfrac{1}{2}m_n(\dot{q}_n^2-\omega_n^2 q_n^2)\right]+\sum_n(-C_n x q_n)\right] \qquad (1.1)
\end{aligned}
$$

where x and q_n are the coordinates of the particle and the oscillators, respectively. The bare frequency Ω is different from the physical frequency Ω_p due to its interaction with the bath, which depends on the cutoff frequency. We will discuss this point in more detail at the end of Sec. II. For problems discussed here we are interested in how the environment affects the system in some averaged way. The quantity containing this information is the reduced density matrix of the system obtained from the full density operator of the system + environment by tracing out the environmental degrees of freedom. The equation governing this reduced density matrix is the master equation. Our central task is to derive this master equation for the Brownian particle in a general environment. We can get an overall though simplified picture of this system by invoking the fluctuation-dissipation relation and analyzing the spectral density of the environment.

The evolution of the combined system + environment can be characterized by different time scales. For simplicity we will refer to the case in which the isolated Brownian particle is a harmonic oscillator (extensions to the case of an unstable potential or a free particle are straightforward). In this case we have four basic time scales [30,3,4,7]: first, the scale associated with the natural frequency Ω of the isolated system; second, the relaxation time scale corresponding to frequency γ_0 determined largely by the coupling strength between the system and the bath; third, a "memory time" that is usually associated with the highest frequency (Λ) present in the reservoir; finally, a time scale $\tau_\beta=\hbar\beta^{-1}$ associated with the temperature of the bath $T=(k_B\beta)^{-1}$, which measures the relative importance of quantum to thermal effects. This multiplicity of time scales makes the problem very complicated. In most cases one has to assume some relation between the different scales in order to simplify the calculations.

The effect of the environment on the dynamics of the system can be seen as the interplay of the dissipation and fluctuation phenomena. (These two concepts will be quantified later.) For the quantum Brownian-motion problem with linear coupling, both fluctuations and dissipation are determined by some specific property of the environment, i.e., the "spectral density," which measures the number of oscillators with a given frequency present in the environment and the strength of the interaction between such oscillators and the system,

$$
I(\omega)=\sum_n \delta(\omega-\omega_n)\frac{C_n^2}{2m_n\omega_n} . \qquad (1.2)
$$

Given the spectral density $I(\omega)$ and the initial state of the bath, both dissipation and fluctuation are uniquely determined. In fact, two different environments with the same $I(\omega)$ are effectively equivalent in so far as their influence on the dynamics of the system is concerned. A fully quantum-mechanical (microscopic) treatment of the system + environment allows us to obtain certain general relations between these two (macroscopic) effects, known as the fluctuation-dissipation (FD) relations. The fluctuation-dissipation relations do not depend on the spectral density but only on the state of the environment (i.e., the temperature) and on the nature of the coupling (for a discussion of the quantum fluctuation-dissipation relation as reflected in systems of linear oscillators see, e.g., Ref. [30]).

Different environments are classified according to the functional form of the spectral density $I(\omega)$. On physical grounds, one expects the spectral density to go to zero for very high frequencies. Let us introduce a certain cutoff frequency Λ (a property of the environment) such that $I(\omega)\to 0$ for $\omega>\Lambda$. The environment is classified as ohmic [1–4] if in the physical range of frequencies $(\omega<\Lambda)$ the spectral density is such that $I(\omega)\sim\omega$, as supraohmic if $I(\omega)\sim\omega^n$, $n>1$, or as subohmic if $n<1$. The most studied ohmic case corresponds to an environment which induces a dissipative force linear in the velocity of the system. We have studied the following spectral density as a particular example [2]:

$$I(\omega)=\frac{2}{\pi}M\gamma_0\omega\left[\frac{\omega}{\tilde{\omega}}\right]^{n-1}e^{-\omega^2/\Lambda^2} \tag{1.3}$$

where $\tilde{\omega}$ is another frequency scale usually taken to be Λ.

B. The master equation

Assuming that the system and the environment are initially uncorrelated, we derived the following exact master equation for the reduced density matrix of the system described by the action (1.1):

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\rho_r(x,x',t)=&\left[-\frac{\hbar^2}{2M}\left[\frac{\partial^2}{\partial x^2}-\frac{\partial^2}{\partial x'^2}\right]+\frac{1}{2}M\Omega^2(x^2-x'^2)\right]\rho_r(x,x't)+\frac{1}{2}M\delta\Omega^2(t)(x^2-x'^2)\rho_r(x,x',t)\\ &-i\hbar\Gamma(t)(x-x')\left[\frac{\partial}{\partial x}-\frac{\partial}{\partial x'}\right]\rho_r(x,x',t)-iM\Gamma(t)h(t)(x-x')^2\rho_r(x,x',t)\\ &+\hbar\Gamma(t)f(t)(x-x')\left[\frac{\partial}{\partial x}+\frac{\partial}{\partial x'}\right]\rho_r(x,x',t)\ . \end{aligned} \tag{1.4}$$

The terms in the first square brackets make up the Liouvillian. The second term depicts a time-dependent frequency shift $\delta\Omega^2(t)$. The third is a dissipative term with a time-dependent dissipative constant $\Gamma(t)$. The last two are the diffusive terms with time-dependent coefficients $\Gamma(t)h(t)$ and $\Gamma(t)f(t)$. The time dependence of these coefficients is rather complicated [see Eq. (2.41)], but, given a particular form of the spectral density and the initial state of the environment, they can be explicitly calculated. The coefficients vanish at the initial time t_0 because of the assumed uncorrelated condition. One of the nice but somewhat unexpected features of this equation is that though it depicts non-Markovian processes it is not an integrodifferential equation but just an ordinary differential equation. All the non-Markovian behavior is embodied in the time dependence of the coefficients (however, note that the time axis is not homogeneous since the time $t=t_0$ is a privileged instant). This equation depicts the quantum Brownian motion of a particle linearly coupled to a general nonohmic environment. Some important aspects of the behavior of the Brownian motion at low temperatures and strong damping were discussed by Haake and Reibold [27] who earlier derived via the canonical quantization method an equation for the Wigner distribution function for a particular type of environment (the Drude's model) which has features (e.g., time-dependent coefficients) similar to our general master equation (1.4).

Let us briefly mention the relation between our equation (1.4) and other master equations found in the literature. Unruh and Zurek's [7] master equation is valid for arbitrary temperature but restricted to a purely ohmic environment with a linear spectral density. Our equation reduces to theirs in that limit. However, the purely ohmic environment is an idealized and somewhat unphysical case because it does not have a high-frequency cutoff. This unphysical assumption about the nature of the environment leads to pathological properties in the time-dependent coefficients: the dissipative coefficient and the frequency shift are not continuous functions (the frequency shift is divergent) and the diffusive coefficients involve ill-defined frequency integrals (sum-rule divergences [4]). Unruh and Zurek obtained a finite result by introducing a cutoff in the divergent integral involving the noise kernel alone but not in the dissipation kernel. We believe that this is an incorrect regularization procedure as it violates the fluctuation-dissipation relation. Instead, a more consistent and physically sound procedure is to regularize the divergent quantities with a high-frequency cutoff in the spectral density of the environment. This affects the fluctuations and the dissipation in a balanced manner. An environment regularized in this way is appropriate for processes which take place in a very short time scale. Under such treatments, for a model described in Eq. (1.3) with $n=1$, all the coefficients in Eq. (1.4) become continuous functions of time. Thus, the master equation we derived for this regularized environment differs from the regularized version of Unruh and Zurek's equation. However, for some physically relevant choice of the parameters Λ, Ω, γ_0, and β, the coefficients of our exact master equation can be approximated by those obtained by Unruh and Zurek. This is possible, roughly speaking, when the cutoff frequency is large compared with the natural frequency Ω and the relaxation frequency γ_0 since in these circumstances the dissipation can be considered approximately local. Therefore, in practical terms, Unruh and Zurek's equation still has a wide range of applicability.

Another feature (called to our attention by Ambegaokar [31] after this work was submitted for publication) worth noticing is that the master equations derived in Refs. [1] and [7] both have the pathology that the density matrix loses its positivity at times shorter than $\tau_\beta=\hbar/(k_B T)$. This violation is essentially due to the action of the friction term therein at short times. At $t<\tau_\beta$ quantum effects become dominant over thermal effects, and this is the time range when the master equation (2.13a) of Calderia and Leggett [1] derived for high temperature is not expected to be valid. Similar pathological behavior is observed in the master equation (2.13b) of Unruh and Zurek [7]. In that case the friction coefficient is assumed to be constant, which can become dominant at short times (within certain appropriately chosen parameters). Our master equation (2.40) does not have this pathological behavior. This can be verified with the results in Sec. III. From Figure 1 we see that the friction coefficient is a time-dependent function that vanishes initially together with its first derivative. By contrast, the diffusion coefficient displayed in Figs. 3 and 4 grows faster initially (it has a nonvanishing first derivative). Therefore, the initial behavior of (2.40) is diffusion dominated and it is for this that the positivity of the density matrix is preserved.

C. Decoherence

One of the several statistical effects we mentioned in the beginning which can be studied with the master equation derived here is the loss of coherence in quantum systems interacting with a general environment. This subject is of basic importance in theoretical physics and of central concern in the quantum theory of measurement. It has received much recent attention in connection with the experimental possibility of observing quantum interference effects in macroscopic systems [32,33] and the theoretical inquiry into the emergence of time in the classical limit of quantum cosmology [9,15]. Since this topic has been discussed in detail by many authors in these respective fields, notably Zurek [5], Joos and Zeh [6], Gell-Mann and Hartle [11], and more recently Unruh and Zurek [7], we will be very brief here.

Macroscopic bodies and measurement devices normally interact with huge environments and this interaction may produce the loss of quantum coherence thus suppressing the possibility of observing quantum interference effects between macroscopically distinguishable states. A key role in this process is played by the correlations established between the system (in this case the macroscopic body) and the environment during the evolution. If the system-environment interaction is such that the states $|s_n\rangle$ for which the system manifests macroscopic behavior become correlated to states of the environment that are approximately orthogonal to each other, then the reduced density matrix of the system can evolve into the form

$$\rho_r \simeq \sum_n |c_n|^2 |s_n\rangle\langle s_n| \tag{1.5}$$

which describes a statistical mixture of noninterfering states (or classical branches). The reduced density matrix becomes diagonal in a particular basis chosen by the dynamics, called the "pointer basis" by Zurek [5], which approximately coincides with the eigenstates of the interaction Hamiltonian between the system and the environment. One can say that decoherence is achieved when the reduced density matrix becomes "approximately" diagonal in a fixed (i.e., time-independent) basis of the Hilbert space of the system. In the QBM problem with interaction (1.1), the system is a simple particle and the pointer basis consists of the position eigenstates. If the reduced density matrix is diagonalized in the sense that $\rho_r(x,x')\simeq 0$ for $|x-x'|\simeq\Delta$, then it will not be possible to observe interference effects between states with wave functions centered around positions that differ by more than Δ.

