Exact results for a damped quantum-mechanical harmonic oscillator

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Exact calculations for a quantum oscillator linearly coupled to a thermal reservoir are presented. Explicit results (variances and correlations) for the response and the spontaneous fluctuations are evaluated for two different models of the heat bath; a reservoir with a spectrum which is similar to that of acoustic phonons and another which is analogous to optic phonons. The low-temperature behavior is shown to depend sensitively on the spectral density of the thermal reservoir. The mass and the frequency of the oscillator become renormalized through the coupling to the bath. These renormalizations are intrinsically frequency dependent. Moreover, the commonly used form of Ehrenfest's equation for the dynamics of the linearly damped oscillator is shown to only be a reasonable approximation within certain frequency regimes.

I. INTRODUCTION

The dynamics of a quantum-mechanical particle coupled to a heat bath has been the subject of great interest, and has a long history.[1-4] These systems form archetypes for many important processes, where quantum-mechanical systems equilibrate with a heat bath. The coupling to the heat bath can have important consequences on the dynamics of the system, by altering the effective potential in which the particle moves, as well as by allowing energy to be exchanged with the thermal reservoir, thereby allowing the system to attain thermal equilibrium. Recently, there has been a resurgence of interest in this problem.[5-11] Caldeira and Legget[5,7] have shown that the coupling to the heat bath can be eliminated, at the expense of including a retarded term into the effective Lagrangian. The motion of a particle subjected to this kind of dynamics presents us with both technical and conceptual difficulties. Perhaps, the greatest difficulty is that of reconciling our classical notions of energy dissipation with our quantum-mechanical notions. For example, it is well known that a quantum system in its ground state cannot dissipate energy, whereas a system in the excited state can. This dissipation of energy can be completely dissociated from the value of the expectation value of the linear momentum of the particle. Likewise, both the ground state and the excited states can have finite mean square fluctuations in the momentum. Even the energy which is dissipated can come from changes in the energy associated with both the displacement and momentum degrees of freedom. Our classical concepts relate the dissipation of energy directly to the presence of a nonzero momentum.

In order to clarify some of these issues, we shall address the simplest model of a quantum-mechanical system that one can envisage.[2] Namely, we shall investigate some of the dynamic properties of a harmonic oscillator, which is coupled via its displacement q, to a thermal reservoir composed of an infinite number of independent harmonic oscillators. This form for the heat bath, was used by Caldeira and Leggett[5,7] in the problem of macroscopic quantum tunneling. The independent oscillators are assumed to represent all the normal modes of the infinite heat bath. As a consequence, we expect that the normal-mode frequencies and the coupling strengths should form a continuum. However, in order to reconcile the equations of motion for the path of minimum action of the quantized system with the classical motion of a particle in the presence of damping, they[5,7] were forced to restrict the coupling functional of the heat bath to a certain class modeling Ohmic dissipation. Recently, a phenomenological approach to the quantum theory of a harmonic oscillator with Ohmic dissipation has been put forward by Grabert *et al.*[6] We show how previous calculations provide a microscopic basis for the results obtained in Ref. 6. Also we consider the case of a different, non-Ohmic heat-bath coupling.

In Sec. II, we present a microscopic Hamiltonian containing a linear coupling to a heat bath formed of harmonic oscillators, and calculate the exact frequency-dependent susceptibility. In Sec. III, we evaluate the dynamic correlation functions for two different types of dissipative mechanisms. We consider in model A the case of Ohmic dissipation regularized by a Drude cutoff and in model B, a dissipative mechanism resulting from a coupling similar to optical phonons. Our results are discussed in Sec. IV.

II. THE MODEL SYSTEM

The model consists of a particle of mass M, labeled by position variable q and momentum p. The particle is governed by the Hamiltonian first introduced by Ullersma,[2] it moves in a harmonic potential

$$\frac{p^2}{2M}+\frac{M}{2}\omega_0^2q^2 \,. \tag{2.1}$$

The heat bath consists of an infinite number of harmonic oscillators, the normal modes. The mass and the frequency of the nth heat-bath oscillator are m_n and ω_n, respectively. The Hamiltonian which governs the heat bath is

$$\sum_{n=1}^{N}\left[\frac{\pi_n^2}{2m_n}+\frac{m_n\omega_n^2}{2}\phi_n^2\right], \tag{2.2}$$

where ϕ_n and π_n are the position and momentum coordinates of the nth normal mode.

The particle is coupled to the heat bath by a term in the Hamiltonian, which is both linear in the particle position q and linear in the heat-bath normal coordinates ϕ_n

$$\sum_{n=1}^{N}\lambda_n\phi_n q \ . \tag{2.3}$$

We also assume that the Poincaré recurrence time of the heat bath is much longer than any time scale of physical interest. This is achieved by taking the number of normal modes N to infinity.

