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Caldeira–Leggett master equation and medium temperatures

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The Markovian approximation of quantum dissipation has been reconsidered in the model of Caldeira and Leggett [Physica A 121 (1983) 587]. Their high temperature master equation has been generalized to medium temperatures. Two additional damping terms in the master equation have been derived and shown to assure the Lindblad form of the equation. A transient term in the density matrix has been found and expressed in a simple form.

1. Introduction

Several years ago, Caldeira and Leggett [1] (CL) constructed an exactly soluble model for quantum dissipation. They assumed a simple quantum system coupled to a bosonic reservoir, i.e., to an infinite number of quantum oscillators at thermal equilibrium. A similar model was considered later by Unruh and Zurek [2]. The reduced dynamics of the simple quantum system turned out to be dissipative due to the interaction with the reservoir. The statistical operator ρ of the damped particle satisfies a generalized master equation of the form

$$\rho(t) = \hat{S}(t)\,\rho(0)\,, \qquad t > 0\,, \tag{1}$$

where $\hat{S}$ is the evolution *superoperator* preserving positivity and normalization of ρ. For *high* temperatures, CL approximated eq. (1) by the Markovian master equation

$$\dot{\rho}(t) = \hat{L}(t)\,\rho(t)\,, \tag{2}$$

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where $\hat{L}$ is the Liouville superoperator, also given by CL.

In our paper, we try to generalize the Markovian approximation for *medium* temperatures, too. We recalculate the Liouville operator $\hat{L}$ from the exact CL evolution operator $\hat{S}$. Our result differs from CL's one by additional damping terms known from Dekker's earlier phenomenological calculations [3]. Our $\hat{L}$ is of the Lindblad [4,5] form, which assures its mathematical consistency, while, on the other hand, the CL master equation would violate the positivity of the statistical operator ρ, see refs. [6,7].

2. The generalized master equation

Assume a certain quantum particle with Heisenberg canonical operators $q(t)$ and $p(t)$. For concreteness, we think of a quantum oscillator, so that canonical equations are the following:

$$\dot{q} = (1/M)p\,, \qquad \dot{p} = -M\omega^2 q\,. \tag{3}$$

The quantum state will be represented by the statistical operator ρ.

Consider, on the other hand, a certain bosonic reservoir and single out a certain harmonic coordinate $Q(t)$ of it. Let us introduce the auto-correlation function of $Q(t)$,

$$\alpha(t) = \frac{1}{\hbar}\langle Q(t)\,Q(0)\rangle_T\,, \tag{4}$$

where symbols $\langle\ldots\rangle_T$ stand for equilibrium expectation values at temperature T.

At $t = 0$, let us couple the reservoir and the particle together, by switching on the interaction Hamiltonian

$$H_{\mathrm{I}} = qQ\,. \tag{5}$$

Having solved the coupled dynamic equations and then having traced over reservoir states, one obtains a generalized master equation of the form (1). If at $t = 0$ the particle and the reservoir were uncorrelated (to the opposite case see, e.g., ref. [8]) then the evolution superoperator $\hat{S}$ is given the following exact form:

$$\hat{S}(t) = \hat{T}\exp\Big(-\frac{1}{\hbar}\int_0^t \mathrm{d}\tau \int_0^\tau \mathrm{d}s\,\{\mathrm{i}[q_+(\tau) - q_-(\tau)]\alpha_{\mathrm{I}}(\tau - s)\,[q_+(s) + q_-(s)]$$
$$+ [q_+(\tau) - q_-(\tau)]\alpha_{\mathrm{R}}(\tau - s)\,[q_+(s) - q_-(s)]\}\Big)\,, \tag{6}$$

where α_R, α_I are the real and imaginary parts, respectively, of the correlation function (4). Now is the time to explain the superoperator notation applied above. A usual operator, say q, becomes superoperator when it is appended by a $+/-$ index, indicating q is to be applied to the statistical operator ρ from the left/right, respectively. Furthermore, symbol $\hat{T}$ prescribes time-ordering for $q_+(t)$ while anti-time-ordering for $q_-(t)$, cf. ref. [9].

