Relaxation spectrum of quantum harmonic motion in the presence of nonlinear dissipative-diffusive couplings

M. A. Despósito and E. S. Hernández
Departamento de Física, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, 1428 Buenos Aires, Argentina
(Received 03 June 1992)

We analyze the behavior of a damped quantum harmonic oscillator immersed in a heat bath with a nonlinear coupling. For this purpose, we construct a generalized master equation (GME) for the reduced density of the oscillator. We specialize the results for a quadratic coupling in the presence of a bosonic reservoir and an Ohmic dissipation model, analyzing the evolution equation for the mean value of the oscillator coordinate. In the asymptotic case we obtain a gain-loss master equation whose transition rates are polynomials in the number of quanta. No explicit solutions other than the equilibrium one can be written, since the standard methods do not apply. The equilibrium solution is investigated and the eigenvalues of the corresponding spectral problem are numerically computed to study the effect of the nonlinearity on the evolution of the system. By means of the Wigner transformation of the GME, we extract a third-order partial derivative equation that represents the semiclassical evolution of the damped oscillator. In the classical limit this is a nonlinear Fokker-Planck equation.

PACS number(s): 05.40.+j, 05.70.Ln, 03.65.Sq

I. INTRODUCTION

In several fields of physics, mostly related to quantum optics, condensed matter, or nuclear theory, one encounters harmonic motion perturbed by some stochastic interaction with a macroscopic object. This situation typically corresponds to the residual coupling between one or various normal modes of a quantum fluid or many-body system to the remaining, i.e., unresolved, microscopic degrees of freedom. The usual approaches to formulate this problem in the frame of statistical mechanics resort to either the quantum Langevin equation [1] or to a reduction of the Liouville–von Neumann description of quantum mechanics [2, 3] that gives rise to irreversible evolution ruled by generalized master equations (GME's) [4–6] as illustrated in a series of previous works for different selections of the deterministic coupling to a heat reservoir. In any case, the relaxation dynamics is that of the so-called quantal Brownian motion [3, 7, 8] and one can assert that the damped evolution of a harmonic oscillator immersed into an arbitrary heat bath is fairly well understood insofar as the Markovian limit is concerned. The non-Markovian case has been investigated as well [9–12] and for various models of the thermal environment one can set a simple rule to estimate the characteristic decay time. The common feature to the above-mentioned and other authors' models [1, 4, 13–16] of damped quantal harmonic motion—the latter concerning oscillator reservoirs—resides in the structure of the dissipative coupling which is, in every case, a linear function of the decaying coordinate and/or momentum. This choice makes room only for nearest-neighbor transitions between states in the oscillator spectrum, and the asymptotic master equation that describes the time evolution of the level occupation probabilities is the well-known one-step chain [17] whose spectral problem can be analytically solved in the Markovian regime [9, 17]. We believe then it is of interest to investigate the kind of lifetime spectrum associated with multiphonon transitions, in other words, with nonlinear interactions between the quantum harmonic coordinates and its macroscopic environment. A typical example that arises from quantum optics is the model of two-photon absorption from a single-mode field inside a cavity [18, 19].

For the above-stated purpose, in Sec. II we devise a particular model that generalizes the previous ones for nonlinear couplings between the system and the reservoir. We construct the corresponding generalized master equation for the reduced density matrix and obtain the law of motion of the harmonic coordinate. In Sec. III we specialize the above results for a quadratic coupling and analyze the Markovian limit and the Ohmic dissipation model, concentrating most of the discussion on the evolution of averaged observables. In Sec. IV we obtain the gain-loss master equation that emerges in the asymptotic limit and discuss its solutions. The semiclassical version of the model is developed in Sec. V using the Wigner transformation. A summary of our results is given in Sec. VI.

II. GENERALIZED QUANTUM MASTER EQUATIONS

We consider a quantum harmonic oscillator with natural frequency ω_0 and mass m immersed into an arbitrary heat bath. The exact motion of the composite system is described by the Hamiltonian

$$H = H_S + H_B + H_{SB} \ , \tag{2.1}$$

where

$$H_S = \frac{P^2}{2m} + \frac{m\omega_0^2}{2}Q^2 \tag{2.2}$$

is the isolated oscillator Hamiltonian and H_B is the isolated reservoir Hamiltonian. The interaction term is assumed to be of the form

$$H_{SB} = \lambda F(Q)B \ , \tag{2.3}$$

where λ is a parameter that measures the average strength of the interaction, $F(Q)$ is an arbitrary function of the oscillator coordinate, and the operator B belongs to the operator space of the reservoir and contains infinite summations over all particles in the environment. The structure of this Hamiltonian is an extension of the "fully coupled oscillator model" [14] where only the harmonic coordinate and not the momentum is affected by the interaction with the microscopic degrees of freedom. However, at this point no reference to an explicit model for the thermal bath is put forward.

Starting from the Liouville–von Neumann equation of motion for the total density operator, the use of standard projection operator techniques complemented by the usual Born (weak-coupling) aproximation yields a GME for the reduced density operator ρ of the oscillator. If we assume that no correlations between the oscillator and the heat bath exist at $t = 0$, and that the latter is initially in thermal equilibrium, i.e.,

$$\rho_B(0) = \rho_B^{\rm eq} = \frac{e^{-\beta H_B}}{{\rm Tr}(e^{-\beta H_B})} \ , \tag{2.4}$$

where ρ_B is the reduced density of the heat bath and $\beta = 1/k_B T$ is related to the equilibrium temperature of the reservoir, the corresponding GME takes the form [20]

$$\begin{aligned}\dot\rho(t) + \frac{i}{\hbar}[H_S,\rho(t)] = &-\frac{\lambda^2}{\hbar^2}\int_0^t d\tau [F(Q), e^{-iH_S\tau/\hbar}[F(Q),\rho(t-\tau)]e^{iH_S\tau/\hbar}]{\rm Re}\{\Phi(\tau)\} \\ &-\frac{i\lambda^2}{\hbar^2}\int_0^t d\tau [F(Q), e^{-iH_S\tau/\hbar}[F(Q),\rho(t-\tau)]_+ e^{iH_S\tau/\hbar}]{\rm Im}\{\Phi(\tau)\} \ ,\end{aligned} \tag{2.5}$$

where $[\,,\,]$ and $[\,,\,]_+$, respectively, denote the commutator and anticommutator, while ${\rm Re}\{\Phi(\tau)\}$ and ${\rm Im}\{\Phi(\tau)\}$ are the real and imaginary parts of the correlation function

$$\Phi(t) = {\rm Tr}_B[B(t)B\rho_B^{\rm eq}] \tag{2.6}$$

for the bath operator B evolving in time by the motion of the reservoir.