The heat-bath coupling (2.3) introduces a negative shift in the (squared) frequency of the oscillator

$$\Delta\omega^2=-\sum_{n=1}^{N}\lambda_n^2/Mm_n\omega_n^2$$

for frequencies $\omega\simeq\omega_0$ which are much smaller than the largest characteristic frequency of the heat bath ω_B. We assume that $\Delta\omega^2$ is finite, which corresponds to assuming that the spectral density associated with the coupling to the heat bath

$$\sum_{n=1}^{N}\lambda_n^2/Mm_n\delta(\omega-\omega_n)$$

varies as a higher power of ω, than ω^2, for $\omega\to 0$. In contrast to Ref. 5, our model does not include a counter-term canceling this induced frequency shift.

A general formula for the exact response function has been given by Ullersma,[2] in a series of four papers. We find it convenient to rederive his results, by recasting them into the response function formalism, in order to make direct comparison with the recent work (Refs. 5—11) easier.

We shall calculate the dynamic susceptibility[12] defined by

$$\chi_{A,B}(t)=i\Theta(t)\langle[\hat{A}(t),\hat{B}(0)]_-\rangle \tag{2.4}$$

from the equation of motion

$$i\frac{\partial}{\partial t}\chi_{A,B}(t)=-\delta(t)\langle[\hat{A}(t),\hat{B}(0)]_-\rangle +i\Theta(t)\langle[[\hat{A}(t),\hat{H}(t)]_- ,\hat{B}(0)]_-\rangle \ . \tag{2.5}$$

Here and in the following we choose the units in which $\hbar=1$.

This represents the response function for the changes in $\hat{A}$ which occur when an external force F_B, which couple to $\hat{B}$ is introduced. The relationship between the change in A, $\hat{\delta}A$, and the driving force is[12]

$$\delta\langle\hat{A}(t)\rangle=\int_{-\infty}^{t}\chi_{A,B}(t-t')F_B(t')dt' \ .$$

The resulting set of coupled equations are

$$i\frac{\partial}{\partial t}\chi_{qq}(t)=\frac{i}{M}\chi_{pq}(t) \ , \tag{2.6}$$

$$i\frac{\partial}{\partial t}\chi_{pq}(t)=i\delta(t)-iM\omega_0^2\chi_{qq}(t)-i\sum_{n=1}^{N}\lambda_n\chi_{\phi_n q}(t) \ , \tag{2.7}$$

$$i\frac{\partial}{\partial t}\chi_{\phi_n q}(t)=\frac{i}{m_n}\chi_{\pi_n q}(t) \ , \tag{2.8}$$

$$i\frac{\partial}{\partial t}\chi_{\pi_n q}(t)=-im_n\omega_n^2\chi_{\phi_n q}(t)-i\lambda_n\chi_{qq}(t) \ . \tag{2.9}$$

These equations form a closed set, and can be solved. We define the frequency-dependent susceptibility by

$$\chi_{A,B}(\omega)=\int_0^{\infty}dt\, e^{i\omega t}\chi_{A,B}(t) \ . \tag{2.10}$$

Fourier transforming Eqs. (2.6)—(2.9) yield

$$\omega\chi_{qq}(\omega)=\frac{i}{M}\chi_{pq}(\omega) \ , \tag{2.11}$$

$$\omega\chi_{pq}(\omega)=i-iM\omega_0^2\chi_{qq}(\omega)-i\sum_{n=1}^{n}\lambda_n\chi_{\phi_n q}(\omega) \ , \tag{2.12}$$

$$\omega\chi_{\phi_n q}(\omega)=\frac{i}{m_n}\chi_{\pi_n q}(\omega) \ , \tag{2.13}$$

$$\omega\chi_{\pi_n q}(\omega)=-im_n\omega_n^2\chi_{\phi_n q}(\omega)-i\lambda_n\chi_{qq}(\omega) \ . \tag{2.14}$$

From these, we find that the frequency-dependent susceptibility is of the form

$$\chi_{qq}(\omega)=-\frac{1}{M}[\omega^2-\omega_0^2-\Pi(\omega)]^{-1} \tag{2.15}$$

in which the "self-energy" $\Pi(\omega)$ is given by

$$\Pi(\omega)=\sum_{n=1}^{N}\frac{\lambda_n^2}{Mm_n}(\omega^2-\omega_n^2)^{-1} \ . \tag{2.16}$$

The imaginary part of $\Pi(\omega)$ is given by

$$\begin{aligned}\mathrm{Im}\Pi(\omega)&=\sum_{n=1}^{N}\frac{\lambda_n^2}{2Mm_n\omega_n}\mathrm{Im}\left[\frac{1}{\omega-\omega_n}-\frac{1}{\omega+\omega_n}\right]\\&=-\sum_{n=1}^{N}\frac{\pi\lambda_n^2}{2Mm_n\omega_n}[\delta(\omega-\omega_n)-\delta(\omega+\omega_n)] \ .\end{aligned} \tag{2.17}$$

