

## Master equation for a particle coupled to a two-level reservoir

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(Received 16 September 1994)

We study the quantum dissipative dynamics of a particle coupled linearly to a set of two-level systems (the heat bath) via the master equation method, which we extract from the path integral formalism independently from the form of the bath spectral density. We compare our results with the standard models based on bosonic heat baths, showing their main differences and similarities. In particular, we study special forms for the spectral density of the bath which give results quite different from the standard models.

The study of quantum open systems is one of the most important issues of statistical quantum mechanics, because of its application to many different subjects such as thermalization (tendency to thermal equilibrium), loss of quantum coherence and quantum Brownian motion. This kind of theoretical approach has been used with success in order to study macroscopic quantum tunneling,<sup>1,2</sup> evolution of the early universe,<sup>3</sup> and measurement theory,<sup>4</sup> among others.

The field of quantum Brownian motion had a major revival after the work of Caldeira and Leggett<sup>1</sup> on the study of a particle coupled to a set of harmonic oscillators via the method devised by Feynman and Vernon<sup>5</sup> using path integrals. The path integral method allows the tracing over the oscillators variables (the heat bath) and the studying of the coordinate of interest. As it is already well known, the dissipation and diffusion of a particle coupled linearly to a heat bath depend essentially on the spectral density,  $J(\omega)$ , of the heat bath (which is related to the response function of the reservoir at some frequency  $\omega$ ). In the Caldeira-Leggett model,<sup>1</sup> the dissipation is supposed to be Ohmic, that is, the spectral density of the bath has the form

$$J_0(\omega) = \eta_0 \omega \theta(\omega_c - \omega), \quad (1)$$

where  $\omega_c$  is a suitable cutoff frequency. With this special choice for the spectral density, Caldeira and Leggett showed that the semiclassical dynamics of the system is described by the Langevin equation with a dissipation coefficient  $\eta_0$ .

However, the study of open quantum systems has a long history with many branches. One of the main streams of research is based on the study of master equations (such as the Fokker-Planck equation) for the dynamical evolution of quantum systems, which is used in quantum optics.<sup>6,7</sup> In the seventies, Lindblad gave a general mathematical criteria for the classification and existence of such master equations.<sup>8</sup> More recently, the methods of master equations has been used extensively in the

literature.<sup>9,10,12</sup> Actually, Caldeira and Leggett obtained the equation for the evolution of the reduced density matrix,  $\rho_s$  (the density matrix after the trace over the oscillators bath), with the Ohmic spectral density (1) and in the high temperature limit ( $k_B T \gg \hbar\omega_c$ ) which, in the position representation [ $\rho_s(x, y, t) = \langle x | \rho_s(t) | y \rangle$ ], reads,<sup>1</sup>

$$i\hbar \frac{d\rho_s(x, y, t)}{dt} = \left[ -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} \right) - i\hbar \Gamma (x - y) \left( \frac{\partial}{\partial x} - \frac{\partial}{\partial y} \right) + V_R(x) - V_R(y) - i D_{pp} (x - y)^2 \right] \rho_s(x, y, t), \quad (2)$$

where  $m$  is the mass of the particle,  $V_R$  is the renormalized external potential, and  $D_{pp} = 2\eta_0 k_B T / \hbar$ ,  $\Gamma = \eta_0 / m$ , are the diffusion coefficient in momentum space and the effective dissipation coefficient, respectively.

In this paper, we address the problem of the master equation for a different kind of bath which was proposed recently in the literature by Caldeira *et al.*<sup>13</sup> and has distinct features from the models described above. In the model proposed in Ref. 13, the particle interacts with a heat bath composed of two-level systems. The Hamiltonian of interest can be written as a sum of three terms,  $H = H_s + H_i + H_b$ , where  $H_s$  is the Hamiltonian for a particle in an external potential  $V(x)$ ,  $H_s = p^2/2m + V(x)$ ,  $H_i$  gives the interaction between the particle and the bath,  $H_i = -\sum_n J_n x \sigma_{x_n}$ , and the bath Hamiltonian is  $H_b = \sum_n (\hbar\omega_n/2) \sigma_{z_n}$ , where  $\sigma_{x_n}$  and  $\sigma_{z_n}$  are the usual Pauli matrices and  $J_n$  is the coupling constant for the particle with the  $n$ th two-level system.

