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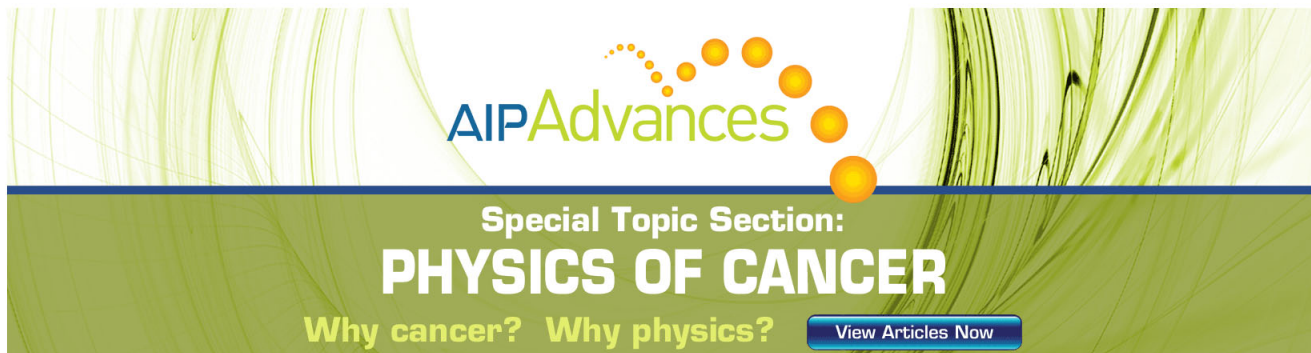
Memory effects in the relaxation of quantum open systems

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A close examination of the validity of the Markovian approximation in the context of relaxation theory is presented. In particular, we examine the question of positivity of various approximations to the reduced dynamics of an open system in interaction with a heat reservoir. It is shown that the Markovian equations of motion obtained in the weak coupling limit (Redfield equations) are a consistent approximation to the actual reduced dynamics only if supplemented by a slippage in the initial conditions. This slippage captures the effects of the non-Markovian evolution that takes place in a short transient time, of the order of the relaxation time of the isolated bath.

I. INTRODUCTION

Because of the remarkable success of the phenomenological Bloch equations in the description of quantum relaxation processes,[1] the derivation of a quantum master equation from a microscopic model is of fundamental importance. This task has proven to be unexpectedly complicated and full of mathematical subtleties.[2] In fact, no single attempt to complete this derivation seems to be fully satisfactory.[3,4]

One of the most elegant approaches to this program is the projection operator technique inaugurated by Zwanzig.[5] This procedure allows us to rewrite the equations of motion for the reduced density matrix of an open system interacting with a heat bath in the form of a generalized master equation (i.e., there are memory effects present). This form is particularly useful as a starting point for successive approximations. One of the most frequent approximations (consistent with the success of Bloch-type equations in accounting for experimental results) is to assume that all the memory effects in the dynamics of the open system are rapidly dissipated by the bath, and that the reduced equations of motion become Markovian (i.e., local in time).[5–7,2]

This approximation has been criticized in the literature,[3,7,8] since it breaks the positivity of the reduced dynamics (that is, it leads to negative values for population variables). In particular, for the case of an open system weakly coupled to its environment, Dümcke and Spohn[8] have suggested that the only Markovian approximation consistent with the requirement of positivity of the dynamics is the one proposed by Davies,[9] which unfortunately does not comply with the symmetry of the Hamiltonian and hence is physically unacceptable.

In this paper, we argue that the Markovian approximation that preserves the symmetry of the Hamiltonian is in fact correct, provided that we take into account nonlocal memory effects that take place in a very short time scale. It is only after this transient time that the reduced dynamics are properly described by the standard Markovian evolution. These effects will be the object of the investigation carried out in this paper. In Sec. II, we shall examine the various Markovian approximations in detail, comparing them and assessing their consistency with physical requirements. In Sec. III the origin of the brief non-Markovian evolution regime will be clarified. Finally, Sec. IV will be devoted to the effect of initial conditions on the magnitude of the nonlocal memory effects.

II. THE QUANTUM MASTER EQUATION

The starting point for the derivation of the quantum master equation is the reversible dynamics (generated by a Hamiltonian) of a large macroscopic system. The objective is to obtain equations that describe the irreversible approach of reduced quantities (referring to a small number of degrees of freedom) to their equilibrium values, from the complete reversible dynamics. The project, as described by Zwanzig,[5] can be summarized as follows: First, we divide the universe into the system of interest and a reservoir. This division is arbitrarily dictated by the fact that we are interested in performing measurements of observables of the system alone, regardless of the state of the environment. Then, by means of an appropriate technique, we shall obtain a generalized Fokker–Planck equation for the reduced density matrix of the open system in interaction with the bath, or, equivalently, a generalized Langevin equation for the system observables. This can be exactly accomplished by using a suitably defined projection operator. The function of the projection operator is twofold. First, it separates the dynamics into a "relevant" and an "irrelevant" part. Second, it provides a definition for the temperature at which the evolution takes place.

