Generalized-master-equation analysis of a ferromagnet model*

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The method of generalized master equations (GME) is used to investigate the nonequilibrium properties of a mean-field ferromagnet model in interaction with a bath. The Zwanzig projection techniques, modified to include coarse graining, provide the tool for obtaining various GME's at various levels of description. Results obtained by Goldstein and Scully and by Wang are shown to follow from the GME's in the long-time limit and an undesirable assumption, which was necessary in an earlier analysis, is eliminated. Explicit expressions are calculated for several quantities relevant to the evolution of the probabilities and their moments. Short-time results, characteristic of the underlying microscopic equations and inaccessible to the traditional analysis, are shown to follow from the GME, with a specific illustration for a simple two-spin system. This work thus complements the earlier analysis of Goldstein and Scully.

I. INTRODUCTION, MODEL, AND TECHNIQUE

Studies of nonequilibrium properties of a uniform-coupling model of a ferromagnet in interaction with a bath have been recently reported.[1,2] Techniques based on the Zwanzig derivation[3] of generalized master equations (GME) have been recently developed and applied[4] to problems of the oscillatory approach to equilibrium in the Kac-Dresden model[5] and the description of excitation transfer in molecular aggregates.[6] In the present paper the model studied in Refs. 1 and 2 (albeit in a generalized form) is analyzed with the help of the techniques presented in Refs. 4 and 6.

The system under investigation has the Hamiltonian[1,2]

$$H = H_f + H_b + V \,, \tag{1.1}$$

where

$$H_f = -(2JS^z S^z + 2\mu BS^z) \,, \tag{1.2}$$

$$H_b = \sum_\alpha \epsilon_\alpha a_\alpha^\dagger a_\alpha \,, \tag{1.3}$$

$$V = \sum_\alpha \lambda_\alpha (S^+ a_\alpha + S^- a_\alpha^\dagger + S^+ a_\alpha^\dagger + S^- a_\alpha)$$

$$\equiv \sum_\alpha \lambda_\alpha (V_\alpha^{+-} + V_\alpha^{-+} + V_\alpha^{++} + V_\alpha^{--}) \,. \tag{1.4}$$

Following the customary notation $\vec{S} = \sum_{i=1}^N \vec{s}_i$, $\vec{S}$ and $\vec{s}_i$ have respective Cartesian components S^x, S^y, S^z and s_i^x, s_i^y, s_i^z, the expressions $S_\pm^x \pm iS^y$ are abbreviated as $S^\pm$, etc. The above model incorporates a trivial generalization of the one studied in Refs. 1 and 2 in that the latter does not contain the first two terms in Eq. (1.4). The reservoir particles, created by $a_\alpha^\dagger$, are taken to be bosons. It should be noted that due to the uniform-coupling nature of the model the various terms in Eq. (1.4) are independent of the spin locations.

The GME technique of the description of the time evolution exploits the equation

$$\frac{\partial P_\xi(t)}{\partial t} = \int_0^t dt' \sum_\mu [w_{\xi\mu}(t-t')P_\mu(t') - w_{\mu\xi}(t-t')P_\xi(t')] \,, \tag{1.5}$$

which is more general than the customary Pauli master equation (PME)

$$\frac{\partial P_\xi(t)}{\partial t} = \sum_\mu [F_{\xi\mu}P_\mu(t) - F_{\mu\xi}P_\xi(t)] \tag{1.6}$$

in that it is non-Markoffian and describes the evolution correctly for times shorter than are accessible to the PME, although at large times its predictions can coincide with those of the PME. The derivation of Eq. (1.5) and the relevant discussions have been repeated in the literature almost more often than necessary, and we shall therefore not present them here. A lucid discussion may be found in the original Zwanzig article.[3] It suffices to state here that Eq. (1.5) is an exact consequence of the Liouville equation under the initial diagonality condition (also called the initial random-phase assumption), and under the weak-coupling approximation, which involves retaining the first term in a perturbation scheme, the "memory-possessing transition probability" $w_{\xi\mu}(t)$ is given in the Zwanzig argument[3] by

$$w_{\xi\mu}(t) = 2\,|\langle \xi | V | \mu \rangle|^2 \cos\omega_{\xi\mu} t \,. \tag{1.7}$$

It may be helpful to recall here that in this version of the GME the probabilities P_ξ are diagonal elements $\langle \xi | \rho | \xi \rangle$ of the density matrix ρ in a representation of the eigenstates (ξ, μ, etc.) of a part H_0 of the total Hamiltonian $H_0 + V$, that $\omega_{\xi\mu}$ is the difference $E_\xi - E_\mu$ of the eigenvalues of H_0, and that $\hbar$ has been equated to unity.