Thus, a commonly proposed way to analyze decoherence is by examining how the nondiagonal elements of the reduced density matrix evolve under the master equation. The diffusion terms are mainly responsible for their rapid disappearance in the coordinate representation. (Other approaches to the study of decoherence which do not use the master equation include the recent one proposed by Gell-Mann and Hartle and earlier work of Griffiths, Omnes, and others [11]. The basic idea there is to examine the conditions for defining a probability measure on the space of histories of the system.)

For the QBM problem we have obtained here some preliminary results on the effect of nonohmic environments on decoherence. In Sec. III we analyzed numerically the time dependence of the coefficients in our master equation for various supraohmic and subohmic environments. Examining the behavior of the diffusive coefficient we can show that in all cases a strong peak appears in a short time $t\simeq\Lambda^{-1}$, whereas the long-time behavior depends markedly on the spectral density. For example, the diffusive coefficient for the supraohmic environment defined by Eq. (1.3) with $n=2$ in the limit of weak coupling and high temperature behaves like

$$\Gamma(t)h(t)\simeq\frac{4\gamma_0}{\hbar\beta}\Lambda t e^{-\Lambda^2 t^2}\cos\Omega t+O(\Omega/\Lambda)\ . \tag{1.6}$$

Owing to the presence of this initial jolt, the diagonal components of the reduced density matrix diminish rapidly and quantum coherence is reduced in a time scale of the order of Λ^{-1} by an amount similar to that for an ohmic environment. However, in the long-time regime the diffusive coefficient vanishes, as distinct from the ohmic case where the coefficient is asymptotically proportional to the temperature.

From our numerical analysis, which is restricted to short times, the initial jolt observed in Ref. [7] appears in all examples under very different conditions. We suspect that this is a special consequence of the assumed uncorrelated initial condition. As already noted by earlier authors, this condition is unlikely to be attained experimentally. For realistic applications it would be important to consider more physical initial conditions such as that treated in Refs. [25,4]. There it is assumed that the system and the environment are in equilibrium and that at some initial instant $t=0$ one performs an imperfect measurement on the system retaining part of the preexisting correlations. For correlated initial conditions the initial jolt might not be as pronounced. In the absence of the jolt, the more delicate aspects of the environment's influence on decoherence can become more apparent. In fact, previous results obtained in another context seem to point in that direction [2].

II. THE MASTER EQUATION

A. The functional approach

We will briefly review here the Feynman-Vernon [22] influence functional method for deriving the master equation. Readers who are familiar with it can skip this subsection. The method provides an easy way to obtain a functional representation for the evolution operator J_r for the reduced density matrix $\hat{\rho}_r$. Let us start first with the evolution operator J for the full density matrix $\hat{\rho}$ defined by

$$\hat{\rho}(t)=J(t,t_0)\hat{\rho}(t_0) \ . \tag{2.1}$$

As the full density matrix $\hat{\rho}$ evolves unitarily under the action of Eq. (1.1), the evolution operator J has a simple path-integral representation. In the position basis, the matrix elements of the evolution operator are given by

$$\begin{aligned} J(x,q,x',q',t|x_i,q_i,x_i',q_i',0)&=K(x,q,t|x_i,q_i,0)K^*(x',q',t|x_i',q_i',0)\\ &=\int_{x_i}^{x}Dx\int_{q_i}^{q}Dq\exp\left[\frac{i}{\hbar}S[x,q]\right]\int_{x_i'}^{x'}Dx'\int_{q_i'}^{q'}Dq'\exp\left[-\frac{i}{\hbar}S[x',q']\right] \ , \end{aligned} \tag{2.2}$$

where the operator K is the evolution operator for the wave functions. In the second equation, the path integrals are over all histories compatible with the boundary conditions. We have used q to represent the full set of environmental coordinates q_n and the subscript i to denote the initial variables.

The reduced density matrix is defined as

$$\rho_r(x,x')=\int_{-\infty}^{+\infty}dq\int_{-\infty}^{+\infty}dq'\rho(x,q;x',q')\delta(q-q')$$

and is propagated in time by the evolution operator J_r:

$$\rho_r(x,x',t)=\int_{-\infty}^{+\infty}dx_i\int_{-\infty}^{+\infty}dx_i'\,J_r(x,x',t|x_i,x_i',0)\rho_r(x_i,x_i',0) \ . \tag{2.3}$$

By using the functional representation of the full density-matrix evolution operator given in Eq. (2.2), we can also represent J_r in path-integral form. In general, the expression is very complicated since the evolution operator J_r depends on the initial state. If we assume that at a given time $t=0$ the system and the environment are uncorrelated, i.e.,

$$\hat{\rho}(t=0)=\hat{\rho}_s(0)\times\hat{\rho}_e(0) \ , \tag{2.4}$$

then the evolution operator for the reduced density matrix does not depend on the initial state of the system and can be written [22] as

$$\begin{aligned} J_r(x_f,x_f',t|x_i,x_i',0)&=\int_{x_i}^{x_f}Dx\int_{x_i'}^{x_f'}Dx'\exp\left[\frac{i}{\hbar}(S[x]-S[x'])\right]F[x,x']\\ &=\int_{x_i}^{x_f}Dx\int_{x_i'}^{x_f'}Dx'\exp\left[\frac{i}{\hbar}A[x,x']\right] \ , \end{aligned} \tag{2.5}$$

where the subscript f denotes final variables, and $A[x,x']$ is the effective action for the open quantum system. The factor $F[x,x']$, called the "influence functional," is defined as

$$\begin{aligned} F[x,x']&=\int_{-\infty}^{+\infty}dq_f\int_{-\infty}^{+\infty}dq_i\int_{-\infty}^{+\infty}dq_i'\int_{q_i}^{q_f}Dq\int_{q_i'}^{q_f}Dq'\exp\left[\frac{i}{\hbar}(S_b[q]+S_{\rm int}[x,q]-S_b[q']-S_{\rm int}[x',q'])\right]\rho_b(q_i,q_i',0) \ ,\\ &=\exp\left[\frac{i}{\hbar}\delta A[x,x']\right] \end{aligned} \tag{2.6}$$

where $\delta A[x,x']$ is the influence action. Thus $A[x,x']=S[x]-S[x']+\delta A[x,x']$.

It is obvious from its definition that if the interaction term is zero, the influence functional is equal to unity, and the influence action is zero. In general, the influence functional is a highly nonlocal object. Not only does it depend on the time history, but—and this is the more important property—it also irreducibly mixes the two sets of histories in the path integral of Eq. (2.5). Note that the histories x and x' could be interpreted as moving forward and backward in time, respectively. Viewed in this way, one can see the similarity of the influence functional (IF) and the generating functional in the closed-time-path (CTP) integral formalism [23]. The Feynman rules derived in the CTP method are very useful for computing the IF. We shall treat the field-theoretic problems in later papers.

In those cases where the initial decoupling condition (2.4) is satisfied, the influence functional depends only on the initial state of the environment. We will further assume that the environment is initially in thermal equilibrium at a temperature β^{-1} (the influence-functional method can be extended to more general conditions, such as thermal equilibrium between the system and the environment [25], or correlated initial states [4,26]).

For the problem described by Eq. (1.1), the influence functional can be computed exactly [22,3]. The result is

$$F[x,x']=\exp\left[-\frac{i}{\hbar}\int_0^t ds_1\int_0^{s_1} ds_2[x(s_1)-x'(s_1)]\eta(s_1-s_2)[x(s_2)+x'(s_2)]\right.$$
$$\left.-\frac{1}{\hbar}\int_0^t ds_1\int_0^{s_1} ds_2[x(s_1)-x'(s_1)]\nu(s_1-s_2)[x(s_2)-x'(s_2)]\right] . \tag{2.7}$$

The kernels η and ν are generally nonlocal and are defined as

$$\nu(s)=\int_0^{+\infty} d\omega\, I(\omega)\coth\frac{1}{2}\beta\hbar\omega\cos\omega s \tag{2.8a}$$

and

$$\eta(s)=\frac{d}{ds}\gamma(s) , \tag{2.8b}$$

where

$$\gamma(s)=\int_0^{+\infty} d\omega\,\frac{I(\omega)}{\omega}\cos\omega s . \tag{2.8c}$$

Here $I(\omega)$ is the spectral density defined in Eq. (1.2).

The influence functional (2.7) and the corresponding influence action can be written in a compact way:

$$A[x,x']=S[x]-S[x']+\delta A[x,x'] ,$$
$$\delta A[x,x']=-2\int_0^t ds_1\int_0^{s_1} ds_2\Delta(s_1)\eta(s_1-s_2)\Sigma(s_2)$$
$$+i\int_0^t ds_1\int_0^{s_1} ds_2\Delta(s_1)\nu(s_1-s_2)\Delta(s_2) \tag{2.9}$$

with the use of the "center-of-mass" and "relative" coordinates,

$$\Sigma=\tfrac{1}{2}(x+x'),\quad \Delta=x-x' . \tag{2.10}$$

The evolution operator given in Eq. (2.5) generates a non-Markovian dynamics since it fails in general to satisfy the relation

$$J_r(t_2,t_0)=J_r(t_2,t_1)J_r(t_1,t_0)$$

for the reason that the operator $J_r(t_2,t_1)$ depends on the state of the system in time t_1, unless that time is the one for which the system and the environment were decoupled. The non-Markovian behavior is, in fact, a direct consequence of the nonlocality of the influence functional.

As pointed out by many authors (see, for example, Refs. [3,4]), the real and imaginary parts of $A[x,x']$ can be interpreted as being responsible for dissipation and noise, respectively. The real part of the exponent in Eq. (2.7) is determined by $\nu(s)$, the noise (or fluctuation) kernel. The name becomes apparent when we realize that the term $\exp[-(x-x')\nu(x-x')]$ can be interpreted as coming from the interaction between the system and a stochastic force ξ that is linearly coupled to the system and has a probability density given by $P[\xi]=\exp(-\xi\nu^{-1}\xi)$. On the other hand, the kernel $\eta(s)$ in (2.7) is known as the dissipation kernel. The motivation for the name comes from the fact that the imaginary part of the exponent in Eq. (2.7) introduces a modification in the real saddle-point trajectories of the path integral in Eq. (2.5). Strictly speaking only the nonsymmetric part of the η kernel should be associated with dissipation. Thus, all of the symmetric part can be absorbed in a nonlocal potential (that does not contribute to the mixing of the x and x' histories). There is no such symmetric part in the η kernel of our problem although it does appear in other cases [28].

