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We consider the problem of a single quantum oscillator coupled linearly to a heat bath of independent harmonic modes. An exact solution is presented for the system-oscillator observables of interest. The exact results are then used to evaluate the utility of a variational approach to the problem that has proven useful recently in elucidating the dynamics of dissipatively coupled systems. We find that the variational approach does provide a good description for most, but not all, observables of interest. Both the exact and the variational treatment demonstrate the important role played by the low-frequency bath modes in determining qualitative features of the dynamical behavior.

I. INTRODUCTION

A large number of papers have been written recently addressing the dissipative dynamics of relatively simple, one-particle quantum mechanical systems which are linearly coupled to a bath of independent quantum oscillators.[1-7] In view of the work that has been done over the years on electron–phonon interactions and related areas, it is perhaps not suprising that many results of these recent calculations have been known for a long time; nonetheless, considerable progress has been made recently in understanding how subtle changes in the nature of the bath can bring about qualitative changes in the dynamical behavior of the subsystem. As an example of such behavior, we note the recent interest in the dynamics of the two-state tunneling problem where it has been shown that zero-temperature dynamical localization of the tunneling species can occur when certain conditions on the bath are satisfied.[1-4] This localization "transition" has been demonstrated by many workers adopting quite different approaches including path integrals, instantons, renormalization group methods, and also more standard quantum statistical methods. As an example of the latter, Silbey and Harris,[4] and more recently Parris and Silbey,[5] have analyzed the tunneling problem using a variational, small polaron transformation to determine an appropriate zeroth order Hamiltonian, and then treating the full dynamics perturbatively. The results of these calculations agree in all essential details with those obtained by the other, also approximate, methods mentioned above.

In this paper we apply the same basic variational approach to a different problem, one for which an exact dynamical solution exists, viz., the linearly coupled harmonic oscillator. This allows us to compare the results of an exactly soluble model with those obtained from the variational treatment, thereby providing a good test of the latter, while at the same time developing further insight into the general problem of dissipative quantum systems.

We find that the variational approach, coupled with the lowest nontrivial order of perturbation theory, does in fact provide a good description of the problem, reproducing the essential features of the exact calculations in most details. Indeed, the exact calculations and the variational treatment both show that although nothing so severe as localization occurs in the oscillator problem, some very interesting qualitative changes do occur when the characteristics defining the bath are altered. As in the two-state problem, this behavior is very sensitive to the low frequency characteristics of the bath, becoming most pronounced in the case of an Ohmic bath.

The paper is laid out as follows. In Sec. II we introduce the model and its Hamiltonian. In Sec. III the equations of motion are solved and expressions for the absorption and emission spectra, the oscillator population, and the mean-square particle position are obtained and considered for a rather general form of heat both chosen specifically to allow for a variation of the low frequency characteristics of the bath. In Sec. IV we outline the variational approach to the problem by introducing an appropriate unitary transformation, reexpressing the observables obtained in Sec. II in terms of averages with respect to the transformed Hamiltonian, and calculating the averages using perturbation theory. The effects associated with particular baths are again discussed and in the last section we summarize our results.

II. THE MODEL

The system we treat is a single oscillator of frequency Ω coupled to a bath of independent harmonic modes. The Hamiltonian of the entire system may be written

$$H = \Omega a^{\dagger} a + \sum_{\nu} \omega_{\nu} (b^{\dagger}_{\nu} b_{\nu} + 1/2)$$

$$+ \sum_{\nu} g_{\nu} (a^{\dagger} + a)(b^{\dagger}_{\nu} + b_{\nu})$$

$$+ \sum_{\nu} (g^2_{\nu}/\omega_{\nu})(a^{\dagger} + a)^2, \qquad (2.1)$$

where $a^{\dagger}$ and $b^{\dagger}$ are standard, boson creation operators for

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the system oscillator of frequency Ω and the bath mode of frequency ω_v, respectively; the coupling constants g_v determine the strength of the linear coupling between the central oscillator and the vth bath mode. The last term in Eq. (2.1) has been included to avoid a renormalization of the oscillator frequency: it could have easily been included in the definition of Ω, but including it at this point leads to a simplification of later expresssions and also allows us to consider a wider range of parameter space. For an elucidation of this point, including a discussion of instances when it is physically important to include such a term, see the paper of Caldiera and Leggett.[1]