The GME (2.5) contains the reversible and irreversible contributions that arise from the total Hamiltonian. In general, this kind of matrix equation is rather difficult to handle and is not suitable for approximations consistent with the requirements of a master equation. On the other hand, it contains much more information than that which is experimentally available. For this reason, it is much more useful to use a c-number representation of the matrix equation, like the evolution of the averaged observables, the asymptotic master equation, or a semiclassical equation. Later on in this work, we analyze and discuss these kinds of representation.

Since the mean value of an arbitrary operator A belonging to the oscillator space is $\langle A\rangle_t = {\rm Tr}_S\{A\rho(t)\}$, from Eq. (2.5) we get

$$\begin{aligned}\langle\dot A\rangle_t - \frac{i}{\hbar}\langle[H_S,A]\rangle_t = &-\frac{\lambda^2}{\hbar^2}\int_0^t d\tau\langle[e^{iH_S\tau/\hbar}[A,F(Q)]e^{-iH_S\tau/\hbar},F(Q)]\rangle_{t-\tau}{\rm Re}\{\Phi(\tau)\} \\ &-\frac{i\lambda^2}{\hbar^2}\int_0^t d\tau\langle[e^{iH_S\tau/\hbar}[A,F(Q)]e^{-iH_S\tau/\hbar},F(Q)]_+\rangle_{t-\tau}{\rm Im}\{\Phi(\tau)\} \ .\end{aligned} \tag{2.7}$$

Therefore, for any kind of function $F(Q)$, the evolution of the mean values for the oscillator displacement and momentum is given by

$$\langle\dot Q\rangle_t = \frac{1}{m}\langle P\rangle_t \ , \tag{2.8}$$

$$\langle\dot P\rangle_t = -m\omega_0^2\langle Q\rangle_t + \frac{i\lambda^2}{\hbar}\int_0^t d\tau\langle[F'(Q(-\tau)),F(Q)]\rangle_{t-\tau}{\rm Re}\{\Phi(\tau)\} - \frac{\lambda^2}{\hbar}\int_0^t d\tau\langle[F'(Q(-\tau)),F(Q)]_+\rangle_{t-\tau}{\rm Im}\{\Phi(\tau)\} \ , \tag{2.9}$$

where we use the fact that $[F(Q),P] = i\hbar F'(Q)$. Note that in this model (in contrast to the rotating wave approximation case [1, 14]) the mean values of momentum and velocity are proportional to each other. This relation is also valid from the operators themselves, as one can easily verify by writing down the Heisenberg equation of motion for the operator Q from the total Hamiltonian (2.1).

III. QUADRATIC COUPLING

We now assume that the coupling between the oscillator and the heat bath is quadratic in the former, i.e., $F(Q) = Q^2$. From Eqs. (2.8) and (2.9) one obtains that the mean value of the oscillator displacement obeys the integro-differential equation

$$\begin{aligned} m\langle \ddot{Q} \rangle_t = & -m\omega_0^2 \langle Q \rangle_t \\ & + \frac{4\lambda^2}{m\omega_0} \int_0^t d\tau \sin(\omega_0 \tau) \mathrm{Re}\{\Phi(\tau)\} \langle Q \rangle_{t-\tau} \\ & - \frac{4\lambda^2}{\hbar} \int_0^t d\tau \cos(\omega_0 \tau) \mathrm{Im}\{\Phi(\tau)\} \langle Q^3 \rangle_{t-\tau} \\ & - \frac{4\lambda^2}{\hbar\omega_0} \int_0^t d\tau \sin(\omega_0 \tau) \mathrm{Im}\{\Phi(\tau)\} \langle \{\dot{Q}, Q^2\} \rangle_{t-\tau} , \end{aligned} \tag{3.1}$$

where $\{\,,\,\}$ stands for the symmetrized product and we use the fact that $m\dot{Q} = P$. In contrast to the linear coupling case [21], this equation contains the real part of the bath correlation function that in the case of a bosonic reservoir, as we will see later, depends on the temperature. Moreover, Eq. (3.1) includes the higher moments $\langle Q^3 \rangle$ and $\langle \{\dot{Q}, Q^2\} \rangle$ and the evolution equation for these moments involves again higher moments. In connection with this, note that only in the linear coupling model [21], i.e., $F(Q) = Q$, do Eqs. (2.8) and (2.9) involve the mean values $\langle Q \rangle$ and $\langle P \rangle$ alone, and this makes possible an analytical approach.

A. Markovian regime

The equation of motion (3.1) is a nonlinear and non-Markovian integro-differential equation. In this form it is untractable. To further simplify the problem we make the Markov assumption [22]. In this approximation one can replace the density $\rho(t-\tau)$ into the integrals of Eq. (3.1) by

$$\rho(t-\tau) \approx e^{iH_S\tau} \rho(t) e^{-iH_S\tau} , \tag{3.2}$$

and the upper limit in the integrals by infinity. In this case one can verify that

$$\langle Q \rangle_{t-\tau} = \cos(\omega_0\tau) \langle Q \rangle_t - \frac{1}{m\omega_0} \sin(\omega_0\tau) \langle P \rangle_t \tag{3.3}$$

