Hazards of reservoir memory

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We add memory effects to the master equation describing a harmonic oscillator embedded in a reservoir. Solving the time evolution exactly, we show that the model is sensible only in the Markovian limit. Thus we issue a warning against indiscriminate introduction of memory effects in master equations and call for a systematic method to obtain corrections to Markovian time evolution.

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I. INTRODUCTION

The introduction of irreversible equations from basic physical principles has posed a challenging and illuminating problem for a long time. When quantum theory arose, this problem acquired new actuality, and Pauli seems to have been the first to present such a master equation for irreversible time evolution [1].

Later the problem of magnetic induction of the nuclear spin (nuclear magnetic resonance) required a foundation for the phenomenological equation introduced by Bloch. Such derivations were soon provided by Wangsness and Bloch [2] and later by Redfield [3]. The phenomenological equations assumed that the time evolution would be determined solely by the instantaneous state of the system; this is termed Markovian evolution in physics literature. The microscopic derivations, however showed that this derives from assumptions about the correlation time scales of the reservoirs to which the spin couples. It is far from evident that the time evolution has the assumed Markovian property. Thus the interest turned to more general approaches to the relaxation behavior of a system of interest embedded in another one serving as a reservoir.

When a physical system is put into contact with a reservoir, the reservoir degrees of freedom can be eliminated exactly to produce a master equation that formally ascribes all time evolution to the degrees of freedom of the system of interest [4–6]. This result, however, is only formal; the solution of the equation still requires the solution of the full problem of coupled system-reservoir dynamics. To achieve real irreversible time evolution, one needs to apply further approximations, which eliminate the reversible, short time evolution and push all recurrences beyond the time scales under investigations. Two such assumptions are the weak-field and the short-memory approximations, and consequently the derivations of the master equations are said to be carried out in the Born-Markov limit.

The weak-interaction approximation asserts that we need treat the system-reservoir interaction in second order of perturbation theory only. Thus the reservoir is taken to pursue its own time evolution without regard to the much smaller system coupled to it. This assumption is inherent in the very naming of the reservoir. It is, however, also assumed to respond instantly, so that we do not need to consider the possible delay in its action on the system of interest; this causes the system evolution to depend only on the instantaneous state of the system. In physics this is called a Markovian behavior, even if its exact mathematical meaning is somewhat obscure. The validity conditions for general master equations are discussed by Fano [7].

In this paper we want to draw the attention to the fact that the two assumptions cannot be considered independent; we cannot indiscriminately assume that the reservoir carries memory of its interaction and at the same time remains unaffected by the interaction. We do this by introducing *ad hoc* memory effects into the standard Lindblad form of the damped harmonic oscillator [8]. We can then solve the time evolution exactly and show that the result violates physically reasonable conditions. This we take to mean that one cannot simply add memory effects to dissipative behavior and retain the physical sense of the equations. We have, however, no suggestion how to improve on the Markovian limit, which seems to give reasonable results in most cases. There are cases when even this can lead to problems, for a review consult [9].

In perturbative derivations it is often found that the ensuing master equation is not of the Lindblad form. In fact, there are cases where the physically well-justified fluctuation-dissipation theorem is not compatible with this form. This does not guarantee that the density matrix retains its positivity during the time evolution. There are indications, see Refs. [10,11], that this affects only the initial time evolution. However, when approximative methods, e.g., numerical approaches, are used, this type of instability makes the procedure dangerous and often nonapplicable. A time-evolution generator with unstable eigenelements, will always tend to amplify small errors and disqualify all approximate approaches.

Here we address the problem of a reservoir with memory and damping times not much longer than the periods of the secular motion induced by the Hamiltonian. Such systems are found in laser-excited molecular-dynamic experiments. Here the Markovian approximation is not acceptable. A phenomenological way to introduce damping with memory is to use an environment consisting of Brownian oscillators [12], but this method rapidly becomes unwieldy to apply in computations. Thus we would like to use our physical intuition to add memory effects, but the present work shows that this cannot be carried out indiscriminately. We start by an operator of the Lindblad form; this is expected to give stable evolution for all times. By adding a physically reasonable delay function, we show that the benevolent behavior of the Lindblad form is destroyed. To amend this we would need a criterion analogous to the Lindblad one for master equations with memory. As far as we know, such results have not been formulated.