The sign in Eq. (2.17) is determined by the causality condition, i.e., that $\chi_{AB}(\omega)$ is analytic in the upper half of the complex ω plane. We can express the real part of the $\Pi(\omega)$ in terms of the imaginary part through the Kramers-Kronig relation:

$$\mathrm{Re}\Pi(\omega)=\sum_{n=1}^{N}\frac{\lambda_n^2}{2Mm_n}\mathrm{P}\int d\omega'\frac{1}{\omega-\omega'}\times\left[\frac{\delta(\omega'-\omega_n)+\delta(\omega'+\omega_n)}{\omega'}\right] .$$

On taking the principal part integral (P) outside the summation, we find the Kramers-Kronig relation

$$\mathrm{Re}\Pi(\omega)=-\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\mathrm{P}\frac{1}{\omega-\omega'}\mathrm{Im}\Pi(\omega') \ , \tag{2.18}$$

Equations (2.15)—(2.18) represent the exact expression for the frequency-dependent response function in terms of the microscopic parameters of the Hamiltonian. The above results are also contained in the work of Ullersma,[2] although in a less transparent form. We note that $\mathrm{Re}\Pi(\omega)$ is finite at low values of ω but vanishes at larger ω, indicating a different response occurring for low and high frequencies.

The spontaneous fluctuations of the system are characterized by the anticommutator correlation function

$$S_{A,B}(t)=\tfrac{1}{2}\langle[\hat{A}(t),\hat{B}(0)]_{+}\rangle \; . \tag{2.19}$$

The Fourier transform of this, the spectral density

$$S_{A,B}(\omega)=\int dt\, e^{i\omega t}S_{A,B}(t)\; ,$$

is related to the imaginary part of the dynamic susceptibility through the fluctuation-dissipation theorem. This relation takes the form[13]

$$S_{A,B}(\omega)=[N(\omega)+\tfrac{1}{2}]2\,\mathrm{Im}\chi_{A,B}(\omega)\; , \tag{2.20}$$

where $N(\omega)$ is the Bose-Einstein distribution function

$$N(\omega)=(e^{\beta\omega}-1)^{-1}\; .$$

Hence, knowing $\chi_{qq}(\omega)$ we can obtain the dynamic correlation function from an inverse Fourier transform

$$\begin{aligned} S_{qq}(t)&=\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{-i\omega t}S_{qq}(\omega)\\ &=-\frac{1}{M}\int_{0}^{\infty}\frac{d\omega}{\pi}\coth\left[\frac{\beta\omega}{2}\right]\cos(\omega t)\\ &\quad\times\frac{\mathrm{Im}\Pi(\omega)}{[\omega^2-\omega_0^2-\mathrm{Re}\Pi(\omega)]^2+[\mathrm{Im}\Pi(\omega)]^2}\; , \end{aligned} \tag{2.21}$$

where we have used the property

$$\mathrm{Im}\chi_{qq}(\omega)=-\mathrm{Im}\chi_{qq}(-\omega)\; .$$

In Sec. III, we shall investigate the consequences of various models for the heat bath. Our procedure will be to find $\mathrm{Re}\Pi(\omega)$ for a given $\mathrm{Im}\Pi(\omega)$ via Eq. (2.18). Then we may examine the effects on $S_{qq}(t)$ as expressed by Eq. (2.21).

III. SPECTRAL DENSITY AND DYNAMIC CORRELATION FUNCTIONS

We shall examine the consequences of various models of the thermal-reservoir coupling. The imaginary part of the "self-energy" $\Pi(\omega)$ is related to the spectral density $J(\omega)$ introduced in Ref. 5 as follows:

$$\mathrm{Im}\Pi(\omega)=-\mathrm{sgn}\omega\frac{J(\omega)}{M}\; . \tag{3.1}$$

A. Ohmic dissipation

For the case of Ohmic dissipation we consider the spectral function suggested by Caldeira and Leggett,[5,7] $J(\omega)=M\Gamma\omega/(1+\omega^2/\omega_B^2)$. The frequency ω_B represents the largest characteristic frequency of the thermal reservoir. This frequency usually corresponds to the time scales of microscopic processes in the heat bath. In this case we obtain

$$\mathrm{Im}\Pi(\omega)=-\Gamma\omega\left[\frac{\omega_B^2}{\omega^2+\omega_B^2}\right]\; , \tag{3.2a}$$

$$\mathrm{Re}\Pi(\omega)=-\Gamma\omega_B\left[\frac{\omega_B^2}{\omega^2+\omega_B^2}\right]\; , \tag{3.2b}$$

where the real part of $\Pi(\omega)$ has been obtained from the Kramers-Kronig relation (2.18).

