Hysteresis in a quantum spin model

Varsha Banerjee, Sushanta Dattagupta, and Parongama Sen
School of Physical Sciences, Jawaharlal Nehru University, New Delhi 110 067, India
(Received 24 April 1995)

We study the hysteresis effects in an Ising system in an external field rotating in the transverse plane, the latter introducing nontrivial quantum effects. The rate equations for the components of magnetization are derived in the mean field approximation by using a microscopic system-plus-reservoir approach. The area of the hysteresis loop is obtained by solving these equations numerically, and its scaling behavior with respect to temperature (T) and strength of the external field (Γ) is studied.

PACS number(s): 05.70.Ln, 75.60.−d, 75.10.Jm

I. INTRODUCTION

When an external field applied to a system is sinusoidal in time, the response is not instantaneous but delayed, leading to hysteresis, which is a typical nonequilibrium phenomenon. At a rudimentary level, hysteresis manifests itself as the competition between experimental time scales, determined by the frequencies of the applied perturbation and internal time scales, which are governed by relaxation phenomena, activated rate processes, decay of metastable states, and so on. Since metastable states occur quite naturally in connection with first-order phase transitions, hysteresis is particularly noticeable near such transitions and is often used to mark their onset [1]. While the phenomenon of hysteresis is intrinsically classical, our interest here is to study its occurrence in quantum systems, especially as the latter are characterized by new routes to relaxation. Thus a quantum system has additional time scales associated with tunneling, which can link different minima of the free-energy surface. In this paper, we study such a quantum model in the context of hysteresis, in which we have to consider the competition of the probe frequency with not just heat-bath-induced relaxation rates but with tunneling frequencies as well.

As far as hysteresis in classical systems is concerned, there have been several recent attempts to provide a satisfactory statistical mechanical treatment. In most of the model studies, the scaling of the hysteresis loop area with the probe frequency and the temperature as well as the evidence of a dynamic phase transition have been the issues of interest. Rao, Krishnamurthy, and Pandit [2] considered the hysteretic response of a three-dimensional $(\phi^2)^2$ model with $O(N)$ symmetry in the large-N limit by numerical integration of the equations of motion. Dhar and Thomas [3] obtained the corrected solution of the dynamical equations of Rao, Krishnamurthy, and Pandit. Rao, Krishnamurthy, and Pandit also studied a two-dimensional nearest-neighbor ferromagnetic Ising model by Monte Carlo simulation for different lattice sizes. Lo and Pelcovits [4] extended this study to large system sizes and observed the evidence of a dynamic phase transition. Acharyya and Chakrabarti [5] studied the hysteretic response and the scaling behavior of Ising models in $d=2$–4 dimensions by Monte Carlo simulations. Our aim is to extend these studies to appropriate quantum models and investigate similar scaling phenomena.

It should be clear at the outset that only a single degree of freedom (in contact with a thermal bath, of course) is sufficient for observing hysteresis. This is evident from the recent work of Simon and Libchaber [6] in which a single Brownian particle is constrained to move in a double-well (mechanical) potential subject to an external sinusoidal bias [7]. However, the real interest in hysteresis, perhaps due to its historical development in the context of magnetic domains, lies in systems that show cooperative phenomena of many degrees of freedom accompanied by phase transitions. The simplest statistical mechanical system that exhibits cooperative as well as quantum effects is described by an Ising model in a transverse field. This model has been rejuvenated in recent years by its physical realization in a variety of condensed matter systems. Two prominent examples are (i) hydrogen bonded ferroelectric crystals such as KH_2PO_4, known as KDP, in which the two available sites for the proton in the O—H $\cdots$ O bond are mapped onto the two states of an Ising spin $\sigma_z=\pm 1$; the transverse field then mimics the tunneling of the proton between these two sites [8]; and (ii) rare earth magnetic systems such as $LiRF_4$ (R stands for rare earth) in which an externally applied field transverse to the axis of symmetry of the crystal field lifts the degeneracy of the lowest Kramers doublet [9]. Motivated by these experimental possibilities as well as the previous theoretical analysis of hysteresis in Ising models, as mentioned in the preceding paragraph, we base our present study of hysteresis on an Ising model that is subject to a sinusoidally varying field in the transverse plane. We may suggest, for the purpose of possible verification of our results, that a time-varying field can be created in the laboratory either by pressure modulation in the KDP crystal or by simply applying an oscillatory magnetic field to the rare earth system of $LiRF_4$.

In the present paper, we imagine that our transverse Ising system is in contact with a thermal bath and adopt a microscopic system-plus-reservoir approach in order to bring out the irreversible effects of the bath on the dynamical evolution of the system variables, i.e., the components of the magnetization, in the case at hand. The coupling between the system and the reservoir is

1063-651X/95/52(2)/1436(11)/$06.00

chosen such that the kinetic equation of motion of the magnetization, in the absence of the transverse term, is the same as that obtained in the Glauber model [10]. We then employ a mean field approximation directly in the microscopic Hamiltonian and *derive* the rate equations for the components of the magnetization. This is in contrast to a recent approach to hysteresis in the transverse Ising model by Acharyya, Chakrabarti, and Stinchcombe [11] (referred to as ACS henceforth). ACS *begin* their study from *phenomenological* rate equations, which are solved by numerical and approximate analytical techniques. Our derived rate equations turn out to be different from the phenomenological equations of ACS and we make appropriate comments where necessary, highlighting these differences. We then obtain the scaling exponents of the hysteresis loop area as a function of temperature T, the probe frequency ω, and the amplitude Γ of the transverse field.

The paper is organized as follows. In Sec. II, the basic model Hamiltonian is discussed and its mean field limit obtained. Various terms describing the interaction with the heat bath are also assessed. We then obtain in Sec. III the rate equations treating the rotating transverse field as a small perturbation to the combined system of Ising spins plus the heat bath using the linear-response theory (LRT). Next, in Sec. IV we obtain a master equation for the complete density matrix in the presence of large quantum fluctuations (LQFs), using a cumulant expansion scheme that treats the system-bath interaction perturbatively, and rewrite the corresponding rate equations. Numerical results, summary, and concluding remarks are included in Sec. V.

II. MODEL AND FORMALISM

A. The Hamiltonian in the mean field approximation

The Hamiltonian describing the Ising model composed of N interacting spins in a rotating transverse field may be written as

$$H_s = -\sum_{i,j} J_{ij}\sigma_{zi}\sigma_{zj} - \Gamma\cos 2\omega t\sum_i \sigma_{xi} - \Gamma\sin 2\omega t\sum_i \sigma_{yi} , \quad (1)$$

where J_{ij} is the interaction strength between spins i and j, σ's are the Pauli matrices, and Γ is the strength of the transverse field rotating with frequency ω. The rotating field selected as above introduces an x-y symmetry in the Hamiltonian in addition to making it quantum mechanical. In the mean field approximation, the Hamiltonian can be expressed as

$$H_s \simeq -h\sigma_z - \Gamma_x(t)\sigma_x - \Gamma_y(t)\sigma_y , \quad (2)$$

where the site-independent mean field $h=\sum_j J_{ij}\langle\sigma_{zj}\rangle$, $\Gamma_x(t)=\Gamma\cos 2\omega t$, and $\Gamma_y(t)=\Gamma\sin 2\omega t$.