In order to solve the problem, we apply the formalism of a damping basis introduced by Briegel and Englert [13] and elaborated in some detail by the present authors [14]. They also give the eigenoperators for a spin-$\frac{1}{2}$ system based on Pauli operators. This case was earlier noted also in Ref. [15]. The spectrum of the Lindblad operator is discussed from a more mathematical point of view in Ref. [16].

The use of eigenoperators for the Lindblad evolution allows an exact solution of the problem with memory, and looking at specific initial conditions we can show that nonphysical behavior emerges. Not all cases display such behavior; in particular, the Markovian limit emerges essentially correctly. The fact that basic physical requirements may be violated proves that the approach is flawed, and dooms all results derived from this type of approach to be unreliable. We can even pinpoint the source of the problem, but we have no suggestion how to amend it.

In Sec. II, we introduce the master equation with memory effects added and show how the conventional Markovian result follows. Section III summarizes the formal results we need to derive our solutions to the master equation with memory effects retained.

Section IV presents the general solution and by particularizing it to a simple initial state we can see by inspection that the result violates obvious physical requirements. Thus we conclude that no reliable results can be obtained from equations of the type we have introduced. We also see what condition leads to the unphysical behavior, and show in Sec. V that when these conditions do not prevail, we can obtain a physically acceptable behavior compatible with Markovian evolution. Finally, Sec. VI discusses the results and the ensuing problematic situation.

II. THE MARKOVIAN LIMIT OF RESERVOIR INTERACTIONS

We assume that elimination of a reservoir has lead to the master equation of a type

$$\frac{d\hat{\rho}(t)}{dt}=\int_0^t K(t-t')\mathcal{L}\hat{\rho}(t')dt'=\int_0^t K(t')\mathcal{L}\hat{\rho}(t-t')dt', \tag{1}$$

where $\hat{\rho}(t)$ is the density operator of the system of interest and the Lindblad operator is defined by

$$\mathcal{L}\hat{\rho}=2\hat{a}\hat{\rho}\hat{a}^{\dagger}-\hat{a}^{\dagger}\hat{a}\hat{\rho}-\hat{\rho}\hat{a}^{\dagger}\hat{a}. \tag{2}$$

The form assumes the reservoir to be at zero temperature but our argument is not affected by this. We also omit the unitary time evolution deriving from the Hamiltonian; this has no effect on our argument. For a free-oscillator Hamiltonian it only implies that we work in a rotating frame.

We assume the memory kernel to be of second order in the coupling V as follows

$$K(t-t')=V^2k(t-t'); \tag{3}$$

if $k(t)$ is replaced by a δ function $\delta(\gamma t)$, the ordinary Marovian result emerges. The parameter γ refers to the bandwidth of the reservoir spectrum.

Equation (1) assumes that we look at the time evolution over some extended interval; the very short times display the details of the interaction. We also assume that the coupling is weak, i.e., $V\rightarrow 0$, but in such a way that the scaled time variable

$$\tilde{t}=V^2t \tag{4}$$

remains finite. Long ago, van Hove [17] pointed out that this is the limit in which irreversible behavior emerges.

In terms of this variable, Eq. (1) becomes

$$\frac{d\hat{\rho}}{d\tilde{t}}=\lim_{V\rightarrow 0}\int_0^{\tilde{t}/V^2}K(t')\mathcal{L}\hat{\rho}(\tilde{t}-V^2t')dt' =\left[\int_0^{\infty}K(t')dt'\right]\mathcal{L}\hat{\rho}(\tilde{t}), \tag{5}$$

which is the ordinary Markovian limit.

If we want to evaluate the corrections to the limit, we might try to utilize the expansion

$$\hat{\rho}(\tilde{t}-V^2t')=\sum_{k=0}^{\infty}\frac{(-V^2t')^k}{k!}\left[\frac{d^k\hat{\rho}(\tilde{t})}{d\tilde{t}^k}\right]. \tag{6}$$

This retains the Markovian character of the equation, but at the expense of the introduction of higher derivatives in the density operator. This is known to be a dangerous route, which in the case of radiation damping causes the well-known "run-away" solutions [18]. It seems to us, that either one goes to the Markovian limit or alternatively the full problem needs to be solved. We will approach this in the following, but first we need to summarize the tools developed in our earlier paper [14].