The noise and dissipation kernels can always be related by some integral equation known as the fluctuation-dissipation relation. For the QBM case, it can be written as

$$\nu(s)=\int_{-\infty}^{+\infty} ds' K(s-s')\gamma(s') , \tag{2.11a}$$

where the kernel $K(s)$ is

$$K(s)=\int_0^{+\infty}\frac{d\omega}{\pi}\omega\coth\tfrac{1}{2}\beta\hbar\omega\cos\omega s . \tag{2.11b}$$

In the classical or high-temperature limit, the kernel K is proportional to the delta function $K(s)=2k_BT\delta(s)$ and the FD relation is equivalent to the well-known Einstein formula. The quantum-mechanical FD relations have been analyzed in detail by many authors [30]. Here we just want to mention one of the notable features. Contrary to the classical case, the quantum-mechanical relations predict that fluctuation and dissipation have very different time scales (i.e., the fluctuation correlation time can be very different from the memory time). The memory time scale (for the non-Markovian case) in the dissipation kernel is related to Λ^{-1} while the fluctuation correlation time is in general the maximum of Λ^{-1} and $\hbar\beta$. Then, the noise correlation time diverges at low temperature (in the sense that the correlations do not decay exponentially but as some power law). Some macroscopic effects at low temperatures are attributable to this fact (see Ref. [30] for an interesting analysis of the low-temperature excess in the population of the Brownian oscillator caused by this purely quantum effect).

B. The master equation under restricted conditions: Previous results

The problem defined by the action (1.1) with linear coupling can be solved exactly. The path integral in Eq. (2.5) can be computed since it is a Gaussian. However, for physical considerations, the master equation for the time evolution of the reduced density matrix is often more useful than the exact solution for the evolution operator. Indeed, from the master equation we can extract some qualitative features about the evolutionary behavior of the system more readily, i.e., features that are independent of the initial condition, and for exact details it can be numerically integrated.

Although many authors alluded to attributes of the master equation and some have obtained approximate versions of it, to our knowledge, an exact master equation for the QBM in a general environment is not yet known. We will describe here in more detail the two cases we mentioned in the Introduction. Using the path-integral approach, Caldeira and Leggett [3] found the master equation for a purely ohmic environment at high temperature. Such a model is defined by a spectral density like that given in Eq. (1.3). If we consider the temperature to be such that $\hbar\beta \ll \Lambda^{-1}$ and then let $\Lambda \to \infty$ (the order in which we take the limits is important), the noise and dissipation kernels (2.8) are simplified to

$$\nu(s)=\frac{2Mk_BT\gamma_0}{\hbar}\delta(s) \tag{2.12a}$$

and

$$\eta(s)=\frac{d}{ds}\gamma(s)=M\gamma_0\delta'(s)\ . \tag{2.12b}$$

The master equation is easily obtained from the path integral since in that case the influence functional is local and the evolution is Markovian. The equation obtained by Caldeira and Leggett is (from now on, we avoid writing the mass of the oscillator by rescaling the variables $x \to M^{1/2}x$):

$$\begin{aligned}i\hbar\frac{\partial}{\partial t}\rho_r(x,x',t)=&\left[-\frac{\hbar^2}{2}\left[\frac{\partial^2}{\partial x^2}-\frac{\partial^2}{\partial x'^2}\right]+\frac{1}{2}\Omega^2(x^2-x'^2)\right]\rho_r(x,x',t)\\&-i\hbar\gamma_0(x-x')\left[\frac{\partial}{\partial x}-\frac{\partial}{\partial x'}\right]\rho_r(x,x',t)-i2k_BT\gamma_0(x-x')^2\rho_r(x,x',t)\ .\end{aligned} \tag{2.13a}$$

Unruh and Zurek considered an ohmic environment at arbitrary temperature. For an environment with spectral density $I(\omega)=\gamma_0\omega$ their master equation reads

$$\begin{aligned}i\hbar\frac{\partial}{\partial t}\rho_r(x,x',t)=&\left[-\frac{\hbar^2}{2}\left[\frac{\partial^2}{\partial x^2}-\frac{\partial^2}{\partial x'^2}\right]+\frac{1}{2}\Omega^2(x^2-x'^2)\right]\rho_r(x,x',t)\\&-i\hbar\gamma_0(x-x')\left[\frac{\partial}{\partial x}-\frac{\partial}{\partial x'}\right]\rho_r(x,x',t)-i\gamma_0h(t)(x-x')^2\rho_r(x,x',t)\\&+\hbar\gamma_0f(t)(x-x')\left[\frac{\partial}{\partial x}+\frac{\partial}{\partial x'}\right]\rho_r(x,x',t)\ ,\end{aligned} \tag{2.13b}$$

where f and h are two time-dependent functions that are determined by the parameters of the model (temperature, etc.). They harbor the non-Markovian behavior.

C. The master equation in a general environment: Derivation from the path integral

Our derivation of (1.4) is based on the use of the functional-integral representation for the evolution operator of the reduced density matrix given in Eq. (2.5). Using the path integral to obtain the master equation is conceptually equivalent to deriving the Schrödinger equation from the functional representation of the quantum-mechanical propagator. The only (but very important) complication here arises from the nonlocality of the integrand.

To obtain the master equation we have to find the time derivative of the evolution operator of the density matrix. One is tempted at first to write the path-integral form of the propagator $J_r(t+dt,t)$, expand the expression in powers of dt, and subtract $J_r(t,t)$ to get the desired time derivative. However, this naive procedure is incorrect because of the nonlocality of the influence functional: the propagator $J_r(t+dt,t)$ depends on the state of the system at time t. For the ohmic environment at high temperature, Caldeira and Leggett [3] derived the master equation Eq. (2.13a) from the path integral following the standard textbook approach, but that derivation was possible only because, in that approximation, the problem becomes local.

Our procedure goes as follows: To compute the time derivative of $J_r(t,0)$, we will use the functional representation for $J_r(t+dt,0)$ given in Eq. (2.5), expand the result in powers of dt, and subtract $J_r(t,0)$. The time derivative of the reduced density matrix is directly obtainable from that of the propagator. The assumption of an initially uncorrelated condition is important since it makes the evolution operator $J_r(t,0)$ independent of the state of the system at time $t=0$. We can schematically divide our derivation into five steps.

(1) The first step consists of taking the functional representation of $J_r(t+dt,0)$ given by Eq. (2.5) and dividing each of the path integrals into two parts. We introduce two intermediate points x_m, x_m' at time t and integrate over them, thus writing

$$\int_{0;x_0}^{t+dt;x_f} Dx=\int_{-\infty}^{+\infty} dx_m \int_{0;x_0}^{t;x_m} D\bar{x} \int_{t;x_m}^{t+dt;x_f} D\tilde{x} \; . \tag{2.14}$$

There is a similar expression for the sum over x' histories.

The original histories $x(\tau)$ are functions defined on the $(0,t+dt)$ time interval that satisfies the boundary conditions $x(0)=x_0$ and $x(t+dt)=x_f$. The new set of histories $\bar{x}(\tau)$ and $\tilde{x}(\tau)$ are functions defined respectively on the $(0,t)$ and $(t,t+dt)$ intervals. They satisfy the boundary conditions $\bar{x}(0)=x_0$, $\bar{x}(t)=x_m=\tilde{x}(t)$ and $\tilde{x}(t+dt)=x_f$. The integrand in Eq. (2.5) can be written easily in terms of the new set of histories as follows:

$$A[x,x']=A[\bar{x},\bar{x}']+A[\tilde{x},\tilde{x}']+A_i[\bar{x},\bar{x}',\tilde{x},\tilde{x}'] \; , \tag{2.15}$$

where A_i is a term that mixes the $\tilde{x}$ histories with the $\bar{x}$ histories. This term appears due to the nonlocality of the influence functional. It is in fact what complicates this calculation.

(2) The second step of the derivation consists of approximating the path integral over the $(\tilde{x},\tilde{x}')$ histories by some (time-dependent) constant multiplying the value of the integrand evaluated on the "straight-line histories" defined by

$$\tilde{x}(s)=x_m+(x_f-x_m)\frac{s-t}{dt}=x_m+\beta_x\frac{s-t}{dt} \tag{2.16}$$

and similarly for $\tilde{x}'$ (with $\beta_{x'}$). To compute the time derivative of J_r one takes the limit $dt\rightarrow 0$. Using the previous equations we can write

$$\int_{(0;x_i,x_i')}^{(t+dt;x_f,x_f')} Dx\,Dx'\exp(iA[x,x'])=N(t)\int_{-\infty}^{+\infty}dx_m\int_{-\infty}^{+\infty}dx_m'\exp(iA[\tilde{x},\tilde{x}'])$$
$$\times\int_{(0;x_i,x_i')}^{(t;x_m,x_m')} D\bar{x}\,D\bar{x}'\exp(iA[\bar{x},\bar{x}'])\exp(iA_i[\bar{x},\bar{x}',\tilde{x},\tilde{x}']) \; , \tag{2.17}$$

where $N(t)$ is a normalization constant. Henceforth we will set $\hbar=1$ except for the final equation. We will also use $\tilde{x}$ for the straight-line history defined in Eq. (2.16) (the same holds for $\tilde{x}'$).

We have to expand every term in the last equation in powers of dt keeping only the first-order contribution. It is easy to show that

$$A[\tilde{x},\tilde{x}']\simeq\frac{1}{2\,dt}(\beta_x^2-\beta_x'^2)-\frac{1}{2}\Omega^2 dt(x_f^2-x_f'^2)+\cdots \tag{2.18}$$

and

$$A_i[\bar{x},\bar{x}',\tilde{x},\tilde{x}']\simeq -dt\int_0^t ds\,J_\Sigma(s)\bar{\Sigma}(s)$$
$$+idt\int_0^t J_\Delta(s)\bar{\Delta}(s)+\cdots \; , \tag{2.19}$$

where the two sources in (2.19) are given by

$$J_\Sigma(s)=\frac{2}{dt}\int_t^{t+dt}ds'\tilde{\Delta}(s')\eta(s'-s)$$
$$\simeq 2(x_f-x_f')\eta(t-s)+\cdots \tag{2.20}$$

and

$$J_\Delta(s)=\frac{1}{dt}\int_t^{t+dt}ds'\tilde{\Delta}(s')\nu(s'-s)$$
$$\simeq(x_f-x_f')\nu(t-s)+\cdots \; . \tag{2.21}$$

Here, the ellipses stand for terms of higher order in dt or β^2.