As it was shown in Ref. 13, the dynamics of the particle can be evaluated in the path integral formalism via the  $\mathcal{J}$ .<sup>5</sup> Assuming that initially, at some time  $t = 0$  the particle and the bath are decoupled, the time evolution of the system can be written as

$$\rho_s(x, y, t) = \int_{-\infty}^{+\infty} dx_0 \int_{-\infty}^{+\infty} dy_0 \mathcal{J}(x, y, t | x_0, y_0, 0) \times \rho_s(x_0, y_0, 0), \quad (3)$$

where the superpropagator is given by

$$\mathcal{J}(t, 0) = \int_{x_0}^x \mathcal{D}x(s) \int_{y_0}^y \mathcal{D}y(s) \times \exp \frac{i}{\hbar} \{S[x(s)] - S[y(s)]\} F[x(s), y(s)]. \quad (4)$$

In the last equation,  $F[x(s), y(s)]$  is the influence functional,<sup>5</sup> and  $S[x(s)]$  is the free action for the particle,

$$S[x(s)] = \int_0^t ds \left[ \frac{m\dot{x}^2(s)}{2} - V[x(s)] \right].$$

In this paper, we will be interested in the case where the external potential is harmonic, that is,  $V[x(s)] = \frac{1}{2} m \Omega_0^2 x^2(s)$ .

In the weak coupling limit, the influence functional reads,<sup>13</sup>

$$F[q(s), Q(s)] = \exp - \frac{i}{\hbar} \left[ \int_0^t ds_1 \int_0^{s_1} ds_2 2 q(s_1) \times Q(s_2) \eta(s_1 - s_2) \right] \times \exp - \frac{1}{\hbar} \left[ \int_0^t ds_1 \int_0^{s_1} ds_2 q(s_1) \times q(s_2) \nu(s_1 - s_2) \right], \quad (5)$$

where

$$q(s) = x(s) - y(s), \quad Q(s) = \frac{1}{2} [x(s) + y(s)], \quad (6)$$

and the kernels in (5) are given in terms of the spectral density as

$$\nu(s) = \int_0^\infty d\omega J(\omega) \cos \omega s \quad (7)$$

and

$$\eta(s) = - \int_0^\infty d\omega J(\omega) \tanh \frac{\hbar\omega}{2k_B T} \sin \omega s. \quad (8)$$

For this particular model, the spectral density is written as  $J(\omega) \equiv \sum_n (J_n^2/\hbar) \delta(\omega - \omega_n)$ .

Since the double path integral in (4) is quadratic, it can be evaluated completely in terms of the initial and final coordinates given by the transformation (6),

$$\mathcal{J}(t, 0) = Z(t) \exp(i/\hbar) [ (b_1 Q_0 + b_2 Q) q - (b_3 Q_0 + b_4 Q) q_0 ] \times \exp - (1/\hbar) [a_{11} q^2 + a_{12} q_0 q + a_{22} q_0^2], \quad (9)$$

where the coefficients  $b_n$  ( $n = 1, \dots, 4$ ) and  $a_{nm}$  ( $n, m = 1, 2$ ) are given by the solution of the following equations:

$$\frac{d^2 \kappa_n(s)}{ds^2} + 2 \int_0^s ds_1 \eta(s - s_1) \kappa_n(s_1) + \Omega_0^2 \kappa_n(s) = 0,$$

with the boundary conditions  $\kappa_1(s=0) = \kappa_2(s=t) = 1$ ,  $\kappa_1(s=t) = \kappa_2(s=0) = 0$ . Then the unknown functions in (9) are defined as

$$b_1(t) = m (d\kappa_1/ds)|_{s=t}, \quad b_2(t) = m (d\kappa_2/ds)|_{s=t}, \\ b_3(t) = m (d\kappa_1/ds)|_{s=0}, \quad b_4(t) = m (d\kappa_2/ds)|_{s=0},$$

and

$$a_{nm}(t) = \frac{1}{1 + \delta_{nm}} \int_0^t ds_1 \times \int_0^{s_1} ds_2 \kappa_n(s_1) \nu(s_1 - s_2) \kappa_m(s_2).$$

Also the normalization factor in (9) is given by

$$Z(t) = b_4/2\pi\hbar.$$

Using the above equations, we can derive a set of identities,

$$\frac{\dot{b}_3}{b_4 b_1} = -\frac{1}{m}, \quad \dot{a}_{22} = -\frac{\dot{b}_3 a_{12}}{b_1}, \quad \frac{\dot{b}_4}{b_2 b_4} = -\frac{1}{m} \quad (10)$$

(the dot over the functions denotes a derivative with respect to  $t$ ), which we shall use later.