III. SUMMARY OF FORMAL RESULTS

In this section we present the formal eigenelements of the Lindblad operator (2) satisfying

$$\mathcal{L}\hat{A}_{\nu}=\lambda_{\nu}\hat{A}_{\nu}. \tag{7}$$

These operators have been proved to form a complete set of operators in which to expand the density operator, a damping basis [13].

The operators are found to be labeled by two nonnegative integers $\{m,l\}$ and are given by

$$\hat{A}_m^l=\sum_{n=0}^{m}(-1)^n\frac{m!}{(m-n)!}\sqrt{\left[\frac{l!}{n!(n+l)!}\right]}|n\rangle\langle n+l|, \tag{8}$$

where $|n\rangle$ is the ordinary oscillator eigenstate. The corresponding eigenvalue has the form

$$\lambda_m^l = -(2m+l), \tag{9}$$

which guarantees the decay of the system towards the unique ground state

$$\hat{A}_0^0 = |0\rangle\langle 0|. \tag{10}$$

The eigenvalues (9) have earlier been obtained for the case of laser cooling [19], Sec. V D.

We can also define a complete set of adjoint operators $\hat{B}_m^{l\,\dagger}$ by requiring that

$$\mathrm{Tr}(\hat{B}_m^{l\,\dagger}\hat{A}_{m'}^{l'}) = \delta_{ll'} \quad \delta_{mm'}, \tag{11}$$

giving

$$\hat{B}_m^l = \frac{(-1)^m}{m!}\sum_{n=m}^{\infty}\sqrt{\left(\frac{n!(n+l)!}{l!}\right)}\frac{1}{(n-m)!}|n\rangle\langle n+l|. \tag{12}$$

In terms of these operators we can expand the density operator as

$$\rho = \sum_{m=0}^{\infty}\sum_{l=0}^{\infty}\eta_l(\rho_{ml}\hat{A}_m^l + \rho_{ml}^*\hat{A}_m^{l\,\dagger}), \tag{13}$$

where the parameter

$$\eta_l = 1 - \frac{1}{2}\delta_{l0} \tag{14}$$

is introduced to take care of the fact that

$$\hat{A}_m^0 = (\hat{A}_m^0)^\dagger. \tag{15}$$

It also follows that the imaginary part of every ρ_{m0} does not enter the expansion and hence we may choose these elements real. The coefficients are given by

$$\rho_{ml} = \mathrm{Tr}(\hat{B}_m^{l\,\dagger}\hat{\rho}). \tag{16}$$

These results were earlier obtained by Briegel and Englert [13], who have also used them to discuss a variety of problems in cavity QED [20–26]. Here we want to utilize the formalism to derive the solution of the memory-function master equation (1)

IV. SOLUTION OF THE NON-MARKOVIAN EVOLUTION

In order to obtain the solution to the master equation (1) we evaluate its Laplace transform to

$$s\overline{\rho}(s) - \hat{\rho}(0) = \overline{K}(s)\,\mathcal{L}\,\overline{\rho}(s) \tag{17}$$

with the solution

$$\overline{\rho}(s) = \frac{1}{s-\overline{K}(s)\,\mathcal{L}}\hat{\rho}(0) = \sum_{m,l}\eta_l\left[\frac{1}{s+\overline{K}(s)\,(2m+l)}\right] \times(\rho_{ml}\hat{A}_m^l + \rho_{ml}^*\hat{A}_m^{l\,\dagger}). \tag{18}$$

If we assume the simplest possible memory function

$$K(t-t') = V^2\exp(-\gamma|t-t'|), \tag{19}$$

then we obtain the Laplace transform

$$\overline{K}(s) = \frac{V^2}{s+\gamma}. \tag{20}$$

The poles of the expression (18) are then at the positions

$$s = -\frac{\gamma}{2} \pm i\sqrt{V^2(2m+l) - \left(\frac{\gamma}{2}\right)^2} \equiv -\frac{\gamma}{2} \pm i\Omega(m,l). \tag{21}$$