We can keep terms only up to first order in β_i^2 in all of the previous equations because in Eq. (2.17) we have an integration over β_x and $\beta_{x'}$ (we can change integration variables from x_m to β_x, as is obvious from Eq. (2.16)]. Due to the existence of the first term in Eq. (2.18), the integrand will be highly oscillating in the $dt\rightarrow 0$ limit. The only relevant contribution to the integral over β_i will come from a region around zero with a width $\beta_x\sim dt^{1/2}$ (the same is valid for $\beta_{x'}$). Thus, terms up to first order in dt correspond to order β^2 also, but we can safely forget about higher-order ones.

A simple manipulation allows us to reorganize Eq. (2.17) as follows:

$$J_r(x_f,x_f',t+dt|x_i,x_i'0)\simeq N(t)\int_{-\infty}^{+\infty}d\beta_x\int_{-\infty}^{+\infty}d\beta_{x'}\exp\left[\frac{i}{2\,dt}(\beta_x^2-\beta_x'^2)\right]\times\{1-i\,dt[V(x_f)-V(x_f')]\}J_r(x_m,x_m',t|x_i,x_i',0;[\mathbf{b}])\;. \tag{2.22}$$

The last term of this equation comes from the last term of (2.17):

$$\tilde{J}_r(x_m,x_m',t|x_i,x_i'0;[\mathbf{b}])=\int_{(0;x_i,x_i')}^{(t;x_m,x_m')}D\bar{x}\,D\bar{x}\,'\exp\left[i\left[A\,[\bar{x},\bar{x}\,']-dt\int_0^t ds\,J_\Sigma(s)\Sigma(s)+i\,dt\int_0^t ds\,J_\Delta(s)\Delta(s)\right]\right]\;, \tag{2.23}$$

where we have introduced a vectorlike notation defining

$$\mathbf{b}=\begin{bmatrix}J_\Sigma\\ J_\Delta\end{bmatrix}\;.$$

Note that $\tilde{J}_r(\mathbf{b})$ can be interpreted as the evolution operator under the action of two external sources.

(3) The third step of the derivation consists of computing the path integral in Eq. (2.23). We want to show that it is possible to write $\tilde{J}_r(\mathbf{b})$, the evolution operator under the action of two sources, as a product of two terms:

$$\tilde{J}_r(x_m,x_m',t|x_i,x_i',0;[\mathbf{b}])=J_r(x_m,x_m',t|x_i,x_i',0)\times W[x_m,x_m',x_i,x_i',dt]\;. \tag{2.24a}$$

The first term is the evolution operator with no source and the second one is a function of the end points. This is expected since the sources $\mathbf{b}$ are functions of the end points through Eqs. (2.20) and (2.21). This, the third step of the calculation, is the most complicated one. Our approach reproduces the familiar results for Markovian cases. In fact, in an ohmic environment at high temperature, the sources J_Δ and J_Σ are proportional to local distributions like $\delta(t-s)$ or its derivatives. Then, using Eqs. (2.12) and the explicit form of the sources given by Eqs. (2.20) and (2.21), we can show that the function W in (2.24a) is given by:

$$W=1+i\,dt\,\Gamma_0\left[\Delta_f\dot{\sigma}_f+\frac{i\Delta_f^2}{\beta\hbar}+\cdots\right]\;, \tag{2.24b}$$

where $\dot{\Sigma}_f=(\beta_x+\beta_{x'})/dt$. In Eq. (2.24 b) β stands for the inverse temperature, not the integration variable. Substituting this result into Eq. (2.22), expanding the integrand in powers of β_i, performing the integrations and subtracting $J_r(t,0)$ we easily obtain the same master equation Eq. (2.13a) in this Markovian limit. We are, in fact, redoing the calculation of Caldeira and Leggett in a slightly different way.

In the general non-Markovian case, to complete the third step of our calculation, we have to compute the path integral in Eq. (2.23) and identify the function W defined in (2.24a). This function will carry a nonstandard dependence on the end points. Until now we have made no assumption on the particular form of the external potential in $S[x]$. In fact, Eqs. (2.22) and (2.23) could be derived for any kind of potential. If it is quadratic, as in Eq. (1.1), the calculation can be done exactly since the path integral has a Gaussian integrand. For a nonquadratic potential, to compute the function W we have to make some approximations. In the path-integral formulation, it is easy to do perturbative calculations, e.g., for cases with weak self-interaction.

Let us schematically describe how to compute the path integral in Eq. (2.23). We start by reparametrizing the paths, writing

$$\begin{aligned}&\Sigma(s)=\chi_1(s)+\Sigma_{\rm cl}(s)\;,\\ &\Delta(s)=\chi_2(s)+\Delta_{\rm cl}(s)\end{aligned} \tag{2.25a}$$

where the "classical paths" $\binom{\Sigma}{\Delta}_{\rm cl}$ are solutions to the equations of motion derived from the real part of $A[\Sigma,\Delta]$. The equations governing these functions are

$$\begin{aligned}&\ddot{\Sigma}_{\rm cl}(s)+\Omega^2\Sigma_{\rm cl}(s)+2\int_0^s ds'\eta(s-s')\Sigma_{\rm cl}(s')=0\;,\\ &\Sigma_{\rm cl}(0)=\Sigma_i\quad\text{and}\quad\Sigma_{\rm cl}(t)=\Sigma_m\end{aligned} \tag{2.25b}$$

and

$$\begin{aligned}&\ddot{\Delta}_{\rm cl}(s)+\Omega^2\Delta_{\rm cl}(s)+2\int_s^t ds'\eta(s'-s)\Delta_{\rm cl}(s')=0\;,\\ &\Delta_{\rm cl}(0)=\Delta_i\quad\text{and}\quad\Delta_{\rm cl}(t)=\Delta_m\;.\end{aligned} \tag{2.25c}$$

After the path reparametrization, Eq. (2.23) can be rewritten as

$$\tilde{J}_r(x_m,x_m',t|x_i,x_i',0;[\mathbf{b}])=\tilde{J}_r(0,0,t|0,0,0;[\mathbf{b}])\exp\left[i\left[A[\Sigma_{\rm cl},\Delta_{\rm cl}]-dt\int_0^t ds\,J_\Sigma(s)\Sigma_{\rm cl}(s)+i\,dt\int_0^t ds\,J_\Delta(s)\Delta_{\rm cl}(s)\right]\right]\;, \tag{2.26}$$

where

$$\tilde{J}_r(0,0,t|0,0,0;[\mathbf{b}])=\int_{0;\chi_1=0}^{t;\chi_1=0}D\chi_1\int_{0;\chi_2=0}^{t;\chi_2=0}D\chi_2\exp\left[i\left[\int_0^t ds_1\int_0^t ds_2\tfrac{1}{2}\boldsymbol{\chi}(s_1)\hat{O}(s_1,s_2)\boldsymbol{\chi}(s_2)+\int_0^t ds\,\boldsymbol{\chi}(s)\cdot\mathbf{B}(s)\right]\right]\;. \tag{2.27}$$

In this last functional integral, we have introduced the vectors

$$\chi=\begin{bmatrix}\chi_1\\ \chi_2\end{bmatrix} , \tag{2.28a}$$

$$\mathbf{B}=\begin{bmatrix}-dt\,J_\Sigma\\ i\,dt\,J_\Delta+i\tilde{J}_\Delta\end{bmatrix} , \tag{2.28b}$$

where $\tilde{J}_\Delta$ is a new source which appears because of the nonlocality of the influence functional. It couples the "classical paths" to the χ_i paths

$$\tilde{J}_\Delta(s)=\int_0^t ds'\Delta_{\rm cl}(s')\nu(s-s') . \tag{2.28c}$$

The matrix operator $\hat{O}$ in Eq. (2.27) is defined as follows:

$$\begin{aligned}
&O_{11}(s_1,s_2)=0,\quad O_{22}(s_1,s_2)=2i\nu(s_1,s_2) ,\\
&O_{12}(s_1,s_2)=\left[\frac{d^2}{ds_1^2}+\Omega^2\right]\delta(s_1-s_2)+2\theta(s_2-s_1)\eta(s_1-s_2) ,\\
&O_{21}(s_1,s_2)=\left[\frac{d^2}{ds_1^2}+\Omega^2\right]\delta(s_1-s_2)+2\theta(s_1-s_2)\eta(s_1-s_2) .
\end{aligned} \tag{2.28d}$$

The Gaussian path integral in Eq. (2.27) can be computed in terms of the inverse of the operator $\hat{O}$, which we will call $G=\hat{O}^{-1}$. One can easily show that $G_{22}=0$ and (with some patience) deduce the following result valid up to first order in dt:

$$\tilde{J}_r(0,0,t|0,0,0;[\mathbf{b}])\simeq Z_0(t)\left[1+\frac{dt}{2}\int_0^t ds_1\int_0^t ds_2 J_\Sigma(s_1)\left[G_{12}(s_1,s_2)+G_{21}(s_2,s_1)\right]\tilde{J}_\Delta(s_2)\right] , \tag{2.29}$$

where $Z_0(t)$ is a normalization constant. The Green's functions G_{ab} satisfy the following equations:

$$\frac{d^2}{ds_1^2}G_{12}(s_1,s_2)+\Omega^2G_{12}(s_1,s_2)+2\int_0^{s_1}d\tau\,\eta(s_1-\tau)G_{12}(\tau,s_2)=\delta(s_1-s_2) \tag{2.30a}$$

with the boundary conditions $G_{12}(0,s_2)=G_{12}(s_1,t)=0$. The equations for G_{21} are analogous.

