PHYSICAL REVIEW E VOLUME 51, NUMBER 6 JUNE 1995

Quantum dissipation is a dynamical collective effect

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(Received 10 February 1994; revised manuscript received 7 February 1995)

We show that the dissipative dynamics observed in a small quantum system coupled to a large one (the bath) is a consequence of increasing the size of the bath. We exemplify this effect with a quantum harmonic oscillator coupled to N harmonic oscillators. We find that revivals in the level population exist and give an estimate of their period. For large values of N, the level population decays exponentially coming into thermal equilibrium. We conclude that quantum dissipation is a *dynamical collective effect.* Finally, we discuss extensions beyond the harmonic oscillator.

PACS number(s): 05.30.–d, 05.40.+j

I. INTRODUCTION

The dissipative behavior of quantum systems has been extensively studied over the past years [1–16]. It has often been claimed that quantum mechanics cannot provide new insights into the problem since it fails to take into account the irreversible increase of entropy observed in real life. In some cases modifications of the Schrödinger equation have been proposed to reproduce dissipative dynamics [17–21] but no satisfactory conclusions have been reached as yet. On the other hand, traditional formalisms based on Master or Langevin equations [22–24] which are currently being used to simulate quantum dissipation, involve several approximations; thus their conclusions are also unsatisfactory as a final answer to the problem. Besides, it has been speculated that the mean value of the population of a single quantum oscillator coupled to a bath of N harmonic oscillators should revive after a certain relaxation time [25] but no evidence has been reported so far. The main reasons for this failure is that this effect is a consequence of both the discreteness of the energy spectrum and the quantum correlations and the standard treatments of the problem mentioned above do not take adequate account of both.

In the present paper, we show a first-principles quantum dissipative dynamics without resorting to biased approximations. Moreover, we show that a quantum harmonic oscillator coupled to a bath of N harmonic oscillators shows a dissipative evolution without referring to a continuum energy spectrum or to a Markovian approximation. Quite contrary to the widespread belief that dissipation is an effect of loss of memory, the usual exponential decay is seen as a result of increasing the size of the bath. We also demonstrate that the expected revivals exist, and they are a consequence of all quantum correlations inherent to this model. Furthermore, we conclude from our treatment, based on first principles, that quantum dissipation is a dynamical collective effect which has nothing to do with loss of memory, randomness or any other ad hoc hypothesis needed to obtain this physical effect.

Let us summarize briefly the basic concepts of the maximum entropy principle (MEP) approach that will be used hereafter. Within the MEP context, the density matrix $\hat{\rho}$ is obtained from the knowledge of the expectation values of, say, the $M+1$ operators $\hat{O}_j$ ($\hat{O}_0 = \hat{I} =$ identity operator),

$$\langle \hat{O}_j \rangle = \mathrm{Tr}\,[\,\hat{\rho}(t)\,\hat{O}_j\,]\,,\quad j = 0, 1, \ldots, M\,, \tag{1.1}$$

in the form

$$\hat{\rho}(t) = \exp\left(-\lambda_0 \hat{I} - \sum_{j=1}^{M} \lambda_j \hat{O}_j\right), \tag{1.2}$$

where the $M+1$ Lagrange multipliers λ_j are determined to fulfill Eq. (1.1) [26–28]. The density operator $\hat{\rho}$ maximizes the entropy $S(\hat{\rho})$ given by

$$S(\hat{\rho}) = -\mathrm{Tr}\,[\,\hat{\rho}\,\ln\hat{\rho}\,] = \lambda_0 \hat{I} + \sum_{j=1}^{M} \lambda_j \langle \hat{O}_j \rangle \tag{1.3}$$

in units of the Boltzmann constant. If we further impose the condition that the evolution of $\hat{\rho}(t)$ obeys the Liouville equation, the entropy turns out to be an invariant of motion. This fact stems from the well-known result of quantum mechanics, which asserts that the evolution of any function of a density matrix which evolves according to the Liouville equation also obeys that equation. Thereby there emerges a very strong requirement concerning the operators used to construct the density matrix. It is found that the *relevant* operators entering Eq. (1.2) are those which close a semi-Lie algebra under commutation with the Hamiltonian [26]

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$$[\hat{H}, \hat{O}_i] = i\hbar \sum_{j=0}^{q} g_{ji} \hat{O}_j , \tag{1.4}$$

where g_{ji} are the elements (c numbers) of a $q \times q$ matrix G. This equation defines mathematically the concept of relevant operators and the elements of the G matrix. The Liouville equation can be replaced by a set of coupled equations for the expectation values of the relevant operators as follows:

$$\frac{d\langle \hat{O}_j \rangle_t}{dt} = -\sum_{i=0}^{q} g_{ij} \langle \hat{O}_i \rangle , \quad j = 0, 1, \ldots, q . \tag{1.5}$$