We further introduce the notation $\Omega(m) \equiv \Omega(m, l=0)$. When these singularities are utilized, the Laplace transform (18) can be inverted [8] to give

$$\begin{aligned}\hat{\rho}(t) = {} & \rho_{00}\hat{A}_0^0 + \sum_{m=1}^{\infty}\exp\left(-\frac{\gamma t}{2}\right)\rho_{m0}\hat{A}_m^0\left\{\cos[\Omega(m)t]\right. \\ & \left. + \frac{\gamma}{2\Omega(m)}\sin[\Omega(m)t]\right\} + \sum_{m=0}^{\infty}\sum_{l=1}^{\infty}\exp\left(-\frac{\gamma t}{2}\right) \\ & \times\left\{\rho_{ml}\hat{A}_m^l\left\{\cos[\Omega(m,l)t] + \frac{\gamma}{2\Omega(m,l)}\right.\right. \\ & \left.\left.\times\sin[\Omega(m,l)t]\right\} + \mathrm{h.c.}\right\}.\end{aligned} \tag{22}$$

Here we have, in particular,

$$\rho_{00} = 1; \quad \hat{A}_0^0 = |0\rangle\langle 0|. \tag{23}$$

For small values of $\{m,l\}$ the frequencies $\Omega(m,l)$ are imaginary when

$$V^2 \ll \frac{\gamma^2}{4}, \tag{24}$$

but for larger values they become real; the solution written down above holds for all cases.

When the solution is described by damped oscillations, the result derived above contains clearly unphysical features. This is most easily seen if we assume the initial density matrix to be in a pure number state $\hat{\rho}(0) = |n\rangle\langle n|$ when the initial state is given by (see Ref. [14])

$$\rho_{ml} = \frac{(-1)^n n!}{m!(n-m)!}\delta_{l0} \quad (m \geqslant n). \tag{25}$$

Introducing this into the solution and calculating the probability of remaining in the state $|n\rangle$ we find

$$\langle n|\hat{\rho}(t)|n\rangle = \rho_{n0}\langle n|\hat{A}_n^0|n\rangle \exp\left(-\frac{\gamma t}{2}\right)\left\{\cos[\Omega(n)t] + \frac{\gamma}{2\Omega(n)}\sin[\Omega(n)t]\right\}$$
$$= \exp\left(-\frac{\gamma t}{2}\right)\left\{\cos[\Omega(n)t] + \frac{\gamma}{2\Omega(n)} \times \sin[\Omega(n)t]\right\}. \tag{26}$$

It is obvious that this result is meaningless, because it will take negative values for real frequencies $\Omega(n)$. Thus whenever

$$2nV^2 > \frac{\gamma^2}{4} \tag{27}$$

we obtain negative probabilities. This result appears, because then the effective coupling to the reservoir $\sqrt{n}V$ exceeds the width of the reservoir spectrum γ. And for all values of V and γ, there are some n values above which this occurs, making the whole procedure dangerous and unreliable. Thus we conclude that the basic equation (1) is fundamentally flawed and should not be used. A more sophisticated approach to memory effects is needed, but we do not know how to device such an approach without solving the full problem of system-reservoir coupling.

V. THE PERTURBATIVE LIMIT

In the case that we have

$$2nV^2 \ll \frac{\gamma^2}{4}, \tag{28}$$

we can expand the root in Eq. (21) as

$$\tilde{\Omega}(n) = -i\Omega(n) = \frac{\gamma}{2}\sqrt{1-\left(\frac{8nV^2}{\gamma^2}\right)} = \frac{\gamma}{2} - \frac{2nV^2}{\gamma} - \frac{4n^2V^4}{\gamma^3} + \cdots. \tag{29}$$

Introducing this into the solution (26) we obtain

$$\langle n|\hat{\rho}(t)|n\rangle = \exp\left(-\frac{\gamma t}{2}\right)\left\{\cosh[\tilde{\Omega}(n)t] + \frac{\gamma}{2\tilde{\Omega}(n)}\sinh[\tilde{\Omega}(n)t]\right\}. \tag{30}$$

For large times this becomes

$$\langle n|\hat{\rho}(t)|n\rangle = \exp\left(-\frac{2nV^2}{\gamma}t\right)\left(1+\frac{2nV^2}{\gamma^2}\right). \tag{31}$$