The Hamiltonian (2.1) has been studied in one form or another by many workers,[6-9] being an important example, classical and quantum mechanical, of a tractable model exhibiting stochastic behavior. It has, therefore, proven to be useful in the development of the theory of Brownian motion. Indeed, it was in that context that Kac, Ford, and Mazur investigated conditions under which instantaneous dissipation occurs, i.e., under which the reduced system coordinate obeys a strict Langevin equation of motion.[8] Such considerations lead to a particular choice of the spectral function $J(\omega) \equiv \Sigma_v g_v^2 \delta(\omega - \omega_v) = \eta\omega$ for all bath frequencies, taken in the limit in which the width of the bath ω_c is much larger than any frequency of interest, i.e., $\omega_c/\Omega \to \infty$. While this choice of $J(\omega)$ is important in the context for which it was obtained, it (or the same form with large but finite ω_c) has often—for a variety of reasons (sometimes, but not always, physically motivated)—been taken as a standard form to use in much of the subsequent work on coupled quantum oscillators. Indeed quite recent statements appear in the literature to the effect that, for the coupled oscillator, the precise form of $J(\omega)$ is unimportant provided that it is dense about the frequency Ω of the system oscillator and that the spectral width of the bath is sufficiently large. If this were true, then it would be in stark contrast to recent developments in the problem of a two-level system coupled linearly to a bath where it is found that some rather striking differences in behavior do, in fact, occur with changes in the low frequency form of $J(\omega)$. Indeed, these differences become most dramatic when $J(\omega)$ is linear in ω at low frequency (what has been referred to in the literature as the Ohmic case); this is precisely the limiting behavior, however, of the form suggested by Ford, Kac, and Mazur and that which has been commonly used for the quantum oscillator problem.

It is one of the points of this paper to emphasize the qualitative dynamical differences that do occur as the form of $J(\omega)$ is varied from the Ohmic case to a form which may be more relevant to other physical phenomena besides Brownian motion [such as, e.g., impurities in crystals where the density of phonon states and nature of the coupling lead to a dependence on ω of $J(\omega)$ that is of a power higher than the first]. To this end, and recognizing the critical role played by the low frequency modes, we will, in this paper, consider the following form for $J(\omega)$:

$$J(\omega) = \eta\omega_c (\omega/\omega_c)^s \theta(\omega_c - \omega), \qquad (2.2)$$

where $\theta(x)$ denotes the step function, the dimensionless constant η is a measure of the average squared coupling, and

we will be primarily interested in integer values of s. This form allows us to consider, with s variable, the Ohmic case ($s = 1$) as well as other cases of interest. For example, a d-dimensional acoustic phonon bath with deformation potential coupling corresponds at low frequency to Eq. (2.2) with $s = d$. While this does correspond to the Ohmic case for $d = 1$, it gives $s = 3$ for normal solids.

III. SOLUTION OF THE EQUATIONS OF MOTION

We now follow the procedure of Lindenberg and West,[6] whereby writing down the Heisenberg equations of motion for the operators a, $a^\dagger$ along with those for the set of operators b_v, $b_v^\dagger$ we may, through standard means, eliminate the dependence of the former on the latter to obtain a set of linear (but nonlocal) equations for $a(t)$ and $a^\dagger(t)$:

$$a(t) = -i\Omega a(t) - if(t) - ik(t)[a^\dagger(0) + a(0)]$$
$$-i\Omega \int_0^t d\tau\, k(t-\tau)[a(\tau) - a^\dagger(\tau)], \qquad (3.1a)$$

$$a^\dagger(t) = i\Omega a^\dagger(t) + if(t) + ik(t)[a^\dagger(0) + a(0)]$$
$$-i\Omega \int_0^t d\tau\, k(t-\tau)[a(\tau) - a^\dagger(\tau)]. \qquad (3.1b)$$

Thus, by eliminating the bath variables exactly, we have introduced into the equations describing the uncoupled dynamics two terms. The first, involving the function $f(t)$ defined via the expression

$$f(t) \equiv \sum_v g_v [b_v^\dagger(0)\exp(i\omega_v t) + b_v(0)\exp(-i\omega_v t)], \qquad (3.2)$$

is a fluctuating, operator-valued, force term which, with the bath initially in thermal equilibrium, is of zero mean value. The second term involves $a(t)$ and $a^\dagger(t)$ in a convolution and describes the manner in which energy of the system is dissipated into the bath. The kernel appearing in Eq. (3.1) is given by

$$k(t-\tau) \equiv 2\sum_v (g_v^2/\omega_v)\cos[\omega_v(t-\tau)]$$
$$= 2\int_0^\infty d\omega\, \omega^{-1} J(\omega)\cos[\omega(t-\tau)], \qquad (3.3)$$

which we have expressed in terms of the spectral function $J(\omega)$ introduced in the last section. When $k(t)$ is proportional to a delta function, i.e., when $J(\omega)/\omega$ is equal to a constant for all ω [the limit $s \to 1$, $\omega_c \to \infty$ of Eq. (2.2)], then the convolution term in Eq. (3.1) is just proportional to the velocity operator, and hence on a form suggestive of classical friction [and thus the reference to this form of $J(\omega)$ as an Ohmic bath]. As mentioned previously, however, in many real systems $J(\omega)$ does not take this form and we therefore make no such restriction.