We motivate our study of hysteresis through a phase diagram corresponding to the static Hamiltonian

$$H_{s0} = -h\sigma_z - \Gamma\sigma_x . \quad (3)$$

In the mean field limit [12] the equilibrium solution of the magnetization corresponding to Eq. (3) is given by

$$m_x = \frac{\Gamma}{h_0}\tanh(\beta h_0) \quad (4a)$$

and

$$m_z = \frac{h}{h_0}\tanh(\beta h_0) , \quad (4b)$$

where $h_0=\sqrt{h^2+\Gamma^2}$. The phase diagram of this model indicating the transition from the ferromagnetic to the paramagnetic regime with regard to m_z as the order parameter is shown in Fig. 1. It is clear that disorder can be accentuated by varying either the temperature or the strength Γ of the transverse field as the latter has the effect of tilting the magnetization away from the z axis. The presence of oscillations increases the values of Γ_c and T_c but maintains the qualitative features of the static phase diagram. The effect of oscillations is discussed in detail in Sec. V. Our study of hysteresis encompasses regions on either side of the phase transition line in the presence of oscillations.

In order to motivate the mathematical formalism to study the kinetics of the model, we first consider a time-independent Hamiltonian in the absence of the transverse field

$$H_s = -h\sigma_z . \quad (5)$$

We comment here that even in the presence of a time-dependent transverse field, we can still arrive at an equation resembling Eq. (5) by appropriate rotations in the spin space and use the formalism developed below. This will be discussed in detail in Sec. IV.

The Hamiltonian in Eq. (5) describes the reversible dynamics of the system only. In order to introduce kinetics into the model, we imagine that the spin system is in con-

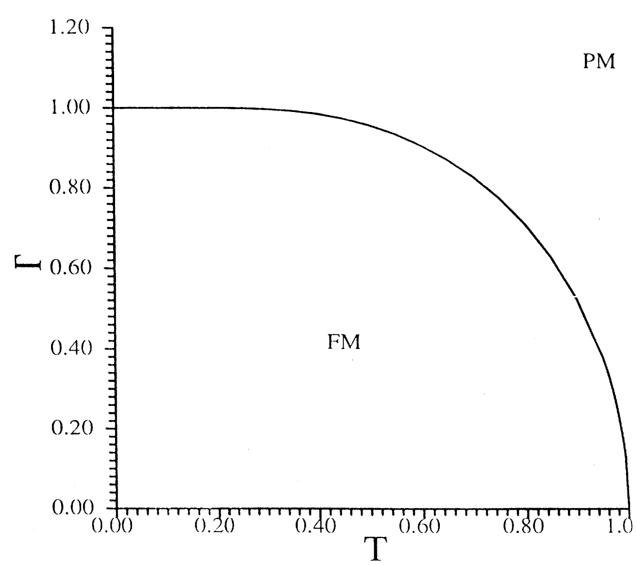

FIG. 1. Phase diagram of the Ising model with a transverse field in the mean field approximation indicating the ferromagnetic (FM) to paramagnetic (PM) transition.

tact with a heat bath that drives thermal fluctuations into the system. It is customary to imagine that the dynamics arises from additional coupling terms to the heat bath that are off diagonal in the representation in which σ_z is diagonal. This is then in the spirit of the kinetic Ising model of the Glauber type. The physical meaning of the Glauber terms is evident. They cause spontaneous spin flips, which in the context of hydrogen-bonded ferroelectrics mimic the hopping of the hydrogen or the proton from one site to another in the O—H · · · O bond while in the context of lithium rare earth ferrites, they represent transitions within the ground-state doublet mediated by spin lattice relaxations. Motivated by our preceding comments, we generalize the Hamiltonian as in Eq. (5) to

$$H_0 = H_s + V + H_B \ , \tag{6}$$

where H_B is the bath Hamiltonian and V describes the interaction between the spin subsystem and the heat bath. In accordance with our stated objective, we assume the following type of interaction between the spin subsystem and the heat bath:

$$V = g\hat{b}(\sigma_x + \sigma_y) \ . \tag{7}$$

In Eq. (7), $\hat{b}$ is an operator that acts on the Hilbert space of the heat bath and g is a multiplicative coupling constant. The specific form of the interaction is chosen so that the coupling of H_s with the heat bath is purely off diagonal and results in an appropriate dynamics in the limit when the transverse field is zero.

B. Mathematical formulation

As a first step towards obtaining the required rate equations, we derive a master equation for the density matrix. We start from the Liouville equation of motion

$$\frac{d\rho(t)}{dt} = -i[H_0, \rho(t)] \ , \tag{8}$$

where H_0 is the total Hamiltonian defined in Eq. (6). In the interaction picture the evolution is governed by

$$i\frac{d\rho_I(t)}{dt} = [V_I(t), \rho_I(t)] = V_I^{\times}(t)\rho_I(t) \ , \tag{9}$$

where

$$\rho_I(t) = \exp[i(H_s + H_B)t]\rho(t)\exp[-i(H_s + H_B)t] \tag{10}$$

and

$$V_I(t) = \exp[i(H_s + H_B)t]V\exp[-i(H_s + H_B)t] \ , \tag{11}$$

$V_I^{\times}(t)$ being the Liouville operator associated with $V_I(t)$. The solution of Eq. (9) can be formally written as

$$\rho_I(t) = \left[\exp_T\left[-i\int_0^t V_I^{\times}(t')dt'\right]\right]\rho_I(0) \ , \tag{12}$$

with $\exp_T$ denoting a time-ordered series with the operators for the latest time at the left. Note that at $t=0$, $\rho_I(0) = \rho(0)$. Combining Eqs. (10) and (12), we have

$$\rho(t) = e^{-i(H_s + H_B)t}\left\{\left[\exp_T\left[-i\int_0^t dt' V_I^{\times}(t')\right]\right]\rho(0)\right\} \times e^{i(H_s + H_B)t} \ . \tag{13}$$

The rate equations for magnetization m_μ ($\mu = x, y, z$) are obtained from

$$\frac{dm_\mu}{dt} = \mathrm{Tr}\left[\frac{d\rho(t)}{dt}\sigma_\mu\right] \ , \tag{14}$$

where

$$m_\mu = \mathrm{Tr}[\rho(t)\sigma_\mu] \tag{15}$$

and $\rho(t)$ is given in Eq. (13). However, it is easier to work in terms of a reduced density matrix for the spin system alone:

$$\rho_s(t) = \mathrm{Tr}_b \rho(t) \ , \tag{16}$$

where Tr_b denotes a trace operation over the degrees of freedom of the heat bath. Thus, from Eq. (13),

$$\rho_s(t) = e^{-iH_s t}\mathrm{Tr}_b\left\{\left[\exp_T\left[-i\int_0^t dt' V_I^{\times}(t')\right]\right]\rho(0)\right\}e^{iH_s t}$$
$$\cong e^{-iH_s t}\left[\exp_T\left[-i\int_0^t dt'\langle V_I^{\times}(t')\rangle - \int_0^t dt'\int_0^t dt''\langle V_I^{\times}(t')V_I^{\times}(t'')\rangle_T\right]\rho_s(0)\right]e^{iH_s t} \ . \tag{17}$$

The angular brackets $\langle\ \rangle$ refer to an averaging over the bath degrees of freedom. In writing Eq. (17) we have assumed that the density matrix can be factorized as

$$\rho(0) \cong \rho_b \otimes \rho_s \tag{18}$$

and have used the cumulant expansion theorem [13]. The physical ground for writing Eq. (18) is that at $t=0$, the spin system is assumed to be decoupled from the heat bath; it is at that instant that the perturbation V, which couples the spin system to the bath, is switched on. The subsequent time evolution of $\rho_s(0)$ is what we are interested in.