Once more there is some arbitrariness as to which projection operator should be chosen, and a variety of criteria can be adopted (see Romero-Rochin and Oppenheim[4] for a discussion on the subject).

In order to be more explicit, consider the dynamics generated by the Hamiltonian $H = H_s + H_b + \lambda V_{sb}$, where H_s is the Hamiltonian for the free system, H_b is the Hamiltonian of the isolated bath, and λV_{sb} is the interaction between them (λ is a dimensionless parameter measuring the strength of the coupling). The time evolution of the total density matrix for the system is given by

$$\rho(t) = \exp(-iH^X t)\rho(0), \tag{1}$$

where $H^X O = [H, \mathcal{O}]$, i.e., the commutator of the Hamiltonian with an arbitrary operator $\mathcal{O}$. Assume that we have chosen a projector $\mathcal{P}$ (Hermitian, idempotent, $\mathcal{P} + \mathcal{Q} = 1$). This projector divides the density matrix into a relevant part $\rho_1(t) = \mathcal{P}\rho(t)$, and an irrelevant part $\rho_2(t) = \mathcal{Q}\rho(t)$, with $\rho(t) = \rho_1(t) + \rho_2(t)$. The equation of motion for the relevant part of the density matrix has the form of a generalized Fokker–Planck equation (note that *generalized* is used to indicate that the equation includes memory effects, i.e., it is non-Markovian),

$$i\dot{\rho}_1(t) = \mathcal{P}H^X \exp\{-i\mathcal{Q}H^X t\}\rho_2(0) + \mathcal{P}H^X \rho_1(t)$$
$$- i \int_0^t d\tau \mathcal{P}H^X \exp\{-i\mathcal{Q}H^X \tau\}$$
$$\times \mathcal{Q}H^X \rho_1(t-\tau). \tag{2}$$

Note that the right-hand side of the equation consists of three terms, the first of which is explicitly dependent on the initial conditions. The usual assumption is that this term vanishes after a short time, the characteristic relaxation time of the bath τ_b (usually, on the order of ps or faster). Alternatively, we may take the viewpoint that the projection operator selects a very special kind of initial conditions, for which $\rho_2(0)$ vanishes identically.

As an example, consider the following two proposals for a projection operator, encountered in the literature. The first is

$$\mathcal{P}_0 \mathcal{O} = \rho_b^{eq} \operatorname{Tr}_b \mathcal{O},$$

where

$$\rho_b^{eq} = \frac{\exp\{-\beta H_b\}}{\operatorname{Tr}_b(e^{-\beta H_b})}, \tag{3}$$

and Tr_b indicates "trace over the bath degrees of freedom" ($\mathcal{O}$ is an arbitrary system-bath operator). It corresponds to the choice of factorized initial conditions, in which the system is in an arbitrary state and the bath is in equilibrium with respect to H_b,

$$\rho(0) = \rho_1(0) = \rho_b^{eq}\sigma(0),$$

where $\sigma(t) \equiv \operatorname{Tr}_b[\rho(t)]$ is the reduced density matrix for the system. This is in fact the projector that we shall use throughout most of this paper.

A second choice is given by[4]

$$\mathcal{P}\mathcal{O} = \tfrac{1}{2}(\tilde{\rho}\operatorname{Tr}_b \mathcal{O} + \operatorname{Tr}_b \mathcal{O}\tilde{\rho}^+),$$

with

$$\tilde{\rho} = \rho_e W_e^{-1},$$
$$\tilde{\rho}^+ = W_e^{-1}\rho_e,$$

and

$$\rho_e = \frac{e^{-\beta H}}{\operatorname{Tr}_{bs}(e^{-\beta H})}, \quad W_e = \operatorname{Tr}_b(\rho_e),$$

which has the advantage of separating the streaming and dissipative parts on the right-hand side of Eq. (2).

We note that although the appearance of Eq. (2) is very promising, we have done nothing but reformulate the problem. In order to come closer to a solution, we have to deal with two difficulties: on one hand, the equation is nonlocal in time. On the other, the tensor kernel of the convolution is unknown; furthermore, its exact form requires our solving the full dynamics.

Both these problems can be approximately solved in the weak coupling limit (λ small). We shall approximate the kernel by its expansion to second order in the weak coupling parameter λ, which can be easily calculated. This limit also provides a separation of time scales; the relaxation time of the bath, τ_b, which is assumed to be fast, and a slower time scale corresponding to the relaxation of the system when it is coupled to the bath or heat reservoir τ_R. The latter scale is of order $\tau_R \sim (1/\lambda^2) \gg \tau_b$. It has been pointed out by several authors[3,8,7,10] that even though such approximation preserves the Hermiticity and the trace of $\rho(t)$, in general it does not preserve positivity. This implies that if we start with an arbitrary reduced density matrix, the approximate time evolution might map $\sigma(0)$ into an unphysical $\sigma(t)$ whose eigenvalues lie outside the interval [0,1] in contradiction with their physical interpretation as populations of states.