Equation (2.2) and its conjugate are straightforwardly solved by taking Laplace transforms. Introducing matrix notation we write the solution as

$$\mathbf{a}(t) = \mathcal{M}(t)\mathbf{a}(0) + \int_0^\infty d\tau\, \mathcal{G}(t-\tau)\mathbf{f}(\tau), \qquad (3.4)$$

where

$$\mathbf{a}(t) = \begin{pmatrix} a(t) \\ a^\dagger(t) \end{pmatrix}, \quad \mathbf{f}(t) = \begin{pmatrix} -if(t) \\ if(t) \end{pmatrix}, \qquad (3.5)$$

and where we define the 2×2 matrices $\mathscr{G}(t)$ and $\mathscr{M}(t)$ through their Laplace transform:

$$\mathscr{G}(z) \equiv \int_0^\infty d\tau\, \mathscr{G}(\tau) e^{-z\tau}$$

$$= \frac{1}{D(z)} \begin{pmatrix} z - i\Omega + \Omega k(z) & \Omega k(z) \\ \Omega k(z) & z + i\Omega + \Omega k(z) \end{pmatrix} \qquad (3.6)$$

with

$$D(z) = z^2 + \Omega^2 + 2\Omega z k(z);$$
$$\mathscr{M}(z) = \mathscr{G}(z)\{1 + \mathscr{K}(z)\}$$

and where the 2×2 matrix $\mathscr{K}(z)$ has elements $\mathscr{K}_{11} = \mathscr{K}_{12} = -ik(z)$; $\mathscr{K}_{22} = \mathscr{K}_{21} = ik(z)$. Equation (3.4) gives, exactly, the time dependence of $a(t)$ and $a^\dagger(t)$ in terms of the initial operators $a(0)$, $a^\dagger(0)$, $b_\nu^\dagger(0)$, and $b_\nu(0)$. We comment in passing, that it is straightforward, but surprisingly difficult excercise to show how Eq. (3.4) yield the correct boson commutation relations for $a(t)$ and $a^\dagger(t)$ at all times.

We will be interested in evaluating certain time-dependent expectation values of operators formed from products of $a(t)$ and $a^\dagger(t)$ at different times. This requires, naturally, the initial density matrix of the system, which should ideally be determined by experimental considerations. In what follows, however, we write the initial density matrix as a product of that corresponding to an equilibrium bath, and a particular system density matrix in which the system oscillator is in its *ground state*. Insofar as we will be primarily focusing on the long-time properties of the system, corresponding to equilibrium correlation functions and averages, the initial density matrix is not expected to play a major role provided there is a well defined temperature associated with the bath at $t = 0$.

Let us first consider, then, the two-time position correlation function

$$S(t,\tau) \equiv \langle q(t)q(t+\tau)\rangle$$

$$= \langle [a^\dagger(t)a^\dagger(t+\tau) + a^\dagger(t)a(t+\tau)$$
$$+ a(t)a^\dagger(t+\tau) + a(t)a(t+\tau)]\rangle, \qquad (3.7)$$

where we have defined $q(t) = a^\dagger(t) + a(t)$. Our goal is to obtain useful expressions for this quantity in the limit $t \to \infty$, since it leads, through a Fourier transform, to the absorption and emission spectra which are directly observable quantities. A formal but cumbersome expression for $S(t,\tau)$ is readily obtained from the solution (3.4) for $a(t)$, in terms of matrix elements of $\mathscr{M}$ and $\mathscr{G}$. The second term, e.g., can be written, for the stated initial conditions,

$$\langle a^\dagger(t)a(t')\rangle$$
$$= \mathscr{M}_{21}(t)\mathscr{M}_{12}(t')$$
$$+ \int_0^t d\tau \int_0^{t'} d\tau'\, \mathscr{S}_2(t-\tau)\mathscr{S}_1(t'-\tau')\langle f(\tau)f(\tau')\rangle, \qquad (3.8)$$

in which $\mathscr{S}_1(t) \equiv \mathscr{G}_{11}(t) - \mathscr{G}_{12}(t)$ and $\mathscr{S}_2(t) \equiv \mathscr{G}_{22}(t) - \mathscr{G}_{21}(t)$. The fluctuating force-correlation function appearing in Eq. (3.8) is also readily calculated. From the definition (3.2) we find with an initially thermal bath distribution:

$$\langle f(t)f(\tau)\rangle = \int_0^\infty d\omega\, J(\omega)\{n_\omega \exp[i\omega(t-\tau)]$$
$$+ (n_\omega + 1)\exp[-i\omega(t-\tau)]\}, \qquad (3.9),$$

where $n_\omega = \{\exp(\beta\omega) - 1\}^{-1}$ is the Planck function for the number of quanta in an oscillator of frequency ω at temperature $T = 1/k\beta$.