This version of the GME has been used in Wang's analysis[2] of the present problem, and it will be shown below that the relevant equations in Ref. 2 can be obtained with considerable economy of ef-

fort as a direct consequence of Eq. (1.7). However, there exists another version of the GME[4,6,7] which is more appropriate to the problem at hand. It involves a coarse-graining operation which is built into the projection operator employed to obtain the GME. It replaces Eq. (1.7) with another equation whose particular form depends on the particular definition of the projection operator, i.e., on the amount and nature of the coarse graining employed. If the coarse graining is defined as an equal-weight summation over the states ξ, μ into groups ξ', μ', one replaces ξ, μ in Eq. (1.5) with ξ', μ' and replaces Eq. (1.7) with [4,6]

$$\mathcal{W}_{\xi'\mu'}(t)=\left(\sum_{\xi\subset\xi'}1\right)^{-1}2\sum_{\substack{\xi\subset\xi'\\ \mu\subset\mu'}}|\langle\xi|V|\mu\rangle|^2\cos\omega_{\xi\mu}t. \tag{1.8}$$

If $|\xi\rangle\equiv|\xi'\rangle|a\rangle$, the coarse graining may be defined as a trace over the $|a\rangle$ space. If the operation is modified with the introduction of thermal factors $e^{-\beta E_a}/Z$, where E_a is an energy corresponding to $|a\rangle$ and Z is the normalizing constant, Eq. (1.7) is replaced[8] with

$$\mathcal{W}_{\xi'\mu'}(t)=(Z)^{-1}2\sum_{a,b}e^{-\beta E_b}|\langle\xi'|\langle a|V|b\rangle|\mu'\rangle|^2\times\cos\omega_{\xi\mu}t. \tag{1.9}$$

A detailed discussion of the derivation of these equations has been given elsewhere.[4] They follow from the expression $\mathcal{P}Le^{-it(1-\mathcal{P})L}(1-\mathcal{P})L$ ($\mathcal{P}$ and L are the projection operator and the Liouville operator, respectively), from which $\mathcal{W}_{\xi\mu}(t)$ is obtained[2-4,6-8] when the meaning of $\mathcal{P}$ is suitably modified. The primary element in the nonequilibrium analysis of the model specified by Eqs. (1.1)–(1.4) is therefore an evaluation of $\mathcal{W}(t)$ as given in equations like (1.7)–(1.9). This constitutes the first part of the calculations presented below.

II. EXPLICIT EXPRESSIONS

Taking H_0 as the sum H_f+H_b of the ferromagnetic and bath Hamiltonians and writing $|\xi\rangle=|s,n\rangle$, $|\mu\rangle=|s',n'\rangle$, one observes that the energy difference $\omega_{\xi\mu}$ appearing in Eqs. (1.7)–(1.9) is given by

$$\omega_{\xi\mu}=E_{s',n'}-E_{s,n}=-2J(S'-S)\left(S'+S+\frac{\mu B}{J}\right)+\sum_\alpha(n'_\alpha-n_\alpha)\epsilon_\alpha\ . \tag{2.1}$$

In view of the particular nature of the interaction V [see Eq. (1.4)], one need consider only four types of states $|s',n'\rangle$ to analyze Eq. (1.7). Write $|s,n\rangle=|s\rangle|n\rangle$ and define (in keeping with the notation in Ref. 2) states $|s_j^+\rangle=s_j^+|s\rangle$, $|s_j^-\rangle=s_j^-|s\rangle$, $|n_\alpha^+\rangle=a_\alpha^\dagger|n\rangle$, $|n_\alpha^-\rangle=a_\alpha|n\rangle$. Here $s_j^\pm$ yields zero if the state $|s\rangle$ on which it acts has $s_j=\pm\frac{1}{2}$, and if $s_j=\mp\frac{1}{2}$ it yields the state $|s_j^\pm\rangle$, which is identical to $|s\rangle$ except in having its spin at the jth location reversed. The nature of the states $|n_\alpha^\pm\rangle$ is obvious from the definition of the familiar operators $a_\alpha^\dagger$ and a_α. Dropping the spin location index one then has four types of states $|s',n'\rangle$: $|s^+,n_\alpha^-\rangle$, $|s^-,n_\alpha^+\rangle$, $|s^+,n_\alpha^+\rangle$, and $|s^-,n_\alpha^-\rangle$. These are precisely the states (and the only states) that are connected to $|s,n\rangle$ by the respective terms $\lambda_\alpha V_\alpha^{+-}$, $\lambda_\alpha V_\alpha^{-+}$, $\lambda_\alpha V_\alpha^{++}$, and $\lambda_\alpha V_\alpha^{--}$ of the interaction V in Eq. (1.4). The first of these terms gives rise to the matrix element