In order to elucidate this point, consider a particular Hamiltonian describing the interaction between a nondegenerate two-level system and its environment

$$H = -\frac{\Delta}{2}\sigma_z + H_b + \lambda V\sigma_x; \quad \Delta > 0. \tag{4}$$

We shall also assume (somewhat optimistically) that we have been able to obtain an analytical form for the equations of motion for the elements of the density matrix to all orders in λ, and that the Markovian approximation is valid. Although this program is possible in theory, in practice it becomes a forbiddingly difficult task to carry out. (However, see Larid et al.[11] for this derivation beyond weak coupling, up to fourth order in λ. If we stop at second order in the perturbation parameter, we obtain the usual Redfield equations.[6] See also Harris and Stodolsky.[12]) The equations of motion for the elements of the density matrix in the basis set that diagonalizes σ_z, $\sigma_z| \pm \rangle = \pm | \pm \rangle$, are

$$\dot{\sigma}_{++}(t) = -A\Gamma\sigma_{++}(t) + \Gamma\sigma_{--}(t),$$
$$\dot{\sigma}_{--}(t) = A\Gamma\sigma_{++}(t) - \Gamma\sigma_{--}(t), \tag{5}$$

for the diagonal terms, where $A = \sigma_{--}^{eq}/\sigma_{++}^{eq}$, and Γ is a real constant. For the off-diagonal terms

$$\dot{\sigma}_{+-}(t) = i\Delta\sigma_{+-} - C\sigma_{+-}(t) + C^*\sigma_{-+}(t),$$
$$\dot{\sigma}_{-+}(t) = -i\Delta\sigma_{-+} + C\sigma_{+-}(t) - C^*\sigma_{-+}(t), \tag{6}$$

with $C = \gamma + i\delta w$, γ and δw real. These are usually referred to as Redfield equations.

Note that these expressions have been written solely on the basis of the symmetry of the Hamiltonian and that the

equations are local in time. It shall be convenient to rewrite these equations in the form of a Bloch vector, defined as

$$z(t) = \sigma_{++}(t) - \sigma_{--}(t),$$

$$x(t) = \sigma_{+-}(t) + \sigma_{-+}(t), \tag{7}$$

$$y(t) = i[\sigma_{+-}(t) - \sigma_{-+}(t)],$$

leading to

$$\dot{z}(t) = -(1+A)\Gamma z(t) + (1-A)\Gamma, \tag{8}$$

$$\dot{x}(t) = \Delta y(t), \tag{9}$$

$$\dot{y}(t) = -(\Delta - 2\delta w)x(t) - 2\gamma\, y(t). \tag{10}$$

We remark that, even though Eqs. (8) and (10) are approximate, Eq. (9) is exact for this Hamiltonian. It is also straightforward to check that such equations do not in general preserve positivity. The relations that the coefficients in Eqs. (8)–(10) have to fulfill, lest the Markovian map should be nonpositive are (from Alicki and Lendi[10])

(I) $2\gamma = (1+A)\Gamma$,

(II) $4(\delta w)^2 + (A-1)^2\Gamma^2 < (1+A)^2\Gamma^2 - 4\gamma^2$.

Both conditions cannot be simultaneously fulfilled unless $\delta w = 0$ and $A = 1$. This fact can also be checked directly by solving the set of Eqs. (8)–(10),

$$z(t) = (z(0) - z_{eq})\exp[-(1+A)\Gamma t] + z_{eq},$$

$$x(t) = \left\{ x(0)\cos wt + \left[\frac{\Delta}{w}y(0) + \frac{\gamma}{w}x(0)\right]\sin wt \right\}e^{-\gamma t}, \tag{11}$$

$$y(t) = \left\{ y(0)\cos wt - \left[\frac{\gamma}{w}y(0) + \frac{\Delta - 2\delta w}{w}x(0)\right]\sin wt \right\}e^{-\gamma t},$$

with the definition $w^2 = \Delta(\Delta - 2\delta w) - \gamma^2$.

In particular, for the weak-coupling case (that is, Γ, $A\Gamma$, and C approximated by their expansion truncated to second order in λ), the explicit expressions for these coefficients are

$$A\Gamma = \lambda^2 \int_{-\infty}^{\infty} d\tau e^{-i\Delta\tau}\langle \hat{V}(\tau)V \rangle = e^{-\beta\Delta}\Gamma,$$

$$\Gamma = \lambda^2 \int_{-\infty}^{\infty} d\tau e^{i\Delta\tau}\langle \hat{V}(\tau)V \rangle, \tag{12}$$

$$C = \lambda^2 \int_{0}^{\infty} d\tau e^{-i\Delta\tau}\langle [\hat{V}(\tau), V]_+ \rangle,$$