The class of $\mathrm{Im}\Pi(\omega)$ which vanishes as $\omega\to 0$ like ω, represents an idealization of an Ohmic heat bath. First we note that the coupling term (2.3) induces transitions where a phonon is created or destroyed in the harmonic oscillator simultaneously with the creation or destruction of one phonon in the normal modes of the thermal reservoir. Of all the possible processes, only those which conserve energy will persist as real dissipation processes. Since our heat bath has a finite density of normal modes spanning a wide range of frequencies, our harmonic oscillator can dissipate arbitrarily small amounts of energy as ω_0 tends to zero. The linearity of $\mathrm{Im}\Pi(\omega)$ in ω is required in order that the system approximately satisfies an Ehrenfest equation similar to the classical equation of a damped oscillator:

$$\ddot{q}+(\omega_0^2-\Gamma\omega_B)q+\Gamma\dot{q}=0\; . \tag{3.3}$$

The conditions under which this approximation holds has been discussed extensively in Refs. 2 and 3. With $\Pi(\omega)$ given in (3.2), the dynamical susceptibility $\chi_{qq}(\omega)$, (2.15), assumes the form

$$\chi_{qq}(\omega)=\frac{1}{M}\left[(\omega_0^2-\Gamma\omega_B)-\omega^2-\frac{i\omega\omega_B\Gamma}{\omega_B-i\omega}\right]^{-1} \tag{3.4}$$

which is *identical* to the response function of the phenomenological Drude-regularized classical equation

$$\ddot{q}+(\omega_0^2-\Gamma\omega_B)q+\Gamma\int_{-\infty}^{t}dt'\,\omega_B e^{-\omega_B(t-t')}\dot{q}(t')=0\; . \tag{3.5}$$

Thus, this equivalence justifies the phenomenological approach put forward in Ref. 6 in which the regularization (3.5) was utilized. Note, that the inclusion of a counterterm for the frequency shift, in the Hamiltonian, $-\frac{1}{2}M(\Delta\omega)^2$, where

$$\begin{aligned}(\Delta\omega)^2&\equiv\lim_{\omega\to 0}\mathrm{Re}\Pi(\omega)\\ &=-\Gamma\omega_B\end{aligned} \tag{3.6}$$

would yield the renormalized frequency $(\omega_0^2-\Gamma\omega_B)\to\omega_0^2$ as implied in Ref. 6.

For the frequencies of physical interest, we find a mass renormalization, given by

$$\begin{aligned}\tilde{M}&=M\left[1-\frac{\partial}{\partial\omega^2}[\mathrm{Re}\Pi(\omega)]\right]_{\omega=0}\\ &=M\left[1-\frac{\Gamma}{\omega_B}\right]\end{aligned} \tag{3.7}$$

when $\omega/\omega_B \ll 1$. Likewise, we find that the frequency of the oscillator is shifted to the renormalized value $\tilde{\omega}_0$ given by

$$\tilde{\omega}_0^2 = \frac{\omega_0^2 - \Gamma\omega_B}{1-\Gamma/\omega_B} . \tag{3.8}$$

These results are similar to those found by Ullersma[2] as well as those implied in Refs. 5 and 7, apart from the mass renormalization factors. Since our basic premise is that of $\Gamma/\omega_B \ll 1$ and $\omega_0/\omega_B \ll 1$, the mass renormalization is a relatively unimportant effect at low frequencies. However, the frequency shift can be of major consequence. One implication is that Γ/ω_B and $(\omega_0/\omega_B)^2$ must be regarded as being of the same order of smallness. At microscopic time scales, where $\omega > \omega_B$, the real part $\Pi(\omega)$ vanishes, and the system responds at the bare frequency ω_0. The poles of $\chi_{qq}(\omega)$ are most readily found from consideration of (3.2). The analytic structure is determined from the solutions of the cubic equation

$$F(\omega) \equiv \omega^3 + i\omega_B\omega^2 - \omega_0^2 - i\omega_B(\omega_0^2 - \Gamma\omega_B) = 0 . \tag{3.9}$$

The roots ω_1, ω_2, and ω_3 must satisfy the equations

$$\begin{aligned} &\omega_1+\omega_2+\omega_3 = -i\omega_B , \\ &\omega_1\omega_2+\omega_1\omega_3+\omega_2\omega_3 = -\omega_0^2 , \\ &\omega_1\omega_2\omega_3 = i\omega_B(\omega_0^2-\Gamma\omega_B) . \end{aligned} \tag{3.10a}$$

For $(\omega_0/\omega_B)^2 > \Gamma/\omega_B$ we find that the roots all lie in the lower half of the complex ω plane. The approximate poles are given by

$$\begin{aligned} &\omega_1 \simeq -i\omega_B \left[1-\frac{\Gamma}{\omega_B}\right] , \\ &\omega_2 \simeq \omega_B \left\{ \left[\left[\frac{\omega_0}{\omega_B}\right]^2 - \frac{\Gamma}{\omega_B} \right]^{1/2} - \frac{i}{2}\frac{\Gamma}{\omega_B} \right\} , \\ &\omega_3 \simeq -\omega_B \left\{ \left[\left[\frac{\omega_0}{\omega_B}\right]^2 - \frac{\Gamma}{\omega_B} \right]^{1/2} + \frac{i}{2}\frac{\Gamma}{\omega_B} \right\} \end{aligned} \tag{3.10b}$$

up to order $(\omega_0/\omega_B)^2$ and Γ/ω_B. As can be inferred from Eqs. (3.3), (3.8), or (3.10), when $(\omega_0/\omega_B)^2 > \Gamma/\omega_B$ the system is unstable.