II. MODEL

In order to study the relaxation problem we will consider a quantum harmonic oscillator coupled to a quantum-mechanical heat bath. The coupling between both systems is assumed to be bilinear and we will use the rotating wave approximation. The Hamiltonian reads [23]

$$\hat{H} = \Omega \hat{a}^\dagger \hat{a} + \sum_{j=1}^{N} \omega_j \hat{b}_j^\dagger \hat{b}_j + \sum_{j=1}^{N} (\gamma_j \hat{a}^\dagger \hat{b}_j + \gamma_j^* \hat{b}_j^\dagger \hat{a}) , \tag{2.1}$$

$\hbar = 1$, where γ_j are the constants coupling the single oscillator to the reservoir, ω_j is the energy of the jth mode, and Ω is the energy of the single harmonic oscillator. $\hat{a}^\dagger$, $\hat{b}_j^\dagger$ ($\hat{a}$, $\hat{b}_j$) are creation (annihilation) boson operators. The coupling coefficients γ_j are assumed to be small as compared with Ω or ω_j [23]. Thus, only the oscillators with $\omega_j \approx \Omega$ will be significantly coupled. As mentioned in Ref. [23], in most physical problems N will be a large *finite* number (i.e., $N \approx 10^{23}$). Thus we shall study this problem for a given N without replacing the sums by integrals. We show that exact results for the $N \to \infty$ can be obtained.

The set of relevant operators which satisfy Eq. (1.4) reads

$$\hat{\Delta} \equiv \hat{a}^\dagger \hat{a} , \tag{2.2a}$$

$$\hat{B}_j \equiv \hat{b}_j^\dagger \hat{b}_j , \tag{2.2b}$$

$$\hat{F}_j \equiv i(\gamma_j \hat{a}^\dagger \hat{b}_j - \gamma_j^* \hat{b}_j^\dagger \hat{a}) , \tag{2.2c}$$

$$\hat{I}_j \equiv \gamma_j \hat{a}^\dagger \hat{b}_j + \gamma_j^* \hat{b}_j^\dagger \hat{a} , \tag{2.2d}$$

$$\hat{\mathcal{F}}_{j,k} \equiv i(\gamma_j^* \gamma_k \hat{b}_j^\dagger \hat{b}_k - \gamma_j \gamma_k^* \hat{b}_k^\dagger \hat{b}_j) , \tag{2.2e}$$

$$\hat{\mathcal{I}}_{j,k} \equiv \gamma_j^* \gamma_k \hat{b}_j^\dagger \hat{b}_k + \gamma_j \gamma_k^* \hat{b}_k^\dagger \hat{b}_j , \tag{2.2f}$$

where j, $k = 1, \ldots, N$. $\hat{\Delta}$, $\hat{B}_j$, $\hat{F}_j$, $\hat{I}_j$ are operators representing the population of the single harmonic oscillator, the populations of the modes of the heat bath, the current between the mode j and the oscillator, and the interaction between them, respectively. The operators $\hat{\mathcal{F}}_{j,k}$ and $\hat{\mathcal{I}}_{j,k}$ represent the current and the interaction energy between the modes j and k of the reservoir. It is important to notice that although different modes are not coupled by the Hamiltonian, their quantal correlations [Eqs. (2.2e)–(2.2f)] will appear in the evolution equations [6,10]. Using the fact that $\hat{\mathcal{I}}_{j,j} = 2|\gamma_j|^2 \hat{B}_j$, $\hat{\mathcal{I}}_{j,k} = \hat{\mathcal{I}}_{k,j}$, and $\hat{\mathcal{F}}_{j,k} = -\hat{\mathcal{F}}_{k,j}$, it can be easily proved that the number of independent operators is $(N+1)^2$. The above mentioned operators can be thought of as microscopic ones. A macroscopic description can be straightforwardly obtained by summing over the modes of the bath (i.e., the energy of the bath reads $\sum_{j=1}^{N} \omega_j \hat{B}_j$). A detailed study in terms of these variables will be presented elsewhere.

