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

Paulo C. Marques¹ and A.H. Castro Neto^{2,3}

¹ Instituto de Física da Universidade de São Paulo

C.E.P. 01452-990, C.P. 20516, São Paulo, S.P., Brazil.

² Institute for Theoretical Physics

University of California in Santa Barbara

Santa Barbara, CA, 93106-4030

³ Department of Physics

University of Illinois at Urbana-Champaing

1110 W. Green St, Urbana, IL, 61801

Abstract

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 sim-

ilarities. In particular, we study special forms for the spectral density of the

bath which give results quite different from the standard models.

PACS number(s): 03.65Bz, 05.40+j, 03.65.Db

Typeset using REVT_EX

1

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), lost of quantum coherence and quantum brownian motion. This kind of theoretical approach has been used with success in order to study macroscopic quantum tunneling [1,2], evolution of the early universe [3] and measurement theory [4], among others.

The field of quantum brownian motion had a major revival after the work of Caldeira and Leggett [1] on the study of a particle coupled to a set of harmonic oscillators via the method devised by Feynman and Vernon [5] using path integrals. The path integral method allows the trace over the oscillators variables (the heat bath) and the study 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 ω). In the Caldeira-Leggett model [1] the dissipation is supposed to be ohmic, that is, the spectral density of the bath has the form,

$$J_0(\omega) = \eta_0 \,\omega \,\theta(\omega_c - \omega),\tag{1}$$

where ω_c is a suitable cut-off 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 η_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 [6,7]. In the seventies, Lindblad gave a general mathematical criteria for the classification and existence of such master equations [8]. More recently, the methods of master equations has been used extensively in the literature [9,10,12]. Actually, Caldeira and Leggett obtained the equation for the evolution of the reduced density matrix, ρ_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 [1],

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

where m is the mass of the particle, V_R is the renormalized external potential and

$$D_{pp} = \frac{2\eta_0 k_B T}{\hbar} , \qquad \Gamma = \frac{\eta_0}{m} ,$$

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.* [13] 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),

$$H_s = \frac{p^2}{2m} + V(x),$$

 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,

$$H_b = \sum_{n} \frac{\hbar \omega_n}{2} \, \sigma_{z_n}$$

where σ_{x_n} and σ_{z_n} are the usual Pauli matrices and J_n is the coupling constant for the particle with the nth two-level system.

As it was shown in [13], the dynamics of the particle can be evaluated in the path integral formalism via the superpropagator, J, [5]. 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,

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

where the superpropagator is given by,

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

In the last equation, F[x(s), y(s)] is the influence functional [5], 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 [13],

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

where,

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

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

$$\nu(s) = \int_0^\infty d\omega \ J(\omega) \cos \omega s \tag{7}$$

and

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

For this particular model the spectral density is written as,

$$J(\omega) \equiv \sum_{n} \frac{J_n^2}{\hbar} \delta(\omega - \omega_n).$$

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), the result is:

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

where the coefficients b_n (n = 1, ..., 4) and a_{nm} (n, m = 1, 2) are given by the solution of the 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,

$$\kappa_1(s=0) = \kappa_2(s=t) = 1 \qquad \kappa_1(s=t) = \kappa_2(s=0) = 0.$$

Then the unknown functions in (9) are defined as,

$$b_1(t) = M \frac{d\kappa_1}{ds} \Big|_{s=t} \qquad b_2(t) = M \frac{d\kappa_2}{ds} \Big|_{s=t}$$

$$b_3(t) = M \frac{d\kappa_1}{ds} \Big|_{s=0} \qquad b_4(t) = M \frac{d\kappa_2}{ds} \Big|_{s=0}$$

and,

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

Also the normalization factor in (9) is given by,

$$Z(t) = \frac{b_4}{2\pi\hbar}.$$

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

$$\frac{\dot{b}_3}{b_4 b_1} = -\frac{1}{M} \qquad \dot{a}_{22} = -\frac{\dot{b}_3 a_{12}}{b_1} \qquad \frac{\dot{b}_4}{b_2 b_4} = -\frac{1}{M} \tag{10}$$