In their pioneering work [1] CL derived and presented formula (6) in path-integral formalism (see their equation (3.9)), which is equivalent to our T-product formalism. For brevity, we introduce the standard notations [9]

$$q_\Delta = q_+ - q_- , \qquad q_c = \tfrac{1}{2}(q_+ + q_-) , \tag{7}$$

hence eq. (6) reads

$$\hat{S}(t) = \hat{T}\exp\left(-\frac{1}{\hbar}\int_0^t \mathrm{d}\tau \int_0^\tau \mathrm{d}s\,[2\mathrm{i}q_\Delta(\tau)\,\alpha_I(\tau-s)\,q_c(s) + q_\Delta(\tau)\,\alpha_R(\tau-s)\,q_\Delta(s)]\right) . \tag{8}$$

The CL model of reservoir and the choice of coupling led to the following correlation functions (cf. eqs. (3.10), (3.11) and (3.23) of ref. [1]):

$$\alpha_R(\tau) = \frac{\eta}{\pi}\int_0^\Omega \omega \coth(\hbar\omega/2kT)\cos(\omega\tau)\,\mathrm{d}\omega , \tag{9a}$$

$$\alpha_I(\tau) = -\frac{\eta}{\pi}\int_0^\Omega \omega \sin(\omega\tau)\,\mathrm{d}\omega , \tag{9b}$$

where the coupling constant η plays the role of viscosity coefficient, the cutoff Ω is the maximum frequency of reservoir oscillators.

Eq. (6), applied to eq. (1), gives the exact solution for the dynamics of the quantum particle's damped motion. Remember that $q_\pm(\tau)$, $q_\pm(s)$ are the solutions of the particle Heisenberg equations of motion (3).

3. Markovian approximation, medium and high temperatures

From now on, we consider high and medium temperatures satisfying the condition

$$kT \gtrsim \hbar\Omega . \tag{10}$$

It is rather straightforward to see that the correlation function (4) falls for large time separations,

$$\alpha(\tau) \approx 0 \qquad \text{if } |\tau| \gg \tau_c . \tag{11}$$

For the CL reservoir (9a,b), the characteristic time of the memory τ_c of the reservoir can be chosen as

$$\tau_c = 1/\Omega , \tag{12}$$

provided condition (10) is fulfilled.

To prepare the Markovian approximation, write the correlation functions (9a,b) in the following forms:

$$\alpha_R(\tau) = \frac{2\eta kT}{\hbar} \tilde{\delta}(\tau) - \frac{\eta\hbar}{6kT} \tilde{\delta}''(\tau) + \ldots , \tag{13a}$$

$$\alpha_I(\tau) = \eta \tilde{\delta}'(\tau) , \tag{13b}$$

where the ellipse stands for the third (and higher) powers of the inverse temperature $1/T$ times the fourth (and higher) time derivatives of the function $\tilde{\delta}$. This latter is defined by

$$\tilde{\delta}(\tau) \equiv \frac{1}{\pi} \int_0^{\Omega} \mathrm{d}\omega \cos(\omega\tau) , \tag{14}$$

i.e. it is a smoothed delta-function of a width of about $\tau_c = 1/\Omega$ and of height

$$\tilde{\delta}(0) = \Omega/\pi . \tag{15}$$

(The expansion (13a) has its counterpart in eq. (3.19) of ref. [1].)

We are now prepared to summarize the concrete rules of the Markovian approximation, which will be applied in the forthcoming section. (i) Following ref. [1], we take $\tilde{\delta}(\tau) \approx \delta(\tau)$ but, whenever $\tilde{\delta}(0)$ enters explicitly, we shall retain its regularized value (15). (ii) *Opposite to* ref. [1], we shall retain the first *two* terms on the rhs of eq. (13a) and then neglect the higher order ones.

Step (i) assumes that non-stationary features of the particle dynamics, if finer than the reservoir memory τ_c, will not be described. This approximation is still useful provided

$$\omega \ll 1/\tau_c , \tag{16a}$$

i.e. the *dynamic* acceleration (cf. eq. (3)) of the damped particle is small at the time scale of the reservoir's memory. A similar condition must be satisfied for the *frictional* deceleration. The corresponding mathematical condition is

$$\gamma \equiv \eta/2M \ll 1/\tau_c \tag{16b}$$

though this fact can only be justified later, in section 4.