Assuming invariance under time translation, we can write

$$\rho_s(t) = e^{-iH_s t} \times \left[\exp_T\left[-\int_0^t (t-\tau)\langle V_I^{\times}(\tau)V_I^{\times}(0)\rangle dt\right] \times \rho_s(0)\right]e^{iH_s t} \ . \tag{19}$$

There has been an additional assumption in writing Eq. (19), viz.,

$$\langle V_I^\times(t')\rangle=\langle V_I^\times(0)\rangle=\langle V_I^\times\rangle=0 \,. \tag{20}$$

This can always be ensured by an appropriate choice of the coupling term V. The assumption Eq. (20) is necessitated by the physical requirement of the model that at a large enough time, the system should equilibrate to a situation governed by the Hamiltonian H_s alone. Using a short-time approximation for the bath correlation functions of the kind $\langle \hat{b}(\tau)\hat{b}(0)\rangle$, viz., that correlation functions die out after a time short compared to any other "times" of physical interest in H_s, the upper limit in the integrals in Eq. (19) can be extended to ∞. This enables us to further write the equation of motion as

$$\frac{d}{dt}\rho_s(t)=-i[H_s,\rho_s(t)] -e^{-iH_st}\left[\int_0^\infty d\tau\langle V_I^\times(\tau)V_I^\times(0)\rangle\right] \times e^{iH_st}\rho_s(t)\,. \tag{21}$$

This is the desired master equation. We make no attempt to calculate the bath correlation function in Eq. (21). Instead we simply parametrize it in terms of a phenomenological relaxation rate by making use of Kubo relations as discussed in Appendix A. We can now derive the equations of motion using Eqs. (14) and (21).

III. LINEAR-RESPONSE THEORY

As a first step towards our understanding of the effect of quantum transitions in the presence of the transverse field on spin relaxation we consider the linear-response regime in which the transverse field is a small perturbation to the Ising system. The total Hamiltonian in this case is hence given by

$$H_0=H_s+V+H_B+H_t \,, \tag{22}$$

where

$$H_s=-h\sigma_z \,, \tag{23}$$

$$H_t=-\Gamma\cos(2\omega t)\sigma_x-\Gamma\sin(2\omega t)\sigma_y \,, \tag{24}$$

and H_B and V are bath and interaction Hamiltonians, respectively. The interaction V as defined earlier by Eq. (7) ensures that the coupling term is completely off diagonal with respect to H_s leading to the correct Glauber kinetics in the absence of the transverse field.

The relaxation dynamics of the components of magnetization can be obtained from the equation of motion of the reduced density operator defined in Sec. II B [Eq. (21)] as

$$\frac{dm_\mu}{dt}=\mathrm{Tr}_s\left[\frac{d\rho_s(t)}{dt}\sigma_\mu\right] . \tag{25}$$

When the transverse field is zero, the reversible dynamics of the system is governed by H_s alone. Using Eq. (21) and after some lengthy algebra involving the matrix representation of Liouville operators and regrouping of terms as correlation function of heat bath operators (Appendix A), we arrive at the rate equation

$$\frac{dm_z}{dt}=-2\lambda[m_z-\tanh\beta h]\,, \tag{26a}$$

$$\frac{dm_x}{dt}=-\lambda m_x+2hm_y\,, \tag{26b}$$

$$\frac{dm_y}{dt}=-\lambda m_y-2hm_x\,. \tag{26c}$$

The presence of a perturbation in the form of a transverse field contributes additional terms, linear in Γ, to these dynamical equations [Eq. (26)]. In the linear-response regime, the time-dependent contribution to the Hamiltonian (H_t) is presumed to affect only the reversible dynamics of H_s and does not affect the relaxation governed by the coupling terms. That is, the transverse field being small is assumed to have no effect on the heat bath dynamics. Using the formalism developed in Sec. II B, it is straightforward to see that with the additional contribution, the equation of motion is

$$\frac{d\rho_s(t)}{dt}=-i[H_s,\rho_s(t)] -e^{-iH_st}\int_0^\infty d\tau\langle V_I^\times(\tau)V_I^\times(0)\rangle e^{iH_st}\rho_s(t) -i[H_t,\rho_s(t)]\,. \tag{27}$$

The first two terms correspond to relaxation in the pure Ising system [leading to Eqs. (26)] while the last term is a consequence of the perturbing transverse field. The contribution to dynamics due to these terms can be calculated easily using the properties of Pauli matrices. The resulting equations governing spin relaxation in linear-response theory (LRT) are

$$\frac{dm_z}{dt}=-2\lambda[m_z(t)-\tanh(\beta h)] -2\Gamma_x(t)m_y(t)+2\Gamma_y(t)m_x(t)\,, \tag{28a}$$

$$\frac{dm_x}{dt}=-\lambda m_x(t)+2hm_y(t)-2\Gamma_y(t)m_z(t)\,, \tag{28b}$$

$$\frac{dm_y}{dt}=-\lambda m_y(t)-2hm_x(t)+2\Gamma_x(t)m_z(t)\,. \tag{28c}$$

In the classical limit ($\Gamma_x=\Gamma_y=0$), the above equations of motion reduce to the well known mean field equations for Ising dynamics [cf. Eq. (26)]. We note here that the relaxation rate associated with m_z is twice that of m_x and m_y. This is attributed to the choice of our interaction Hamiltonian and the x-y symmetry therein.