The static correlation functions $S_{qq}(0)$ and $S_{pp}(0)$ can be evaluated from integrals of the form (2.21), with the aid of the identity[14]

$$\coth\left[\frac{\beta\omega}{2}\right] = \frac{2}{\beta\omega} + \frac{1}{\pi i}\left[\psi\left[1+\frac{i\beta\omega}{2\pi}\right] - \psi\left[1-\frac{i\beta\omega}{2\pi}\right]\right] \tag{3.11}$$

in which ψ is the digamma function. Further, $\mathrm{Im}\chi_{qq}(\omega)$ can be expressed as partial fractions as

$$\mathrm{Im}\chi_{qq}(\omega) = \frac{i}{2M}\sum_{n=1}^{3}\left[\left.\frac{\dfrac{\partial F(\omega)}{\partial\omega_0^2}}{\dfrac{\partial F(\omega)}{\partial\omega_n}}\right|_{\omega=\omega_n} \frac{1}{\omega-\omega_n} - \left.\frac{\dfrac{\partial F^*(\omega)}{\partial\omega_0^2}}{\dfrac{\partial F^*(\omega)}{\partial\omega_n^*}}\right|_{\omega=\omega_n^*} \frac{1}{\omega-\omega_n^*} \right] , \tag{3.12}$$

where $F(\omega)$ is defined in Eq. (3.9) and ω_n and ω_n^* are the roots and complex conjugate roots, respectively. Since $\psi(1+i\beta\omega/2\pi)$ and $\psi(1-i\beta\omega/2\pi)$ are, respectively, analytic in the lower and upper half of the complex ω plane, the integrals can be deformed to yield a contribution from the contours at infinity plus contributions from the poles at ω_n and ω_n^*. The contours at infinity do not contribute to the integral, since $\chi_{qq}(\omega)$ vanishes faster than ω^{-3}. Thus we find the exact result

$$S_{qq}(0) = \frac{1}{2M}\left[\frac{2}{\beta(\omega_0^2-\Gamma\omega_B)} + \frac{2}{\pi i}\sum_{n=1}^{3} \left.\frac{\dfrac{\partial F(\omega)}{\partial\omega_0^2}}{\dfrac{\partial F(\omega)}{\partial\omega_n}}\right|_{\omega=\omega_n} \psi\left[1+\frac{i\beta\omega_n}{2\pi}\right] \right] . \tag{3.13}$$

In deriving this expression, we have utilized the properties of the roots ω_n, namely,

$$\begin{aligned} &\omega_1^* = -\omega_1 , \\ &\omega_2^* = -\omega_3 , \\ &\omega_3^* = -\omega_2 . \end{aligned} \tag{3.14}$$

The expression (3.13) is an exact result. In the limit $\Gamma \to 0$, we find that (3.13) simplifies to

$$\begin{aligned} S_{qq}(0) &= \frac{1}{2M\omega_0}\left[\frac{2}{\beta\omega_0} + \frac{2}{\pi}\mathrm{Im}\psi\left[1+\frac{i\beta\omega_0}{2\pi}\right]\right] \\ &= \frac{1}{2M\omega_0}\coth\left[\frac{\beta\omega_0}{2}\right] \end{aligned} \tag{3.15}$$

as is expected for a simple Harmonic oscillator. Likewise, we find $S_{pp}(0)$, since the equations of motion yield

$$\chi_{pp}(0) = M^2\omega^2\chi_{qq}(0) . \tag{3.16}$$

The contours at infinity vanish again since $\mathrm{Im}\Pi(\omega)$ decays as ω^{-1}; hence, $\mathrm{Im}\chi_{qq}(\omega)$ vanishes as ω^{-5} for larger ω. The net result is

$$S_{pp}(0)=\frac{M}{2}\left[\frac{2}{\beta}\sum_{n=1}^{3}\omega_n\left.\frac{\dfrac{\partial F(\omega)}{\partial\omega_0^2}}{\dfrac{\partial F(\omega)}{\partial\omega_n}}\right|_{\omega=\omega_n}+\frac{2}{\pi i}\sum_{n=1}^{3}\omega_n^2\left.\frac{\dfrac{\partial F(\omega)}{\partial\omega_0^2}}{\dfrac{\partial F(\omega)}{\partial\omega_n}}\right|_{\omega=\omega_n}\psi\left[1+i\frac{\beta\omega_n}{2\pi}\right]\right] \tag{3.17}$$

which is a well-defined, real quantity. The first term in the square brackets is just $2/\beta$. We note that at high temperatures, (3.13) and (3.17) simplify to give