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

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

$$\frac{\partial \rho_{s}(q,Q,t)}{\partial t} = \left[\frac{\dot{Z}}{Z} + \frac{i}{\hbar} \dot{b}_{2} q Q - \frac{1}{\hbar} \dot{a}_{11} q^{2} \right] \rho_{s}(q,Q,t)
+ \frac{i}{\hbar} \dot{b}_{1} q \int_{-\infty}^{+\infty} dq_{0} \int_{-\infty}^{+\infty} dQ_{0} Q_{0} J(t,0) \rho_{s}(q_{0},Q_{0},0)
- \left[\frac{i}{\hbar} \dot{b}_{4} Q + \frac{1}{\hbar} \dot{a}_{12} q \right] \int_{-\infty}^{+\infty} dq_{0} \int_{-\infty}^{+\infty} dQ_{0} q_{0} J(t,0) \rho_{s}(q_{0},Q_{0},0)
- \frac{i}{\hbar} \dot{b}_{3} \int_{-\infty}^{+\infty} dq_{0} \int_{-\infty}^{+\infty} dQ_{0} q_{0} J(t,0) \rho_{s}(q_{0},Q_{0},0)
- \frac{1}{\hbar} \dot{a}_{22} \int_{-\infty}^{+\infty} dq_{0} \int_{-\infty}^{+\infty} dQ_{0} q_{0}^{2} J(t,0) \rho_{s}(q_{0},Q_{0},0)$$
(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,

$$q_0 J(t,0) = \left[\frac{b_2}{b_4} q + i\hbar \frac{1}{b_4} \frac{\partial}{\partial Q} \right] J(t,0)$$

$$(12)$$

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

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

$$i\hbar \frac{d\rho_s(x,y,t)}{dt} = \left[-\frac{\hbar^2}{2M} \left(\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} \right) + \frac{M\Omega_R^2}{2} (x^2 - y^2) \right] \rho_s(x,y,t)$$

$$- i\hbar \Gamma(t) (x - y) \left(\frac{\partial}{\partial x} - \frac{\partial}{\partial y} \right) \rho_s(x,y,t)$$

$$- i D_{pp}(t) (x - y)^2 \rho_s(x,y,t)$$

$$+ \hbar \left[D_{xp}(t) + D_{px}(t) \right] (x - y) \left(\frac{\partial}{\partial x} + \frac{\partial}{\partial y} \right) \rho_s(x,y,t)$$
(13)

is the master equation for the reduced density matrix of a particle coupled to a two-level reservoir. Observe that the term which 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 [10].

The coefficients that appear in (13) are given by,

$$\Omega_R^2 = \frac{\dot{b}_1 \ b_2}{b_1} - \dot{b}_2$$

is the renormalized frequency for the harmonic potential,

$$\Gamma(t) = b_2 + \frac{\dot{b}_1}{2 b_1} \tag{14}$$

is the dissipation coefficient,

$$D_{pp}(t) = \dot{a}_{11} - 4 a_{11} b_2 + \dot{a}_{12} \frac{b_2}{b_4} - \frac{\dot{b}_1}{b_1} \left[2 a_{11} + a_{12} \frac{b_2}{b_4} \right]$$
 (15)

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

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

is the diffusion coefficient which mix 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 [1] unless we choose a *temperature dependent* spectral density of the form,

$$J_1(\omega) = \eta_1 \,\omega \, \coth \frac{\hbar \omega}{2k_B T} \,\theta(\omega_c - \omega) \tag{17}$$

as it was first realized in Ref. [13] (it reduces to the spectral density (1) when $T \to 0$). 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,

$$\nu(s) \approx \frac{2\eta_1 k_B T}{\hbar} \delta(s)$$
 $\eta(s) = \eta_1 \frac{d\delta(s)}{ds}.$

In this case the diffusion and the dissipation are markovian while at low temperatures the diffusion is clearly non-markovian. Moreover, the coefficients that appear in (14) - (16) are given by,

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

as expected.