where $\hat{V}(t) = e^{iH_b t}Ve^{-iH_b t}$ is in the interaction representation with respect to the bath Hamiltonian, $[A,B]_+ \equiv AB + BA$ is an anticommutator, and $\langle \mathcal{O} \rangle = \mathrm{Tr}_b(\rho_b^{eq}\mathcal{O})$ is the thermal average of the bath operator $\mathcal{O}$. In the weak coupling case, condition (I) for positivity is fulfilled [i.e., $(1 + A)\Gamma = 2\mathrm{Re}(C)$], but not condition (II) [since $\mathrm{Im}(C)\neq 0$]. In order to be more specific, we shall carry out a numerical calculation which will explicitly show the eigenvalues of the reduced density matrix straying away from the interval [0,1]. The model chosen for the environ-
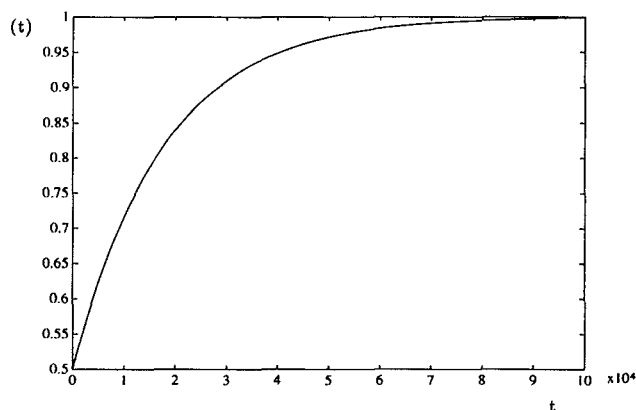

FIG. 1. Relaxation of the population variable $z(t)$ from its initial value $z(0) = 0.5$ to its equilibrium value $z_{eq} = 1$, according to Redfield equations. The parameters for this and following simulations are $\eta = 0.01$; $\Delta = 0.1$; $w_c = 1$; $T = 0$, unless otherwise indicated.

ment is a Debye bath of independent harmonic oscillators, and linear coupling between the bath and the system,

$$H_b = \frac{1}{2} \sum_\alpha\, (p_\alpha^2 + w_\alpha^2 x_\alpha^2),$$

$$\lambda V = \sum_\alpha c_\alpha x_\alpha. \tag{13}$$

The spectral strength for this bath (assuming that the deformation potential approximation is valid) is $\mathcal{J}(w) = \Sigma_\alpha(c_\alpha^2/2w_\alpha)\delta(w_\alpha - w) = \eta(w^3/w_c^2)\exp[-(w/w_c)]$. η is a dimensionless friction constant (of order λ^2), and w_c is an appropriate cutoff frequency. The following parameters have been used in the simulation: $\eta = 0.01$; $\Delta = 0.1$; $w_c = 1$; $T = 0$. Energies are measured in units of w_c and time in units of w_c^{-1}. For this set of parameters, $\delta w = 2 \times 10^{-3}$ and $\Gamma = 5.7 \times 10^{-5}$; $A = 0$. If the cutoff frequency for the bath is $w_c \approx 100$ cm^{-1} (i.e., τ_b is on the order of ps), the relaxation rate for the system τ_R is on the order of ns, which is reasonable from a experimental point of view. This is also consistent with the requirement that $\tau_R \gg \tau_b$, so that the time scales are well separated and the Markovian approximation is valid.

Figure 1 shows the evolution of the system population variable in the $\{|\pm\rangle\}$ basis, $z(t)$. In Fig. 2 (solid line), we present the simulation for the time evolution of the determinant of the reduced density matrix, given a particular set of initial conditions [$x(0) = 0$; $y(0) = \sqrt{3}/2; z(0) = 0.5$]. We observe that it soon becomes negative, signaling that one of its eigenvalues is lower than zero and the other is larger than one. As expected, the amount by which the positivity is broken is of order λ^2.

The solution proposed by Dümcke and Spohn[8] to the lack of positivity of Redfield equations is to substitute for this set of weak coupling equations another (positivity preserving) set, which is equivalent to the same order in λ. The details of how to obtain such an approximation can be found in Refs. 8 and 9. Here we shall just quote the results for the Hamiltonian under consideration. The equations
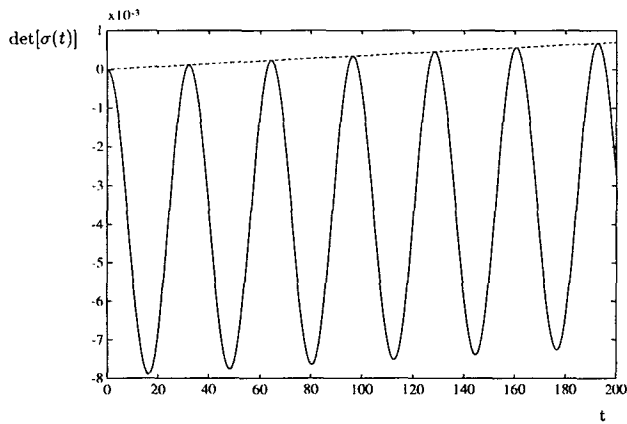
FIG. 2. Comparison between the standard weak coupling evolution (full line) and Dümcke and Spohn's proposal (dashed line). The quantity plotted is the determinant of the reduced density matrix of the system. The initial conditions which have been chosen are $x(0)=0$; $y(0) = \sqrt{3}/2$; $z(0) = 0.5$, which implies that the determinant initially vanishes.