It is straightforward to show using Tauberian theorems for the Laplace transform, that the matrix elements $\mathscr{M}_{ij}(t) \to 0$ as $t \to \infty$, provided the bath is of finite spectral width, which we assume. Thus in the long-time limit the only contribution to Eq. (3.8) is from the convolution. Substituting Eq. (3.9) into Eq. (3.8) and taking the limit $t \to \infty$, gives, after some slight manipulation, a useful integral representation for $I_1(\tau) \equiv \lim_{t\to\infty} \{\langle a^\dagger(t)a(t+\tau)\rangle\}$:

$$I_1(\tau) = \int_0^\infty d\omega \frac{J(\omega)\{n_\omega(\omega+\Omega)^2\exp(-i\omega\tau) + (n_\omega+1)(\omega-\Omega)^2\exp(i\omega\tau)\}}{|D(i\omega)|^2}, \qquad (3.10)$$

where the Laplace transforms which have appeared arise quite naturally when the upper limits of integration in Eq. (3.8) are taken to infinity. Note that $I_1(0)$, by definition, is just the long-time limit of the number of quanta in the system oscillator. We will examine this quantity in more detail shortly.

Expressions similar to Eq. (3.8) are readily obtained for the other terms in Eq. (3.7). They allow us to write

$$S(\infty,\tau) = 4\Omega^2 \int_0^\infty d\omega \frac{J(\omega)\{n_\omega \exp(-i\omega\tau) + (n_\omega+1)\exp(i\omega\tau)\}}{|D(i\omega)|^2} \qquad (3.11)$$

for the long-time limit of $S(t,\tau)$. The Fourier transform of Eq. (3.11) then gives, for positive frequencies, the absorption spectrum $S_a(\omega)$ and, for negative frequencies, the emission spectrum $S_e(\omega)$:

$$S(\omega) = \int_{-\infty}^\infty d\tau \exp(-i\omega\tau)S(\infty,\tau), \qquad (3.12a)$$

$$S_a(\omega) = 4\Omega^2 J(\omega)(n_\omega + 1)|D(i\omega)|^{-2}, \quad \omega > 0, \qquad (3.12b)$$

$$S_e(\omega) = 4\Omega^2 J(\omega)(n_\omega)|D(i\omega)|^{-2}, \quad \omega > 0. \qquad (3.12c)$$

To proceed further we need to calculate the quantity $D(i\omega)^2$ which appears in Eqs. (3.10)–(3.12) and is defined following Eq. (3.6). Thus we need the following expression for the Laplace transform $k(z)$ evaluated at $z = i\omega$:

$$k(i\omega) = 2\int_0^\infty dt \exp(-i\omega t)\int_0^\infty d\xi\, \xi^{-1}J(\xi)\cos(\xi t)$$

$$= \pi J(\omega)/\omega - 2i\omega\mathscr{P}\int_0^\infty d\xi\, \xi^{-1}J(\xi)\{\omega^2 - \xi^2\}^{-1},$$

$$(3.13).$$

where $\mathscr{P}$ denotes principal value. With the choice (2.2) for $J(\omega)$, Eq. (3.12) along with Eq. (3.13) gives, in terms of the dimensionless variable $x \equiv \omega/\omega_c$, and dimensionless oscillator frequency $\delta = \Omega/\omega_c$,

$$|D(i\omega)|^2 = \omega_c^4\{[x^2 - 4\delta\gamma_S(x) - \delta^2]^2 + (2\pi\delta\eta x^s)^2\},$$

$$(3.14)$$

where for $s = 1$, 2, and 3,

$$\gamma_s(x) = \eta x \tanh^{-1}(x), \quad s = 1, \qquad (3.15b)$$

$$= \eta x^2/2 \ln[x^2/(1-x^2)], \quad s = 2, \qquad (3.15b)$$

$$= -\eta x^2\{1 - x\tanh^{-1}(x)\}, \quad s = 3. \qquad (3.15c)$$

We can now examine the spectra defined in Eq. (3.12). In Figs. 1 and 2 we have plotted the emission spectrum as a function of frequency for different values of the relevant parameters. Figure 1 corresponds to the Ohmic case ($s = 1$) and Fig. 2 corresponds to a three-dimensional bath ($s = 3$). The differences are striking. We infer from Eq. (3.12), e.g., that for small ω, $S_e(\omega)$ goes to zero as $\omega \to 0$ for any $s > 1$, but goes to a finite value in the Ohmic case. We see also from Fig. 1 that the Ohmic case shows a very strong sensitivity to the strength η of the interaction; it changes from what is essentially a Lorentzian peak at the oscillator frequency when η is small to a function which, in fact, has a maximum of $\omega = 0$ for values of η that are not particularly large. Indeed, it is clear from Fig. 1 that the position of the absolute maximum of S_e changes discontinuously as η is increased. For $s > 1$, on the other hand, it would appear from Fig. 2 that the spectra remain peaked in the neighborhood of Ω, with the usual broadening and shifting typically associated with phonon

