Nonequilibrium phase transition in the kinetic Ising model: Divergences of fluctuations and responses near the transition point

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The nonequilibrium dynamic phase transition in the kinetic Ising model in the presence of an oscillating magnetic field is studied by Monte Carlo simulation. The fluctuation of the dynamic order parameter is studied as a function of temperature near the dynamic transition point. The temperature variation of appropriately defined ''susceptibility'' is also studied near the dynamic transition point. Similarly, the fluctuation of energy and appropriately defined ''specific heat'' is studied as a function of temperature near the dynamic transition point. In both cases, the fluctuations (of dynamic order parameter and energy) and the corresponding responses diverge (in power law fashion) near the dynamic transition point with similar critical behavior (with identical exponent values). [S1063-651X(97)02906-1]

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I. INTRODUCTION

The physics of the equilibrium phase transition in the Ising model is well understood [1]. However, the mechanism behind the nonequilibrium phase transition has not yet been explored rigorously, and the basic phenomenology is still undeveloped. It is quite interesting to study how the system behaves if it is driven out of equilibrium. The simplest prototype example is the kinetic Ising model in an oscillating magnetic field. In this context, the dynamic response of the Ising system in the presence of an oscillating magnetic field has been studied extensively [2–7] in the last few years. The dynamic hysteresis [2–4] and the nonequilibrium dynamic phase transition [5–7] are two important aspects of the dynamic response of the kinetic Ising model in the presence of an oscillating magnetic field. The nonequilibrium dynamic phase transition in the kinetic Ising model in the presence of an oscillating magnetic field was first studied by Tome and Oliviera [5]. They solved the mean-field (MF) dynamic equation of motion (for the average magnetization) of the kinetic Ising model in the presence of a sinusoidally oscillating magnetic field. By defining the dynamic order parameter as the time-averaged magnetization over a full cycle of the oscillating magnetic field, they showed that, depending upon the value of the field amplitude and the temperature, the dynamic order parameter takes a nonzero value from a zero value. In the field amplitude and temperature plane there exists a distinct phase boundary separating dynamic ordered (nonzero value of order parameter) and disordered (order parameter vanishes) phases. A tricritical point [separating the nature (discontinuous continuous) of the transition], on the phase boundary line, was also observed by them [5]. However, one may argue that such a MF transition is not truly dynamic in origin since it exists even in the quasistatic (or zero frequency) limit. This is because, if the field amplitude is less than the coercive field (at a temperature less than the transition temperature without any field), then the response magnetization varies periodically but asymmetrically even in the zero frequency limit; the system remains locked to one well of the free energy, and cannot go to the other one, in the absence of fluctuation.

The true dynamic nature of this kind of phase transition (in the presence of fluctuation) was studied by Lo and Pelcovits [6]. They studied the dynamic phase transition in the kinetic Ising model in the presence of an oscillating magnetic field by Monte Carlo (MC) simulation which allows the microscopic fluctuations. Here the transition disappears in the zero frequency limit; due to the fluctuations, the magnetization flips in the direction of the magnetic field and the dynamic order parameter (time-averaged magnetization) vanishes. However, they [6] did not report any precise phase boundary. Acharyya and Chakrabarti [7] studied the nonequilibrium dynamic phase transition in the kinetic Ising model in the presence of an oscillating magnetic field by extensive MC simulation. They [7] also identified that this dynamic phase transition (at a particular nonzero frequency of the oscillating magnetic field) is associated with the breaking of the symmetry of the dynamic hysteresis $(m-h)$ loop. In the dynamically disordered phase (where the value of the order parameter vanishes) the corresponding hysteresis loop is symmetric, and loses its symmetry in the ordered phase (giving a nonzero value of dynamic order parameter). They [7] also studied the temperature variation of the ac susceptibility components near the dynamic transition point. The major observation was that the imaginary (real) part of the ac susceptibility gives a peak (dip) near the dynamic transition point (where the dynamic order parameter vanishes). The important conclusions were (i) this is a distinct signal of phase transition, and (ii) this is an indication of the thermodynamic nature of the phase transition. The Debye relaxation of the dynamic order parameter and the critical slowing down were studied very recently [11] both by MC simulation and by solving the dynamic MF equation [5] of motion for the average magnetization. The specific-heat singularity [11] near the dynamic transition point is also an indication of the thermodynamic nature of this dynamic phase transition. It is

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worth mentioning here that the statistical distribution of the dynamic order parameter was studied by Sides *et al.* [8]. The nature of the distribution changes (from bimodal to unimodal) near the dynamic transition point. They also observed [8] that the fluctuation of the hysteresis loop area becomes considerably larger near the dynamic transition point.

In the case of equilibrium phase transitions, the fluctuation-dissipation theorem (FDT) states (due to the applicability of Gibbs formalism) that the mean square fluctuations of some intrinsic physical quantities (say, energy, magnetization etc.) are directly related to some responses (specific heat, susceptibility etc.) of the system. Consequently, near the ferropara transition point, both the fluctuation of magnetization and the susceptibility show the same singular behavior. If it is of power law type, the same singular behavior will be characterized by the same exponent. This is also true for the fluctuation of energy and the specific heat. These are the consequences of the fluctuation-dissipation theorem [1]. Here the main motivation is to study the fluctuations and corresponding responses near the dynamic transition temperature.