and

$$\begin{aligned} \cos(\omega_0\tau)\langle Q^3 \rangle_{t-\tau} + \frac{\sin(\omega_0\tau)}{m\omega_0} \langle \{PQ^2\} \rangle_{t-\tau} \\ = \cos^2(\omega_0\tau) \langle Q^3 \rangle_t - \frac{\sin(2\omega_0\tau)}{m\omega_0} \langle \{PQ^2\} \rangle_t \\ + \frac{\sin^2(\omega_0\tau)}{m^2\omega_0^2} \langle \{P^2 Q\} \rangle_t , \end{aligned} \tag{3.4}$$

which enable us to write the Markovian version of the evolution equation (3.1) as

$$\begin{aligned} m\langle \ddot{Q} \rangle_t = & -\left(m\omega_0^2 - \frac{2\lambda^2}{m\omega_0} \int_0^\infty d\tau \sin(2\omega_0\tau) \mathrm{Re}\{\Phi(\tau)\} \right) \langle Q \rangle_t - \frac{4\lambda^2}{\hbar} \left(\int_0^\infty d\tau \cos^2(\omega_0\tau) \mathrm{Im}\{\Phi(\tau)\} \right) \langle Q^3 \rangle_t \\ & - \frac{4\lambda^2}{m\omega_0^2} \left(\int_0^\infty d\tau \sin^2(\omega_0\tau) \mathrm{Re}\{\Phi(\tau)\} \right) \langle \dot{Q} \rangle_t + \frac{4\lambda^2}{\hbar\omega_0} \left(\int_0^\infty d\tau \sin(2\omega_0\tau) \mathrm{Im}\{\Phi(\tau)\} \right) \langle \{\dot{Q}, Q^2\} \rangle_t \\ & - \frac{4\lambda^2}{\hbar\omega_0^2} \left(\int_0^\infty d\tau \sin^2(\omega_0\tau) \mathrm{Im}\{\Phi(\tau)\} \right) \langle \{(\dot{Q})^2, Q\} \rangle_t . \end{aligned} \tag{3.5}$$

As expected [23], one can see that the coupling with the macroscopic environment introduces both a mechanism of dissipation and a renormalization of the original potential of the system.

Taking into account the coefficients that appear in the linear coupling model [21], we can rewrite Eq. (3.5) as

$$\begin{aligned} m\langle \ddot{Q} \rangle_t = & -[m\omega_0^2 + 4\delta(2\omega_0)] \langle Q \rangle_t + m[\omega_r^2(2\omega_0) + \omega_r^2(0)] \langle Q^3 \rangle_t - 4\nu(2\omega_0) \langle \{\dot{Q}, Q^2\} \rangle_t \\ & + \frac{2}{m\omega_0^2} [C(2\omega_0) - C(0)] \langle \dot{Q} \rangle_t - \frac{m}{\omega_0^2} [\omega_r^2(2\omega_0) - \omega_r^2(0)] \langle \{(\dot{Q})^2, Q^2\} \rangle_t , \end{aligned} \tag{3.6}$$

where

$$C(\omega) = \lambda^2 \int_0^\infty d\tau \cos(\omega\tau) \mathrm{Re}\{\Phi(\tau)\} , \tag{3.7}$$

$$\nu(\omega) = -\frac{2\lambda^2}{\hbar\omega} \int_0^\infty d\tau \sin(\omega\tau) \mathrm{Im}\{\Phi(\tau)\} , \tag{3.8}$$

are, respectively, the diffusion and friction coefficients,

$$\omega_r^2(\omega) = -\frac{2\lambda^2}{\hbar m} \int_0^\infty d\tau \cos(\omega\tau) \mathrm{Im}\{\Phi(\tau)\} \tag{3.9}$$

is a renormalized frequency, and

$$\delta(\omega) = -\frac{\lambda^2}{m\omega} \int_0^\infty d\tau \sin(\omega\tau) \mathrm{Re}\{\Phi(\tau)\} \tag{3.10}$$

is a correction to the unperturbed stiffness.

From their definitions, one can demonstrate (see the appendix) that the diffusion and friction coefficients are related by the quantum fluctuation-dissipation relationship

$$C(\omega) = \frac{\hbar\omega}{2} \coth\left(\frac{\beta\hbar\omega}{2}\right) \nu(\omega) , \tag{3.11}$$

which in the classical limit reduces to the usual form

$$C(\omega) = k_B T \nu(\omega) \ . \tag{3.12}$$

B. Bosonic reservoir and Ohmic dissipation model

We now consider that the reservoir consists of harmonic oscillators[1, 7, 14] and the coupling is linear in every microscopic coordinate. In this case, we choose the operator B of the coupling Hamiltonian (2.3) as

$$B = \sum_j c_j (b_j^\dagger + b_j) \ , \tag{3.13}$$

where $b_j^\dagger$ and b_j are, respectively, the creation and annihilation operators for the boson of frequency ω_j, and c_j are real coupling constants. For this model, one can verify that the correlation function is given by

$$\Phi(t) = 2\sum_j c_j^2 \left\{ \coth\left(\frac{\beta\hbar\omega_j}{2}\right)\cos(\omega_j t) - i\sin(\omega_j t) \right\} \ . \tag{3.14}$$

Note that the imaginary part of the correlation function only depends on the reservoir characteristics, while the real part also includes the reservoir temperature.

As usual, the bath is described in the continuous limit by its density of states $g(\omega)$. The Ohmic dissipation model [15, 24] is obtained by setting down

$$g(\omega)c^2(\omega) \propto \omega\, f_c(\omega/\gamma) \ , \tag{3.15}$$

where γ is essentially the phonon bandwidth of the heat bath excitations that couple to the oscillator, and $f_c(\omega/\gamma)$ is a cutoff function such that $f_c(0) = 1$ and significantly decreases within a frequency range of order γ. If we choose a Lorentzian cutoff [14–16, 23], we get

$$g(w)c^2(\omega) = \alpha\frac{\hbar}{2\pi}\frac{\gamma^2\omega}{\gamma^2+\omega^2} \ , \tag{3.16}$$

and therefore [20]

$$\mathrm{Im}\{\Phi(t)\} = -\alpha\frac{\hbar\gamma^2}{2}e^{-\gamma t} \ , \tag{3.17}$$

$$\mathrm{Re}\{\Phi(t)\} = \alpha\frac{\hbar\gamma^2}{2}\left\{ \cot\left(\frac{\beta\hbar\gamma}{2}\right)e^{-\gamma t} - \sum_{k=1}^{\infty}\frac{8\pi k\ e^{-(2\pi k t)/(\beta\hbar)}}{(\beta\hbar\gamma)^2-(2\pi k)^2} \right\} \ . \tag{3.18}$$