FIG. 2. Normalized emission spectra [Eq. (3.12c)] corresponding to a bath of the form (2.2) with $s = 3$, as a function of frequency for different values of the coupling strength η. We have taken $\delta = 0.1$ and $\theta = 0.5$. We have plotted curves in order of decreasing position of the maxima corresponding to values of $\eta = 0.1$, 0.5 1.0 and 5.0, respectively.

interactions. In fact at very low temperatures a shoulder does appear on the low energy side of the peak which, as we shall see, has important implications for the number of quanta in the system oscillator at long times. Nonetheless, for $s > 1$ the results are *qualitatively* insensitive to the strength of η, in contrast to the behavior discussed above for $s = 1$. Similar remarks hold for the absorption spectra at high temperature when $n_\omega \gg 1$. At low temperatures the dominant contribution to the absorption spectra is from the zero temperature limit of Eq. (3.12b) wherein $n_\omega \to 0$.

Using Eqs. (3.14) and (3.15) in conjunction with Eq. (3.10) we may also investigate the long-time limit of the number of quanta in the oscillator. We find from an analysis of the resulting integral that

$$N(T) \equiv \lim_{t\to\infty}\langle a^\dagger(t)a(t)\rangle$$

$$= \{\exp(\beta\Omega) - 1\}^{-1} + \mathscr{N}(T) + N(T=0),$$

$$(3.16)$$

where the zero temperature limit, given by

$$N(T=0) = \int_0^1 \frac{\eta x^s(x-\delta)^2\, dx}{[x^2 - 4\delta\gamma_s(x) - \delta^2]^2 + (2\pi\delta\eta x^s)^2}$$

$$(3.17)$$

has the following limiting behavior for $(\Omega/\omega_c) = \delta \ll 1$:

$$N(T=0) = \eta\{\ln(1/\delta) - (1+\gamma) + \mathscr{O}(\delta)\}, \quad s = 1,$$

$$= \frac{\eta}{s-1}\{1 + \mathscr{O}(\delta)\}, \quad s > 1. \qquad (3.18)$$

The finite temperature behavior is a bit more difficult to extract. We note first that in the integral defining $N(T)$:

$$N(T) - N(0) = \int_0^1 \frac{2\eta x^s(x^2 + \delta^2)n(x/\theta)dx}{[x^2 - 4\delta\gamma_s(x) - \delta^2]^2 + [2\pi\delta\eta x^s]^2},$$

$$(3.19)$$

where we have introduced the dimensionless temperature
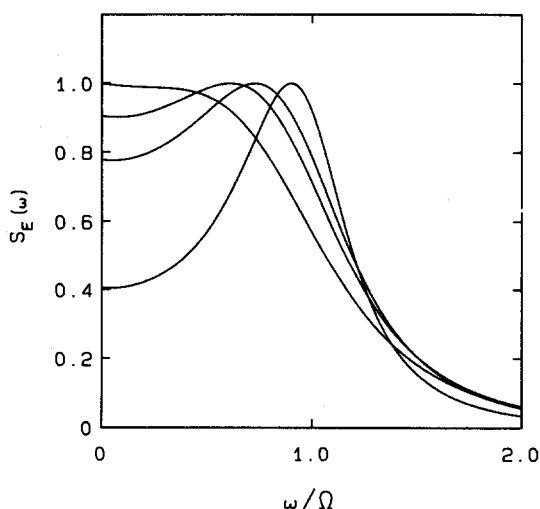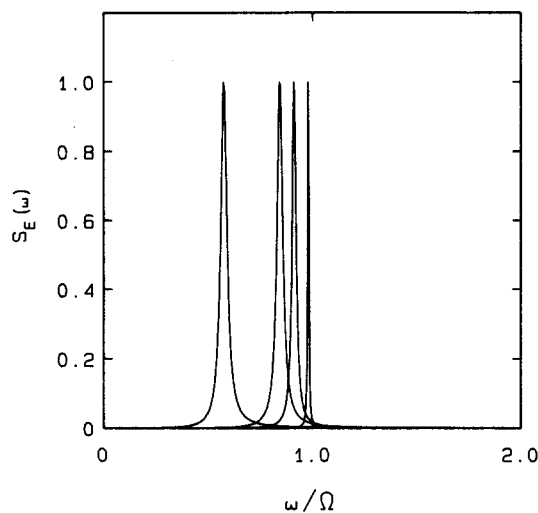

FIG. 1. Normalized emission spectra [Eq. (3.12c)] correponding to an ohmic bath ($s = 1$) as a function of frequency for different values of the coupling strength η. We have taken $\delta = 0.1$ and $\theta = 0.5$. The curves which peak from right to left correspond to values of $\eta = 0.1$, 0.12, 0.15, and 0.20, respectively.