$$\langle s_j^+,n_\alpha^-|\lambda_\alpha V_\alpha^{+-}|s,n\rangle=\lambda_\alpha\sqrt{n_\alpha}\ , \tag{2.2}$$

which is independent of the spin location index. Other matrix elements may be calculated in a similar manner. One also observes that for the above four types of states, one may write in Eq. (2.1) $S'-S=\pm1$ and $S'+S=2S\pm1$ if $s'=s^\pm$. Also $n_\alpha^\pm-n_\alpha=\pm1$. With the definition[9]

$$\Delta_\pm=E_{s^\pm}-E_s=\mp2J(2S\pm1)\mp\mu B \tag{2.3}$$

one can write the energy differences $\omega_{\xi\mu}$ between $|s,n\rangle$ and the above four types of states as sums and differences of the quantities $\Delta_\pm$ and ϵ_α. These energy differences and the matrix elements like (2.2) are all that is required to write down the GME for the evolution of the probabilities $P_{s,n}$. Equation (1.5) takes the form

$$\frac{\partial P_{s,n}(t)}{\partial t}=\int_0^t dt'\sum_{\alpha,j}\{\mathcal{W}^{+-}(t-t')P_{s_j^+,n_\alpha^-}(t')+\mathcal{W}^{-+}(t-t')P_{s_j^-,n_\alpha^+}(t')+\mathcal{W}^{--}(t-t')P_{s_j^-,n_\alpha^-}(t')+\mathcal{W}^{++}(t-t')P_{s_j^+,n_\alpha^+}(t')-[\mathcal{W}^{+-}(t-t')+\mathcal{W}^{-+}(t-t')+\mathcal{W}^{++}(t-t')+\mathcal{W}^{--}(t-t')]P_{s,n}(t')\}\ . \tag{2.4}$$

The quantities $\mathcal{W}^{+-}$, etc., are all functions of S and n_α relevant to the state $|s,n\rangle$ and are defined through

$$\mathcal{W}^{+-}(t)=2\lambda_\alpha^2 n_\alpha\cos(\Delta_+-\epsilon_\alpha)t\ , \tag{2.5}$$

$$\mathcal{W}^{-+}(t)=2\lambda_\alpha^2(n_\alpha+1)\cos(\Delta_-+\epsilon_\alpha)t\ , \tag{2.6}$$

$$\mathcal{W}^{++}(t)=2\lambda_\alpha^2(n_\alpha+1)\cos(\Delta_++\epsilon_\alpha)t\ , \tag{2.7}$$

$$\mathcal{W}^{--}(t)=2\lambda_\alpha^2 n_\alpha\cos(\Delta_--\epsilon_\alpha)t\ . \tag{2.8}$$

These expressions are a straightforward consequence of Eq. (1.7). If, in keeping with the model in Ref. 2, one omits the terms given in Eqs. (2.5) and (2.6) and notes[9] that our quantities $P_{s,n}(t)$, ϵ_α, Δ_+, and Δ_- are equivalent to the quantities $\rho(s,n,t)$, ω_α, $-\Delta E_+$, and ΔE_- in Ref. 2, one immediately obtains Eq. (3.12) in the latter as a special case of our Eq. (2.4).

III. COARSE-GRAINED GME (MICROSCOPIC)

When the detailed evolution of the states $|s,n\rangle$ is not under investigation and it is only the states $|s\rangle$ that are of interest, a summation is ordinarily

performed[2] over the states $|n\rangle$. The closed nature of the evolution equation is naturally lost because of this summation, i.e., the evolution of the P_s is given not in terms of $P_{s'}$ but in terms of $P_{s'n'}$, which are entitles external to the space of entities P_s. To circumvent this problem the assumption.

$$P_{s,n}(t) = P_s(t)P_n(\infty) \tag{3.1}$$

is made,[2] whereby the bath is assumed to be forever in the (thermalized) state $P_n(\infty)$, in spite of its interaction with the ferromagnetic system. It will be now shown that the assumption implied by Eq. (3.1) above [Eqs. (3.13) and (4.1) of Ref. 2) can be completely avoided with the help of the coarse-grained GME.