$$S_{qq}(0)=\frac{k_BT}{M(\omega_0^2-\Gamma\omega_B)} \tag{3.18}$$

$$S_{pp}(0)=Mk_BT\ . \tag{3.19}$$

This result is somewhat unexpected since, at high temperatures, a fair amount of thermal excitation should occur in the microscopic models of the heat bath ($k_BT\gg\omega_B$). Since, the oscillator responds at these large frequencies exactly as an undamped oscillator at frequency ω_0, one might expect that the spontaneous fluctuations in $S_{qq}(0)$ should occur at the unrenormalized microscopic frequency instead of the renormalized frequency $\tilde{\omega}_0^2=\omega_0^2-\Gamma\omega_B$. It is also surprising, in that at high temperatures, the energy is not partitioned equally between the momentum and position degrees of freedom of the microscopic Hamiltonian (2.1). Of course, the discrepancy is resolved after examining the energies of the coupling term (2.3) and reapportioning its high-temperature contribution between the bath and the oscillator. It is interesting to note that the unrenormalized mass M appears in the above expressions for $S_{qq}(0)$ and $S_{pp}(0)$. In the expression for $S_{qq}(0)$, this can be understood as being due to the cancellation of the factor in (3.7) (the effective mass) with the denominator of (3.8) (the renormalized frequency). In the zero temperature limit we find

$$S_{qq}(0)=\frac{1}{M\pi}\frac{\tan^{-1}[(\omega_0^2-\Gamma\omega_B)^{1/2}]}{(\omega_0^2-\Gamma\omega_B)^{1/2}}\ ,\quad T\to 0 \tag{3.20}$$

and

$$S_{pp}(0)=\frac{M}{\pi}(\omega_0^2-\Gamma\omega_B)^{1/2}\tan^{-1}[(\omega_0^2-\Gamma\omega_B)^{1/2}]+\frac{M\Gamma}{\pi}\ln\left[\frac{\omega_B^2}{\omega_0^2-\Gamma\omega_B}\right],\quad \Gamma\omega_B<\omega_0^2\ . \tag{3.21}$$

The result for $S_{qq}(0)$ is similar to that obtained in Refs. 5, 6, and 9. The authors of Ref. 5 have shown that in the absence of a finite ω_B, $S_{pp}(0)$ should diverge logarithmically. This divergence was regularized in Ref. 6 by use of a phenomenological Drude model for the frequency-dependent damping [see (3.5)].

We shall now address the long-time behavior of $S_{qq}(t)$ at $T=0$. Since the integrals are dominated by the low-frequency behavior we find the asymptotic behavior

$$S_{qq}(t)\sim\frac{\Gamma}{\pi M(\omega_0^2-\Gamma\omega_B)^2t^2}\ .$$

This is similar to the result of Grabert *et al.*[6] In Figs. 1 and 2 we depict $\mathrm{Im}\chi_{qq}(\omega)$ and the normalized $S_{qq}(t)$, at $T=0$.

B. Non-Ohmic dissipation

Thus far we have considered the behavior of the harmonic oscillator which is coupled to a heat bath which has several idealized features. Namely, that the spectral

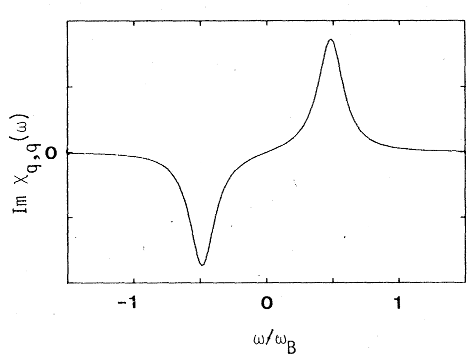

FIG. 1. The imaginary part of the frequency-dependent susceptibility for choice of $\mathrm{Im}\Pi(\omega)$ given by Eq. (3.2a). We express all quantities in terms of the dimensionless units ω/ω_B, ω_0/ω_B, and Γ/ω_B. We exhibit the case where $\omega_0/\omega_B=0.5$ and $\Gamma/\omega_B=0.1$.

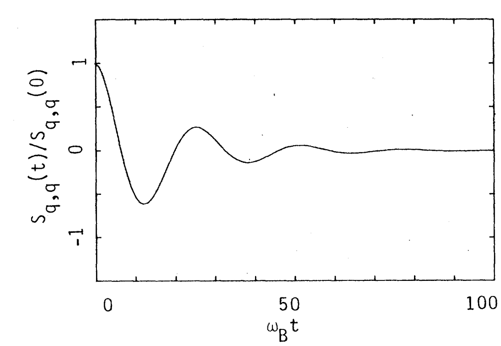

FIG. 2. Time dependence of $S_{qq}(t)$. We have normalized it to the initial value $S_{qq}(0)$. Parameters are the same as in Fig. 1. Temperature T is taken to be zero.

density of the heat bath spans an extremely large frequency range which extends all the way down to $\omega=0$. This has the consequence that no matter how small the characteristic frequency of the oscillator ω_0 is, energy can be dissipated into the heat bath. This can be seen by examining the transitions that are induced by the coupling term (2.3). The transitions involve a change in the state of the harmonic oscillator by one quantum number, and there is a concomitant change in the quantum number of one normal mode of the heat bath. Those transitions which do not conserve energy are only virtual transitions while those that do conserve the energy of the entire system persist as real processes that dissipate energy. The requirement that energy is conserved means that a *single transition* can only represent a real dissipative process if the normal modes of the thermal reservoir have a finite spectral weight at the frequency ω_0.