for the diagonal terms remain unchanged, whereas, for the off-diagonal elements, the equations become

$$\dot{\sigma}_{+-}(t) = i\Delta\sigma_{+-} - C\sigma_{+-}(t),$$

$$\dot{\sigma}_{-+}(t) = -i\Delta\sigma_{-+} - C^*\sigma_{-+}(t), \tag{14}$$

which, in terms of a Bloch vector is

$$\dot{x}(t) = (\Delta - \delta w)y(t) - \gamma x(t), \tag{15}$$

$$\dot{y}(t) = -(\Delta - \delta w)x(t) - \gamma y(t). \tag{16}$$

The only condition for positivity in this case is $(1+A)\Gamma \leqslant 2\gamma$, which is immediately fulfilled in the weak coupling case [as $(1+A)\Gamma = 2\gamma$]. The explicit solution for $x(t)$, $y(t)$ is

$$x(t) = [x(0)\cos(wt) + y(0)\sin(wt)]e^{-\gamma t},$$

$$y(t) = [y(0)\cos(wt) - x(0)\sin(wt)]e^{-\gamma t}, \tag{17}$$

where $w = \Delta - \delta w$. The dashed line in Fig. 2 gives the time evolution for the determinant of the system reduced density matrix, for the same parameters and initial conditions as in the corresponding Redfield case. It shows how the behavior is modified from one approximation to the other, with Dümcke and Spohn's map becoming a completely positive one.

We note, however, that the oscillations of the determinant have been suppressed in the latter approximation. This is related to the fact that Eqs. (15) and (16) cannot be obtained naturally from a Hamiltonian such as Eq. (4). Henceforth, we shall argue this approximation is arbitrary, in the sense that it fixes the lack of positivity of the Markovian map [Eqs. (5) and (6)] but is inconsistent with the symmetry of the problem.

III. NONLOCAL EFFECTS

In the previous section, it has been shown that even if we are able to obtain a Markovian master equation valid to infinite order in perturbation theory, we encounter the fun-

damental difficulty that the reduced dynamics do not preserve the positivity of the density matrix. In addition, the alternatives proposed in the literature are obtained by rather arbitrary procedures and present further drawbacks.

In our proposal, we emphasize that the Markovian master equation is valid only after a transient time, on the order of the relaxation time of the isolated bath and independent of λ. During this transient regime, *correlations* (in a sense that shall be specified later on) are being built between the bath and the system, implying that the evolution is complex and highly non-Markovian. The former fact is well-known in the literature.[13] However, its relevance to the present discussion has not been stressed in past work. These nonlocal effects are also important because they seem to restrict a class of density matrices that can evolve under the Markovian master equation. That is, not all physical reduced density matrices (that is, Hermitian, with unit trace and non-negative eigenvalues) can be chosen as initial conditions for Redfield equations.

In this fashion, the problem of positivity seems to be resolved, without abandoning the symmetry restrictions imposed by the Hamiltonian. The conditions obtained by Alicki and Lendi[10] for positivity preserving maps were derived based on the assumption that the set of all physical reduced density matrices ($\mathscr{S}$) should be mapped into itself by the dynamics. However, we argue that only a subset can actually evolve under the Markovian dynamics, and that it is only elements of this subset that have to be mapped into $\mathscr{S}$.

As an illustration of these points, we proceed to perform numerical calculations on the Hamiltonian Eq. (4). Since these effects take place at a very short time scale, we expect that second order perturbation theory should be adequate.[2] [Note that this approximation is different from the one we make in the derivation of Redfield equations, in which we effectively resum terms of order $(\lambda^2 t)^n$.] The results for the Bloch vector are

$$x(t) = x(0)[\cos\Delta t + \Theta_1(t)] + y(0)[\sin\Delta t - \Theta_2(t)],$$

$$y(t) = y(0)[\cos\Delta t - \Theta_3(t)] - x(0)[\sin\Delta t - \Theta_2(t)],$$

$$z(t) = z(0)[1 - \Theta_4(t)] - \Theta_5(t), \tag{18}$$

with the values

$$\Theta_1(t) = 2\lambda^2 \int_0^t d\tau \left[\frac{1}{\Delta}\sin\Delta(t-\tau) - (t-\tau)\cos\Delta(t-\tau) \right]$$
$$\times \mathrm{Re}\langle \hat{V}(\tau)V \rangle,$$