For this purpose one replaces the diagonalizing projection operator[3] $\mathcal{P}_1$, which gives, for any operator O,

$$\langle s,n|\mathcal{P}_1 O|s',n'\rangle = \langle s,n|O|s,n\rangle\delta_{s,s'}\delta_{n,n'} , \tag{3.2}$$

by the new operator $\mathcal{P}_2$, which gives

$$\langle s,n|\mathcal{P}_2 O|s',n'\rangle$$

$$= Z^{-1}e^{-\beta E_n}\sum_{\{n\}}\langle s,n|O|s,n\rangle\delta_{s,s'}\delta_{n,n'} , \tag{3.3}$$

where

$$Z = \sum_{\{n\}} e^{-\beta E_n} .$$

Equation (3.3) has, as a consequence, Eq. (1.9), with ξ', μ', a, b, ξ, μ replaced with s, s', n, n' (s,n), $(s',n',)$, etc. A straightforward calculation yields for $P_s \equiv \sum_n P_{s,n}$

$$\frac{\partial P_s(t)}{\partial t} = \int_0^t dt' \sum_j \{\mathcal{W}^+(t-t')P_{s_j^+}(t') + \mathcal{W}^-(t-t')P_{s_j^-}(t') - [\mathcal{W}^+(t-t')+\mathcal{W}^-(t-t')]P_s(t')\} \tag{3.4}$$

as the new GME with

$$\mathcal{W}^{\pm}(t) = \eta_c(t)\cos\Delta_{\pm}t - \eta_s(t)\sin\Delta_{\pm}t , \tag{3.5}$$

where

$$\eta_c(t) = 2\sum_\alpha \lambda_\alpha^2[2\bar{n}(\epsilon_\alpha)+1]\cos\epsilon_\alpha t , \tag{3.6}$$

$$\eta_s(t) = 2\sum_\alpha \lambda_\alpha^2 \sin\epsilon_\alpha t , \tag{3.7}$$

$$\bar{n}(\epsilon_\alpha) = Z^{-1}\sum_{\{n\}} e^{-\beta E_n} n_\alpha = (e^{\beta\epsilon_\alpha}-1)^{-1} . \tag{3.8}$$

Once again reduction of Eq. (3.4) above to Eq. (3.18) of Ref. 2 is immediate when the first two terms in Eq. (1.4) are dropped. The form of Eq. (3.4) is then unchanged, but Eq. (3.5) is replaced with

$$\mathcal{W}^{\pm}(t) = \eta_c^{\pm}(t)\cos\Delta_{\pm}t \mp \eta_s^{\pm}(t)\sin\Delta_{\pm}t , \tag{3.9}$$

with

$$\eta_c^{+}(t) = 2\sum_\alpha \lambda_\alpha^2[\bar{n}(\epsilon_\alpha)+1]\cos\epsilon_\alpha t , \tag{3.10}$$

$$\eta_c^{-}(t) = 2\sum_\alpha \lambda_\alpha^2\bar{n}(\epsilon_\alpha)\cos\epsilon_\alpha t , \tag{3.11}$$

$$\eta_s^{+}(t) = 2\sum_\alpha \lambda_\alpha^2[\bar{n}(\epsilon_\alpha+1)]\sin\epsilon_\alpha t , \tag{3.12}$$

$$\eta_s^{-}(t) = 2\sum_\alpha \lambda_\alpha^2\bar{n}(\epsilon_\alpha)\sin\epsilon_\alpha t . \tag{3.13}$$

It is interesting to observe that the equations are actually simplified [see Eqs. (3.5)–(3.7)] by the generalization of the model adopted in this paper. This is so because then only the combinations $\eta_c^+ + \eta_c^- = \eta_c$ and $\eta_s^+ - \eta_s^- = \eta_s$ appear in the expressions. It is trivial to see that Eq. (3.4) with Eqs. (3.9)–(3.13) is identical to Eq. (3.18) of Ref. 2.

IV. COARSE-GRAINED GME (MACROSCOPIC)

As was done earlier,[2] one may now perform the appropriate summation on Eq. (3.4) and obtain a macroscopic evolution equation for the probability $\sum_{s\subset S} P_s = P(S,t) \equiv P(m,t)$ that the total S has a value $m \equiv S$. One does not require an assumption analogous to Eq. (3.1) here because $\mathcal{W}^{\pm}$ is independent of the spin locations and depends on the ferromagnetic state only through $\Delta_{\pm}$, which contains S [see Eqs. (3.5) and (2.3)]. We shall, however, show here how the macroscopic evolution equation may be obtained directly without the help of the intermediate equations derived above. The projection operator we shall now employ is $\mathcal{P}_3$, which gives for any operator O,

$$\langle s,n|\mathcal{P}_3 O|s',n'\rangle$$

$$= \left(\sum_{s\subset S} 1\right)^{-1}\sum_{s\subset S} Z^{-1}e^{-\beta E_n}\sum_{\{n\}}\langle s,n|O|s,n\rangle\delta_{s,s'}\delta_{n,n'} , \tag{4.1}$$

which, in addition to the diagonalization performed by $\mathcal{P}_1$ [see Eq. (3.2)] and the summation with thermal factors over the $\{n\}$ performed by $\mathcal{P}_2$ [see Eq. (3.3)] performs an equal-weight summation ($s\subset S$) over those $\{s\}$ states which have a total S^z value equal to S. The resulting GME, with $m = S$,