In brief, we point out that the fulfillment of condition (16a) justifies step (ii) as well. It can be shown that the neglected higher order terms in eq. (13a) are proportional to increasing powers of the ratio ω/T. The smallness of these terms is assured by condition (16a) combined with condition (10).

4. Calculation of the Liouville operator and the initial slip

We are going to calculate the Markovian approximation of the exact evolution superoperator $\hat{S}(t)$. Let us write eq. (8) into the form

$$\hat{S}(t) = \hat{T}\exp[\hat{\Sigma}(t)] \tag{17}$$

and assume the time lapse is much greater than the reservoir memory:

$$t \gg \tau_c \equiv 1/\Omega\ . \tag{18}$$

We have to calculate the superoperator $\hat{\Sigma}(t)$, i.e. the double integral on the rhs of eq. (8). We substitute eqs. (13a) and (13b) into it. Then we apply the Markovian approximation explained in the preceding section.

The first term contributes as

$$\begin{aligned}\hat{\Sigma}_R^{(0)}(t) &\equiv -\frac{2\eta kT}{\hbar^2}\int_0^t \mathrm{d}\tau \int_0^\tau \mathrm{d}s\; q_\Delta(\tau)\,\tilde{\delta}(\tau-s)\,q_\Delta(s) \\ &\approx -\frac{\eta kT}{\hbar^2}\int_0^t \mathrm{d}\tau\,[q_\Delta(\tau)]^2\ .\end{aligned} \tag{19}$$

The second term yields

$$\begin{aligned}\hat{\Sigma}_R^{(1)}(\mathrm{t}) &\equiv \frac{\eta}{6kT}\int_0^t \mathrm{d}\tau \int_0^\tau \mathrm{d}s\; q_\Delta(\tau)\,\tilde{\delta}''(\tau-s)\,q_\Delta(s) \\ &\approx \frac{\eta}{6kT}\left(-\frac{\Omega}{\pi}[q_\Delta(0)]^2 - \frac{\Omega}{\pi}\int_0^t \mathrm{d}\tau\, q_\Delta(\tau)\,\dot{q}_\Delta(\tau) - \frac{1}{2}\int_0^t \mathrm{d}\tau\,[\dot{q}_\Delta(\tau)]^2\right)\,,\end{aligned} \tag{20}$$

where we have ignored a term $(\eta/6kT)\ [q_\Delta \dot q_\Delta]_0^t$. Its contribution is small as compared to the second integral on the rhs, due to condition (18).

The imaginary part (13b) yields the following contribution:

$$\hat\Sigma_{\rm I}^{(1)}(t) \equiv -2\frac{\eta}{\hbar}\int_0^t \mathrm{d}\tau \int_0^\tau \mathrm{d}s\ q_\Delta(\tau)\ \tilde\delta'(\tau-s)\ q_{\rm c}(s)$$

$$\approx \frac{\eta}{\hbar}\left(\frac{\Omega}{\pi}\int_0^t \mathrm{d}\tau\ [q_+^2(\tau)-q_-^2(\tau)] - \int_0^t \mathrm{d}\tau\ q_\Delta(\tau)\ \dot q_{\rm c}(\tau)\right). \tag{21}$$

At the conditions of Markovian approximation (cf., in particular, conditions (10) and (16a)) one has thus obtained the following result:

$$\hat\Sigma(t) \approx \hat\Sigma_{\rm R}^{(0)}(t) + \hat\Sigma_{\rm R}^{(1)}(t) + \mathrm{i}\hat\Sigma_{\rm I}^{(1)}(t)\ , \qquad t \gg \tau_{\rm c}\ . \tag{22}$$