With this we derive an expression for the function W in Eq. (2.24a) as

$$\begin{aligned}
W[x_m,x_m';x_i,x_i',dt]=1+\frac{dt}{2}\Bigg[&-2i\int_0^t ds\,J_\Sigma(s)\Sigma_{\rm cl}(s)-\int_0^t ds\,J_\Delta(s)\Delta_{\rm cl}(s)\\
&+\int_0^t ds_1\int_0^t ds_2 J_\Sigma(s_1)[G_{12}(s_1,s_2)+G_{21}(s_2,s_1)]\tilde{J}_\Delta(s_2)\Bigg] .
\end{aligned} \tag{2.31}$$

Some more work is required to finish the third step of the derivation: the dependence of W on the end points is hidden in the classical solutions $\Sigma_{\rm cl}$ and $\Delta_{\rm cl}$. In order to make this dependence explicit, we can write the classical solutions in terms of elementary functions $u_a(s)$ and $v_a(s)$, $a=1,2$ which are solutions to Eqs. (2.25) satisfying the boundary conditions

$$\begin{aligned}
&u_1(s=0)=1=u_2(s=t) ,\\
&u_1(s=t)=0=u_2(s=0) .
\end{aligned} \tag{2.32}$$

If we define the functions v_a as $v_1(s)=u_2(t-s)$ and $v_2(s)=u_1(t-s)$, we obtain a set of two solutions to Eq. (2.25b). The classical solutions $\Sigma_{\rm cl}$ and $\Delta_{\rm cl}$ can then be written in terms of these elementary functions as

$$\Sigma_{\rm cl}(s)=\Sigma_i u_1(s)+\Sigma_m u_2(s) , \tag{2.33a}$$

$$\Delta_{\rm cl}(s)=\Delta_i v_1(s)+\Delta_m v_2(s) . \tag{2.33b}$$

Substituting (2.31) into Eq. (2.24a) completes the third step of the calculation. Note that the Green's functions G_{ab} can also be written in terms of these elementary functions as

$$G_{12}(s_1,s_2)=[u_1(s_1)u_2(s_2)\theta(s_1-s_2)-u_2(s_1)u_1(s_2)\theta(s_2-s_1)](\dot{u}_1u_2-u_1\dot{u}_2)^{-1}(s_2) . \tag{2.34}$$

A similar expression for G_{21} can be written in terms of v_i. We can now put all the results we have obtained so far into the following equation for the evolution operator $J_r(t+dt,0)$:

$$J_r(x_f,x_f',t+dt|x_i,x_i',0)$$
$$=N(t)\int_{-\infty}^{+\infty}d\beta_x\int_{-\infty}^{+\infty}d\beta_x'\exp\left[\frac{i}{2\,dt}(\beta_x^2-\beta_{x'}^2)\right]\{1+i\,dt[V(x_f)-V(x_f')]\}J_r(x_m,x_m',t|x_i,x_i',0)$$
$$\times(1+dt\{i\Delta_f[d_1(t)\sigma_i+d_2(t)\sigma_f]+[e_2(t)-c_1(t)]\Delta_i\Delta_f+[e_1(t)-c_2(t)]\Delta_f^2\})\ , \tag{2.35}$$

where the time-dependent coefficients are defined as

$$c_i(t)=\int_0^t ds_1\int_0^t ds_2\int_0^t ds_3\,\eta(t-s_1)[G_{12}(s_1,s_2)+G_{21}(s_2,s_1)]\nu(s_2-s_3)u_i(s_3)\ , \tag{2.36a}$$

$$d_i(t)=2\int_0^t ds\,\eta(t-s)u_i(s)\ , \tag{2.36b}$$

$$e_i(t)=\int_0^t ds\,\nu(s)u_i(s)\ . \tag{2.36c}$$

(4) The fourth step of the derivation consists of expanding every term in powers of β_x and $\beta_{x'}$ (using for example $x_m=x_f-\beta_x$), performing the integration and finally subtracting $J_r(t,0)$. After these calculations we obtain

$$i\frac{\partial}{\partial t}J_r(x_f,x_f',t|x_i,x_i',0)=\left\{\left[-\frac{1}{2}\left[\frac{\partial^2}{\partial x_f^2}-\frac{\partial^2}{\partial x_f'^2}\right]+\frac{1}{2}\Omega^2(x_f^2-x_f'^2)\right]\right.$$
$$\left.-\{d_1(t)\Sigma_i\Delta_f+d_2(t)\Sigma_f\Delta_f-i[e_2(t)-c_1(t)]\Delta_i\Delta_f-i[e_1(t)-c_2(t)]\Delta_f^2\}\right\}J_r(x_f,x_f',t|x_i,x_i',0)\ . \tag{2.37}$$

This equation is almost what we want. To obtain the master equation, we would have to multiply both sides by $\rho_r(x_i,x_i',0)$ and integrate over the initial coordinates x_i and x_i'. However, due to the fact that the right-hand side of Eq. (2.37) contains an explicit dependence on the initial coordinates (through the terms containing Σ_i and Δ_i) we still need to do some extra manipulations. This is our fifth step.

(5) Using Eq. (2.26) (for the case $\mathbf{b}=0$), we can derive the following useful relations (they are valid only if the external potential is quadratic; in the more general case we can obtain analogous equations via perturbation theory):

$$\Delta_i J_r(t,0)=\left[\frac{\dot u_2(t)}{\dot u_2(0)}\Delta_f+\frac{i}{\dot u_2(0)}\frac{\partial}{\partial\Sigma_f}\right]J_r(t,0) \tag{2.38a}$$

and

$$\Sigma_i J_r(t,0)=\left[-\frac{\dot u_2(t)}{\dot u_1(t)}\Sigma_f-i\left[\frac{4a_{11}(t)}{\dot u_1(t)}+\frac{2a_{12}(t)}{\dot u_1(t)}\frac{\dot u_2(t)}{\dot u_2(0)}\right]\Delta_f-\frac{i}{\dot u_1(t)}\frac{\partial}{\partial\Delta_f}+\frac{2a_{12}(t)}{\dot u_1(t)\dot u_2(0)}\frac{\partial}{\partial\Sigma_f}\right]J_r(t,0)\ , \tag{2.38b}$$

where we have defined the time-dependent coefficients a_{ij} as

$$a_{ij}(t)=\tfrac{1}{2}\int_0^t ds_1\int_0^t ds_2\,u_i(s_1)\nu(s_1-s_2)u_2(s_2)\ . \tag{2.39}$$

Substituting Eq. (2.38) into Eq. (2.37), multiplying by $\rho_r(x_i,x_i',0)$ and integrating over the initial coordinates, we obtain our final result, the master equation:

$$i\hbar\frac{\partial}{\partial t}\rho_r(x,x't)=\left[-\frac{\hbar^2}{2}\left[\frac{\partial^2}{\partial x^2}-\frac{\partial^2}{\partial x'^2}\right]+\frac{1}{2}\Omega^2(x^2-x'^2)\right]\rho_r(x,x',t)+\frac{1}{2}\delta\Omega^2(t)(x^2-x'^2)\rho_r(x,x',t)$$
$$-i\hbar\Gamma(t)(x-x')\left[\frac{\partial}{\partial x}-\frac{\partial}{\partial x'}\right]\rho_r(x,x',t)-i\Gamma(t)h(t)(x-x')^2\rho_r(x,x',t)$$
$$+\hbar\Gamma(t)f(t)(x-x')\left[\frac{\partial}{\partial x}+\frac{\partial}{\partial x'}\right]\rho_r(x,x',t)\ , \tag{2.40}$$

where the time-dependent coefficients are given by

$$\Gamma(t)=\frac{d_1(t)}{2\dot{u}_1(t)}\ , \tag{2.41a}$$

$$\delta\Omega^2(t)=d_2(t)-2\Gamma(t)\dot{u}_2(t)\ , \tag{2.41b}$$

$$f(t)=2\frac{a_{12}(t)}{\dot{u}_2(0)}+\frac{e_2(t)-c_1(t)}{2\Gamma(t)\dot{u}_2(0)}\ , \tag{2.41c}$$

$$h(t)=\dot{u}_2(t)f(t)+8a_{11}(t)+\frac{e_1(t)-c_2(t)}{\Gamma(t)}\ . \tag{2.41d}$$

The coefficients c_i, d_i, e_i, a_{ij} $(i,j=1,2)$ are defined, respectively, in equations (2.36a)–(2.36c) and (2.39). Their time dependence is generally complicated by integrals of the elementary functions u_i with the noise and/or dissipation kernels.

In Eq. (2.40), the first term on the RHS corresponds to the usual unitary Liouvillian evolution. The second term corresponds to a time-dependent frequency shift (or frequency renormalization). The third term is a dissipative term with a time-dependent dissipative constant $\Gamma(t)$. The last two terms are diffusive terms with time-dependent coefficients. This equation is exact.

It is worth noticing that the frequency shift and the dissipation coefficient depend only on the dissipation kernel while the diffusion coefficients are primarily dependent on the noise kernel. The former two depend on the dissipation kernel in two different ways: first, explicitly through the function d_i and c_i, and second, implicitly through the elementary functions u_i which are determined by the dissipation kernel. All the time-dependent coefficients vanish at $t=0$ when the initial uncorrelated condition is assumed valid.

Let us now briefly explain the implications of the frequency shift $\delta\Omega^2(t)$. The two terms involving the frequency in the equation of motion (2.40) combine as the physical frequency

$$\Omega_p^2(t)=\Omega^2+\delta\Omega^2(t)\ . \tag{2.42}$$

Ω_p^2 acquires a time dependence from $\delta\Omega^2(t)$ and is different from the bare frequency Ω^2. In many physically interesting cases in which the frequency cutoff is much larger than the dynamical frequencies appearing in the action (1.1), the frequency shift approaches a constant value $\delta\Omega^2(\infty)$ at large times. Theoretically, the meaning of frequency renormalization can be understood as follows: We can rewrite the action (1.1) as

$$S=\int_0^t ds\left\{\frac{1}{2}M(\dot{x}^2-\Omega^2x^2)+\sum_n\left[\frac{1}{2}m_n\dot{q}_n^2-\frac{1}{2}m_n\omega_n^2\left[q+\frac{C_n}{m_n\omega_n^2}x\right]^2+\frac{1}{2}\frac{C_n^2}{m_n\omega_n^2}x^2\right]\right\}\ . \tag{2.43}$$

The last term can be viewed as a frequency counterterm Ω_c^2 arising from the interaction of the Brownian particle with the bath oscillators

$$\Omega_c^2=-\frac{1}{2M}\sum_n\frac{C_n^2}{m_n\omega_n^2}=-\int d\omega\frac{I(\omega)}{\omega}\ . \tag{2.44}$$

The bare frequency Ω^2 is thus modified into a renormalized frequency Ω_r^2 given by

$$\Omega_r^2=\Omega^2+\Omega_c^2\ . \tag{2.45}$$

Operationally, in practical calculations, one can start by setting the renormalized frequency Ω_r to a certain value (unity here), assume a spectral density function $I(\omega)$ such as (1.3), calculate Ω_c from (2.44), and compute $\delta\Omega^2(t)$ via the intermediate coefficients $d_i(t)$, $e_i(t)$, $a_{ij}(t)$, $c_i(t)$. In all cases studied, at large times $\delta\Omega^2\simeq\Omega_c^2$ (for the $n=\frac{1}{2}$ cases shown on the figures, it has not yet reached the asymptotic values in the time range of integration). Thus one can view the physical frequency as equal to the renormalized frequency at late times. Note that the distinction between the physical frequency and the renormalized frequency exists for non-Markovian processes only, owing to the nonlocal time-dependence of the coefficients in the master equation. For Markovian processes the frequency shift is time independent and $\Omega_p=\Omega_r$ modulo a constant which can be set to zero.