Thus the evolution equations for the expectation values of the operators defined above are

$$\frac{d\langle \hat{\Delta} \rangle}{dt} = -\sum_{j=1}^{N} \langle \hat{F}_j \rangle, \tag{2.3a}$$

$$\frac{d\langle \hat{B}_j \rangle}{dt} = \langle \hat{F}_j \rangle, \tag{2.3b}$$

$$\frac{d\langle \hat{F}_j \rangle}{dt} = -(\Omega - \omega_j)\langle \hat{I}_j \rangle + 2|\gamma_j|^2 \langle \hat{\Delta} \rangle - \sum_{k=1}^{N} \langle \hat{\mathcal{I}}_{j,k} \rangle, \tag{2.3c}$$

$$\frac{d\langle \hat{I}_j \rangle}{dt} = (\Omega - \omega_j)\langle \hat{F}_j \rangle - \sum_{k=1}^{N} \langle \hat{\mathcal{F}}_{j,k} \rangle, \tag{2.3d}$$

$$\frac{d\langle \hat{\mathcal{F}}_{j,k} \rangle}{dt} = (\omega_k - \omega_j)\langle \hat{\mathcal{I}}_{j,k} \rangle - |\gamma_j|^2 \langle \hat{I}_k \rangle + |\gamma_k|^2 \langle \hat{I}_j \rangle, \tag{2.3e}$$

$$\frac{d\langle \hat{\mathcal{I}}_{j,k} \rangle}{dt} = -(\omega_k - \omega_j)\langle \hat{\mathcal{F}}_{j,k} \rangle + |\gamma_j|^2 \langle \hat{F}_k \rangle + |\gamma_k|^2 \langle \hat{F}_j \rangle, \tag{2.3f}$$

with $j, k = 1, \ldots, N$. Equations (2.3) are the exact dynamical evolution equations of the relevant operators for this problem. Now, following Louisell [23], we specify as the values of the initial conditions and the constants as

$$\omega_k = \Omega + A\, n, \tag{2.4a}$$

$$\gamma_k = \begin{cases} B - C\,|n| & \text{if } n \le n_M \\ 0 & \text{otherwise,} \end{cases} \tag{2.4b}$$

where $n = k - (N+1)/2$ and $n_M = B/C$. Thus we are considering the case with equally spaced modes ($A = \omega_{k+1} - \omega_k$, the energy difference between neighboring levels is the inverse of the density of modes in the reservoir) which are centered at the single oscillator's energy and which have linearly decaying coupling constants (B is the coupling with a mode in resonance and C determines the length of the coupling). Therefore the single harmonic oscillator is in resonance with a mode of the bath for odd N only. The initial conditions are taken as $\langle \hat{\Delta} \rangle_0 = 1$, and $\langle \hat{B}_j \rangle_0 = (e^{\beta\omega_j} - 1)^{-1}$ [$\beta = (k_B T)^{-1}$, where T is the temperature of the reservoir and k_B is the Boltzmann constant] with all the other initial conditions set to zero. This allows comparison with previous results [2,8,22–24]. As is well known, using the master equation formalism, one finds that $\langle \hat{\Delta} \rangle_t$ decays exponentially to an asymptotic value $\langle \hat{\Delta} \rangle_\infty = (e^{\beta\Omega} - 1)^{-1}$ which is statistically indistinguishable from the modes of the reservoir (see, for example, Ref. [4]).

The numerical solution for the temporal evolution of $\langle \hat{\Delta} \rangle_t$ is shown in Fig. 1. We have used $A/\Omega = 6 \times 10^{-4}$, $B/\Omega = 1.25 \times 10^{-3}$, $n_M/N \approx 0.62$, and $\beta = 1/\Omega$ [i.e., $\langle \hat{\Delta} \rangle_\infty = (e - 1)^{-1} \approx 0.58$] [29]. For small N we observe