The main advantage we have achieved is that double time-integrals representing the exact form of $\hat\Sigma(t)$ have been approximated by single integrals. Consequently, we can use the following ansatz:

$$\hat\Sigma(t) \approx \hat\Sigma_{\rm tr} + \int_0^t \mathrm{d}\tau\ \hat L(\tau)\ , \qquad t \gg \tau_{\rm c}\ , \tag{23}$$

where $\hat\Sigma_{\rm tr}$ is a certain *transient* term, and $\hat L$ is the Liouville superoperator, as we shall see below. But first, let us concretize their forms. By comparing eq. (23) with eqs. (19)–(22), we get the transient term $\hat\Sigma_{\rm tr}$ in the form

$$\hat\Sigma_{\rm tr} = -\frac{\eta\Omega}{6kT}[q_+(0)-q_-(0)]^2\ . \tag{24}$$

The Liouville superoperator takes the Dekker form [3]

$$\hat L = -\frac{\mathrm{i}}{\hbar}(H_+'-H_-') - \frac{\mathrm{i}}{\hbar}\gamma(q_+-q_-)(p_++p_-)$$
$$-\frac{1}{\hbar^2}[D_{pp}(q_+-q_-)^2 + D_{qq}(p_+-p_-)^2 + 2D_{pq}(q_+-q_-)(p_+-p_-)]\ , \tag{25}$$

where, for brevity, we have suppressed notations of time arguments in $\hat L(t)$, $q(t)$ and $p(t)$. The latter stands, of course, for $\dot q(t)$ times the mass M.

The reservoir has renormalized the particle Hamiltonian by adding the inverse harmonic oscillator potential [1] to it,

$$H' = -\frac{\eta\Omega}{\pi} q^2 . \tag{26a}$$

The four damping constants of Dekker's phenomenology turn out to take the following values:

$$\gamma = \frac{\eta}{2M} , \tag{26b}$$

$$D_{pp} = \eta kT , \tag{26c}$$

$$D_{qq} = \frac{\eta\hbar^2}{12M^2kT} , \tag{26d}$$

$$D_{pq} = \frac{\eta\Omega\hbar^2}{12\pi MkT} . \tag{26e}$$

(Eqs. (26a,b) correspond to ref. [1], eqs. (3.37), (3.36), respectively, while the coefficient (26c) appears first in eq. (5.1) of ref. [1].)

It remains to interpret the transient term $\hat{\Sigma}_{tr}$ and to prove that $\hat{L}$ of eq. (23) plays the role of a Liouville operator indeed. Let us substitute eq. (23) into eq. (17):

$$\hat{S}(t) \approx \left(T \exp \int_0^t d\tau\, \hat{L}(\tau)\right) \exp(\hat{\Sigma}_{tr}) , \qquad t \gg \tau_c . \tag{27}$$

It is worthwhile to recall the effect of T-ordering: the transient factor gets to the very right. Invoking the generalized master equation (1), we are going to interpret the effect of the evolution superoperator (27). The coupling to the reservoir at $t = 0$ changes the quantum state of the particle after a transient period $t \approx \tau_c$:

$$\rho(0) \to \exp(\hat{\Sigma}_{tr})\, \rho(0) \equiv \exp\left(-\frac{\eta\Omega}{6\pi kT} [q_+(0) - q_-(0)]^2\right) \rho(0) . \tag{28}$$

In the spirit of the recent paper by Suarez et al. [10], this *initial slippage* destroys non-Markovian non-stationary features built in the initial state. After this transient period the statistical operator satisfies the stationary Markovian master equation (2) with the Liouville superoperator (25):

$$\dot{\rho} = \hat{L}\rho \equiv -\frac{\mathrm{i}}{\hbar}[H',\rho] - \frac{\mathrm{i}}{\hbar}\gamma[q,\{p,\rho\}] \\ -\frac{1}{\hbar^2}(D_{pp}[q,[q,\rho]] + D_{qq}[p,[p,\rho]] + 2D_{qp}[q,[p,\rho]]) . \tag{29}$$

Hence, the main result of the paper has been presented by eqs. (28), (29) together with eqs. (26a–e). In particular, the master equation (29) is expected to be valid for medium and high temperatures (10), and for small dynamic and frictional accelerations. Consider the quantum expectation value $v \equiv \mathrm{tr}(\rho p)/M$ of the velocity. The master equation (29) together with the Heisenberg equation (3) lead to the well-known classical equation of motion

$$\dot{v} = -\omega_{\mathrm{R}}^2 q - 2\gamma v , \tag{30}$$

where $\omega_{\mathrm{R}}^2 = \omega^2 - 4\gamma\Omega/\pi$ (cf. eq. (3.37) of ref. [1]). Thus the dynamic acceleration is characterized by the renormalized frequency [1] ω_{R}, while the frictional deceleration is characterized by the relaxation constant γ. In summary, the master equation (29) is valid for

$$\omega_{\mathrm{R}}, \gamma \ll \Omega \lessapprox kT/\hbar , \tag{31}$$

although we cannot exclude the possibility that further restrictions are necessary.