$$\Theta_2(t) = 2\lambda^2 \int_0^t d\tau (t-\tau)\sin\Delta(t-\tau)\mathrm{Re}\langle \hat{V}(\tau)V \rangle,$$

$$\Theta_3(t) = 2\lambda^2 \int_0^t d\tau \left[\frac{1}{\Delta}\sin\Delta(t-\tau) + (t-\tau)\cos\Delta(t-\tau) \right]$$
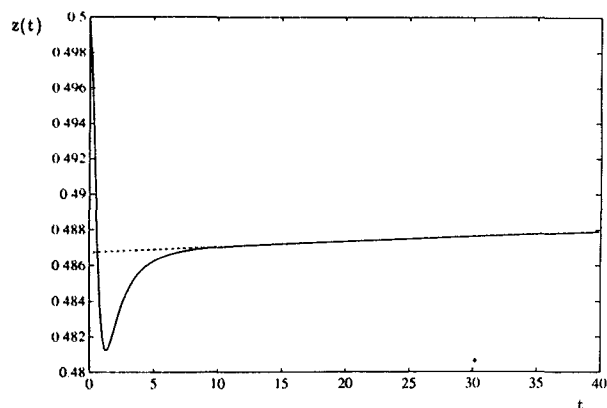$$\times \mathrm{Re}\langle \hat{V}(\tau)V \rangle,$$

FIG. 3. Short time dynamics of the population variable $z(t)$ obtained by two different approximations. (i) The full line corresponds to the result of second order perturbation theory. (ii) The broken line corresponds to the standard Redfield equations and *slipped* initial conditions. In both cases $z(0) = 0.5$.

$$\Theta_4(t) = 4\lambda^2 \int_0^t d\tau(t-\tau)\cos\Delta\tau \, \mathrm{Re}\langle\widehat{V}(\tau)V\rangle,$$

$$\Theta_5(t) = 4\lambda^2 \int_0^t d\tau(t-\tau)\sin\Delta\tau \, \mathrm{Im}\langle\widehat{V}(\tau)V\rangle.$$

The results are plotted in Figs. 3 and 4, for the same parameters as in the previous section ($\eta = 0.01$; $\Delta = 0.1$; $w_c = 1$; $T = 0$). We remark that the hypothesis that the memory effects take place on a very short time scale is in fact correct. After $t > 10w_c^{-1}$, the local Redfield equations seem to take over the dynamics. This picture suggests that we could extrapolate the Markovian evolution back to zero time to find a different set of *slipped* initial conditions $\widetilde{x}(0)$, $\widetilde{y}(0)$, $\widetilde{z}(0)$. If we were to use these slipped initial conditions together with the quantum master equation, we should get the same dynamics as in the case when we evolve the true initial conditions $x(0)$, $y(0)$, $z(0)$ with the
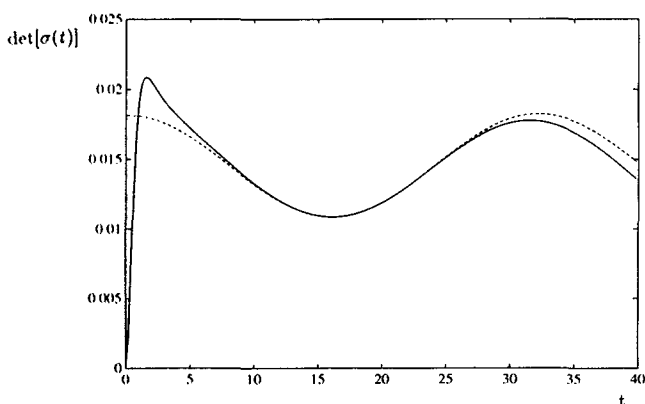

FIG. 4. Short time dynamics of $\det[\sigma(t)]$. The same initial conditions as in Fig. 2 have been used. The full line corresponds to second order perturbation theory and the dashed line to Redfield equations with slipped initial conditions. The discrepancy for $t > 30$ is due to the breakdown of perturbation theory.
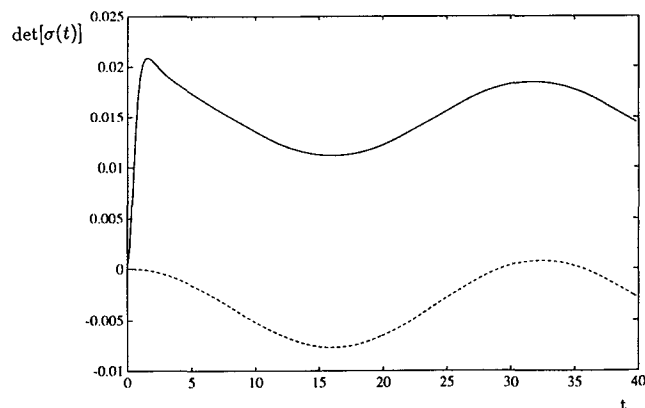