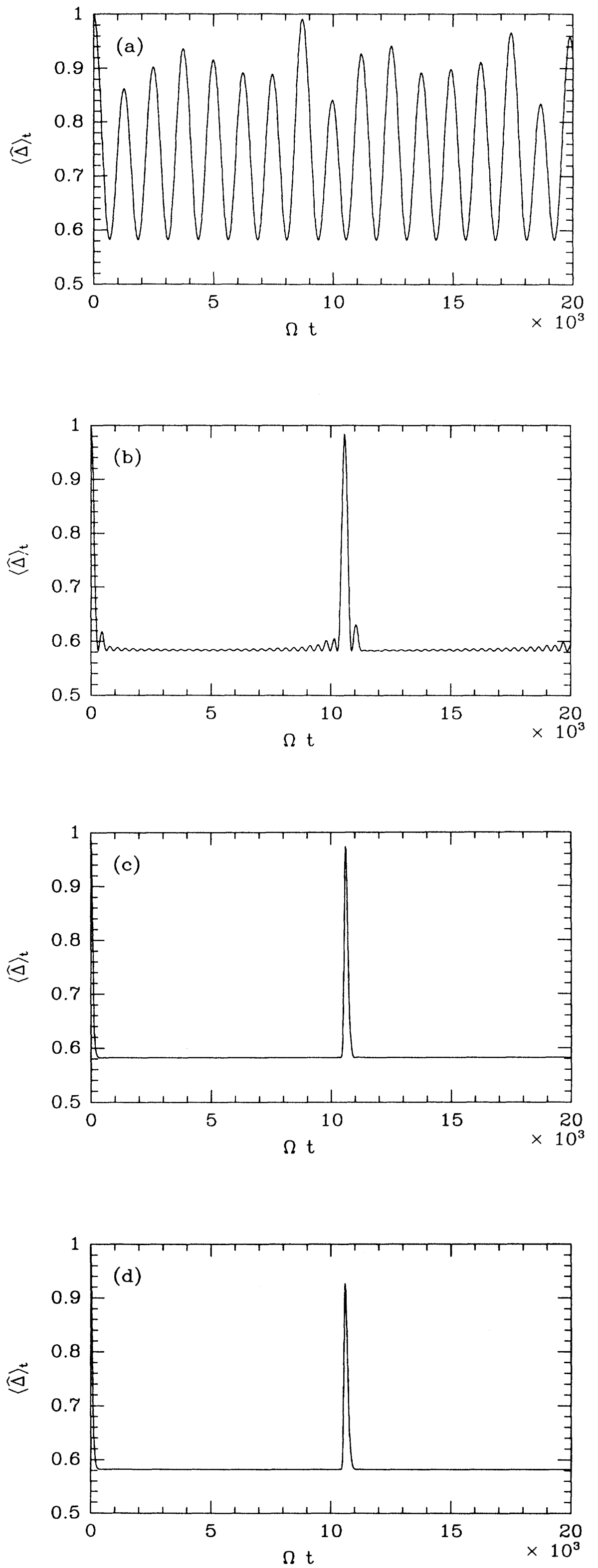

FIG. 1. Temporal evolution of $\langle\hat{\Delta}\rangle_t$. (a) $N = 5$, $C/\Omega = 1.55 \times 10^{-4}$. (b) $N = 31$, $C/\Omega = 2.5 \times 10^{-5}$. (c) $N = 99$, $C/\Omega = 7.8 \times 10^{-6}$. (d) $N = 151$, $C/\Omega = 5.1 \times 10^{-6}$. In all cases, $A/\Omega = 6 \times 10^{-4}$, $B/\Omega = 1.25 \times 10^{-3}$, and $\beta = 1/\Omega$.

an oscillatory behavior. Note, however, that the lowest value of $\langle\hat{\Delta}\rangle_t$ is $\langle\hat{\Delta}\rangle_\infty$ [see Fig. 1(a)]. As N grows the oscillations decrease and a huge revival appears [see Fig. 1(b)]. For N large enough, $\langle\hat{\Delta}\rangle_t$ decays to $\langle\hat{\Delta}\rangle_\infty$ and then revives [see Figs. 1(c)–1(d)]. We have obtained numerically that the revival time is

$$t_r \approx 2\pi/A. \tag{2.5}$$

By observing Fig. 1, we conclude that when the number of oscillators of the bath is sufficiently large, the exchange of energy between the systems becomes dissipative. We have observed that this effect is independent of the parameters as well as of the temperature of the bath and is therefore a consequence of its collective dynamics.

In Fig. 2 we show the evolution for small values of Ωt (i.e., $t < t_r$). We consider those values of N for which the system displays a decaying behavior. We observe that for $0^+ < t \lessapprox t'$, $\langle\hat{\Delta}\rangle_t$ evolves like a cosine (see Refs. [30,31]). For $t' \lessapprox t < t_r$, $\langle\hat{\Delta}\rangle_t$ can be fitted by a decaying exponential function. A similar behavior has been described by Fonda *et al.* (see pp. 102 and 105 of Ref. [31]). We have numerically observed that as N grows, the exponential behavior is achieved earlier, that is, $t' \to 0$. In the limit $N \to \infty$,

$$\langle\hat{\Delta}\rangle_t = \langle\hat{\Delta}\rangle_\infty + (1 - \langle\hat{\Delta}\rangle_\infty)\exp(-t/\tau_d) \tag{2.6}$$

with a characteristic time of the decay

$$\tau_d = \frac{A}{2\pi B^2}. \tag{2.7}$$

Moreover, recent simulations with a random distribution for the energy levels show that the decay behavior remains unaltered, as shown in Fig. 2, while the revivals emerge for a larger number of levels.