However, if we insist in 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 non-local form, namely,

$$\nu(s) = -\eta_0 \frac{1}{s^2}$$
 $\eta(s) = \frac{\eta_0 \hbar}{k_B T} \frac{1}{s^3},$

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 the following result for the kernels:

$$\nu(s) = -\eta_0 \frac{1}{s^2} \qquad \eta(s) = \eta_0 \frac{d\delta(s)}{ds},$$

and the only time independent coefficient in the master equation is the dissipation one: $\Gamma(t) = \frac{\eta_0}{m}$. 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,

$$J_2(\omega) = \eta_2 \,\theta(\omega_c - \omega), \tag{19}$$

which is very common in applications in quantum optics [6,14] (it should be noticed that η_2 is dimensionally different from η_0 , η_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,

$$\nu(s) = \eta_2 \, \delta(s)$$
 $\eta(s) \approx \frac{\eta_2 \hbar}{2k_B T} \, \frac{d\delta(s)}{ds}.$

and the coefficients in the master equation are given by,

$$\Gamma(t) = \frac{\eta_2 \hbar}{2mk_B T}$$
 $D_{xp}(t) = D_{px}(t) = 0$ $D_{pp}(t) = \eta_2.$

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.

In conclusion, in this paper we obtained the most general master equation for a harmonic oscillator coupled to a reservoir consisting on two-level systems. 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. [13] 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 $T \to 0$). We showed that the usual ohmic spectral density produces a different kind of behavior from the usual oscillator model [1]. 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.

ACKNOWLEDGMENTS

We would like to thank Amir O. Caldeira, Carlos O.Escobar and Andrew Matacz for many helpful comments and suggestions. P.C.M. wishes to thank Fundação de Amparo à Pesquisa no Estado de São Paulo for financial support. A.H.C.N. acknowledges CNPq (Brazil) for financial support. This research was supported in part by the National Science Foundation under Grants No. PHY89-04035 and DMR91-22385.

REFERENCES

- A.O.Caldeira and A.J.Leggett, Ann. Phys. (N.Y.) 149, 374, (1983); Physica A 121, 587, (1983).
- [2] A.J.Leggett, S.Chakravarty, A.T.Dorsey, M.P.A.Fisher, A.Garg and W.Zwerger, Rev.Mod.Phys. 59, 1, (1987).
- [3] M.Gell-Mann and J.B.Hartle, in Complexity, Entropy and the Physics of Information,
 ed. by W.H.Zurek (Addison-Wesley, Reading, (1990)); Phys.Rev.D 47, 3345, (1993);
 B.L.Hu and A.Matacz, in Proc.Int.Workshop on Fluctuations and Order: A New Synthesis, Los Alamos (1993).
- [4] W.H.Zurek, Phys.Rev.D 24, 1516, (1981); 26, 1862, (1982).
- [5] R.P. Feynman and F.L. Vernon, Annals of Physics 24, 118, (1963).
- [6] W.H.Louisell, Quantum Statistical Properties of Radiation, (John Wiley, New York, 1973) and references therein.
- [7] R.Zwanzig, J.Stat.Phys. 9, 215, (1973).
- [8] G.Lindblad, Commun.Math.Phys. 48, 119, (1976).
- [9] W.G.Unruh and W.H.Zurek, Phys.Rev.D 40, 1071, (1989).
- [10] B.L.Hu, J.P.Paz and Y.Zhang, Phys.Rev. D 45, 2843, (1992); Phys.Rev. D 47, 1576, (1993); B.L.Hu and A.Matacz, University of Maryland preprint 93-210 (1993).
- [11] J.P.Paz in *The Physical Origin of Time Asymmetry* ed. J.J.Halliwell, Cambridge Univ. Press, 1994.
- [12] M.R.Gallis, Phys.Rev. A 48, 1028, (1993); M.R.Gallis and G.N.Fleming, Phys.Rev. A 42, 38, (1990).
- [13] A.O. Caldeira, A.H. Castro Neto and T. Oliveira de Carvalho, *Phys. Rev.* B 48, 13974,

(1993).

[14] A. H. Castro Neto and A. O. Caldeira, Phys.Rev.A 42, 6884, (1990).