The master equation is obtained using the simplified method proposed by Paz.<sup>11</sup> Taking the derivative of (3), with respect to  $t$ , it is straightforward to show that

$$\frac{\partial \rho_s(q, Q, t)}{\partial t} = \left[ \frac{\dot{Z}}{Z} + \frac{i}{\hbar} \dot{b}_2 q Q - \frac{1}{\hbar} \dot{a}_{11} q^2 \right] \rho_s(q, Q, t) + \frac{i}{\hbar} \dot{b}_1 q \int_{-\infty}^{+\infty} dq_0 \int_{-\infty}^{+\infty} dQ_0 Q_0 \mathcal{J}(t, 0) \rho_s(q_0, Q_0, 0) \\ - \left[ \frac{i}{\hbar} \dot{b}_4 Q + \frac{1}{\hbar} \dot{a}_{12} q \right] \int_{-\infty}^{+\infty} dq_0 \int_{-\infty}^{+\infty} dQ_0 q_0 \mathcal{J}(t, 0) \rho_s(q_0, Q_0, 0) \\ - \frac{i}{\hbar} \dot{b}_3 \int_{-\infty}^{+\infty} dq_0 \int_{-\infty}^{+\infty} dQ_0 q_0 Q_0 \mathcal{J}(t, 0) \rho_s(q_0, Q_0, 0) \\ - \frac{1}{\hbar} \dot{a}_{22} \int_{-\infty}^{+\infty} dq_0 \int_{-\infty}^{+\infty} dQ_0 q_0^2 \mathcal{J}(t, 0) \rho_s(q_0, Q_0, 0). \quad (11)$$

Although (11) seems quite complicated, we can simplify it by taking derivatives of (9) with respect to the end points,  $q$  and  $Q$ , which lead to the following relations:

$$q_0 \mathcal{J}(t, 0) = [(b_2/b_4) q + i\hbar (1/b_4) (\partial/\partial Q)] \mathcal{J}(t, 0), \quad (12)$$

$$Q_0 \mathcal{J}(t, 0) = [-(b_2/b_1) Q - i (a_{12} b_2/b_1 b_4) q + \hbar (a_{12}/b_1 b_4) (\partial/\partial Q) - i (2 a_{11}/b_1) q - i\hbar (1/b_1) (\partial/\partial q)] \mathcal{J}(t, 0).$$

By substituting (12) in (11) and using (10) and (3), we find after some straightforward algebra that

$$\begin{aligned} i\hbar \frac{d\rho_s(x, y, t)}{dt} = & \left[ -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} \right) + \frac{m\Omega_R^2}{2} (x^2 - y^2) \right] \rho_s(x, y, t) - i\hbar \Gamma(t) (x - y) \left( \frac{\partial}{\partial x} - \frac{\partial}{\partial y} \right) \rho_s(x, y, t) \\ & - i D_{pp}(t) (x - y)^2 \rho_s(x, y, t) + \hbar \left[ D_{xp}(t) + D_{px}(t) \right] (x - y) \left( \frac{\partial}{\partial x} + \frac{\partial}{\partial y} \right) \rho_s(x, y, t) \end{aligned} \quad (13)$$

is the master equation for the reduced density matrix of a particle coupled to a two-level reservoir. Observe that the term that represents the diffusion in real space,  $D_{xx}$ , is absent in this model, since the kernels in (7) and (8) depend only on the time interval  $s_1 - s_2$  [see Eq. (5)]. This is a general feature of stationary kernels.<sup>10</sup>

The coefficients that appear in (13) are given by  $\Omega_R^2 = (\dot{b}_1 b_2/b_1) - \dot{b}_2$ , which is the renormalized frequency for the harmonic potential,

$$\Gamma(t) = -\frac{1}{2} [(b_2/m) + (\dot{b}_1/2 b_1)], \quad (14)$$

which is the dissipation coefficient,

$$\begin{aligned} D_{pp}(t) = & \dot{a}_{11} - 4 a_{11} b_2 + \dot{a}_{12} (b_2/b_4) \\ & - (\dot{b}_1/b_1) [2 a_{11} + a_{12} (b_2/b_4)], \end{aligned} \quad (15)$$

which is the diffusion coefficient in momentum space (it gives the fluctuation in  $\hat{x}^2$ ), and

$$D_{xp}(t) = D_{px}(t) = \frac{1}{4} \left[ \frac{\dot{a}_{12}}{b_4} - \frac{\dot{b}_1 a_{12}}{b_1 b_4} - 4 a_{11} \right] \quad (16)$$

is the diffusion coefficient which mixes the real space and the momentum space (it gives the fluctuation in  $\hat{x}\hat{p} + \hat{p}\hat{x}$ ).

The first observation is that the kernels in (7) and (8) do not have the same form as for the case of the oscillator bath,<sup>1</sup> unless we choose a *temperature dependent* spectral density of the form

$$J_1(\omega) = \eta_1 \omega \coth(\hbar\omega/2k_B T) \theta(\omega_c - \omega), \quad (17)$$

as it was first realized in Ref. 13 [it reduces to the spectral density (1) when  $T \rightarrow 0$ ]. With this choice, the bath of oscillators is indistinguishable from the bath of two-level systems. For example, in the *high temperature* limit ( $k_B T \gg \hbar\omega_c$ ), using (17), we find (in what follows, we will look for time scales such that  $s \gg \omega_c^{-1}$ )

$$\nu(s) \approx (2\eta_1 k_B T/\hbar) \delta(s), \quad \eta(s) = \eta_1 [d\delta(s)/ds].$$

Moreover, the coefficients that appear in (14) – (16) are given by

$$\Gamma(t) = \frac{\eta_1}{m}, \quad D_{xp}(t) = D_{px}(t) = 0, \quad D_{pp}(t) = \frac{2\eta_1 k_B T}{\hbar}, \quad (18)$$

as expected.