5. Discussion

Master equation must preserve normalization and positivity of the statistical operator. If the 2×2 matrix of Dekker's coefficients is positive, i.e.

$$\begin{pmatrix} D_{qq} & D_{qp} + \frac{1}{2}\mathrm{i}\hbar\gamma \\ D_{qp} - \frac{1}{2}\mathrm{i}\hbar\gamma & D_{pp} \end{pmatrix} > 0 , \tag{32}$$

then the master equation (29) belongs to the Lindblad class [4,5], which guarantees mathematical consistency including positivity of the statistical operator ρ.

Had we ignored in section 4 the terms $\hat{\Sigma}^{(1)}_{\mathrm{R,I}}$ depending on $\dot{q}$, the only nonzero coefficient would be D_{pp}. This is the simplest Markovian approximation. It yields a mathematically consistent master equation which, however, does not take into account energy dissipation. The CL master equation [1] ignores $\hat{\Sigma}_{\mathrm{R}}^{(1)}$ while it retains $\hat{\Sigma}_{\mathrm{I}}^{(1)}$. It describes dissipation but it violates the positivity condition (32) because $D_{pp}=0$ (and $D_{qp}=0$) in it while $\gamma \neq 0$.

Let us turn back to our master equation (29) with the complete set (26a–e) of nonvanishing Dekker coefficients. Let us calculate the determinant of the matrix (32):

$$D_{pp}D_{qq} - D_{pq}^2 - \hbar^2\gamma^2/4 = \text{const.} \times \left[1 - \frac{1}{3\pi^2}\left(\frac{\hbar\Omega}{kT}\right)^2\right]. \tag{33}$$

It is definitely positive in the medium and high temperature regime (10) and, therefore, our master equation (29) belongs to the Lindblad class.

What can be done with initial slippage (28). Let us write it in coordinate representation,

$$\langle x|\rho|y\rangle \to \exp\left[-\left(\frac{x-y}{2\sigma_{max}}\right)^2\right]\langle x|\rho|y\rangle\,, \tag{34}$$

where

$$\sigma_{\max} \approx \sqrt{\frac{kT}{\eta\Omega}} \approx \sqrt{\frac{\hbar}{\eta}}\sqrt{\frac{kT}{\hbar\Omega}}\,. \tag{35}$$

The transient process (34) performs a fast diagonalization of the particle density operator, in accordance with the results of Hu et al. [11]. In the high temperature limit $kT \gg \hbar\Omega$, the initial slip (28), (34) can be ignored as compared with the similar and quicker effect of the term $D_{pp}[q,[q,\rho]]$ in the master equation (29). This is completely in agreement with the result of Hu et al., who have observed the absence of the *initial jolt* in the exact time dependent coefficient D_{pp} in the high temperature limit.

Presumably the coherence length, i.e. the characteristic length scale at which $\langle x|\rho|y\rangle$ is "diagonal", will never be increased by the stationary process (29) either. Hence $\sigma_{\max}$ (35) is an absolute bound, valid at any not too low temperature (i.e. when $T \gtrsim \hbar\Omega/k$) for the coherent extension of the particle.

6. Outlook

Very recently, stochastic wave function models have been proposed to describe the evolution of various damped quantum systems (see e.g. ref [12]). The new model is physically equivalent to the master equation, advantageous in numeric simulations and represents a concurrent tool to the Wigner functions in investigating the quantum-classical correspondence. Theoretical grounds of the new method have already been known earlier. Every Markovian master equation allows us a unique jump [13] or, alternatively, a unique Gaussian process [14] to use for describing the evolution of the wave function, provided the master equation is of Lindblad type. The Lindblad master equation of the CL model (first published in ref. [7]) opens the way to construct the corresponding stochastic wave function equation and to grasp the fruits of the *quantum state diffusion* [15] method.

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