$$\frac{\partial P(m,t)}{\partial t} = \int_0^t dt' \sum_{m'}[\mathcal{W}_{mm'}(t-t')P(m',t') - \mathcal{W}_{m'm}(t-t')P(m,t')], \tag{4.2}$$

involves the functions $\mathcal{W}_{mm'}$ given by

$$\mathcal{W}_{mm'}(t) = (\tfrac{1}{2}N+m')\mathcal{W}^+(t)\delta_{m',m+1}$$

$$+(\tfrac{1}{2}N-m')\mathcal{W}^{-}(t)\delta_{m',m-1}\ , \tag{4.3}$$

$$\mathcal{W}_{m'm}(t)=(\tfrac{1}{2}N-m)\mathcal{W}^{-}(t)\delta_{m',m+1}$$
$$+(\tfrac{1}{2}N+m)\mathcal{W}^{+}(t)\delta_{m',m-1}\ , \tag{4.4}$$

$\mathcal{W}^{\pm}$ being given by Eq. (3.5). The reduction of Eq. (4.2) with (4.3) and (4.4) to Eq. (3.20) of Ref. 2 is again immediate upon the simplification of our model. It is interesting to observe that while the microscopic GME's [Eqs. (2.4) and (3.4)] do not possess a specially simple form, the nature of the interaction V in the model (each term in V flips only one spin) forces the macroscopic GME to have the simple (one-dimensional) form (4.2), with only nearest-neighbor transition probabilities depicted in Eqs. (4.3) and (4.4). We shall rewrite Eqs. (4.2) through (4.4) as

$$\frac{\partial P(m)}{\partial t}=(\tfrac{1}{2}N+m+1)\mathcal{W}^{+}(m)*P(m+1)$$
$$+(\tfrac{1}{2}N-m+1)\mathcal{W}^{-}(m)*P(m-1)$$
$$-(\tfrac{1}{2}N-m)\mathcal{W}^{-}(m)*P(m)$$
$$-(\tfrac{1}{2}N+m)\mathcal{W}^{+}(m)*P(m)\ , \tag{4.5}$$

where the dependence of $\mathcal{W}^{\pm}$ on m is made explicit and * represents the time convolution, i.e., $A*B=\int_0^\infty dt' A(t-t')B(t')$. It is a straightforward exercise to expand $P(m+1)$, $P(m-1)$, etc., in Eq. (4.5) and obtain a non-Markoffian Fokker-Planck equation which is more general than, but reduces at long times to, the Markoffian Fokker-Planck equation obtained earlier for this problem [Eq. (3.2) of Ref. 1].

V. APPLICATIONS OF THE FORMALISM

Equation (4.5) is the basic equation for the model studied. With its help we shall give two applications of the GME formalism and indicate how its results are more general than, and reduce under the Markoffian approximation to, the predictions of the usual PME analysis.[1,2] The first application is the derivation of equations for moments, which get their importance from that of the quantities[1] $\langle m\rangle=\sum_m mP(m)$ and $\sigma_m^2=\langle m^2\rangle-\langle m\rangle^2$ (the mean magnetization and its mean-square fluctuation, respectively), and the second involves an analysis of a two-spin system.

Equation (4.2) gives the general expression for the rth moment

$$\frac{d\langle m^r\rangle}{dt}=\sum_m \mathcal{a}_r(m)*P(m)\equiv\langle \mathcal{a}_r\rangle_*\ , \tag{5.1}$$

where

$$\mathcal{a}_r(m)=\sum_{m'}\mathcal{W}_{m'm}(m'^r-m^r)\ . \tag{5.2}$$

Equations (4.3) and (4.4) yield, for the model under study,

$$\mathcal{a}_1(m)=\tfrac{1}{2}N[\mathcal{W}^{+}(m)-\mathcal{W}^{-}(m)]-m[\mathcal{W}^{+}(m)+\mathcal{W}^{-}(m)]\ , \tag{5.3}$$

$$\mathcal{a}_2(m)=m(N-1)[\mathcal{W}^{+}(m)-\mathcal{W}^{-}(m)]$$
$$-(2m^2-\tfrac{1}{2}N)[\mathcal{W}^{+}(m)+\mathcal{W}^{-}(m)]\ . \tag{5.4}$$

Equations (5.1) and (5.3) imply, for instance, that

$$\frac{d\langle m\rangle}{dt}=\langle\tfrac{1}{2}N[\mathcal{W}^{+}(m)-\mathcal{W}^{-}(m)]\rangle_*-\langle[\mathcal{W}^{+}(m)+\mathcal{W}^{-}(m)]m\rangle_*\ , \tag{5.5}$$

which is a term-by-term generalization (to the non-Markoffian situation) of Eq. (3.5) of Goldstein and Scully,[1] which we repeat here:

$$\frac{d\langle m\rangle}{dt}=\langle\tfrac{1}{2}N[\Gamma_2(m)-\Gamma_1(m)]\rangle-\langle[\Gamma_2(m)+\Gamma_1(m)]m\rangle\ . \tag{5.6}$$