IV. RATE EQUATIONS FOR ARBITRARILY LARGE TRANSVERSE FIELDS

In this section we consider the situation in which quantum effects dominate because of large values of the strength Γ of the transverse field. It is well known that large quantum fluctuations (LQFs) can destroy the ordered phase of the Ising system, be it a model for a ferromagnet, a ferroelectric, or a spin glass (cf. Fig. 1). The study of nonequilibrium response close to a phase-transition line in such a quantum spin model poses an interesting problem in this context and, to our knowledge, there have been no attempts in this direction. However, the assumptions of the linear-response theory are no longer valid if the strength of the transverse field is "large" and the effect of higher-order terms in Γ must be included in the rate equations [Eq. (28)] derived earlier in Sec. III. Thus motivated, we now treat the transverse field as a part of the subsystem Hamiltonian [as in Eqs. (1) and (2)] and rederive the rate equations to study the effect of large quantum fluctuations on the spin relaxation phenomenon. Our starting point once again is the total Hamiltonian

$$H_0=-h\sigma_z-\Gamma(\sigma_x\cos 2\omega t+\sigma_y\sin 2\omega t)+V+H_B\ . \tag{29}$$

As the transverse coupling is to be treated exactly it is evident that the Hilbert space of the subsystem has to be enlarged now in order to incorporate the terms proportional to both h and Γ within the Hamiltonian H_s. It is expected then that the interaction V with the heat bath ought to be such as to induce relaxation in both these terms. Before we address the issue of what should be the minimal form of V to bring out the requisite physics, we consider the static limit ($\omega=0$) of Eq. (29)

$$H_0=-h\sigma_z-\Gamma\sigma_x+V+H_B\ . \tag{30}$$

We may emphasize that it is quite appropriate to examine the static case first in order to motivate the form of V because after all, the accessible frequencies (ω) in the laboratory are at most of the order of a few kilohertz, whereas the heat-bath-induced rates (triggered through V) are much higher. For instance, proton jump frequencies in KDP or the phonon frequencies (in magnetic systems) are $\geq 10^{12}$ Hz.

The subsystem Hamiltonian corresponding to Eq. (30) is

$$H_s=-h\sigma_z-\Gamma\sigma_x\ . \tag{31}$$

This Hamiltonian can be easily diagonalized by a rotation S_y about the y axis:

$$S_y=\exp\left[-\frac{i}{2}\sigma_y\arctan\frac{\Gamma}{h}\right]\ . \tag{32}$$

The resultant Hamiltonian reads

$$\tilde{H}_s=-h_0\sigma_z,\quad h_0=\sqrt{h^2+\Gamma^2}\ . \tag{33}$$

Equation (33) has the same form as Eq. (5) and therefore it is natural to choose, in the rotated frame, a coupling of the type given in Eq. (7), that is,

$$\tilde{V}=g\hat{b}(\sigma_x+\sigma_y)\ . \tag{34}$$

In the new representation of the rotated quantization axis, $\tilde{V}$ is entirely off diagonal and therefore responsible for inducing Glauber kinetics. It is also easy to see that in the original laboratory frame, the corresponding form of V is

$$V=g\hat{b}\left[\frac{1}{h_0}(h\sigma_x-\Gamma\sigma_z)+\sigma_y\right]\ . \tag{35}$$

We may comment in passing that the subsystem Hamiltonian in Eq. (31) is like the mean field version of an anisotropic Heisenberg model and this symmetry is indeed reflected in the coupling to the heat bath, as in Eq. (35).

We now return to the full time-dependent problem of Eq. (29). The subsystem Hamiltonian (containing the oscillatory terms) can now be diagonalized by first a rotation ωt about the z axis:

$$U_z=\exp(-i\omega t\sigma_z)\ , \tag{36}$$

followed by the transformation S_y [cf. Eq. (32)], which now reads

$$S_y=\exp\left[-\frac{i}{2}\sigma_y\arctan\frac{\Gamma}{(h+\omega)}\right]\ . \tag{37}$$

The transformed Hamiltonian is

$$\tilde{H}_s=-h_0\sigma_z\ , \tag{38}$$

where now

$$h_0=\sqrt{(h+\omega)^2+\Gamma^2}\ . \tag{39}$$

Equation (38) can be interpreted to represent the interaction of a spin with a magnetic field that is the resultant of a field Γ along x and a field h reinforced by a pseudofield ω generated in the rotated frame, along z. Because of this and also our earlier remarks following Eq. (30) about the time-scale separation, we assume V to be given by [cf. Eq. (35)]

$$V=g\hat{b}\left[\frac{(h+\omega)}{h_0}\sigma_x-\frac{\Gamma}{h_0}\sigma_z+\sigma_y\right]\ . \tag{40}$$

What does this imply for the form of $\tilde{V}$ in the rotated frame? Note that

$$\tilde{V}=(U_zS_y)^{-1}V(U_zS_y)\ , \tag{41}$$

which works out to

$$\begin{aligned}\tilde{V}=g\hat{b}\Bigg\{&\sigma_x\left[1+\frac{h}{h_0}\sin(2\omega t)-2\left[\frac{h+\omega}{h_0}\right]^2\sin^2(\omega t)\right]\\&+\sigma_y\left[1-2\sin^2(\omega t)-\left[\frac{h+\omega}{h_0}\right]\sin(2\omega t)\right]\\&+\sigma_z\frac{\Gamma}{h_0}\left[\sin(2\omega t)-2\left[\frac{h+\omega}{h_0}\right]\sin^2(\omega t)\right]\Bigg\}\ .\end{aligned} \tag{42}$$

However, we are only interested in the $\omega=0$ limit of the coupling with the heat bath, in view of our earlier assumed timescale separation. Another formal way of saying the same thing is that we are working within the Markovian limit of heat-bath-induced relaxations [see our comments preceding Eq. (21)]. Hence, in the Markovian approximation, we have

$$\tilde{V}=g\hat{b}(\sigma_x+\sigma_y)\ , \tag{43}$$

which matches with the earlier forms [cf. Eqs. (7) and (34)]. Collecting all the above-mentioned facts together, the full time-dependent problem reduces to a time-independent one in the rotated frame, governed by the Hamiltonian

$$\tilde{H}_0=\tilde{H}_s+\tilde{V}+H_B \ , \tag{44}$$

where $\tilde{H}_s$ and $\tilde{V}$ are given by Eqs. (38) and (43), respectively.

We now rederive the rate equations to study the changes in the components of magnetization in the formalism described and used in Secs. II and III. The equation of motion of the reduced density matrix is Eq. (21) of Sec. II with H_s now defined by Eq. (29). After lengthy algebra involving the properties of Pauli matrices, regrouping of terms and using a short time approximation for the bath correlations characterized by λ (see Appendix B), we arrive at the following rate equations for $\mathbf{m}$ in the LQF regime:

$$\begin{aligned}\frac{dm_x}{dt}=&m_z\left[-\lambda\frac{\Gamma}{h_0^2}(h+\omega)\cos 2\omega t-2\Gamma\sin 2\omega t\right]\\&+m_x\left[-\lambda-\lambda\frac{\Gamma^2}{h_0^2}\cos^2 2\omega t\right]\\&+m_y\left[+2h-\lambda\frac{\Gamma^2}{h_0^2}\cos(2\omega t)\sin(2\omega t)\right]\\&+2\lambda\left[\frac{\Gamma}{h_0}\right]\cos(2\omega t)\tanh\beta h_0 \ ,\end{aligned} \tag{45a}$$

$$\begin{aligned}\frac{dm_y}{dt}=&m_x\left[-\lambda\frac{\Gamma^2}{h_0^2}\sin(2\omega t)\cos(2\omega t)-2h\right]\\&+m_y\left[-\lambda\frac{\Gamma^2}{h_0^2}\sin^2 2\omega t-\lambda\right]\\&+m_z\left[2\Gamma\cos 2\omega t-\lambda\left[\frac{h+\omega}{h_0^2}\right]\Gamma\sin 2\omega t\right]\\&+2\lambda\frac{\Gamma}{h_0}\sin(2\omega t)\tanh\beta h_0 \ ,\end{aligned} \tag{45b}$$

$$\begin{aligned}\frac{dm_z}{dt}=&m_z\left[-2\lambda+\lambda\frac{\Gamma^2}{h_0^2}\right]+2\Gamma\sin(2\omega t)m_x(t)\\&-2\Gamma\cos(2\omega t)m_y(t)+2\lambda\left[\frac{h+\omega}{h_0}\right]\tanh\beta h_0\\&-\lambda\Gamma\left[\frac{h+\omega}{h_0^2}\right]m_x\cos 2\omega t\\&-\lambda\Gamma\left[\frac{h+\omega}{h_0^2}\right]m_y\sin 2\omega t \ .\end{aligned} \tag{45c}$$