We shall now examine the consequences when this energy matching condition is not met. This perhaps could occur in some physical systems where the heat bath is mainly comprised of optical phonons.[15] The thermal reservoir will be characterized by its average frequency ω_B and its dispersion ω_D. The imaginary part of the self-energy is given by

$$\mathrm{Im}\Pi(\omega)=\begin{cases} 0\,, & \omega>\omega_B+\omega_D \\ A(\omega-\omega_B)\,, & \omega_D>|\omega-\omega_B| \\ 0\,, & |\omega_B-\omega_D|>|\omega| \\ -A(\omega+\omega_B)\,, & \omega_D>|\omega+\omega_B| \\ 0\,, & -(\omega_B+\omega_D)>\omega \end{cases} \tag{3.22}$$

where $A(\omega)=(\omega_D^2-\omega^2)^{1/2}$. The intrinsically new situation occurs when $|\omega_0-\omega_B|>\omega_D$. We can evaluate the real part of the self-energy from the Kramers-Kronig relation (2.18) as

$$\mathrm{Re}\Pi(\omega)+2\Gamma\omega_B=\Gamma\begin{cases} B(\omega+\omega_B)-B(\omega-\omega_B)\,, & \omega>\omega_B+\omega_D \\ B(\omega+\omega_B)\,, & |\omega-\omega_B|<\omega_D \\ B(\omega+\omega_B)+B(\omega-\omega_B)\,, & |\omega|<|\omega_B-\omega_D| \\ B(\omega-\omega_B)\,, & |\omega+\omega_B|<\omega_D \\ B(\omega-\omega_B)-B(\omega+\omega_B)\,, & \omega+\omega_B<-\omega_0 \end{cases} \tag{3.23}$$

where $B(\omega)=(\omega^2-\omega_D^2)^{1/2}$. We note that $\mathrm{Re}\Pi(\omega)$ vanishes as $\omega\to\infty$, which indicates that at such large frequencies, the system will respond as an undamped oscillator of frequency ω_0. On the other hand as $\omega\to 0$, the oscillator responds as an undamped oscillator of frequency $\tilde{\omega}$, where

$$\tilde{\omega}^2=\omega_0^2-2\Gamma\omega_B\left\{1-\left[1-\left[\frac{\omega_D}{\omega_B}\right]^2\right]^{1/2}\right\}. \tag{3.24}$$

The magnitude of the frequency shift is of the same order of magnitude as that of (3.8) considered previously. We shall only consider the cases corresponding to a positive value of $\tilde{\omega}^2$. A simple evaluation of $\mathrm{Im}\chi_{qq}(\omega)$ yields continuous spectrum in the frequency ranges

$$|\omega-\omega_B|<\omega_D$$

and

$$|\omega+\omega_B|<\omega_D\,.$$

In addition to these continua, there exists the possibility of having discrete poles of frequencies outside this range, given by the solutions of

$$\omega^2-\omega_0^2=\mathrm{Re}\Pi(\omega)$$

and

$$\mathrm{Im}\Pi(\omega)=0\,. \tag{3.25}$$

When $\tilde{\omega}^2$ given by (3.24) is a positive quantity we find that the spectrum has delta functions at frequencies less $\omega_B-\omega_D$ whenever

$$\omega_0^2-(\omega_B-\omega_D)^2<2\Gamma\omega_B\left[1-\left[1-\frac{\omega_D}{\omega_B}\right]^{1/2}\right].$$

The spectrum will have a delta function at a frequency greater than $\omega_B+\omega_D$ if the criterion

$$(\omega_B+\omega_D)^2-\omega_0^2<2\Gamma\omega_B\left[\left[1+\frac{\omega_D}{\omega_B}\right]^{1/2}-1\right]$$

is satisfied.

For a range of parameters, corresponding to large Γ

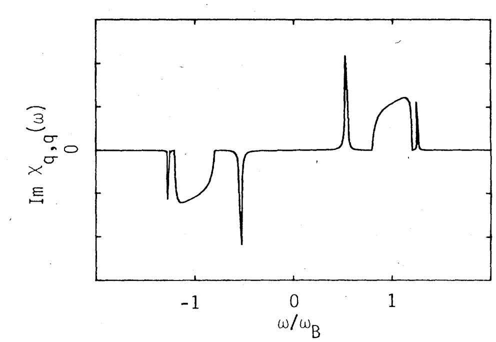

FIG. 3. The imaginary part of the frequency-dependence susceptibility, for a non-Ohmic heat bath. We exhibit the case where $\omega_0/\omega_B=0.9$, $\Gamma/\omega_B=9$, and $\omega_D/\omega_B=0.2$.