Our Eq. (5.5) is identical to Eq. (5.6), except for the replacement of the simple average $\langle\cdots\rangle$ in the latter with the average with the time convolution $\langle\cdots\rangle_*$ in the former. It is straightforward to show that $\int_0^\infty dt\,\mathcal{W}^{+}(m,t)=\Gamma_2(m)$ and $\int_0^\infty dt\,\mathcal{W}^{-}(m,t)=\Gamma_1(m)$, which means that our Eq. (5.5) reduces to the result of Ref. 1 under the Markoffian approximation. Using Eqs. (3.5), (5.1), (5.3), and (5.4), one arrives, after some calculation, at

$$\frac{d\langle m\rangle}{dt}=\langle Q(t)\sin(4Jm+\mu B)t\rangle_*$$
$$-\langle R(t)m\cos(4Jm+\mu B)t\rangle_*\ , \tag{5.7}$$

$$\frac{d\langle m^2\rangle}{dt}=\tfrac{1}{2}N\langle R(t)\cos(4Jm+\mu B)t\rangle_*$$
$$+(2/N)(N-1)\langle Q(t)m\sin(4Jm+\mu B)t\rangle_*$$
$$-2\langle R(t)m^2\cos(4Jm+\mu B)t\rangle_*\ , \tag{5.8}$$

where the m-independent (but bath-dependent) quantities $Q(t)$ and $R(t)$ given by

$$Q(t)=N[\eta_s(t)\cos 2Jt-\eta_c(t)\sin 2Jt]\ , \tag{5.9}$$

$$R(t)=2[\eta_s(t)\sin 2Jt+\eta_c(t)\cos 2Jt]\ , \tag{5.10}$$

have been displayed separately.

As the second application of the formalism we shall consider the simple two-spin system. Then $N=2$, and there are four microscopic (after the coarse graining over the bath) states and three macroscopic states corresponding to values -1, 0, and $+1$ of m. The probability equations at the "macroscopic" level are

$$\frac{\partial P(0)}{\partial t}=2\mathcal{W}^{+}(0)*P(1)+2\mathcal{W}^{-}(0)*P(-1)$$
$$-[\mathcal{W}^{-}(0)+\mathcal{W}^{+}(0)]*P(0)\ , \tag{5.11}$$

$$\frac{\partial P(1)}{\partial t}=\mathcal{W}^{-}(1)*P(0)-2\mathcal{W}^{+}(1)*P(1)\ , \tag{5.12}$$

$$\frac{\partial P(-1)}{\partial t}=\mathcal{W}^{+}(-1)*P(0)-2\mathcal{W}^{-}(-1)*P(-1)\ , \tag{5.13}$$

wherein the $\mathcal{W}$'s are easily calculated from Eq.

(3.5) and from the energy differences

$$-\Delta_+(0) = \Delta_-(1) = 2J + \mu B\,, \tag{5.14}$$

$$-\Delta_-(0) = \Delta_+(-1) = 2J - \mu B\,, \tag{5.15}$$

$$-\Delta_+(1) = 6J + \mu B\,, \tag{5.16}$$

$$-\Delta_-(-1) = 6J - \mu B\,. \tag{5.17}$$

Given the bath functions $\eta_c(t)$ and $\eta_s(t)$, it is straightforward, if tedious, to obtain exact solutions for this system. In order to appreciate the essential changes brought about by the GME formalism, we shall now make some simplifying assumptions which will avoid the considerable algebra that would otherwise result. If the magnetic field B is turned off, Laplace transforms immediately yield the solution of Eq. (5.11) as

$$\tilde{P}(0) = 1/2\epsilon + [P(0,0) - \tfrac{1}{2}]/[\epsilon + 4\tilde{w}(0)]\,, \tag{5.18}$$

where the tilde denotes the Laplace transform, ϵ is the Laplace variable, $w(0)$ equals $w^{\pm}(0)$ with $B=0$, and where use has been made of the conservation of probability in the three-level system: $P(0)+P(1)+P(-1)=1$.