A simpler formula for the time-dependent coefficients in the master equation can be found in the weak-coupling limit. If all the terms containing products of two kernels are neglected (we work up to the second order in the coupling constant between the system and the environment), the following expressions are obtained:

$$\delta\Omega^2(t)=2\int_0^t ds\ \eta(s)\cos\Omega s\ , \tag{2.46a}$$

$$\Gamma(t)=-\frac{1}{\Omega}\int_0^t ds\ \eta(s)\sin\Omega s\ , \tag{2.46b}$$

$$\Gamma(t)f(t)=\frac{1}{\Omega}\int_0^t ds\ \nu(s)\sin\Omega s\ , \tag{2.46c}$$

$$\Gamma(t)h(t)=\int_0^t ds\ \nu(s)\cos\Omega s\ . \tag{2.46d}$$

From the master equation (2.40) it is easy to derive the equation for the Wigner distribution function.

$$F_W(\Sigma,p,t)=\int_{-\infty}^{+\infty}d\Delta\,\rho_r\left[\Sigma-\frac{\Delta}{2},\Sigma+\frac{\Delta}{2},t\right]\exp\left[\frac{i}{\hbar}p\Delta\right]\ . \tag{2.47}$$

It obeys the following Fokker-Planck type equation [27]:

$$\frac{\partial}{\partial t}F_W(\Sigma,p,t)=\left[-p\frac{\partial}{\partial\Sigma}+[\Omega^2+\delta\Omega^2(t)]\Sigma\frac{\partial}{\partial p}+\Gamma(t)\frac{\partial}{\partial p}p+2\Gamma(t)h(t)\frac{\partial^2}{\partial p^2}-2\Gamma(t)f(t)\frac{\partial^2}{\partial\Sigma\partial p}\right]F_W(\Sigma,p,t)\ . \tag{2.48}$$

In summary, the recipe to derive the coefficients of the master equation for QBM in an environment with a spectral density $I(\omega)$ is as follows. First, compute the dissipation kernel using (2.7). Second, solve the classical equations (2.25) that define the elementary functions $u_i(s)$.

These equations are generally nonlocal. In some examples, the precise form of the elementary solutions can be obtained by making use of Laplace-transform techniques; otherwise, numerical work may be necessary. Once we obtain the form of the elementary functions, the third and last step is to compute the coefficients by using the previous formulas, which involve integrations of the noise and dissipation kernels.

III. ANALYSIS AND EXAMPLES

In this section we will first analyze the form of the time-dependent coefficients in the master equation for ohmic and nonohmic environments. Then, as a simple example we calculate the decay of the interference between two Gaussian wave packets in a general environment. This generalizes previous results of Calderia and Leggett [8] for an ohmic environment. Finally, in the discussion we point out that the short-time peak present in all cases is probably an artifact of the factorizable initial condition, and we recommend caution in trusting the generality of previous conclusions on decoherence based on such assumptions.

A. Analysis

1. Ohmic environment

We will assume that the spectral density is given by a function like Eq. (1.3) with $n=1$. It is also possible to consider other ohmic environments with different functional dependence on the cutoff, but as the spectral density is essentially the same in the relevant range $\omega<\Lambda$, all these environments give physically equivalent results. We also analyzed the Drudes model [30], a case for which $I(\omega)\propto\omega(\omega^2+\Lambda^2)^{-1}$, but found no difference from the results obtained for the exponential cutoff.

Before discussing our numerical results, let us first consider the purely ohmic environment without a cutoff, i.e., $I(\omega)=(2/\pi)M\gamma_0\omega$. Despite its unphysical nature, its simplicity enables one to explicitly compute all the coefficients in the master equation. In fact, the dissipation kernel in this case is simply

$$\eta(t)=\gamma'(t)=\gamma_0\delta'(t) \ . \tag{3.1}$$

Using this equation for the formulas given in the last section, one sees that Eq. (2.25a) for the elementary solutions $u_i(s)$ reduces to the following differential equation:

$$\ddot{u}_i+\Omega_r^2u_i+\gamma_0\dot{u}_i=-2\gamma_0\delta(t)u_i(0) \ . \tag{3.2}$$

The functions $u_i(s)$ and the Green functions G_{ab} are thus easily calculable. Using all the equations given in Sec. II, a few algebraic manipulations give the coefficients of the master equation:

$$\Gamma(t)=\gamma_0 \ , \tag{3.3a}$$

$$\delta\Omega^2(t)=-2\gamma_0\delta(0) \ , \tag{3.3b}$$

$$\gamma_0 f(t)=\frac{1}{\Omega}\int_0^t ds\,\sin\tilde{\Omega}s\,e^{-\gamma_0 s}\nu(s) \ , \tag{3.3c}$$

$$h(t)=g(t)-\gamma_0 f(t) \ , \tag{3.3d}$$

where $\tilde{\Omega}^2=\Omega^2-\gamma_0^2$, and

$$\gamma_0 g(t)=\int_0^t ds\,\cos\tilde{\Omega}t\,e^{-\gamma_0 s}\nu(s) \ . \tag{3.3e}$$

The noise kernel is given by

$$\nu(t)=\gamma_0\int_0^{+\infty}\frac{d\omega}{\pi}\omega\coth\tfrac{1}{2}\beta\omega\cos\omega t \ . \tag{3.4}$$

Assuming that the environment does not have a high-frequency cutoff means that the bath can dissipate instantaneously. This unphysical property generates pathology in the coefficients in the master equation in that they are not continuous functions of time, but jump at $t=0$. This initial discontinuity is evident in the dissipative coefficient $\Gamma(t)$ and in the frequency shift of Eqs. (3.3a)–(3.3b). The diffusive coefficients also suffer a similar disease, since the frequency integral in the noise kernel is divergent.

The coefficients that appear in the master equation of Ref. [7] are given precisely by Eq. (3.3). To avoid the divergencies in the frequency integrals and make the diffusive coefficients well defined, Unruh and Zurek used a regularized noise kernel given by

$$\nu(t)=\int_0^{+\infty}\frac{d\omega}{\pi}e^{-\omega^2/\Lambda^2}\omega\coth\tfrac{1}{2}\beta\omega\cos\omega t \ . \tag{3.5}$$

However, this procedure violates the fluctuation-dissipation relation Eq. (2.11) since the dissipative kernel is not modified in a consistent way. Instead, introducing the cutoff in the spectral function (what we have called a regularized ohmic environment) preserves the relation.

We have numerically calculated the coefficients of the master equation given by Eq. (2.41). The general behavior of the two temperature-independent coefficients $\Gamma(t)$ and $\delta\Omega^2(t)$ is depicted in Figs. 1 and 2(a) respectively (see curve *a* in both figures). The parameter space of the problem is rather big and there is a variety of cases that could be analyzed. We only pick a simple representative case to discuss the differences with the results of Unruh and Zurek and compare later with the nonohmic environment. The parameters chosen are such that the renor-

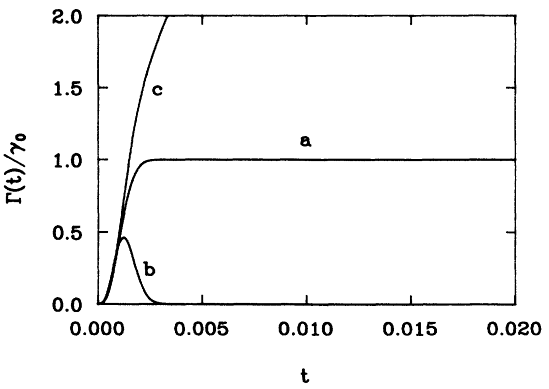

FIG. 1. The dissipative coefficient for the *a* ohmic ($n=1$), *b* supraohmic ($n=3$), and *c* subohmic ($n=\frac{1}{2}$) environments. The parameters are measured in units of the renormalized frequency Ω_r which is set to unity [see Eq. (2.45)]. We consider the cases $\gamma_0=0.3$, $\Lambda=2000$.

malized frequency is fixed to be 1 (i.e., everything is measured in units of this frequency). The relaxation constant is $\gamma_0=0.3$ and the cutoff frequency is $\Lambda=2000$. The bare frequency Ω is determined from the renormalized one using the procedure explained in the previous section. Note that at late times $\Omega_p^2=\Omega^2+\delta\Omega^2\rightarrow\Omega_r^2=1$ [see Fig. 2(b)].

The two coefficients in Figs. 1 and 2 grow very fast on a time scale equal to the inverse cutoff frequency $t=\Lambda^{-1}=5\times10^{-4}$ and approach their asymptotic limit very fast. A similar kind of behavior is observed for other choices of parameters whenever the condition $\Lambda\gg\Omega_r$, γ_0 is satisfied. Otherwise the behavior is highly unstable. Our results for the parameters outside this range differ drastically from Ref. [7], which used (3.3). The coefficients used there are precisely given by the asymptotic form of $\Gamma(t)$ and $\Omega^2+\delta\omega^2(t)$. Thus, despite the inconsistency in the choice of the cutoff, their results are quite accurate in this case.

The behavior of the temperature-dependent diffusive coefficient (Γh) is plotted in Figs. 3 and 4 for low temperature ($T=10$) and high temperature ($T=10^5$), respectively, where curve *a* corresponds to the ohmic case. The corresponding plots for the coefficient (Γf) appear in Figs. 5 and 6. The coefficients again grow very fast in a very short time scale fixed by the cutoff. The initial growth develops into a peak in the low-temperature case and the coefficient tends to a smaller value at late times. In the high-temperature case there is no peak since the coefficient grows steadily until it reaches the expected asymptotic value (i.e., $\Gamma h=2\gamma_0 k_B T$). Both for short and long times, the behavior of the diffusive coefficients in Ref. [7] is in agreement with ours. We also found that the form of the peak is rather parameter independent. The "jolt" that appears in Fig. 3 for the diffusive coefficient has been taken to be responsible for the quick diagonalization of the reduced density matrix.