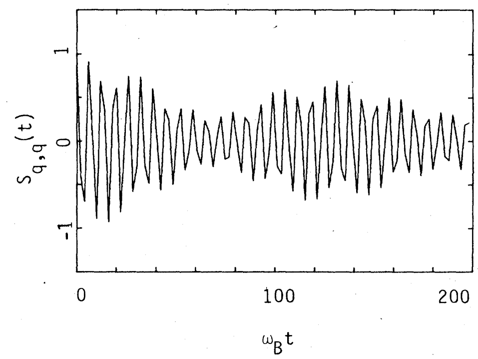

FIG. 4. The time dependence of $S_{qq}(t)$ for the non-Ohmic heat bath coupling of Sec. III B. The correlation function is normalized to its initial value $S_{qq}(t=0)$. Parameters are $\omega_0/\omega_B=0.98$, $\Gamma/\omega_B=15$, and $\omega_D/\omega_B=0.01$. The zero temperature limit is taken.

and small ω_D, it is possible to satisfy both criteria, leading to a response function with poles both above and below the band which corresponds to the spectral density of the thermal reservoirs. This is depicted in Fig. 3. This limit corresponds to the mixing of the various normal modes. Since the dispersion of the heat-bath modes ω_D is small we may consider this as an approximate form of a two-oscillator system. The strong coupling between these two oscillators causes the modes to hybridize and lift the near degeneracy as in mode-crossing systems. The dynamics, depicted in Fig. 4, therefore is representative of two uncoupled harmonic oscillators.

IV. SUMMARY AND CONCLUSIONS

We have examined the exactly soluble model of a harmonic oscillator coupled to a thermal reservoir. We have calculated the response function in terms of the microscopic parameters of the Hamiltonian. The characteristic frequency of the oscillator is renormalized by the coupling to the heat bath. The system responds to perturbations of high frequencies in a manner similar to that of an undamped harmonic oscillator. While for external perturbations of low frequency the characteristic frequency is renormalized by the damping.

We have examined two archetypical models of heat baths; one which resembles a thermal reservoir composed of acoustic phonons. The other model bears more resemblance to a system of optic phonons.

In the case of a heat bath which has a spectral density which extends from $\omega \simeq 0$ up to a cutoff ω_B, we find that the oscillator's frequency is renormalized from ω_0 to $\tilde{\omega}=(\omega_0^2-\Gamma\omega_B)^{1/2}$. Since ω_B is assumed to be greater than ω_0, this reduction together with the restriction that $\tilde{\omega}$ be positive leads to the conclusion that Γ be small. This produces a very restrictive criterion required for the existence of an overdamped limit. In the limit $\omega_B \to \infty$, the overdamped limit does not exist. The spontaneous fluctuations in the position and momentum have been calculated. At low temperatures, the zero-point fluctuations in the displacement are smaller than the corresponding fluctuations in the momentum, due to the presence of a term proportional to the damping which is also logarithmically dependent on the cutoff. This asymmetry is expected simply because we have broken the symmetry of momentum and displacement by introducing a coupling linear in the displacement. At high temperatures, when one expects thermal fluctuations of high frequencies $\omega \sim \omega_B$ to be present with considerable weight one might expect that, since $\Pi(\omega)$ vanishes for these frequencies, the equipartition would involve the unrenormalized frequency ω_0. We find that this is not the case. This implies that the thermal average of the energy associated with the coupling terms is exactly canceled by the counterterms considered by Caldeira and Leggett.[5,7,8]

In the case of a thermal reservoir which has a spectral density similar to that of a system of optical phonons, the response is drastically different. In particular the system responds only to perturbations with frequencies which occur in a narrow frequency range, that corresponds to the spectrum of the thermal reservoir, together with isolated frequencies. The maximum number of these discrete frequencies is two. This extreme limit is that of a very small dispersion in the modes of the thermal reservoir and a large coupling (damping) constant. These two frequencies occur as a result of the mode repulsion of the oscillator and the thermal reservoir, often found in quantum systems.[16] The physics of this system essentially decouples into that of two independent oscillators.

Previous work on this particular subject[5-7] has used the starting point of an Ehrenfest equation. Clearly the Ehrenfest equation does exist for the total system. However, this equation, when contracted onto the single relevant oscillator variable, is not of simple form. The Ehrenfest equation (3.3) for the damped dynamics is not exact, but only holds approximately in restricted regimes of frequencies. In particular, the parameters that enter the Ehrenfest equation should be regarded as being frequency dependent, e.g., as in (3.5). A frequency-dependent mass M and frequency $\tilde{\omega}_0$ should be used [cf. Eqs. (3.7) and (3.8) for low frequencies].

During the final stage of preparation of our manuscript we received a copy of unpublished work from Haake and Reibold[17] on a similar topic. They address the model appropriate for a coupling to a bath of acoustic phonons. Some of our formulas are identical in content with theirs. In particular, they independently come to the same conclusion that an overdamped limit is precluded in this model.

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