The first term in Eq. (5.18) is at once recognized as corresponding to the final equilibrated value $\frac{1}{2}$ of $P(0,t)$, whereas the second term describes the decay of the difference between the initial and final values of $P(0)$. On applying the analysis of Ref. 1 to this two-spin system one obtains

$$P(0,t) = \tfrac{1}{2} + [P(0,0) - \tfrac{1}{2}]\, e^{-4\Gamma t}\,, \tag{5.19}$$

where $\Gamma_{1,2}(0) = \Gamma$ with $B=0$. Equation (5.19) also follows immediately from Eq. (5.18) under the Markoffian approximation

$$w(0,t) \approx \delta(t)\left[\int_0^\infty dt'\, w(0,t')\right] = \delta(t)\Gamma\,.$$

The particular expression

$$w(0,t) = \eta_c(t)\cos 2Jt + \eta_s(t)\sin 2Jt \tag{5.20}$$

has some interesting consequences in Eq. (5.18) which will, however, be discussed elsewhere. In order to observe the effect of relaxing the Markoffian assumption, let us approximate Eq. (5.20) by

$$w(0,t) = \Gamma\gamma\, e^{-\gamma t}\,, \tag{5.21}$$

ignoring the details in Eq. (5.20). This form is reasonable if the bath functions η_c and η_s have strong decays, and it reduces to the Markoffian approximation in the limit $\gamma \to \infty$. Equations (5.18) and (5.21) yield

$$P(0,t) = \tfrac{1}{2} + [P(0,0) - \tfrac{1}{2}] e^{-\gamma t/2}[\cos\Omega t + (\gamma/2\Omega)\sin\Omega t]\,, \tag{5.22}$$

where

$$\Omega = (4\Gamma\gamma - \tfrac{1}{4}\gamma^2)^{1/2}\,. \tag{5.23}$$

Oscillations (for the underdamped case) typical to the GME analysis are exhibited in Eq. (5.22) and are displayed in Fig. 1 along with the result in Eq. (5.19), the initial value of $P(0)$ being taken as 1.

VI. DISCUSSION

With the help of the method of generalized master equations (GME), the present paper complements the thorough treatment of Golstein and Scully[1] of the nonequilibrium properties of the mean-field ferromagnet model in interaction with a bath. The GME's were obtained by various authors[3,7,10] as an intermediate step in the derivation of the Pauli master equation (PME), which forms the basis of all traditional transport analysis. The projection techniques of Zwanzig[3] were introduced into the present problem by Wang,[2] who rederived some of the equations of Goldstein and Scully[1] and applied the general Zwanzig comments to the specific model with the particular purpose of clarifying the place where irreversibility is introduced into the problem. As in the original derivations,[7] however, the analysis in Ref. 2 employs the GME only as an intermediate step. We have developed techniques[4,11] based specifically on the features of the GME which are not shared by the PME, and they have been recently applied[4,6] to several problems. It is in that spirit, and with results that go beyond those of the PME (i.e., of the earlier analysis[1]) that these GME techniques have been applied to the ferromagnet model.

The generalization of the model used earlier,[1,2] implied by our Eq. (1.4), although trivial, is natural and leads to some simplified expressions [compare Eqs. (3.5)–(3.8) with Eqs. (3.9)–(3.13)].

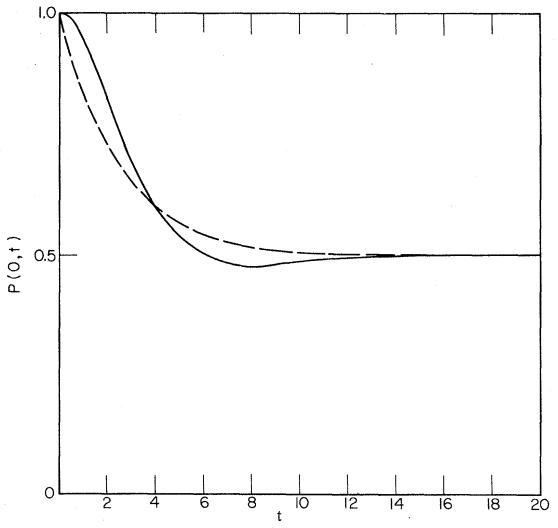

FIG. 1. Probability $P(0,t)$ that the level $m=0$ is occupied, plotted as function of time t. The dashed curve represents the usual analysis and the solid curve is the result of the GME. Units of t are arbitrary.