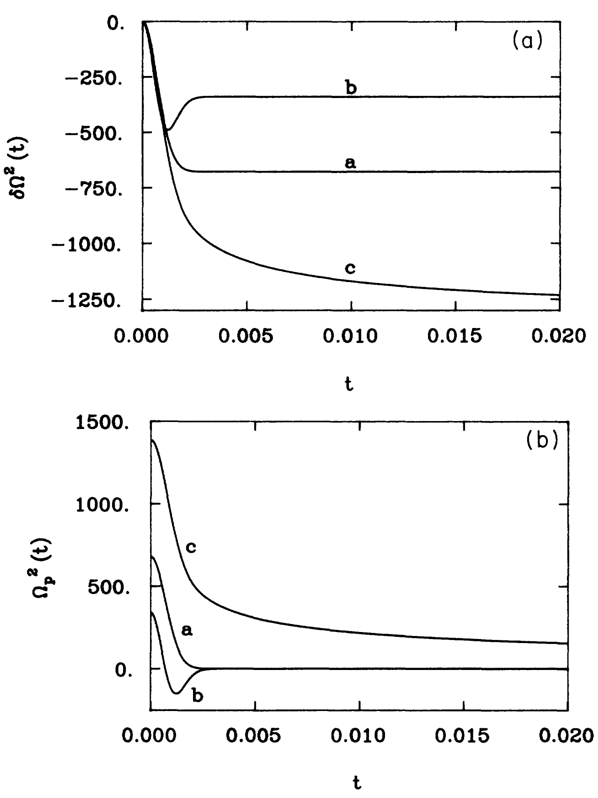

FIG. 2. (a) The frequency shift for the *a* ohmic ($n=1$), *b* supraohmic ($n=3$), and *c* subohmic ($n=\frac{1}{2}$) environments. The parameters are $\Omega_r=1$, $\gamma_0=0.3$, $\Lambda=2000$. The asymptotic value of this coefficient determines the value of the counterterm we have to add in the original action. (b) The physical frequency for the *a* ohmic ($n=1$), *b* supraohmic ($n=3$), and *c* subohmic ($n=\frac{1}{2}$) environments. The parameters are $\Omega_r=1$, $\gamma_0=0.3$, $\Lambda=2000$, $T=10$. The asymptotic value of the physical frequency is equal to the renormalized frequency which is set to unity.

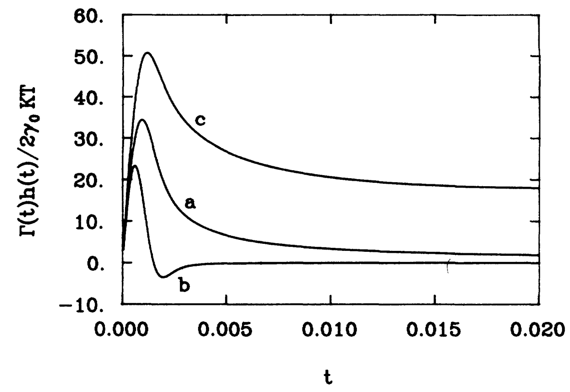

FIG. 3. The coefficient of the normal diffusion term for low temperatures in units of $2\gamma_0 k_B T$. The parameters are $\Omega_r=1$, $\gamma_0=0.3$, $\Lambda=2000$, $T=10$. The three curves correspond to the *a* ohmic ($n=1$), *b* supraohmic ($n=3$) and *c* subohmic ($n=\frac{1}{2}$) environments.

2. Nonohmic environment

Here we will examine the behavior of the coefficients of the master equation for two different nonohmic environ-

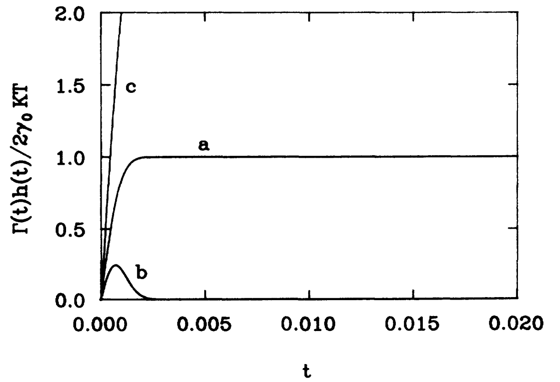

FIG. 4. The coefficient of the normal diffusion term for high temperatures in units of $2\gamma_0 k_B T$. The parameters are $\Omega_r=1$, $\gamma_0=0.3$, $\Lambda=2000$, $T=10^5$. The three curves correspond to the *a* ohmic ($n=1$), *b* supraohmic ($n=3$), and *c* subohmic ($n=\frac{1}{2}$) environments.

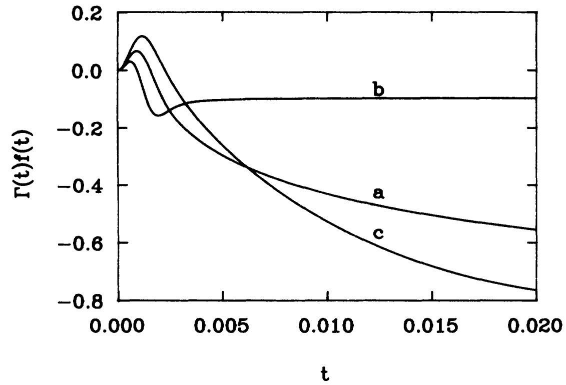

FIG. 5. The coefficient $\Gamma(t)f(t)$ of the second diffusion term in the low-temperature case. The parameters are $\Omega_r=1$, $\gamma_0=0.3$, $\Lambda=2000$, $T=10$. The three curves correspond to the a ohmic ($n=1$), b supraohmic ($n=3$), and c subohmic ($n=\frac{1}{2}$) environments.

ments. They are the supraohmic and the subohmic cases corresponding to a spectral density like Eq. (1.3) with $n>1$ and $n<1$ respectively. We will explicitly consider the $n=3$ and $n=\frac{1}{2}$ cases with the same choice of parameters as in the ohmic case. Here again, the renormalized frequency Ω_r is fixed to unity (the counterterm one has to introduce in the original action depends upon the environment).

From physical considerations we expect the subohmic environment to be more strongly dissipative since in that case the spectral density is greater in the resonant region $\omega\simeq\Omega_r$ than in the ohmic or supraohmic cases. In contrast, the supraohmic environment should be only weakly dissipative since the infrared sector is less important while the ultraviolet is highly suppressed by the cutoff. This qualitative picture is confirmed by our numerical results. The curves b and c of Figs. 1–6 correspond to the supraohmic ($n=3$) and subohmic ($n=\frac{1}{2}$) cases, respectively.

The dissipative coefficient for the supraohmic case displayed in Fig. 1 tends to zero at late times but it develops a jolt in the cutoff time scale. The same coefficient has a rather different behavior in the subohmic environment. In that case it grows fast in the cutoff time scale but seems to continue growing at later times (we still do not fully understand this time dependence which seems to suggest that the environment is acting more and more dissipatively as time goes by). The behavior of the frequency shift shown in Fig. 2 is not surprising and does not differ drastically from the ohmic case (although for the subohmic environment the asymptotic regime is approached slower). The asymptotic value of the frequency shift is what fixes the counterterm we have to use in the original action for a given renormalized frequency.

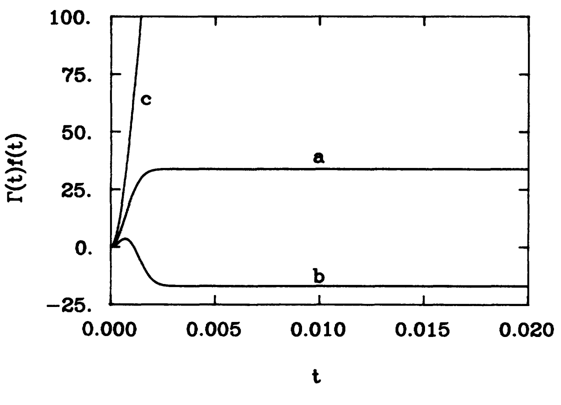

FIG. 6. The coefficient $\Gamma(t)f(t)$ of the second diffusion term in the high-temperature case. The parameters are $\Omega_r=1$, $\gamma_0=0.3$, $\Lambda=2000$, $T=10^5$. The three curves correspond to the a ohmic ($n=1$), b supraohmic ($n=3$) and c subohmic ($n=\frac{1}{2}$) environments.

As for the effects of the environment on decoherence, the relevant quantities to study are the diffusion coefficients plotted in Figs. 3 and 4. There, we can also see that in all cases this coefficient grows in the cutoff timescale and develops a jolt at low temperatures. This peak is sufficient to produce a fast diagonalization of the reduced density matrix which in the very short time scale Λ^{-1} is comparable to the one obtained for the ohmic environment. This initial "jolt" is always there, even for the supraohmic case both at high and low temperature (a case in which the asymptotic value of the diffusive coefficient Γh is zero).

For the supraohmic environment, our numerical calculation confirms the analytic result for the time evolution of the diffusive coefficient under the "weak-coupling" approximation. In fact, if we consider an environment whose spectral density is given by Eq. (1.3) with odd n, the noise kernel is simply

$$\nu_n(s)=\frac{(-1)^{n/2}}{\Lambda^n}\frac{d^n}{ds^n}\nu_0(s) \tag{3.6}$$

and the normal diffusive coefficient, up to first order in γ_0 and Ω/Λ becomes

$$\Gamma h_n(t)=\frac{(-1)^{n/2}}{\Lambda^n}\frac{d^{n-1}}{dt^{n-1}}\nu_0(t)\ . \tag{3.7}$$

In the high-temperature limit, as the expression for the noise kernel simplifies, we obtain for the case $n=2$ the diffusive coefficient:

$$\Gamma h_n(t)\simeq\frac{4\gamma_0}{\beta}\Lambda t e^{-\Lambda^2 t^2}\ . \tag{3.8}$$

Similar expressions are obtained for other values of n. The asymptotic properties of the QBM problem with supraohmic environments have been analyzed by other authors [4] with conclusions that are consistent with ours.

For the subohmic environment the presence of the initial "jolt" is also quite dramatic at low temperatures as can be seen in Fig. 3. (At high temperatures, as in the ohmic case, the peak is not observed. This is because the diffusive coefficient grows steadily until at late times, where its time dependence becomes similar to the dissipative coefficient as displayed in Fig. 1.)

What is the effect of this ubiquitous peak in the diffusive coefficient on decoherence? In a coarse approximation we could solve Eq. (2.40) considering just the influence of the normal diffusive coefficient and obtain

$$\rho_r(x,x',t)\simeq\rho_r(x,x',t_0)\exp\left[-(x-x')^2\int_0^t(\Gamma h)(t')dt'\right] . \tag{3.9}$$

From our results it is easily seen that, in a time scale of the order of Λ^{-1}, the nondiagonal elements of the density matrix are damped by a factor that is similar in all the cases considered ($n=\frac{1}{2},1,3$). For example, for the $n=3$ supraohmic environment in the high-temperature regime, the nondiagonal elements are damped by a factor $\exp\{-[(x-x')^2/\lambda_{\rm dB}^2]\gamma_0/\Lambda\}$ where $\lambda_{\rm dB}$ is the de Broglie wavelength of a particle moving with a momentum $(Mk_BT)^{1/2}$. This damping takes place on a time scale of the order of Λ^{-1} and has the same value as in Unruh and Zurek's ohmic environment. According to the criterion of Refs. [5,7], this is enough to decohere any "macroscopic body." (An example is given by Zurek [5]: with $x-x'=1$ cm, $T=300$ K and $M=1$ g, one gets $(x-x')^2/\lambda_{\rm dB}^2=10^{40}$.) This means that the relaxation time scale can be many orders of magnitude larger than the cutoff scale and the environment can still bring about a strong decoherence.