FIG. 5. Short time dynamics of $\det[\sigma(t)]$ at finite temperature ($K_BT = 0.1$). The full line corresponds to second order perturbation theory and the dashed line to Redfield equations (without slipped initial conditions).

actual non-Markovian dynamics, after a short transient time. This is shown in Fig. 4, where the broken line corresponds to slipped initial condition evolved under the master equation, and the full line corresponds to the actual initial condition evolved under the non-Markovian dynamics. Note also that the determinant $\det[\sigma(t)] = \frac{1}{4}[1 - x(t)^2 - y(t)^2 - z(t)^2]$, which was chosen to be zero for the initial $\{x(0), y(0), z(0)\}$, is slipped towards positive values {i.e., $[1 - \widetilde{x}(0)^2 - \widetilde{y}(0)^2 - \widetilde{z}(0)^2] > 0$} by an amount which seems to be sufficient in all cases to ensure that the Markovian evolution preserves the condition $\det[\sigma(t)] \geqslant 0$, for all times.

In Fig. 5, we present the evolution of the reduced density matrix at a nonzero temperature ($K_BT = 0.1$), without modifying the remaining parameters ($\eta = 0.01$; $\Delta = 0.1$; $w_c = 1$). This simulation demonstrates that memory effects are also present at finite temperatures and that the qualitative features of the evolution are similar to the zero-temperature paradigm; the usual Markovian approximation (i.e., without slippage) leads to a breakdown of positivity. In the true (non-Markovian) evolution, this anomalous behavior is corrected by an initial slippage of $\det[\sigma(t)]$ away from zero, towards positive values; this slippage is followed by a regime in which relaxation proceeds without significant memory effects.

In the next section, we shall suggest a physical interpretation of this process, which will clarify its origin.

IV. PHYSICAL ORIGIN OF THE SLIPPAGE

The common element shared among the different approximations to the time evolution for the reduced quantities associated with the two-level system that have been derived in the previous sections is the assumption that initially system and bath are uncorrelated. The bath is in equilibrium with respect to its own Hamiltonian, and the system is prepared in an arbitrary state (factorization assumption). Hence, it is not unreasonable to posit that in the early time of their joint evolution, system and bath will adjust to each other's state on a fast time scale τ_b.[13] Once
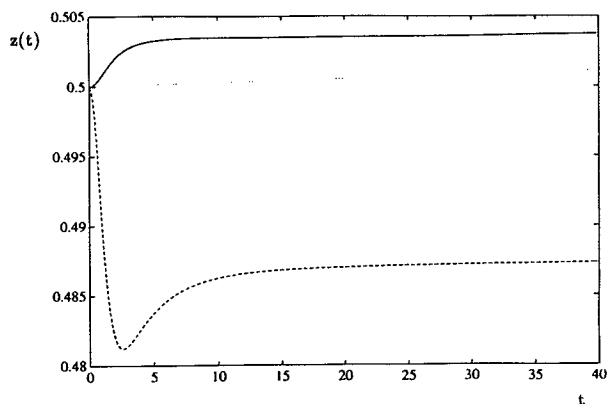
FIG. 6. Effect of initial conditions on slippage. The dashed line corresponds to factorized initial conditions; the full line corresponds to *polaron* initial conditions; and the dotted line is the pure Markovian evolution (assuming no slippage). The parameters used are the same as in the previous simulations ($\Delta=0.1$). For this and the following simulations, the initial conditions are $x(0)=y(0)=0$; $z(0)=0.5$.

these correlations are established, the slow exponential relaxation to equilibrium should be the dominant type of dynamics.

This implies that if we use a different set of initial conditions (or equivalently, a different projection operator for the bath), we should get a different amount of slippage, as the bath would be either "closer" or "further" from the appropriate correlations. The question is, therefore, what are those appropriate correlations?

One of the possibilities that we have explored is that a fairly good approximation to the correlated state should be a polaron; that is, the bath is assumed to be fast enough to equilibrate immediately to the instantaneous state of the two-level system. As the coupling is linear in the oscillators' coordinates, the equilibration simply involves displacements of the oscillators' minima by the amount $c_\alpha/w_\alpha^2\sigma_x$ for the αth oscillator. This pseudoparticle, consisting of the two level system together with the displaced oscillators, has received the name of *polaron*.[14] This scenario will be more likely to occur if the characteristic time scale of the system evolution is much longer than the bath relaxation time (i.e., $w_c \gg \Delta$). In Fig. 6 we have shown the slippage in the population variable $z(t)$ for both polaron (full line) and factorized initial conditions (dashed line) for the case $\Delta=0.1$; $w_c=1$. We note that the slippage for the polaron initial state is smaller in magnitude and opposite in sign to the slippage for the factorized one. In Fig. 7 we present the results of a simulation for an identical system with the same parameters except for $\Delta=0.01$. While the slippage for the factorized initial conditions is of comparable magnitude in both cases, the polaron initial state shows considerably less slippage in the second instance, i.e., in the case that the time scale of the system evolution is much slower than that of the bath.