$\theta = kT/\omega_c$, the integrand is, for small η and δ, very sharply peaked around $x = \delta$, i.e., around the oscillator frequency. In the strict weak-coupling limit when $\eta \to 0$, the integrand becomes proportional to a delta function with strength n_Ω, thus reproducing the first term on the right-hand side of Eq. (3.16). The term denoted $\mathscr{N}(T)$ in Eq. (3.16) represents deviations from this ideal Bose-gas behavior due to the interactions and is in fact of order η. This term is negligible at high temperatures $\theta \gg \delta$, but is in fact dominant at very low temperatures when the peak of the integrand in the neighborhood of the oscillator frequency becomes exponentially smaller, due to the Bose factor, than the region of the integral which lies in the neighborhood of and is less than θ. Since $n(x/\theta)$ cuts off the integral for values of $x \gg \theta$, we can estimate this low temperature contribution by extending the upper limit of Eq. (3.19) to infinity and neglecting the η dependent terms in the denominator. We find that

$$\mathscr{N}(T) \sim 2\eta (kT/\omega_c)^{s-1} (kT/\Omega)^2$$
$$\times \{\Gamma(s+1)\zeta(s+1) + \mathcal{O}[(kT/\Omega)^2]\}, \quad (3.20)$$

where $\Gamma(x)$ is the gamma function and $\zeta(x)$ is the Riemann zeta function.

Notice that the low temperature behavior (3.20) is, to lowest order, independent of the upper frequency cutoff ω_c when $s = 1$, i.e., for the Ohmic bath. This is different than the behavior exhibited for $s > 1$. Indeed, in the latter case the low temperature deviation from the ideal Bose-gas behavior can be made as small as desired merely by increasing the width of the bath. Equation (3.7) indicates, on the other hand, that the zero temperature behavior of the quantity $N(T)$ shows just the opposite behavior. To this order the number of quanta in the system oscillator at zero temperature [Eq. (3.7)] is, for $s > 1$, independent of the upper cutoff frequency ω_c. For the Ohmic case, however, there is a dependence upon the ratio ω_c/Ω. In fact it diverges logarithmically as the width of the bath increases. In Fig. 3 we plot the zero temperature limit of $N(T)$ as a function of the ratio $\delta = \Omega/\omega_c$ for the cases $s = 1, 2$, and 3.
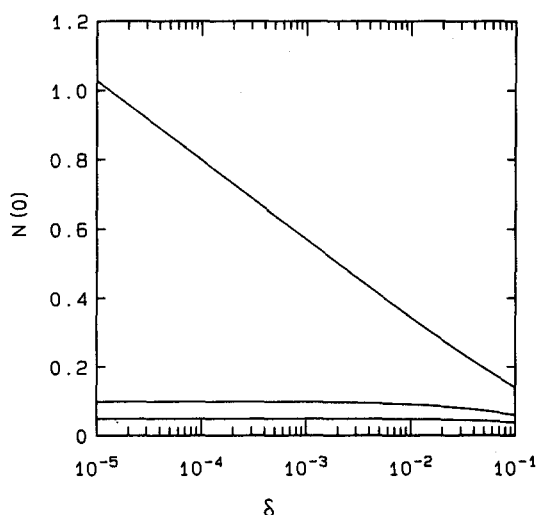

FIG. 3. Zero temperature oscillator population (3.17) for, from top to bottom, values of $s = 1, 2$, and 3, respectively. We have taken $\eta = 0.1$.

IV. VARIATIONAL APPROACH

From the Hamiltonian (2.1) we note that if each bath mode were displaced an amount proportional to $(a + a^\dagger)$, [i.e., $b_\nu + b_\nu^\dagger \to b_\nu + b_\nu^\dagger - f_\nu(a + a^\dagger)$], then the coupling between the bath modes and the system could be made to vanish. To illustrate, let us define new system and bath operators

$$A = UaU^\dagger, \qquad A^\dagger = Ua^\dagger U^\dagger,$$
$$B_\nu = UB_\nu U^\dagger, \qquad B_\nu^\dagger = Ub_\nu^\dagger U^\dagger, \qquad (4.1)$$

where

$$U = \exp\sum_\nu (f_\nu/\omega_\nu)(b_\nu - b_\nu^\dagger)(a + a^\dagger). \qquad (4.2)$$

Then it follows that

$$A = a - \sum_\nu (f_\nu/\omega_\nu)(b_\nu - b_\nu^\dagger)$$
$$= a - \sum_\nu (f_\nu/\omega_\nu)(B_\nu - B_\nu^\dagger),$$
$$A^\dagger = a^\dagger + \sum_\nu (f_\nu/\omega_\nu)(b_\nu - b_\nu^\dagger)$$
$$= a^\dagger \sum_\nu (f_\nu/\omega_\nu)(B_\nu - B_\nu^\dagger),$$
$$B = b_\nu + (f_\nu/\omega_\nu)(a + a^\dagger)$$
$$= b_\nu + (f_\nu/\omega_\nu)(A + A^\dagger),$$
$$B^\dagger = b_\nu^\dagger + (f_\nu/\omega_\nu)(a + a^\dagger)$$
$$= b_\nu^\dagger + (f_\nu/\omega_\nu)(A + A^\dagger). \qquad (4.3)$$