It is easy to see that these equations reduce to the rate equations obtained using linear-response theory in the limit of "small" values of λ, Γ, and T (as compared to h in appropriate units). Terms of order Γ^2 and $\lambda\Gamma$ start contributing significantly as the phase transition line is approached at all values of $T<T_c$, T_c being the critical temperature as defined in the $\omega=0$ or the static limit. The significance of these contributions is evident from the numerical results discussed in Sec. V on scaling of the hysteresis loop area with Γ, ω, and T.

It is difficult to compare the rate equations [Eq. (45)] with those proposed by Acharyya, Chakrabarti, and Stinchcombe [11], viz.,

$$\tau\frac{d\mathbf{m}}{dt}=-\mathbf{m}+[\tanh(h/T)]\frac{\mathbf{h}}{|h|} \ , \tag{46}$$

τ being the macroscopic relaxation time that has been assumed by ACS to be the same for the longitudinal and transverse components of magnetization. They have used heuristic and phenomenological arguments in writing Eq. (46), which is similar to the rate equation for a classical Ising model with Glauber kinetics. However, inclusion of a time-dependent field inside the argument of the tanh function, which arises in the theory from detailed balance factors as shown above, is of questionable basis. Furthermore, such assumptions may lead to unphysical results in the $T\to 0$ limit when quantum effects are important. The only common feature of our Eq. (45) and ACS's Eq. (46) is that both yield correct equilibrium solutions for m_x and m_z, when $\omega=0$ [cf. Eqs. (4a) and (4b)].

V. NUMERICAL RESULTS, SUMMARY, AND CONCLUSION

We numerically solve the coupled dynamical equations for the three components of magnetization in the LRT regime [Eq. (28)] and the LQF regime [Eq. (45)] subject to the initial condition that $m_z(0)=1$ and $m_x(0)=m_y(0)=0$, using the predictor corrector [14] method. In order to incorporate interaction effects, we replace the effective field h by $J(0)m_z$ [later taking $J(0)=1$], as in any mean field calculation. We compute the hysteresis loop area that is measurable in the laboratory:

$$A=\int_0^{\bar{T}}\mathbf{m}\cdot d\mathbf{\Gamma}=\int_0^{\bar{T}}\{m_x d\Gamma_x(t)+m_y d\Gamma_y(t)\} \ . \tag{47}$$

In Eq. (47), the parameter $\bar{T}$ is given by $\bar{T}=\pi/\omega$. The loop area, defined in Eq. (47), is a speciality for the quantum spin model as it relates the energy dissipated in the transverse plane. It is natural then that we look for possible power law scaling in this quantity in order that data points for different parameter values can be made to fall on the same master curve [15].

In Fig. 2, we compare the scaling of area with respect to Γ for LRT (open circles) and LQF (filled circles) for $T=0.5$ and two different relaxation rates: $\lambda=0.1$ [Fig. 2(a), $\omega=5.0$] and $\lambda=5.0$ [Fig. 2(b), $\omega=0.1$]. The data in Fig. 2(a) indicate a power law scaling

$$A\propto\Gamma^{\alpha} \ , \tag{48}$$

where $\alpha\approx 2.03\pm 0.03$ and 2.04 ± 0.03 for the LRT curve and the LQF curve, respectively. The data show a kink at $\Gamma_c\approx 1.3$, perhaps indicative of a dynamic phase transition at this value of ω, which needs further investigation. For large values of λ [Fig. 2(b)], the data indicate a power law fit with $\alpha\approx 1.95\pm 0.05$ and 2.09 ± 0.05 for LRT (open circles) and LQF (filled circles), respectively,

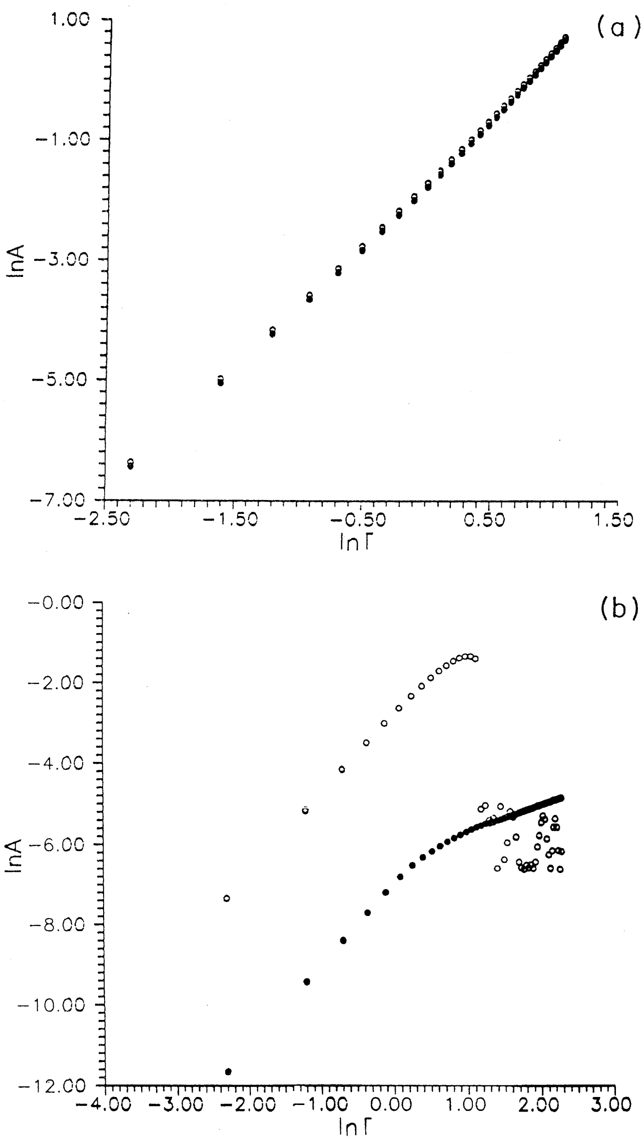

FIG. 2. Scaling of area A with respect to the strength of the transverse field Γ as computed in the linear response regime (open circles) and the large quantum fluctuation regime (filled circles) for two different values of the relaxation rate: (a) $\lambda=0.1$ and (b) $\lambda=5.0$. The values of the exponents have been discussed in the text of Sec. V.

when $\Gamma<\Gamma_c$. However, for large values of Γ, the $\lambda\Gamma$ contribution becomes significant and leads to the breakdown of the LRT. From the upper curve of Fig. 2(b) it is clear that the breakdown of LRT occurs for values of Γ larger than unity. In this regime, the data points based on LRT are extremely erratic and do not seem to conform to any particular scaling behavior. In the LQF regime, on the other hand, the dependence of area on Γ still indicates a power law fit, albeit with a new exponent $\alpha\approx0.64\pm0.02$ [notice the change in the slope in the lower curve of Fig. 2(b)]. Thus Fig. 2(b) justifies our motivation for calculating contributions to the rate equations beyond the LRT regime.