However, if we insist on using the *Ohmic* spectral density, Eq. (1), the kernels in (12) and (13) assume, at *high temperatures* ( $k_B T \gg \hbar\omega_c$ ), a nonlocal form, namely,

$$\nu(s) = -\eta_0 (1/s^2), \quad \eta(s) = (\eta_0 \hbar/k_B T) (1/s^3),$$

and the dynamics is non-Markovian. It is interesting to notice that in the *low temperature* limit ( $k_B T \ll \hbar\omega_c$ ), the use of this Ohmic spectral density gives

$$\nu(s) = -\eta_0 (1/s^2), \quad \eta(s) = \eta_0 [d\delta(s)/ds],$$

and the only time independent coefficient in the master equation is the dissipation one, that is,  $\Gamma(t) = \frac{\eta_0}{m}$ . This shows that the two-level system and the oscillator bath cannot be naively mapped into each other with this spectral density.

Another interesting possibility is a *flat* spectral density of the form

$$J_2(\omega) = \eta_2 \theta(\omega_c - \omega), \quad (19)$$

which is very common in applications in quantum optics<sup>6,14</sup> (it should be noticed that  $\eta_2$  is dimensionally different from  $\eta_0, \eta_1$ ). In this case, the diffusion is purely Markovian (without memory) at any temperature, while the dissipation coefficient presents a transition from Markovian to non-Markovian depending on the temperature scale, that is, substituting (19) in (7) and (8) and taking the *high temperature* limit, we find

$$\nu(s) = \eta_2 \delta(s), \quad \eta(s) \approx (\eta_2 \hbar/2k_B T) [d\delta(s)/ds],$$

and the coefficients in the master equation are given by  $\Gamma(t) = \eta_2 \hbar/2mk_B T$ ,  $D_{xp}(t) = D_{px}(t) = 0$ ,  $D_{pp}(t) = \eta_2$ . Observe that in this case, the dissipation coefficient has temperature dependence (it decreases with the temperature) and the diffusion coefficient is temperature independent. This result must be compared with (18), where the dissipation does not depend on the temperature, but the diffusion increases with the temperature.

As a last comment, we would like to stress that master equation (13) has been derived with the only assumption of weak coupling (although the transport coefficients have been obtained in the asymptotic long time limit). These approximations will generally lead to violations of positivity of the density matrix and, therefore, Eq. (13) may not be a master equation in the strict sense for the model studied in this paper. For a particle coupled linearly to a set of harmonic oscillators (the

Caldeira-Leggett model), Eq. (13) is *exact*, because the problem becomes quadratic. However, Eq. (2), which is a weak coupling approximation for Eq. (13), cannot be written in Lindblad's form and actually violates positivity of the density matrix.<sup>8</sup> This is just an effect of the rough approximations used to simplify it. This problem has been discussed in great detail in the literature of master equations.<sup>15</sup> However, Eq. (13) does not violate positivity for the Caldeira-Leggett model and it is an exact master equation due to the explicit time dependence of the transport coefficients. As it was shown in Refs. 10 and 11, positivity is strictly preserved for the Caldeira-Leggett model when it is solved exactly.

In conclusion, in this paper we obtained a master equation for a harmonic oscillator coupled to a reservoir consisting on two-level systems in the weak coupling limit. We show that the kernels, which generate the diffusion and dissipation coefficients in the master equation, have a

different form from the standard cases of heat baths composed of harmonic oscillators. We confirm the results of Caldeira *et al.*<sup>13</sup> that the results obtained with an oscillator bath can be recovered from a two-level system bath by a temperature dependent spectral density (which reduces to the Ohmic one when  $T \rightarrow 0$ ). We showed that the usual Ohmic spectral density produces a different kind of behavior from the usual oscillator model.<sup>1</sup> We also studied the case of a flat spectral density (usually used in quantum optics), which produces a different kind of diffusion and dissipation for the quantum dynamics of the particle.

We would like to thank A.O. Caldeira, C.O. Escobar, A. Matacz, and J.P. Paz for many helpful comments and suggestions. P.C.M. thanks FAPESP (Brazil) for financial support. This research was supported in part by the NSF under Grant No. PHY94-07194.

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