With these expressions, one can demonstrate that

$$\int_0^\infty dt\, \mathrm{Re}\{\Phi(t)\} = \alpha k_B T \ , \tag{3.19}$$

$$\int_0^\infty dt\, \mathrm{Im}\{\Phi(t)\} = -\alpha\frac{\hbar\gamma}{2} \ , \tag{3.20}$$

which exhibit the link between the reservoir internal correlation and the two sources of energy spread for the current degrees of freedom, namely, the temperature and the phonon bandwidth.

From Eqs. (3.17) and (3.18) we observe that the characteristic memory time of the imaginary part is the inverse γ^{-1} of the bandwidth, while that corresponding to the real part depends on the relationship between γ^{-1} and the thermal relaxation time $\beta\hbar/(2\pi)$. Moreover, it can be shown [20] using the Langevin formalism that the real part is connected with the fluctuations while the imaginary part yields the dissipation. In this sense, the above results agree with those obtained in Ref. [14].

Using (3.17) and (3.18), one can integrate expressions (3.7), (3.8), (3.9), and (3.10) to obtain

$$\nu = \lambda^2\alpha \ , \tag{3.21}$$

$$\omega_r^2 = \lambda^2\alpha\frac{\gamma}{m} \ , \tag{3.22}$$

$$\delta(\omega) = -\lambda^2\alpha\frac{\hbar}{2m}\left[\cot\left(\frac{\beta\hbar\gamma}{2}\right) - \sum_{k=1}^{\infty}\frac{(8\pi k)(\beta\hbar\gamma)^2}{[(\beta\hbar\gamma)^2-(2\pi k)^2][(\beta\hbar\omega_0)^2+(2\pi k)^2]}\right] , \tag{3.23}$$

and $C(\omega)$ is related to ν through the relation (3.11). To obtain the expressions (3.21) to (3.23) we use the fact that $\gamma \gg \omega_0$ in the Markovian case. Note that ν and ω_r do not depend on ω_0. In the classical limit the diffusion coefficient is also independent of ω_0, and in addition, one can set $\delta = 0$.

Therefore, for the Ohmic dissipation model we can write the equation of motion for the position mean value as

$$m\langle\ddot{Q}\rangle_t = -[m\omega_0^2 + 4\delta(2\omega_0)]\,\langle Q\rangle_t + 2m\omega_r^2\,\langle Q^3\rangle_t - 4\nu\,\langle\{\dot{Q},Q^2\}\rangle_t + \frac{2}{m\omega_0^2}[C(2\omega_0)-C(0)]\,\langle\dot{Q}\rangle_t \ , \tag{3.24}$$

and the Markovian version of the GME (2.5) as

$$\begin{aligned}\dot{\rho}(t) = &-\frac{i}{\hbar}[H_S,\rho(t)] + \frac{i}{\hbar}\frac{m\omega_r^2}{2}[Q^2,[Q^2,\rho(t)]_+] - \frac{2}{\hbar^2}\delta[Q^2,[\{QP\},\rho(t)]] - \frac{i}{\hbar}\frac{\nu}{m}[Q^2,[\{QP\},\rho(t)]_+]\\ &-\frac{1}{2\hbar^2}\{C(2\omega_0)+C(0)\}[Q^2,[Q^2,\rho(t)]] + \frac{1}{2\hbar^2m^2\omega_0^2}\{C(2\omega_0)-C(0)\}[Q^2,[P^2,\rho(t)]] \ .\end{aligned} \tag{3.25}$$

IV. ASYMPTOTIC MASTER EQUATION

It can be shown [25] that the decay time of the nondiagonal matrix elements of the reduced density ρ is lower than the characteristic evolution time of its diagonal elements. This behavior can be expected in the weak-coupling limit and is consistent with the adopted Markovian approximation. Consequently, in the near equilibrium (asymptotic) regime one can write the density operator as

$$\rho(t) = \sum_N \rho_N(t)|N\rangle\langle N| \ , \tag{4.1}$$

in the corresponding Fock basis $|N\rangle$ for the oscillator. In this limit, where only the diagonal terms of ρ survive, an algebraic calculation leads us to the asymptotic GME (3.25) in terms of creation and annihilation operators,

$$\begin{aligned}\dot\rho(t) = &-\frac{1}{4m^2\omega_0^2}[C(2\omega_0) - \hbar\omega_0\nu(2\omega_0)]\\ &\times(\Gamma^2\Gamma^{\dagger 2}\rho - 2\Gamma^{\dagger 2}\rho\Gamma^2 + \rho\Gamma^2\Gamma^{\dagger 2})\\ &-\frac{1}{4m^2\omega_0^2}[C(2\omega_0) + \hbar\omega_0\nu(2\omega_0)]\\ &\times(\Gamma^{\dagger 2}\Gamma^2\rho - 2\Gamma^2\rho\Gamma^{\dagger 2} + \rho\Gamma^{\dagger 2}\Gamma^2) \ ,\end{aligned} \tag{4.2}$$

which can be set in the form of a gain-loss master equation

$$\begin{aligned}\dot\rho_N = &\ W^+(N+1)(N+2)\rho_{N+2} + W^- N(N-1)\rho_{N-2}\\ &-[W^+N(N-1) + W^-(N+1)(N+2)]\rho_N \ ,\end{aligned} \tag{4.3}$$

W^+ and W^- being the microscopic transition rates, respectively, associated with the simultaneous annihilation (decay processes) and creation (reexcitation processes) of two quanta. Taking into account the relation (3.11), these transition rates can be written as

$$W^+ = \frac{\hbar\nu}{m^2\omega_0}[n(2\omega_0) + 1] \ , \tag{4.4}$$

$$W^- = \frac{\hbar\nu}{m^2\omega_0}\, n(2\omega_0) \ , \tag{4.5}$$

where $n(\omega_0)$ denotes the average occupation number for oscillator quanta with frequency ω_0 at temperature T. Likewise, these transition rates satisfy

$$\frac{W^-}{W^+} = e^{-2\beta\hbar\omega_0} \ . \tag{4.6}$$

It is important to notice that the results of this section are independent of the choice for the heat bath.