The scaling behavior of area with respect to temperature (T) is indicated in Fig. 3. For high values of T, although the data for the LRT regime is regular, it could not be fitted to any known scaling form. On the other hand, the data for the LQF regime shows a power law scaling

$$A\sim T^{-\beta} \tag{49}$$

with $\beta=0.12\pm0.02$. The loops get thinner as temperature increases and eventually go to zero when spin fluctuations become large and the system becomes paramagnetic. We plot the scaled area $A'=A/(\Gamma^{\alpha}\Gamma^{-\beta})$ against ω in Fig. 4 for six different curves corresponding to different T and Γ values (see the figure caption). This type of data collapse justifies usual attempts to encode different experimental observations in one equation and is the principal significance of scaling [15]. The data indicate that the area initially increases with ω, goes through a maximum, and decreases to zero as ω approaches infinity, when the system can no longer respond to the fast varying field. However, the scaled area A' is skewed as a function of ω and is not a Lorentzian as seen by ACS [11]. This is not a serious issue as the Lorentzian form found by ACS is evidently an artifact of their assumed form for the phenomenological rate equations.

Summarizing, we have considered in this paper the hysteretic response in an Ising model in the presence of quantum effects introduced by an oscillating transverse field. The equations of motion have been obtained by coupling the quantum subsystem to a purely dissipative heat bath. We observe two relaxation rates corresponding to the z and $x(y)$ components of magnetization. The

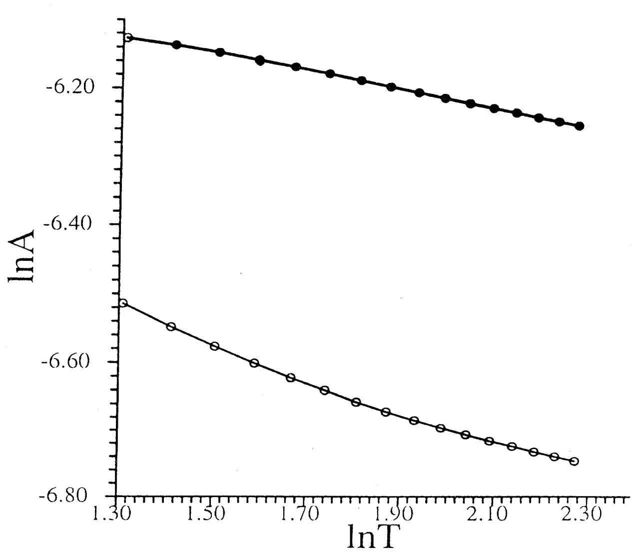

FIG. 3. Variation of area A with respect to temperature T ($T>1.0$ in units of J) in the linear response regime (open circles) and the large quantum fluctuation regime (filled circles). While the data in the linear response regime do not exhibit a power law, the other data indicate a power law variation with an exponent $\beta=0.12\pm0.02$.

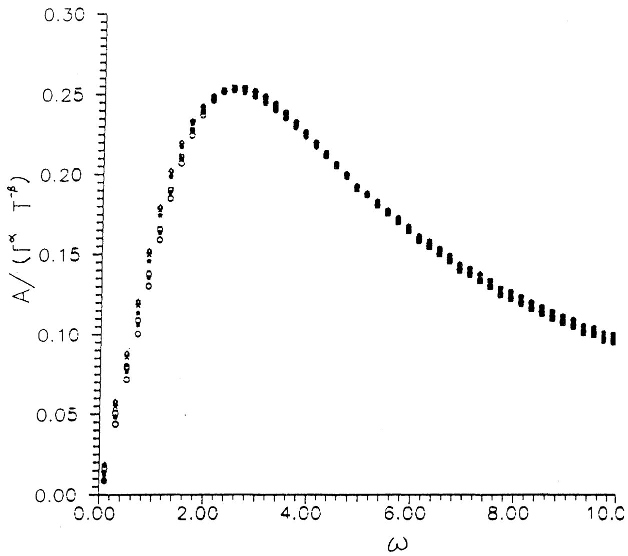

FIG. 4. Scaled area A' ($=A/\Gamma^{\alpha}\Gamma^{-\beta}$) as a function of ω for six sets of data corresponding to different values of the temperature and the strength of the transverse field: $\Gamma=0.1$ ($*$), $\Gamma=0.3$ ($\times$), and $\Gamma=0.5$ ($\Diamond$) (all for $T=4.0$); $\Gamma=0.1$ ($\circ$), $\Gamma=0.3$ ($\blacksquare$), and $\Gamma=0.5$ ($\square$) (all for $T=6.0$). Throughout, $\lambda=5.0$.

scaling exponents of the hysteresis loop area have been obtained. We find a power law scaling with respect to temperature (T) and quantum field (Γ). As a function of frequency (ω), the area goes through a maximum and then reduces to zero for very large values of ω. We conclude with the remark that this approach can be successfully used to study hysteresis in more complicated disordered spin systems such as a quantum spin glass [9,16]. Work in this direction is in progress and is planned to be presented in a forthcoming paper.

ACKNOWLEDGMENTS

V.B. and P.S. acknowledge support of the Council of Scientific and Industrial Research of the Government of India. The authors would also like to thank Muktish Acharyya and Bikas K. Chakrabarti for sending copies of their work prior to publication, which inspired the present study. S. K. Sarkar is acknowledged for a critical reading of the manuscript.