The Hamiltonian (2.1) may then be reexpressed as

$$H = \Omega\left\{A^\dagger A + \frac{1}{2}\right\} - \sum_\nu (g_\nu - f_\nu)^2/\omega_\nu (A + A^\dagger)^2$$
$$+ \sum_\nu \omega_\nu\left\{B_\nu^\dagger B_\nu + \frac{1}{2}\right\} - \Omega\sum_\nu (f_\nu/\omega_\nu)(B_\nu - B_\nu^\dagger)^2$$
$$+ \sum_\nu (g_\nu - f_\nu)(A + A^\dagger)(B_\nu + B_\nu^\dagger)$$
$$- \Omega\sum_\nu (f_\nu/\omega_\nu)(A - A^\dagger)(B_\nu - B_\nu^\dagger). \qquad (4.4)$$

This rather formidable expression simplifies tremendously if $\Omega \ll \omega_\nu$, i.e., in the adiabatic system limit. The choice $f_\nu = g_\nu$ then leads to a set of noninteracting system-bath modes. Unfortunately, this choice can lead to problems if Ω/ω_ν is not small. Consider, e.g., the expectation value of the perturbation term in Eq. (4.4) that is bilinear in the bath modes, taken over the new ground state of the bath for $f_\nu = g_\nu$:

$$-\Omega\left\langle 0\left|\left\{\sum_\nu (g_\nu/\omega_\nu)(B_\nu - B_\nu^\dagger)\right\}^2\right|0\right\rangle$$
$$= \Omega\sum_\nu (g_\nu/\omega_\nu)^2 = \Omega\int d\omega \, J(\omega)/\omega^2.$$

For the Ohmic bath this term is infinite due to an infrared divergence. This suggests that the choice $f_\nu = g_\nu$ is not optimal. A variation approach which leads to useful and interesting results is to take the average of H over the new ground

state (i.e., the vacuum states for the $A^\dagger$ and $B^\dagger$ operators) and minimize the resulting expression:

$$E_0 = \Omega/2 + \sum_\nu (g_\nu - f_\nu)^2/\omega_\nu + \frac{1}{2}\sum_\nu \omega_\nu + \Omega\sum_\nu (f_\nu/\omega_\nu)^2. \quad (4.5)$$

Minimization yields
$$f_\nu = g_\nu (1 + \Omega/\omega_\nu)^{-1} \quad (4.6)$$

so that for small Ω/ω_ν, $f_\nu = g_\nu$, while for for large Ω/ω_ν, $f_\nu = g_\nu\omega_\nu/\Omega$.

With this choice for f_ν, the Hamiltonian becomes

$$H = \Omega\left\{A^\dagger A + \frac{1}{2}\right\} + \sum_\nu \frac{\Omega^2 g_\nu^2}{\omega_\nu(\omega_\nu + \Omega)^2}(A + A^\dagger)^2$$

$$+ \sum_\nu \omega_\nu\left\{B_\nu^\dagger B_\nu + \frac{1}{2}\right\}$$

$$- \Omega\left[\sum_\nu \frac{g_\nu(B_\nu - B_\nu^\dagger)}{(1 + \Omega/\omega_\nu)}\right]^2$$

$$+ \sum_\nu \frac{2\Omega g_\nu}{(\omega_\nu + \Omega)}(A^\dagger B_\nu + A B_\nu^\dagger). \quad (4.7)$$

In what follows, we will treat the free boson Hamiltonian as H_0 and the rest of H as a perturbation.

We can now consider some of the quantities discussed in Sec. III. For example, from Eq. (3.3),

$$N[T] = -\langle a^\dagger a\rangle_H = \left\langle\left[A^\dagger - \sum_\nu (f_\nu/\omega_\nu)(B_\nu - B_\nu^\dagger)\right]\right.$$

$$\times\left.\left[A + \sum_\nu (f_\nu/\omega_\nu)(B_\nu - B_\nu^\dagger)\right]\right\rangle_H. \quad (4.8)$$

To lowest order in the perturbation terms, we find [replacing the thermal density matrix by exp$(-\beta H_0)$]:

$$N(T) = \langle A^\dagger A\rangle_{H_0}$$

$$+ \sum_\nu (f_\nu/\omega_\nu)^2\langle(B_\nu^\dagger B_\nu + B_\nu B_\nu^\dagger)\rangle_{H_0}$$

$$= \frac{1}{\exp(\beta\Omega) - 1} + \int_0^\infty d\omega\frac{J(\omega)(2n_\omega + 1)}{(\omega + \Omega)}. \quad (4.9)$$