The decay and revival times can be independently determined by varying A and B provided an appropriate N is used. For finite N and $t_r > t \gg \tau_d$, $\langle\hat{\Delta}\rangle_t$ is not exactly $\langle\hat{\Delta}\rangle_\infty$ since the bath is slightly out of equilibrium and the

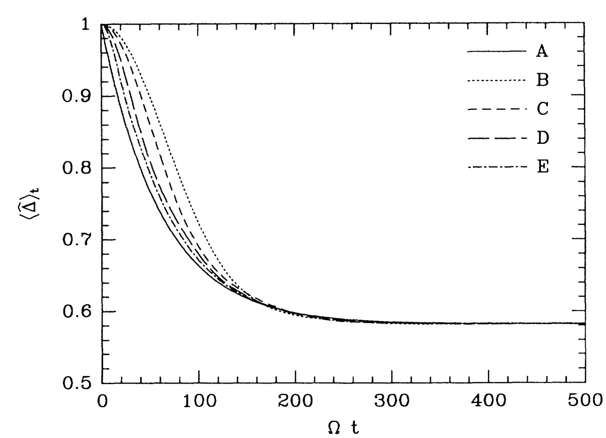

FIG. 2. Temporal evolution of $\langle\hat{\Delta}\rangle_t$. A, Asymptotic behavior given by Eq. (11). B, $N = 99$, $C/\Omega = 7.8 \times 10^{-6}$. C, $N = 151$, $C/\Omega = 5.1 \times 10^{-6}$. D, $N = 301$, $C/\Omega = 2.6 \times 10^{-6}$. E $N = 601$, $C/\Omega = 1.3 \times 10^{-6}$. In all cases $A/\Omega = 6 \times 10^{-4}$, $B/\Omega = 1.25 \times 10^{-3}$, and $\beta = 1/\Omega$.

interaction energy is not zero. We have also found that for large N the evolution described by Eq. (2.6) does not depend on the system being in resonance with any mode. It is important to note that the dependence of τ_d on A and B is exactly the same as the one obtained using the master equation formalism [4,23,24].

We have performed simulations for two-level systems as well as for a system with a random distribution of levels and we have observed that the same collective effect appears. Going beyond the harmonic system implies, in our formalism, that the number of equations increases, since we described the physics of the problem from a Lie algebra based approach which leads to a straightforward generalization of the harmonic oscillator to more complicated models as, for instance, the N-level system.

III. CONCLUSIONS

We have concluded the following: (a) We have obtained the relevant operators for a harmonic oscillator coupled to a quantum-mechanical heat bath [Eq. (2.2)], which allows us to solve exactly the problem at hand. (b) The exact temporal evolution of $\langle\hat{\Delta}\rangle_t$ has been studied. For $t = 0^+$ we have observed a cosinelike behavior. Although we have not made any approximations for large N, we have obtained a decaying exponential approach of $\langle\hat{\Delta}\rangle_t$ to the asymptotic value $\langle\hat{\Delta}\rangle_\infty$ which is expected when the particle is in thermal equilibrium with the bath. (c) $\langle\hat{\Delta}\rangle_t$ shows a revival since the quantum correlations, which naturally appear in our set of relevant operators, were not neglected. (d) We have found the dependence of t_r and τ_d on the constants of the problem. From Eqs. (2.5) and (2.7) we see that both times can be chosen independently (i.e., t_r can be as large as one wants, independent of the value of τ_d). Thus the usual quantum Brownian particle solution can be obtained. As it is well known, in order to achieve irreversible behavior in a literal sense the number of heat-bath oscillators should go to infinity. The approach to this limit is not continuous because it is realized as the divergence of the revival time.

Finally, we would like to emphasize that within our approach, quantum dissipation emerges as a dynamical collective effect, derived from first principles without any approximation. We believe that this conception is brought out clearly and graphically in a numerical simulation of a realistic model where each heat-bath degree of freedom is individually represented.

ACKNOWLEDGMENTS

J.L.G. has benefited from conversations with Professor A. O. Caldeira and also wishes to thank to Dr. D. Domínguez for reading the manuscript and for useful comments. J.A. acknowledges support from Conicet, Argentina. A.N.P. acknowledges support from the Comisión de Investigaciones Científicas de la Provincia de Buenos Aires (CIC). J.A. and A.N.P. acknowledge the support and hospitality of the International Centre for Theoretical Physics (ICTP), Trieste, Italy.

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