B. Example: Decoherence of two Gaussian wave packets

As a simple application of the results obtained above and a concrete example of environment-induced decoherence process, we discuss the damping of the interference between two Gaussian wave packets. This textbook-type problem has been studied before [8] for an ohmic environment; our result generalizes to nonohmic environments.

Let $\psi_{1,2}(x,t)$ be the wave functions of Gaussian wave packets 1 and 2 located initially ($t=0$) at $x=\pm x_0$, respectively, with the same initial spread σ,

$$\psi_{1,2}(x,t=0)=Ne^{-(x\pm x_0)^2/4\sigma^2} , \tag{3.10}$$

where N is a normalization constant. The wave function of the system initially is a superposition of these two wave packets,

$$\psi(x,0)=\psi_1(x,0)+\psi_2(x,0) . \tag{3.11}$$

At $t>0$ as the system begins to interact with the environment it is no longer a pure state but is described by a reduced density matrix, which at all t can be written as the sum of three parts

$$\rho_r(x,x',t)=\rho_{r1}(x,x',t)+\rho_{r2}(x,x',t)+\rho_{r\,\rm int}(x,x',t) . \tag{3.12}$$

If the system and the environment are assumed to be decoupled initially, then the reduced density matrix at $t=0$ is $\rho_r(x,x',0)=\rho(x,x',0)$. For a general environment the time evolution of the reduced density matrix is governed by the master equation (2.40). However, for this problem it is not necessary to solve this equation since, due to the linearity of the problem and to the particular form of the initial state, a closed form for $\rho_r(x,x',t)$ can be found by using the exact expression for the propagator $J_r(x_f,x_f',t|x_i,x_i',0)$. Indeed it can just be read off from Eqs. (2.26) and (2.29) by setting **b** (or J_Δ and J_Σ) equal to zero, i.e.,

$$J_r(x_f,x_f',t|x_i,x_i',0)=Z_0(t)\exp\left[\frac{i}{\hbar}A[\Sigma_{\rm cl},\Delta_{\rm cl}]\right] . \tag{3.13}$$

Using the elementary functions $u_a(s)$ and the coefficients $a_{ij}(t)$ for the classical solutions, we get

$$J_r(x_f,x_f',t|x_i,x_i',0)=Z_0(t)\exp\left[\frac{i}{\hbar}\{[\dot u_1(0)\Sigma_i+\dot u_2(0)\Sigma_f]\Delta_i-[\dot u_1(t)\Sigma_i+\dot u_2(t)\Sigma_f]\Delta_f\}\right]$$
$$\times\exp\left[\frac{-1}{\hbar}\{a_{11}(t)\Delta_i^2+[a_{12}(t)+a_{21}(t)]\Delta_i\Delta_f+a_{22}(t)\Delta_f^2\}\right] . \tag{3.14}$$

By the superposition principle, J_r is also the propagator for ρ_{r1}, ρ_{r2}, and $\rho_{r\,\rm int}$. Since aspects of the decoherence process are already manifest in the behavior of the probability density function, it is sufficient for our purpose of illustration here to just examine the diagonal components of $\rho_r(x,x',t)$. The probability density function can also be written as the sum of three parts:

$$P_r(x,t)=\rho_r(x,x,t)=P_{r1}(x,t)+P_{r2}(x,t)+P_{r\,\rm int}(x,t) , \tag{3.15}$$

where

$$P_{ra}(x,t)=\int_{-\infty}^{+\infty}dx_i\int_{-\infty}^{+\infty}dx_i'\,J_r(x,x,t|x_i,x_i',0)\times\rho_{ra}(x_i,x_i',0) \tag{3.16}$$

and the subscript a denotes 1, 2, or int. Performing the Gaussian integration we get these final results:

$$P_{r1,2}(x,t)=\tilde N(t)\exp\left[-\frac{[x\pm x_0(t)]^2}{2\sigma^2(t)}\right] , \tag{3.17}$$

$$P_{r\,\mathrm{int}}(x,t)=2\sqrt{P_{r1}(x,t)}\sqrt{P_{r2}(x,t)}e^{-D(t)}\cos\phi(t)\ , \tag{3.18}$$

where

$$x_0(t)=-\frac{\dot u_1(0)}{\dot u_2(0)}x_0 \tag{3.19}$$

and

$$\sigma(t)=\left[\frac{\dot u_1^2(0)}{\dot u_2^2(0)}+\frac{2a_{11}(t)}{\sigma^2\dot u_2^2(0)}+\frac{1}{4\sigma^4\dot u_2^2(0)}\right]^{1/2} \tag{3.20}$$

are, respectively, the position and spread of the wave packet at time t,

$$\phi(t)=\frac{2x_0[\dot u_2(0)x+\dot u_1(0)x_0]}{1+8a_{11}(t)\sigma^2+4\dot u_1^2(0)\sigma^4} \tag{3.21}$$

is the oscillatory angle (which is present even in the absence of the environment) and

$$D(t)=\frac{4a_{11}x_0^2}{1+8a_{11}\sigma^2+4\dot u_1^2(0)\sigma^4} \tag{3.22}$$

is the decay factor (which is present only because of the environment). It is this last term depicting the decay of interference between the two wave packets which is usually regarded as providing a measure of decoherence. This function initially vanishes [since $a_{11}(t=0)=0$] and in many physically interesting cases will approach a large constant value given by $x_0^2/2\sigma^2$ [this happens whenever the asymptotic value of a_{11} dominates the denominator of (3.22)]. The interference between the two wave packets is considered sufficiently suppressed when $D(t)$ gets close enough to its asymptotic value. In that case, if the two wave packets are well localized individually, the contribution of $P_{r\,\mathrm{int}}$ will be much smaller than the direct terms $P_{r1,2}$ (although it will never be identically zero due to the fact that the initial wave packets are not orthogonal to each other).

We have numerically computed the decay function $\exp[-D(t)]$ for all the cases described in the previous subsection. The results are shown in Fig. 7 for the high- and low-temperature cases. The suppression of the interference occurs extremely fast in the high-temperature limit. Thus, for the ohmic environment this result is consistent with earlier arguments based on the use of the Markovian master equation in estimating how fast the density matrix diagonalizes. In the low-temperature case, decoherence proceeds much slower and to get a more accurate picture it is necessary to numerically integrate over a longer time span than the one considered above. A detailed study of this problem will be presented elsewhere. It is noteworthy that the interaction with the environment produces decoherence at high temperature even in the case of the supraohmic environment, where the final value of the diffusive coefficient vanishes.

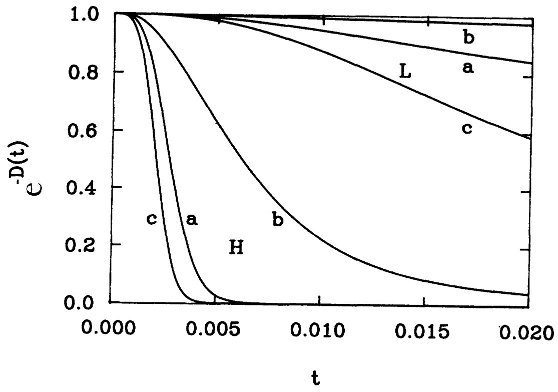

FIG. 7. The decay function $e^{-D(t)}$ for the interference of two Gaussian wave packets located initially at $x_0=\pm0.5$ with spread $\sigma=0.1$ plotted for the *a* ohmic ($n=1$), *b* supraohmic ($n=3$) and *c* subohmic ($n=\frac{1}{2}$) environments at high (H) $T=10^5$ and low (L) $T=10$ temperatures with parameters $\Omega_r=1$, $\gamma_0=0.3$, $\Lambda=2000$.

C. Discussion

We see from the above analysis and example that decoherence occurs in some cases on a very short time scale corresponding to the inverse of the high-frequency cutoff. Duing this time all the coefficients grow fast—including even those that afterwards decay to a vanishing value such as the ones corresponding to the supraohmic environment. The initial "jolt" in the diffusive coefficient is found responsible for the rapid decoherence, be it measured by the suppression of the off-diagonal components of the reduced density matrix, as described in Sec. III A, or the decay of the interference term in the probability density, as described in the above wave-packet example. However, one could question the physical origin and significance of this strong initial jolt. Its persistence for a variety of parameters makes one suspect that it is a consequence of the special initial condition assumed. We are reminded that a totally uncorrelated initial state is assumed in most discussions more for its computational simplicity than for its physical practicality. What happens to the initial jolt if the initial state contains some correlations between the system and the environment? We think it is not unlikely that initial correlations could tend to smooth out the behavior of the coefficients and make the jolt smaller if not eliminated. This is an important question which deserves further exploration, as it may separate the effectiveness of decoherence from the specificity of the initial conditions.

If one tries to compute the decoherence time scale for low temperatures or nonohmic environments it is necessary to take into account the existence of initial correlations or to discount the effect produced by the initial jolt caused by the absence of initial correlations. Previous estimates for the decoherence time made by using the Markovian equations [5] are confirmed by our work and are reliable—in that case (ohmic high-temperature) the initial jolt is not present (as is seen in Fig. 4, curve *a*) and the result is free from this suspicion. In the non-Markovian cases where the jolt is present, its effect on decoherence can be studied along the lines we described here by analyzing the results of longer time runs covering regimes intermediate between the cutoff and the dynamical time scales. It is evident from our results that the behavior in the long-time regime could be drastically different in the sub- and supraohmic cases. This is expected also from previous calculations such as the ones performed by Leggett and collaborators [2]. There they considered the effect of dissipation on the coherent tunneling of a two-level system modeled by a spin-$\frac{1}{2}$ particle bilinearly coupled to a bath of harmonic oscillators with a general spectral density $I(\omega)$. Their results indicate a surprisingly strong dependence on the spectral density: For subohmic environments ($0<n<1$ in our notation) coherence is always lost (the environment, in the words of Ref. [5], "measures" the state of the system and localizes it) while for high supraohmic ($n>2$) environments, coherence is never lost (the "measurement" interaction is not strong enough). There is a crossover region ($1<n<2$) including the ohmic case, in which the behavior of the system depends on the strength of the coupling (the behavior is different in the weak- and strong-coupling regime). Our present study for a general environment brings up, among other issues, such inquiries on the meaning and effectiveness of decoherence and how it could depend on the initial correlations. We plan to pursue some of these issues in the future.

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