APPENDIX A

We start from the equation of motion for the reduced density matrix corresponding to the Hamiltonian given by Eq. (23):

$$\frac{d\rho_s(t)}{dt}=-i[H_s,\rho_s(t)] - e^{-iH_e t}\int_0^{\infty} d\tau\langle V_I^{\times}(\tau)V_I^{\times}(0)\rangle e^{+iH_s t}\rho_s(t)\ , \tag{A1}$$

$$(i)\frac{dm_z(t)}{dt}=\mathrm{Tr}_s\left[\frac{d\rho_s(t)}{dt}\sigma_z\right] \tag{A2}$$

$$=-\mathrm{Tr}_s[e^{-iH_s t}Re^{+iH_s t}\rho_s(t)\sigma_z]\ , \tag{A3}$$

where

$$R=\int_0^{\infty} d\tau\langle V_I^{\times}(\tau)V_I^{\times}(0)\rangle\ , \tag{A4}$$

$$\frac{dm_z(t)}{dt}=-\mathrm{Tr}_s[R\rho_s(t)\sigma_z]\ . \tag{A5}$$

We first evaluate $R\rho_s(t)$

$$R\rho_s(t)=\int_0^{\infty} d\tau\,\mathrm{Tr}_b(\{V_I(\tau),[V_I(0),\rho_b\rho_s(t)]\}) \tag{A6}$$

$$=\int_0^{\infty} d\tau\,\mathrm{Tr}_b\{V_I(\tau)V_I(0)\rho_b\rho_s(t)-V_I(\tau)\rho_b\rho_s(t)V_I(0) - V_I(0)\rho_b\rho_s(t)V_I(\tau)+\rho_b\rho_s(t)V_I(0)V_I(\tau)\}\ . \tag{A7}$$

Now

$$V_I(\tau)=e^{i(H_s+H_B)\tau}V(0)e^{-i(H_s+H_B)\tau} \tag{A8}$$

$$=\frac{1}{2}g\hat{b}(\tau)[\sigma_+e^{-2ih\tau}+\sigma_-e^{2ih\tau}]+\frac{1}{2i}g\hat{b}(\tau)[\sigma_+e^{-2ih\tau}-\sigma_-e^{2ih\tau}]\ . \tag{A9}$$

Substituting (A9) in (A7) we get

$$\begin{aligned}R\rho_s(t)=\frac{g^2}{2}\int_0^{\infty} d\tau[&\langle\hat{b}(\tau)\hat{b}(0)\rangle(\sigma_+\sigma_-e^{-2ih\tau}+\sigma_-\sigma_+e^{2ih\tau})\rho_s(t)+\rho_s(t)\langle\hat{b}(0)\hat{b}(\tau)\rangle(\sigma_+\sigma_-e^{-2ih\tau}+\sigma_-\sigma_+e^{+2ih\tau})\\ &-\langle\hat{b}(0)\hat{b}(\tau)\rangle(\sigma_++\sigma_-)\rho_s(t)(\sigma_+e^{-2ih\tau}+\sigma_-e^{2ih\tau})\\ &+\langle\hat{b}(0)\hat{b}(\tau)\rangle(\sigma_+-\sigma_-)\rho_s(t)(\sigma_+e^{-2ih\tau}-\sigma_-e^{2ih\tau})\\ &-\langle\hat{b}(\tau)\hat{b}(0)\rangle(\sigma_+e^{-2ih\tau}+\sigma_-e^{2ih\tau})\rho_s(t)(\sigma_++\sigma_-)\\ &+\langle\hat{b}(\tau)\hat{b}(0)\rangle(\sigma_+e^{-2ih\tau}-\sigma_-e^{2ih\tau})\rho_s(t)(\sigma_+-\sigma_-)]\ .\end{aligned} \tag{A10}$$

The bath correlation functions can be parametrized in terms of a phenomenological relaxation rate λ using the Kubo relation

$$\int_{-\infty}^{\infty} d\tau\, e^{ih\tau}\langle \hat{b}(\tau)\hat{b}(0)\rangle = e^{\beta h}\int_{-\infty}^{\infty} d\tau\, e^{-ih\tau}\langle \hat{b}(\tau)\hat{b}(0)\rangle \ . \tag{A11}$$

Using (A11) we can write

$$\int_{-\infty}^{\infty} d\tau\, e^{\pm ih\tau}\langle \hat{b}(\tau)\hat{b}(0)\rangle = \lambda \frac{e^{\pm\beta h/2}}{e^{\beta h/2}+e^{-\beta h/2}} \ , \tag{A12}$$

where

$$\lambda = \int_{-\infty}^{\infty} d\tau (e^{ih\tau}+e^{-ih\tau})\langle \hat{b}(\tau)\hat{b}(0)\rangle \tag{A13}$$

$$\equiv \int_{-\infty}^{\infty} d\tau\, e^{ih\tau}[\langle \hat{b}(\tau)\hat{b}(0)\rangle + \langle \hat{b}(0)\hat{b}(\tau)\rangle] \ . \tag{A14}$$

Using Eqs. (A10)–(A14), defining

$$m_\mu(t) = \mathrm{Tr}_s[\rho_s(t)\sigma_\mu] \ , \tag{A15}$$

and using the properties of Pauli spin matrices, Eq. (A5) reduces to

$$\frac{dm_z}{dt} = -2\lambda[m_z - \tanh\beta h] \ , \tag{A16}$$

which is the same as Eq. (26a) in the text

$$(ii)\frac{dm_x}{dt} = \mathrm{Tr}_s\left[\frac{d\rho_s}{dt}\sigma_x\right] \tag{A17}$$

$$= \mathrm{Tr}_s(-i\{[-h\sigma_z,\rho_s(t)]\sigma_x\} - (e^{-iH_st}Re^{iH_st}\rho_s(t)\sigma_s)) \tag{A18}$$

$$= 2hm_y - \mathrm{Tr}_s[Re^{iH_st}\rho_s(t)\sigma_x e^{-iH_st}] \tag{A19}$$

$$= 2hm_y - \mathrm{Tr}_s[R\tilde{\rho}_s(t)e^{iH_st}\sigma_x e^{-iH_st}] \ , \tag{A20}$$

where

$$\tilde{\rho}_s(t) = e^{iH_st}\rho_s(t)e^{-iH_st} \ . \tag{A21}$$

Therefore

$$\frac{dm_x}{dt} = 2hm_y - \mathrm{Tr}_s[R\tilde{\rho}_s(t)[\sigma_x\cos(2ht)+\sigma_y\sin(2ht)] \ . \tag{A22}$$

Repeating steps (A8)–(A14) and simplifying using the commutation rules for the Pauli spin matrices, it is easy to show that

$$\frac{dm_x}{dt} = 2hm_y - \lambda\langle\sigma_x\rangle\cos(2ht) + \lambda\langle\sigma_y\rangle\sin(2ht) \ , \tag{A23}$$

where

$$\langle\sigma_\mu\rangle = \mathrm{Tr}_s[\tilde{\rho}_s(t)\sigma_\mu] \tag{A24}$$

$$= \mathrm{Tr}_s[e^{iH_st}\rho_s(t)e^{-iH_st}\sigma_\mu] \tag{A25}$$

using (A25),

$$\langle\sigma_x\rangle = m_x\cos(2ht) - m_y\sin(2ht) \ , \tag{A26}$$

and

$$\langle\sigma_y\rangle = m_y\cos(2ht) + m_x\sin(2ht) \ . \tag{A27}$$

Therefore

$$\frac{dm_x(t)}{dt} = -\lambda m_x(t) + 2hm_y \tag{A28}$$

which is Eq. (26b). Similarly, it can be shown that

$$\frac{dm_y(t)}{dt} = -\lambda m_y(t) - 2hm_x \tag{A29}$$

which is Eq. (26c) in the text.