The asymptotic master equation (4.3) is a nonlinear one, where the transition probabilities are quadratic polynomials in the number of quanta of the oscillator. Moreover, because the transition occurs only between second neighbors of the oscillator spectrum, the diagonal elements of the density matrix with even (ρ_e) and odd (ρ_o) index are not linked. It is easy to see that for each of these subsystems the corresponding master equation describes a nonlinear one-step process. In connection, note that Eq. (4.3) can be written as

$$\dot\rho = \mathbf{M}\rho \ , \tag{4.7}$$

where ρ denotes here a vector whose components are the diagonal matrix elements of the reduced density and $\mathbf{M}$ is a non-Hermitian pentadiagonal infinite matrix that satisfies $(\mathbf{M})_{N,N\pm1} = 0$. Therefore, by a permutation of rows and columns it can be cast into the decomposable [17] form

$$\mathbf{M}' = \begin{pmatrix} \mathbf{E} & 0 \\ 0 & \mathbf{O} \end{pmatrix} \ , \tag{4.8}$$

where $\mathbf{E}$ and $\mathbf{O}$ are tridiagonal matrices which, respectively, denote the transition matrices governing the evolution of the "noninteracting" subsystems described by ρ_e and ρ_o. In this sense, note that $\mathbf{M}'$ has two linearly independent eigenvectors $\rho_e^{\rm eq}$ and $\rho_o^{\rm eq}$ with zero eigenvalues.

Using the step operator [17] $\mathcal{E}$ defined as

$$\mathcal{E}f(N) = f(N+1), \qquad \mathcal{E}^{-1}f(N) = f(N-1) \ , \tag{4.9}$$

one can write Eq. (4.3) in the stationary case as

$$(\mathcal{E}^2 - 1)[W^+N(N-1) - \mathcal{E}^{-2}W^-(N+1)(N+2)]\rho_N^{\rm eq} = 0 \ . \tag{4.10}$$

This equation states that the expression

$$N(N-1)(W^+\rho_N^{\rm eq} - W^-\rho_{N-2}^{\rm eq}) \tag{4.11}$$

is independent of N and then

$$\rho_N^{\rm eq} = \frac{W^-}{W^+}\rho_{N-2}^{\rm eq} \ . \tag{4.12}$$

Taking into account Eq. (4.6) we may write the equilibrium solution (4.12) as

$$\left.\begin{matrix}\rho_{2N}^{\rm eq}\\ \rho_{2N+1}^{\rm eq}\end{matrix}\right\} = e^{-2\beta\hbar\omega_0 N} \times \left\{\begin{matrix}\rho_0^{\rm eq}\\ \rho_1^{\rm eq} .\end{matrix}\right. \tag{4.13}$$

Consequently, one can assert that the stationary solution possesses the canonical structure with proper normalization factors. These factors can be obtained from the initial conditions considering that the probability must be conserved in each subsystem. Then, using (4.13) one obtains

$$\sum_N \rho_{2N}(0) = \sum_N \rho_{2N}^{\rm eq} = \frac{\rho_0^{\rm eq}}{1 - e^{-2\beta\hbar\omega_0}} \ , \tag{4.14}$$

$$\sum_N \rho_{2N+1}(0) = \sum_N \rho_{2N+1}^{\rm eq} = \frac{\rho_1^{\rm eq}}{1 - e^{-2\beta\hbar\omega_0}} \ , \tag{4.15}$$

where $\rho_N(0)$ denotes the initial occupations. The total normalization condition allows us to write

$$\rho_0^{\rm eq} + \rho_1^{\rm eq} = 1 - e^{-2\beta\hbar\omega_0} \ . \tag{4.16}$$

Therefore, two normalization conditions are needed to completely determine the stationary solution. On the one hand, one realizes that if at $t = 0$ the population is concentrated on just one oscillator state, either even or odd, conditions (4.14) and (4.15) lead to vanishing of the odd or even partner, respectively, on the left-hand side of Eq. (4.16). In such a case, the equilibrium distribution is canonical on the subset where the initial population belongs and the complementary subset remains depopulated. On the other hand, if the initial distribution spreads over at least two states of different parity, the only condition under which (4.13) is an overall canonical distribution over the whole oscillator spectrum is

$$\rho_1^{\rm eq} = \rho_0^{\rm eq}\, e^{-\beta\hbar\omega_0} \ . \tag{4.17}$$

In such a case, Eq. (4.16) gives

$$\rho_0^{\rm eq} = 1 - e^{-\beta\hbar\omega_0} \ , \tag{4.18}$$

which coincides with the canonical partition function. In general according to (4.14) and (4.15), the ratio $\rho_1^{\rm eq}/\rho_0^{\rm eq}$ is determined by the initial odd-even occupation ratio; accordingly, in the majority of cases the distribution (4.13) is noncanonical over the complete Fock space.

Notice that the canonical structure of the equilibrium solution is a consequence of the assumption that the asymptotic density ρ is diagonal or, equivalently, of the weak-coupling hypothesis. In other cases Eq. (4.2) is no longer valid.

Opposite to what happens in the linear coupling case [10], it is not posible to obtain an explicit solution of the master equation (4.3) other than the stationary solution (4.13), since the standard methods [3, 11, 17, 26] do not work in this case. For example, the characteristic function [10] defined as

$$\Psi(z,t) = \sum_{N\geq 0} z^N \rho_N \tag{4.19}$$

can be seen to satisfy the second-order partial derivative equation

$$\frac{\partial}{\partial t}\Psi(z,t) = (1-z^2)\frac{\partial^2}{\partial z^2}[(W^+ - z^2 W^-)\Psi(z,t)] \ , \tag{4.20}$$

and cannot be explicitly integrated.