The fact that the polaron induces a slippage of opposite sign to the one produced by the factorized initial condition suggests that in this case, we overestimate the displacement of the oscillator's minima in order to account for other
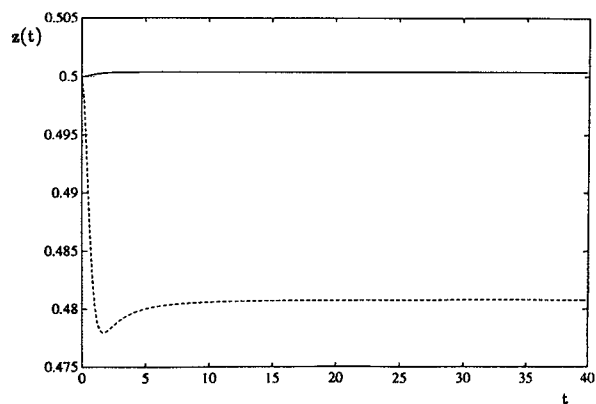

FIG. 7. The same as Fig. 6, except for the value of $\Delta=0.01$.

nonlinear effects that take place during the formation of these system-bath correlations. This can be partially corrected by choosing an initial condition in which the oscillators have been displaced by an amount determined variationally to minimize the free energy at that particular temperature.[15] The simulation in Fig. 8 confirms that for this *variational* polaron initial condition, the nonlocal effects are actually smaller.

Finally, we have also chosen as initial conditions the following case:

$$\rho(0)=U\rho_b^{eq}\sigma(0)U^+$$

where

$$U=\exp(iS);$$

$$S=\sum_\alpha \frac{c_\alpha}{w_\alpha^2-\Delta^2}(p_\alpha\sigma_x-\Delta\ x_\alpha\sigma_y), \qquad (19)$$

where U is the unitary transformation that diagonalizes H to second order in the weak coupling parameter (Fröhlich diagonalization).[16] For this case there is no evolution to lowest order in perturbation theory (see Fig. 8).
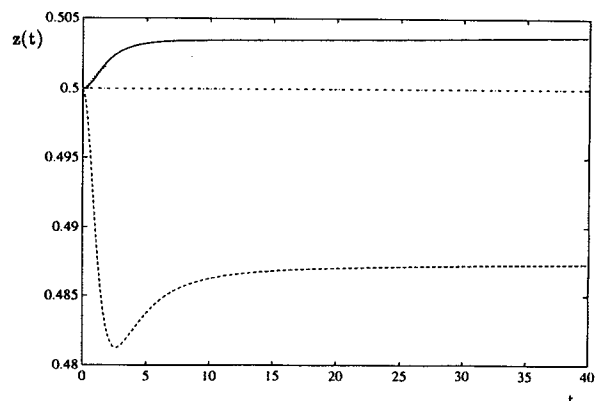

FIG. 8. Effect of initial conditions on slippage. The dashed line corresponds to factorized initial conditions; the full line corresponds to *polaron* initial conditions; the dotted line corresponds to *variational polaron*; and the dash–dot line corresponds to the Fröhlich initial conditions.

It is worth noting that in all cases the duration of this transient regime is roughly the same, confirming the proposition that τ_b is the only time scale relevant for these effects.

V. SUMMARY

The main result of this paper is that the standard Markovian weak coupling approximation for the equations of motion of the reduced density matrix of an open system interacting with its environment is physically consistent. However, there are transient memory effects, which cannot be neglected in a rigorous discussion of the approximation.

It has been shown that these effects can be absorbed in a modification of the initial conditions (*slippage*) upon which the generator for the Markovian evolution acts. The objections raised by the strict nonpositivity of this Markovian map are readily dismissed when a careful examination of the implications of the slippage of the initial conditions is undertaken. In all cases explored, the determinant of the reduced density matrix is shifted in such a way that the Markovian evolution does not lead to the emergence of negative eigenvalues. Unfortunately, the magnitude of the nonlocal effect strongly depends on the particular initial condition and cannot be predicted quantitatively. The analysis has been carried out in great detail for the weak coupling case (in which the slippage is of order λ^2), but the same effects should be present when the coupling is stronger.

The physical origin of this slippage has been ascribed to the fact that initially the bath and the system are not appropriately correlated. During the time that system-bath correlations are being built, we observe that the time evolution is very different from the one predicted by Markovian equations. Only after a transient time, on the order of the relaxation time of the bath, is the evolution well described by a quantum master equation. We should bear in mind that, in the weak coupling case, the solutions of the quantum master equation proposed by Dümcke and Spohn and of the standard one are equivalent. In this regime we are interested only in the effects of order 1 for a timescale of order $1/\lambda^2$. Any difference of order λ^2 in the quantities we are calculating has no relevance from a computational point of view. Nonetheless, the standard approximation should be preferred, as it displays the proper symmetries of the problem.

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