APPENDIX B

Rate equations for LQF

We once again start from the equation of motion of the reduced density matrix corresponding to the Hamiltonian of Eq. (44):

$$\frac{d}{dt}\rho_s(t) = i[H_s,\rho_s(t)] - e^{-iH_st}\int_0^\infty d\tau\langle \tilde{V}^\times(\tau)\tilde{V}^\times(0)\rangle e^{iH_st}\rho_s(t), \tag{B1}$$

where

$$\rho_s(t) = \mathrm{Tr}_b\{\tilde{\rho}(t)\} \text{ and } \tilde{\rho}(t) = S_y^{-1}U_z^{-1}\rho(t)U_zS_y \tag{B2}$$

with the rotations U_z and S_y as given by Eqs. (36) and (37) in the text.

Using $\tilde{\rho}_s(t)=e^{iH_st}\rho_s(t)e^{-iH_st}$, we get

$$\frac{d}{dt}\tilde{\rho}_s(t)=-\int_0^\infty d\tau\langle \tilde{V}^x(\tau)\tilde{V}^x(0)\rangle\tilde{\rho}_s(t) ,$$

which is of the same form as (A4).

We first evaluate the three components of magnetization: (i)

$$m_z(t)=\mathrm{Tr}[\rho(t)\sigma_z]=\mathrm{Tr}[\tilde{\rho}(t)S_Y^{-1}\sigma_zS_Y]$$
$$=\frac{h+\omega}{h_0}\langle\sigma_z(t)\rangle-\frac{\Gamma}{h_0}[\langle\sigma_x(t)\rangle\cos(2h_0t)+\langle\sigma_y(t)\rangle\sin(2h_0t)] , \quad \text{(B3a)}$$

where $\langle\sigma_\mu(t)\rangle=\mathrm{Tr}_s[\tilde{\rho}_s(t)\sigma_\mu(0)]$; similarly, we get (ii)

$$m_x(t)=\mathrm{Tr}_s[\rho_s(t)S_y^{-1}U_z^{-1}\sigma_xU_zS_y]$$
$$=\mathrm{Tr}_s[\tilde{\rho}_s(t)e^{iH_st}S_y^{-1}U_z^1\sigma_xU_ZS_ye^{-iH_st})$$
$$=\langle\sigma_x(t)\rangle\left[\frac{h+\omega}{h_0}\cos(2h_0t)\cos(2\omega t)+\sin(2h_0t)\sin(2\omega t)\right]$$
$$+\langle\sigma_y(t)\rangle\left[\frac{h+\omega}{h_0}\sin(2h_0t)\cos(2\omega t)-\cos(2h_0t)\sin(2\omega t)\right]+\langle\sigma_z(t)\rangle\frac{\Gamma}{h_0}\cos(2\omega t) , \quad \text{(B3b)}$$

and (iii)

$$m_y(t)=-\langle\sigma_x(t)\rangle\left[\sin(2h_0t)\cos(2\omega t)-\frac{h+\omega}{h_0}\sin(2\omega t)\cos(2h_0t)\right]$$
$$+\langle\sigma_y(t)\rangle\left[\cos(2h_0t)\cos(2\omega t)+\frac{h+\omega}{h_0}\sin(2\omega t)\sin(2h_0t)\right]+\langle\sigma_z(t)\rangle\frac{\Gamma}{h_0}\sin(2\omega t) . \quad \text{(B3c)}$$

In terms of $m_\mu(t)$, $\langle\sigma_\mu(t)\rangle$ can be written as

$$\langle\sigma_z(t)\rangle=\frac{(h+\omega)}{h_0}m_z(t)+\frac{\Gamma}{h_0}[m_x(t)\cos(2\omega t)+m_y(t)\sin(2\omega t)] , \quad \text{(B4a)}$$

$$\langle\sigma_x(t)\rangle=-\frac{\Gamma}{h_0}m_z(t)\cos(2h_0t)$$
$$+m_x(t)\left[\frac{h+\omega}{h_0}\cos(2h_0t)\cos(2\omega t)+\sin(2h_0t)\sin(2\omega t)\right]$$
$$+m_y(t)\left[\frac{h+\omega}{h_0}\cos(2h_0t)\sin(2\omega t)-\sin(2h_0t)\cos(2\omega t)\right] , \quad \text{(B4b)}$$

$$\langle\sigma_y(t)\rangle=-\frac{\Gamma}{h_0}m_z(t)\sin(2h_0t)$$
$$+m_x(t)\left[\frac{h+\omega}{h_0}\sin(2h_0t)\cos(2\omega t)-\cos(2h_0t)\sin(2\omega t)\right]$$
$$+m_y(t)\left[\frac{h+\omega}{h_0}\sin(2h_0t)\sin(2\omega t)+\cos(2h_0t)\cos(2\omega t)\right] . \quad \text{(B4c)}$$

The rate equations for the three components of magnetization [Eq. (33)] can be obtained by differentiating Eq. (B3) and making use of Eqs. (B4) and (26) in the text.

[1] G. S. Agarwal and S. R. Shenoy, Phys. Rev. **23**, 2719 (1981).
[2] M. Rao, H. R. Krishnamurthy, and R. Pandit, J. Phys. Condens. Matter **1**, 9061 (1989); Phys. Rev. B **42**, 856 (1990).
[3] D. Dhar and P. B. Thomas, J. Phys. A **25**, 4967 (1992).
[4] W. S. Lo and R. A. Pelcovits, Phys. Rev. A **42**, 3973 (1990).
[5] M. Acharyya and B. K. Chakrabarti, Physica A **192**, 471 (1993); **202**, 467 (1994).
[6] A. Simon and A. Libchaber, Phys. Rev. Lett. **68**, 3375 (1992).

[7] S. K. Sarkar (unpublished); D. Bose and S. K. Sarkar (unpublished).
[8] P. S. Percy, Phys. Rev. B **12**, 2725 (1975).
[9] W. Wu, B. Ellman, T. F. Rosenbaum, G. Appeli, and D. H. Reich, Phys. Rev. Lett. **67**, 2076 (1991).
[10] R. J. Glauber, J. Math. Phys. **4**, 294 (1963); also see S. P. Heims, Phys. Rev. **138**, A587 (1965); K. Kawasaki, *ibid.* **145**, 224 (1966); **148**, 375 (1966); **150**, 232 (1966).
[11] M. Acharyya, B. K. Chakrabarti, and R. B. Stinchcombe, J. Phys. A **27**, 1533 (1994).
[12] R. B. Stinchcombe, J. Phys. C **6**, 2459 (1973).
[13] S. Dattagupta, *Relaxation Phenomena in Condensed Matter Physics* (Academic, Orlando, 1987).
[14] W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, *Numerical Recipes* (Cambridge University Press, Cambridge, 1986).
[15] N. Goldenfeld, *Lectures on Phase Transitions and the Renormalization Group* (Addison-Wesley, Reading, MA, 1992).
[16] V. Banerjee and S. Dattagupta, Phys. Rev. B **50**, 9942 (1994).