Moreover, the evolution equations for the moments

$$\langle N^p\rangle = \sum N^p \rho_N \tag{4.21}$$

can be extracted from Eq. (4.3) and read

$$\begin{aligned}\langle \dot{N^p}\rangle = \sum_{k=1}^{p} 2^k \binom{p}{k}\{\ &\langle N^{p-k+2}\rangle[W^- + (-1)^k W^+] \\ &+\langle N^{p-k+1}\rangle[3W^- + (-1)^{k+1}W^+] \\ &+\langle N^{p-k}\rangle\}\ .\end{aligned} \tag{4.22}$$

These nonlinear moment equations constitute a linked hierarchy in which the motion of the pth moment involves the higher-order $(p+1)$th one and appropriate truncation is needed to obtain some approximate solution. For example, the evolution of the first moment is given by

$$\langle \dot{N}\rangle = 2(W^- - W^+)\langle N^2\rangle + 2(3W^- + W^+)\langle N\rangle + 4W^- \ , \tag{4.23}$$

and one can only extract $\langle N^2\rangle$ as a function of $\langle N\rangle$ in the equilibrium case. The latter can be computed from Eqs. (4.21) and (4.13) [and not from Eq. (4.22)], and reads

$$\langle N\rangle_{\rm eq} = \frac{2e^{-2\beta\hbar\omega_0} - \rho_0^{\rm eq}}{1 - e^{-2\beta\hbar\omega_0}} \ . \tag{4.24}$$

Note that this expression (and therefore all the equilibrium moments) depends on the initial conditions through the relations (4.14) and (4.15).

We now numerically compute the decay rate of the harmonic mode. For this purpose, one can express the oscillator density vector as

$$\rho(t) = \rho^{\rm eq} + \sum_j C_j \mathbf{V}^j e^{-\lambda_j t} \ , \tag{4.25}$$

where $\mathbf{V}^j$ and λ_j are, respectively, the eigenvector and eigenvalues of the spectral problem defined by the matrix $\mathbf{M}'$. To simplify the calculation, the matrices $\mathbf{E}$ and $\mathbf{O}$ have been symmetrized with the usual procedure [26]. In the course of the computations it has been observed that as the parameter $\Theta = k_B T/\hbar\omega_0$ increases, the size of the truncated oscillator spectrum that guarantees the proper behavior of the eigenvalues must be enlarged. In particular, for $\Theta = 100$ the truncation at $N_{\max} = 1000$ is satisfactory. With these prescriptions we have numerically verified that the zero eigenvalue is twofold.

In Fig. 1 we have plotted the six smallest nonvanishing eigenvalues λ_2 to λ_7 as a function of the parameter Θ. We can observe that when $\Theta < 0.5$ these eigenvalues are given by

$$\lambda_n = W^+ n(n-1) \ , \ n = 0,1,2\ldots \ . \tag{4.26}$$

This behavior can be understood if we consider that in this situation, by virtue of Eq. (4.6), the majority of the microscopic processes are decaying events and one can

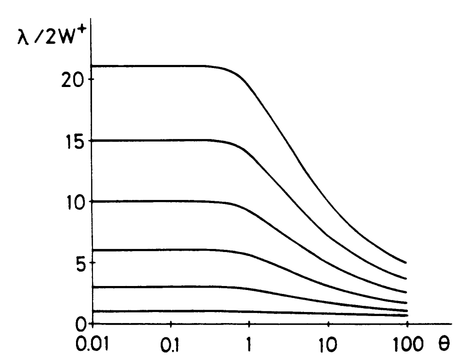

FIG. 1. The six smallest nonvanishing eigenvalues λ_2 to λ_7 that arise from the spectral problem (4.7).

set $W^+ \gg W^- \approx 0$. With this prescription, Eq. (4.20) for the characteristic function reads

$$\frac{\partial}{\partial t}\Psi(z,t) = W^+(1-z^2)\frac{\partial^2}{\partial z^2}\Psi(z,t) \ , \tag{4.27}$$

which can be analytically solved in terms of the Jacobi polynomials [27]. Thus one can verify that the eigenvalues take the form (4.26).

When $\Theta > 0.5$ the eigenvalues decrease with temperature and tend to form a continuum where $\lambda \geq W^+$. Thus, the truncation at finite $N_{\max}$ is not a valid procedure; indeed, for larger values of Θ, the system is a classical one and the GME description should be given up.

V. WIGNER REPRESENTATION

In this section we derive the semiclassical counterpart of Eq. (3.25) according to the Wigner representation [28, 29]. For this purpose we make use of the same prescriptions given in Ref. [12]. From the GME (3.25), and after some algebra, the corresponding equation for the evolution of the Wigner quasiprobability function of the oscillator is

$$\begin{aligned}\frac{\partial}{\partial t}\rho_W(Q,P,t) = \Bigg\{ &-\frac{\partial}{\partial Q}\frac{P}{m} + \frac{\partial}{\partial P}\left((m\omega_0^2 Q + 4\delta(2\omega_0)Q - 2m\omega_r^2 Q^3) + 4\frac{\nu}{m}Q^2 P + \frac{2}{m^2\omega_0^2}[C(0) - C(2\omega_0)]P\right) \\ &-\frac{\partial^2}{\partial Q\partial P}\left(4\delta(2\omega_0)Q^2 + \frac{2}{m^2\omega_0^2}[C(0) - C(2\omega_0)]P\right) \\ &+\frac{\partial^2}{\partial P^2}\left(4\delta(2\omega_0)QP + 2[C(0) + C(2\omega_0)]Q^2 - \hbar^2\frac{\nu}{m}\right) \\ &+\frac{\partial^3}{\partial Q\partial P^2}\hbar^2\frac{\nu}{m}Q + \frac{\partial^3}{\partial P^3}\hbar^2\frac{m\omega_r^2}{2}Q\Bigg\}\rho_W(Q,P,t) \ .\end{aligned} \tag{5.1}$$

Opposite to what happens in the linear coupling case [21], this equation is not a Fokker-Planck one because it contains third-order partial derivatives. Now, Pawula's lemma [30, 31] asserts that the solution for an arbitrary positive initial condition is only positive if the evolution equation is at most a second-order one, or of infinite order. Therefore, in this case the distribution may assume negative values. This is not a contradiction because $\rho_W(Q,P,t)$ is by construction a quasiprobability function [29].