We examine $N(T = 0)$ first. In this limit ($\delta = \Omega/\omega_c$),

$$N(T = 0) = \int_0^\infty d\omega J(\omega)(\omega + \Omega)^{-2}$$

$$= \eta\int_0^1 dx\, x^s(x + \delta)^{-2}$$

$$\approx \eta[\ln(1/\delta) + 1], \quad s = 1,$$

$$\approx \eta(s - 1)^{-1}, \quad s \geqslant 2, \quad (4.10)$$

in agreement with Eq. (3.7). If we now look at $N(T) - N(0)$, we find

$$N(T) - N(0) = (\exp\beta\Omega - 1)^{-1}$$

$$+ 2\int_0^\infty d\omega\frac{J(\omega)(\exp\beta\omega - 1)^{-1}}{(\omega + \Omega)^2}. \quad (4.11)$$

For temperatures low compared to Ω/k_B, we can expand the last integral

$$\int_0^\infty d\omega\frac{J(\omega)(\exp\beta\omega - 1)^{-1}}{(\omega + \Omega)^2}$$

$$= \eta\theta^{s-1}\int_0^{1/\theta} dz\frac{z^s(e^z - 1)^{-1}}{(z + \beta\Omega)^2}$$

$$\approx \eta(kT/\omega_c)^{s-1}(kT/\Omega)^2\Gamma(s + 1)\zeta(s + 1) \quad (4.12)$$

again in agreement with the exact analysis of Eq. (3.9).

Finally, we conclude with a brief discussion of the spectrum calculated using this variational procedure. We assume that the spectrum is given by the Fourier transform of the following *equilibrium* correlation function:

$$I(t) = \langle q(0)q(t)\rangle_H = \langle(a + a^\dagger)[a(t) + a^\dagger(t)]\rangle_H$$

$$= \langle(A + A^\dagger)[A(t) + A^\dagger(t)]\rangle_H. \quad (4.13)$$

This will lead, in second order perturbation theory (weak coupling limit) to Lorentzian lines centered at a renormalized frequency depending on the bath density of states. The renormalized frequencies are obtained more easily. We calculate, again using second order perturbation theory, the change in the energy of the vacuum state $|0\rangle$ and of the state $A^\dagger|0\rangle$; the difference is the new frequency. The relevant perturbation terms are [from Eq. (4.7)]

$$\sum_\nu \frac{\Omega^2 g_\nu^2}{\omega_\nu(\omega_\nu + \Omega)^2}(A + A^\dagger)^2$$

$$+ \sum_\nu \frac{2\Omega g_\nu}{(\omega_\nu + \Omega)}\{A^\dagger B_\nu + A B_\nu^\dagger\}. \quad (4.14)$$

The first term contributes in first order perturbation theory and the second term in second order perturbation theory [to $\mathcal{O}(g_\nu^2)$]. We find

$$\Omega' = \Omega\left\{1 + 2\delta\eta\mathscr{P}\int_0^1 dx\frac{x^{s-1}}{\delta^2 - x^2}\right\} \quad (4.15)$$

so that

$$\Omega'_{s=1} = \Omega\{1 + 2\eta\,\text{arctanh}(\delta)\}, \quad (4.16)$$

$$\Omega'_{s=2} = \Omega\{1 + \eta\delta\ln[\delta^2/(1 - \delta^2)]\}, \quad (4.17)$$

$$\Omega'_{s=3} = \Omega\{1 - 2\eta\delta + \eta\delta^2\ln[(1 + \delta)/(1 - \delta)]\}. \quad (4.18)$$

If we approximate the zeros of $D(i\omega)$ to lowest order in δ [see Eq. (3.14)] we find agreement with these results. Hence the variational procedure yields the correct results (at low order perturbation theory) to order δ^2.

On the other hand, if we compute the widths Γ_s of the optical spectral lines using the Golden Rule, we find

$$\Gamma_s = 4\Omega^2\sum_\nu g_\nu^2/(\omega_\nu + \Omega)^{-2}\delta(\Omega - \omega_\nu)(2n_\nu + 1)$$

$$= \eta\omega_c\left(\frac{\Omega}{\omega_c}\right)^s(2n_\Omega + 1). \quad (4.19)$$

These results are *not* in good agreement with the exact results, in particular for $s = 1$. It is possible that this discrepancy stems from the fact that we have used a different means to calculate the spectra in each case.

We conclude that the variational approach, coupled with the low orders of perturbation theory, provides a good

description of the dynamical behavior of the fully coupled system. It must be used with care, however, particularly when there is strong coupling in bath modes at low frequency, as occurs in the Ohmic case. The general overall agreement of the variational results with the exact calculation, however, lends support to its use as a tool for examining the dissipative dynamics of coupled quantum mechanical systems.

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