The main contribution of this paper lies in deriving *and using* equations like (1.5) which have greater content than equations like (1.6). The procedure consists in defining various projection operators, like $\mathcal{P}_1$, $\mathcal{P}_2$, and $\mathcal{P}_3$, through equations like (3.2), (3.3), and (4.1) and obtaining GME's such as (1.5), (2.4), (3.4), (4.2), (4,5), (5.11), (5.12), and (5.13), with the "memory-possessing transition probabilities" $\mathcal{W}$ given by equations like (1.7), (1.8), and (1.9), with the resulting expressions (2.5)–(2.8), (3.5), (3.9), (4,3), (4.4), and (5.20). The results of the GME's thus derived coincide with those (deduced from the PME's) obtained earlier[1,2] at large times, but differ from them at short times. This wavelike or coherent behavior is a direct manifestation of the underlying microscopic reversibility (contained in the Schrödinger or Liouville equations). It is eliminated by the strong Markoffian approximation made in obtaining the PME. Thus Eq. (4.5) will describe, at sufficiently short times, the wavelike behavior characteristic of the basic equation from which it was derived, but its results will coincide exactly with those of Eq. (3.23) of Ref. 2 or of (3.2) of Ref. 1 at sufficiently long times. The connection between our $\mathcal{W}$'s and their Γ's is given by $\int_0^\infty dt\, \mathcal{W}^+(m) = \Gamma_2(m)$ and $\int_0^\infty dt\, \mathcal{W}^-(m) = \Gamma_1(m)$, and one sees that a "time smoothing" of GME quantities gives the corresponding PME quantities. Similarly, Eqs. (5.6) and (5.19) implied by the earlier analysis[1] [Eq. (5.6) is Eq. (3.5) of Ref. 1] find their generalizations in Eqs. (5.5) and (5.22), respectively.

As a bonus result from the present analysis one obtains the elimination of the undesirable assumption (3.1) that Wang was forced to make[2] [in his Eqs. (3.13) and (4.1)] because of his use of the "fine-grained" GME. To assume that the state of the bath (the reservoir) remains completely unaffected during the entire evolution already destroys reversibility at an earlier stage, even before the Markoffian approximation [Eq. (3.22) of Ref. 2) is made. That assumption cannot be avoided in Ref. 2, but is completely eliminated in the present analysis with the help of the coarse-graining operation. This is so because the coarse-grained GME does not (directly) involve the state of the bath at all! Another advantage of the coarse-grained GME is that one can see clearly how, once the thermodynamic limit is taken, leading to the elimination of Poincaré cycles, a decaying $\mathcal{W}(t)$ results in spite of, and out of, the basic microscopic oscillatory $\mathcal{W}(t)$. This happens through the "Fourier transform" of the V matrix elements implied by equations like (1.8). In fact an expression like (3.5) clearly shows the basic oscillatory nature of the $\mathcal{W}$'s through the cosines and the sines while the irreversibility, brought about by the transition to the macroscopic level of the description (i.e., by the coarse graining), appears in the decaying bath functions η_c and η_s.

The equations for moments for a large system and for the probabilities for a two-spin system have been derived as applications of the formalism developed here. To illustrate the special features of the GME treatment as well as its agreement with the traditional analysis, the probability curves arising from both treatments in the context of the two-spin system (simplifications having been made to reduce the algebra) have been plotted in Fig. 1. The time scale and the values of Γ and γ (0.1 and 0.8, respectively) are chosen arbitrarily. One observes that the solid curve (the GME result) arising out of Eq. (5.22) shows a zero slope at $t=0$ and an oscillation.[12] Both these phenomena are characteristic of the underlying microscopic reversibility (wave like behavior) and neither one can be obtained from the traditional (PME) analysis typified by Eq. (5.19) and represented by the dashed curve. However, one also observes that a time smoothing of the solid curve gives the dashed curve and that the two coincide at long times.

It is important to remark that the additional predictions of the GME presented here would not be very relevant if the time which characterizes the transition to the PME behavior were extremely small (or in practical situations inaccessible). In such cases the treatment of Goldstein and Scully[1] does not need to be complemented by the present analysis.

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[9]In order to facilitate comparison we note that the operators α^+ and α^- defined in Eqs. (2.42) of Ref. 1 have as their respective eigenvalues ΔE_+ and ΔE_- defined in Ref. 2, which equal our $-\Delta_+$ and Δ_-, respectively. Our reason for using $\Delta_\pm$ lies in that they are the energy dif-

ferences between states $|s^{\pm}\rangle$ and $|s\rangle$.

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[11] Techniques based on the non-Markofficity of equations, which are nonlocal in time, have also been used by several authors in the past, e.g., in the theory of liquids [see, e.g., C. A. Croxton, *Liquid State Physics* (Cambridge U. P., London, 1974)] and in the formalism of random walks [see, e.g., H. Scher and M. Lax, Phys. Rev. B 7, 4491 (1973); 7, 4502 (1973); E. W. Montroll and H. Scher, J. Stat. Phys. 9, 101 (1973)]. See also V. M. Kenkre, E. W. Montroll, and M. F. Shlesinger, J. Stat. Phys. 9, 45 (1973) for the connection between GME's and random walks.

[12] The "underdamped" case has been plotted to show clearly the additional features of the GME. The "overdamped" case would not exhibit an oscillation but would still have zero initial slope.