It is interesting to note that the traditional derivation of the Fokker-Planck equation assumes the existence of infinitely small jumps [17], and in the quantum system this hypothesis is clearly not true. In this sense, note that the coefficients of the third-order derivatives are proportional to $\hbar^2$. Consequently, in the classical limit we obtain the following nonlinear Fokker-Planck equation:

$$\begin{aligned}\frac{\partial}{\partial t}\rho_W(Q,P,t) = \Bigg\{ &-\frac{\partial}{\partial Q}\frac{P}{m} + \frac{\partial}{\partial P}\bigg(m\omega_0^2 Q - 2m\omega_r^2 Q^3 \\ &+4\frac{\nu}{m}Q^2 P\bigg) \\ &+\frac{\partial^2}{\partial P^2}4\nu kTQ^2\Bigg\}\rho_W(Q,P,t) \ ,\end{aligned} \tag{5.2}$$

where we use the fact that in that limit $C(0) = C = \nu k_B T$ and $\delta = 0$. This equation coincides with the one obtained in Ref. [32] for the classical system. The fact that the diffusion coefficient depends on the oscillator coordinate is associated with the presence of multiplicative fluctuations [20], a characteristic of nonlinear systems [17, 33].

In the asymptotic regime, Eq. (5.1) can be expressed in angle-action variable representation as

$$\begin{aligned}\frac{\partial}{\partial t}\rho_W(H,t) = \frac{\nu}{m}\frac{2}{m\omega_0^2}\Bigg\{ &\frac{\partial}{\partial H}\left(H^2 + \frac{\hbar^2\omega_0^2}{2} - 2\frac{C(2\omega_0)}{\nu}H\right) \\ &+\frac{\partial^2}{\partial H^2}\left(\frac{C(2\omega_0)}{\nu}H^2 - \hbar^2\omega_0^2 H\right) \\ &+\frac{\partial^3}{\partial H^3}\frac{\hbar^2\omega_0^2}{4}H^2\Bigg\}\rho_W(H,t) \ ,\end{aligned} \tag{5.3}$$

where the missing angle is thoroughly related to the missing off-diagonal matrix density elements of the asymptotic representation (4.1). Equation (5.3) also can be obtained starting from the asymptotic GME (4.2).

It is easy to see that the equilibrium distribution of (5.3) is

$$\rho_W^{\text{eq}}(H) = \frac{2}{\pi}\frac{\nu}{C(2\omega_0)}\exp\left\{-\frac{\nu}{C(2\omega_0)}H\right\} \ , \tag{5.4}$$

which corresponds to a classical canonical distribution for an oscillator in equilibrium at an effective temperature $T_{\text{eff}} = C(2\omega_0)/\nu$. The structure of this distribution is the same as the one obtained in the linear coupling case [12], and both coincide in the classical limit.

VI. SUMMARY AND CONCLUSIONS

In this work we have established a generalized master equation for a quantum harmonic oscillator that interacts with an arbitrary reservoir through a separable coupling, however nonlinear in the oscillator coordinate. The master equation allows one to set down the corresponding Newton-like equation for the mean value of the coordinate. If a quadratic coupling is chosen, several details may be specifically worked out and one finds that Newton's equation contains a temperature-dependent kernel proportional to the real part of the heat-bath correlation, in addition to the third-order moments involving position and velocity. Furthermore, in the Markovian limit the parameters of the GME can be identified as the diffusion and friction coefficients, as well as the corrections to the free-oscillator frequency and stiffness. The fluctuation-dissipation ralationship can then be demonstrated on very general grounds; however, the individual coefficients can only be computed in the frame of a specific model for the heat-bath reservoir. This has been illustrated for an oscillator bath with Ohmic dissipation.

The asymptotic regime of the master equation and mean values is especially interesting, since many general features can be indicated without resorting to numerical solutions. One finds that in spite of nonlinearity that affects the master equation, its moment hierarchy, Newton's law, and the evolution rule for the characteristic function, the equilibrium distribution density matrix can be extracted. Furthermore, the conditions under which it is a canonical distribution may be established. On the other hand, when the spectral problem of the master equation generator is numerically solved, one is able to verify to high accuracy an analytical approximation that holds in the low-temperature limit.

Finally, we have investigated the semiclassical representation of the GME and its classical limit. The evolution equation for the Wigner quasiprobability distribution in oscillator phase space is a non-Fokker-Planck, third-order partial derivative equation. However, its classical limit is a Fokker-Planck one with nonlinear diffusion.

ACKNOWLEDGMENTS

This work was performed under Grant No. PID 97/88 from the Consejo Nacional de Investigaciones Científicas y Técnicas of Argentina, to whom the authors are also grateful for personal financial support.