It is easy to verify that this is the correct Markovian decay rate of the problem, because the master equation is in this limit

$$\frac{d}{dt}\hat{\rho} = \frac{V^2}{\gamma}[2\hat{a}\hat{\rho}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}\hat{\rho} - \hat{\rho}\hat{a}^\dagger\hat{a}], \tag{32}$$

which gives for the initial state $|n\rangle\langle n|$, the equation

$$\frac{d}{dt}\langle n|\hat{\rho}(t)|n\rangle = -\frac{2nV^2}{\gamma}\langle n|\hat{\rho}(t)|n\rangle \tag{33}$$

with the solution (31) except for the shifted initial state. The full result (30) has the physically correct short-time behavior

$$\langle n|\hat{\rho}(t)|n\rangle = 1 - nV^2t^2 + O(t^3). \tag{34}$$

This satisfies the initial time evolution with a smooth onset of the deviation from the correct initial value. The fact that the long-time exponential behavior needs to be corrected for the initial nonexponential onset of the evolution is well known from Brownian-motion-type models, and it has been termed an ''initial slip'' by Haake and Lewenstein [27].

Even if we do not retain terms only to lowest order in V^2, the behavior remains meaningful in the present limit. In the exponential regime of long-time evolution, the result (30) gives an expression of the form

$$\langle n|\hat{\rho}(t)|n\rangle = \exp(-\Gamma t)(1+\varepsilon), \tag{35}$$

where ε is positive and the decay rate is

$$\Gamma = \frac{\gamma}{2}\left(1-\sqrt{1-\left(\frac{8nV^2}{\gamma^2}\right)}\right) = \frac{2nV^2}{\gamma} + \frac{4n^2V^4}{\gamma^3} + \frac{16n^3V^6}{\gamma^5} + O(V^8), \tag{36}$$

which is always positive and implies decay. Thus we find that when the condition (28) is satisfied, the solution is both physically meaningful and asymptotically correct. However, because the condition depends on the initial state, it will eventually be violated for some value of n and thus the solution is not acceptable for an arbitrary initial state.

VI. CONCLUSION

We have discussed the introduction of finite-memory effects in a system dynamics ensuing from the elimination of a reservoir. By choosing the simplest example of a damped harmonic oscillator and an exponentially decaying memory, we have shown that blatantly nonphysical behavior emerges. Only in the Markovian limit, can we claim that the description produces sensible and reliable results. Hence we conclude that such models cannot be utilized with confidence in more complicated situations, where the physical consequences are harder to survey.

The objection may be raised that our conclusions follow from an oversimplified model, and that they are not generic enough to constitute a universally applicable warning against models with memory. We, on the other hand, believe this not to be so; the fact that even a simple and physically fully understood situation produces nonsensical results is indeed a serious warning.

We may try to survey the origin of the nonphysical features. The relation (27) tells us that the bandwidth of the reservoir is less than the rate of change of the system due to the reservoir coupling. The reservoir cannot respond fast enough to follow the evolution induced by the interaction. This is just the limit when the Markovian behavior is expected to break down, but it is also seen to be the limit when the simple introduction of memory effects becomes unphysical. We can understand this, because our simple model (1) introduces the memory as a passive effect. The Markovian limit is the one where all influence the system imposes on the reservoir is lost in its vastness without feeding any effect back. When memory is introduced, the influence on the reservoir undergoes its dynamical evolution, and its effect back on the system is to be modified by this. The passive model we have introduced fails to do this, and the unphysical features may be seen to derive from this fact. This statement, however, does not suggest any way to amend the situation; no systematic corrections to the Markovian limit can be derived from the explanation.

We know that an exact elimination of the reservoir variables can be performed for simple cases [28]. In the Markovian limit, this gives superficially simple results, which however have been shown to be flawed as they stand [29]. The reason seems to be that linear-response theory requires the physically sensible fluctuation-dissipation theorem to hold, but this is not universally compatible with the mathematical requirements on an acceptable Lindblad operator. Remarkably enough, the rotating-wave approximation seems to correct the situation and give a consistent damping behavior for the harmonic oscillator [9].

We have shown that even the mathematicaly reliable and numerically stable Lindblad-operator form leads to instabilities when memory effects are added arbitrarily. We know that there exists an exact memory kernel, but this is usually not identifiable. In applications it thus has to be replaced by physically motivated approximations. We have no universal criteria to judge when this is mathematically safe. This paper analyses such a case in order to find out the hazards that may be inherent in the approach.

The main conclusion of this paper is a warning against the use of approximate models with memory and a challenge to develop systematic corrections to Markovian time evolution in physical systems.

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