APPENDIX

From definitions (3.7) to (3.10) one can easily demonstrate the following relations:

$$C(\omega) \pm \frac{\hbar\omega}{2}\nu(\omega) = \lambda^2 \mathrm{Re} \int_0^\infty d\tau\, e^{\pm i\omega\tau}\Phi(\tau) \ , \tag{A1}$$

$$\mp m\left(\omega\delta(\omega) \pm \frac{\hbar\omega_r^2(\omega)}{2}\right) = \lambda^2 \mathrm{Im} \int_0^\infty d\tau\, e^{\pm i\omega\tau}\Phi(\tau) \ . \tag{A2}$$

Considering the Fourier transform of the correlation function

$$\Phi[\Omega] = \frac{1}{2\pi}\int_{-\infty}^\infty dt\, e^{-i\Omega t}\Phi(t) \ , \tag{A3}$$

which satisfies

$$\Phi[-\Omega] = e^{\beta\hbar\Omega}\Phi[\Omega] \ , \tag{A4}$$

the integrals that appear in Eqs. (A1) and (A2) can be written as

$$\int_0^\infty d\tau\, e^{-i\omega\tau}\Phi(\tau) = \pi\Phi[\omega] + i\mathrm{P}\int_{-\infty}^\infty d\Omega\, \frac{\Phi[\Omega]}{\Omega - \omega} \ , \tag{A5}$$

$$\int_0^\infty d\tau\, e^{i\omega\tau}\Phi(\tau) = \pi e^{\beta\hbar\omega}\Phi[\omega] + i\mathrm{P}\int_{-\infty}^\infty d\Omega\, e^{\beta\hbar\Omega}\frac{\Phi[\Omega]}{\Omega + \omega} \ . \tag{A6}$$

In Eqs. (A5) and (A6) we use the formula

$$\int_0^\infty dx\, e^{\pm i\Delta x} = \pi\delta(\Delta) \pm i\mathrm{P}\left(\frac{1}{\Delta}\right) \ , \tag{A7}$$

where P stands for the Cauchy principal part of the integral.

Inserting (A5) and (A6) into (A1) we obtain the diffusion and friction coefficients in the form

$$C(\omega) = \frac{\lambda^2}{2}\pi\Phi[\omega](1 + e^{\beta\hbar\omega}) \ , \tag{A8}$$

$$\frac{\hbar\omega}{2}\nu(\omega) = \frac{\lambda^2}{2}\pi\Phi[\omega](e^{\beta\hbar\omega} - 1) \ , \tag{A9}$$

and then

$$C(\omega) = \frac{\hbar\omega}{2}\coth\left(\frac{\beta\hbar\omega}{2}\right)\nu(\omega) \tag{A10}$$

is the quantum fluctuation-dissipation relation.

Similary, one can demonstrate that

$$2m\omega\delta(\omega) = \lambda^2\mathrm{P}\int_{-\infty}^\infty d\Omega\,(1 + e^{\beta\hbar\Omega})\frac{\Phi[\Omega]}{\Omega - \omega} \ , \tag{A11}$$

$$\hbar m\omega_r^2(\omega) = \lambda^2\mathrm{P}\int_{-\infty}^\infty d\Omega\,(e^{\beta\hbar\Omega} - 1)\frac{\Phi[\Omega]}{\Omega - \omega} \ . \tag{A12}$$

[1] G.W. Ford, J.T. Lewis, and R.F. O'Connell, Phys. Rev. A **37**, 4419 (1988).
[2] W. Weidlich, Z. Phys. **241**, 325 (1971).
[3] E.S. Hernández and C.O. Dorso, Phys. Rev. C **29**, 1510 (1984).
[4] F. Haake, Springer Tracts Mod. Phys. **66**, 98 (1973).
[5] G.S. Agarwal, Springer Tracts Mod. Phys. **70**, 1 (1974).
[6] K.H. Li, Phys. Rep. **134**, 1 (1986).
[7] A.O. Caldeira, and A.J. Leggett, Physica A **121**, 587 (1983).

[8] H. Grabert, P. Schramm, and G. Ingold, Phys. Rep. **168**, 115 (1988).
[9] E.S. Hernández and H.M. Cataldo, Phys. Lett. A **124**, 489 (1987).
[10] H.M. Cataldo and E.S. Hernández, J. Stat. Phys. **50**, 383 (1988).
[11] H.M. Cataldo and E.S. Hernández, J. Stat. Phys. **53**, 673 (1988).
[12] E.S. Hernández and H.M. Cataldo, Phys. Rev. A **39**, 2034 (1989).
[13] P. Ullersma, Physica **32**, 27 (1966).
[14] K. Lindenberg and B. West, Phys. Rev. A **30**, 568 (1984).
[15] P.S. Riseborough, P. Hanggi, and U. Weiss, Phys. Rev. A **31**, 471 (1985).
[16] Y. Tanimura, Phys. Rev. A **41**, 6676 (1990).
[17] N.G. van Kampen, *Stochastic Processes in Physics and Chemistry* (North-Holland, Amsterdam, 1981).
[18] S. Chaturvedi, P. Drummond, and D.F. Walls, J. Phys. A **10**, 187 (1977).
[19] P.D. Drummond, C.W. Gardiner, and D.F. Walls, Phys. Rev. A **24**, 914 (1981).
[20] M.A. Despósito, Ph.D. thesis, University of Buenos Aires, 1992.
[21] M.A. Despósito, S.M. Gatica, and E.S. Hernández, Phys. Rev. A **46**, 3234 (1992).
[22] It is not our purpose here to establish the conditions that lead to the validity of a Markovian approximation. See, for example, G.W. Ford, H. Kac, and P. Mazur, J. Math. Phys. **6**, 504 (1965).
[23] A.O. Caldeira and A.J. Leggett, Ann. Phys. **149**, 374 (1983).
[24] C. Aslangul, N. Pottier, and D. Saint-James, J. Phys. (Paris) **46**, 2031 (1985).
[25] C.O. Dorso and E.S. Hernández, Phys. Rev. C **26**, 528 (1982).
[26] H. Haken, *Synergetics, an Introduction*, edited by H. Haken, Springer Series in Synergetics Vol. 1 (Springer, Berlin, 1977).
[27] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. Stegun (Dover, New York, 1965).
[28] E.P. Wigner, Phys. Rev. **40**, 249 (1932).
[29] M. Hillery, R.F. O'Connell, M.O. Scully, and E.P. Wigner, Phys. Rep. **106**, 121 (1980).
[30] R.F. Pawula, Phys. Rev. **162**, 186 (1967).
[31] H. Risken, *The Fokker-Plank Equation* (Springer-Verlag, Berlin, 1989).
[32] K. Lindenberg and V. Seshadri, Physica A **109**, 483 (1981).
[33] A. Schenzle and H. Brand, Phys. Rev. A **20**, 1628 (1979).