In this paper, the fluctuations of the dynamic order parameter and the energy are studied as a function of temperature near the dynamic transition point. The temperature variations of ''susceptibility'' and ''specific heat'' are also studied near the transition point. The temperature variation of the fluctuation of the dynamic order parameter and that of the susceptibility are compared. Similarly, the temperature variation of the fluctuation of energy and that of the specific heat are compared. The paper is organized as follows: the model and the simulation scheme are discussed in Sec. II, the results are reported in Sec. III, and Sec. IV contains a summary of the work.

II. MODEL AND SIMULATION

The Ising model with nearest neighbor ferromagnetic coupling in the presence of a time-varying magnetic field can be represented by the Hamiltonian

$$H=-\sum_{\langle ij\rangle} J_{ij}s_i^z s_j^z - h(t)\sum_i s_i^z \tag{2.1}$$

Here, $s_i^z(=\pm 1)$ is the Ising spin variable, J_{ij} is the interaction strength, and $h(t)=h_0\cos(\omega t)$ represents the oscillating magnetic field, where h_0 and ω are the amplitude and the frequency, respectively, of the oscillating field. The system is in contact with an isothermal heat bath at temperature T. For simplicity all $J_{ij}(=J>0)$ are taken equal to unity, and the boundary condition is chosen to be periodic. The temperature (T) is measured in units of J/K, where K is the Boltzmann constant (here K is taken to be unity).

A square lattice of linear size L $(=100)$ has been considered. At any finite temperature T and for a fixed frequency (ω) and amplitude (h_0) of the field, the microscopic dynamics of this system was studied here by Monte Carlo simulation using Glauber single spin-flip dynamics with a particular choice of the Metropolis rate of single spin-flip [12]. Starting from an initial condition where all spins are up, each lattice site is updated here sequentially, and one such full scan over the entire lattice is defined as the unit time step (Monte Carlo step). The instantaneous magnetization (per site), $m(t)=(1/L^2)\Sigma_i s_i^z$, has been calculated. From the instantaneous magnetization, the dynamic order parameter $Q=(\omega/2\pi)\oint m(t)dt$ (time-averaged magnetization over a full cycle of the oscillating field) is calculated. Some of the transient loops have been discarded to obtain the stable value of the dynamical quantities.

III. RESULTS

A. Temperature variations of susceptibility and fluctuation of dynamic order parameter

The fluctuation of the dynamic order parameter is

$$\delta Q^2=(\langle Q^2\rangle-\langle Q\rangle^2),$$

where $\langle\ \rangle$ stands for the averaging over various Monte Carlo samples.

The susceptibility is defined as

$$\chi=-\frac{d\langle Q\rangle}{dh_0}.$$

Here, a square lattice of linear size L $(=100)$ was considered. $\langle Q^2\rangle$ and $\langle Q\rangle$ are calculated using MC simulation. The averaging was done over 100 different (uncorrelated) MC samples.

The temperature variations of the fluctuation of Q, i.e., δQ^2 and susceptibility χ, have been studied here, and both are plotted in Fig. 1. From the figure it is observed that both δQ^2 and χ diverge near the dynamic transition point (where Q vanishes).

This was studied for two different values of field amplitude h_0 [Fig. 1(a) is for h_0 = 0.2 and Fig. 1(b) is for h_0 =0.1]. The dynamic transition temperatures $T_d(h_0)$, at which χ and δQ^2 diverge, are 1.91 ± 0.01 for h_0 = 0.2 and 2.15 ± 0.01 for h_0 = 0.1. These values of $T_d(h_0)$ agree with the phase diagram estimated from vanishing of Q. The $\ln_e(\chi)$ versus $\ln_e(T_d-T)$ and $\ln_e(\delta Q^2)$ versus $\ln_e(T_d-T)$ plots show (insets of Fig. 1) that $\chi\sim(T_d-T)^{-\alpha}$ and $\delta Q^2\sim(T_d-T)^{-\alpha}$. For h_0 = 0.2, $\alpha\sim0.53$ [inset of Fig. 1(a)] and for h_0 = 0.1, $\alpha\sim2.5$ [inset of Fig. 1(b)]. Results show that both χ and δQ^2 diverge near T_d as a power law with the same exponent α, though there is a crossover region (where the effective exponent values are different).

B. Temperature variations of specific heat and fluctuation of energy

The time averaged (over a full cycle) cooperative energy of the system is

$$E=-(\omega/2\pi L^2)\oint\left(\sum_{i,j} s_i^z s_j^z\right)dt,$$

and the fluctuation of the cooperative energy is

$$\delta E^2=(\langle E^2\rangle-\langle E\rangle^2).$$

The specific-heat C [11] is defined as the derivative of the energy (defined above) with respect to the temperature, and

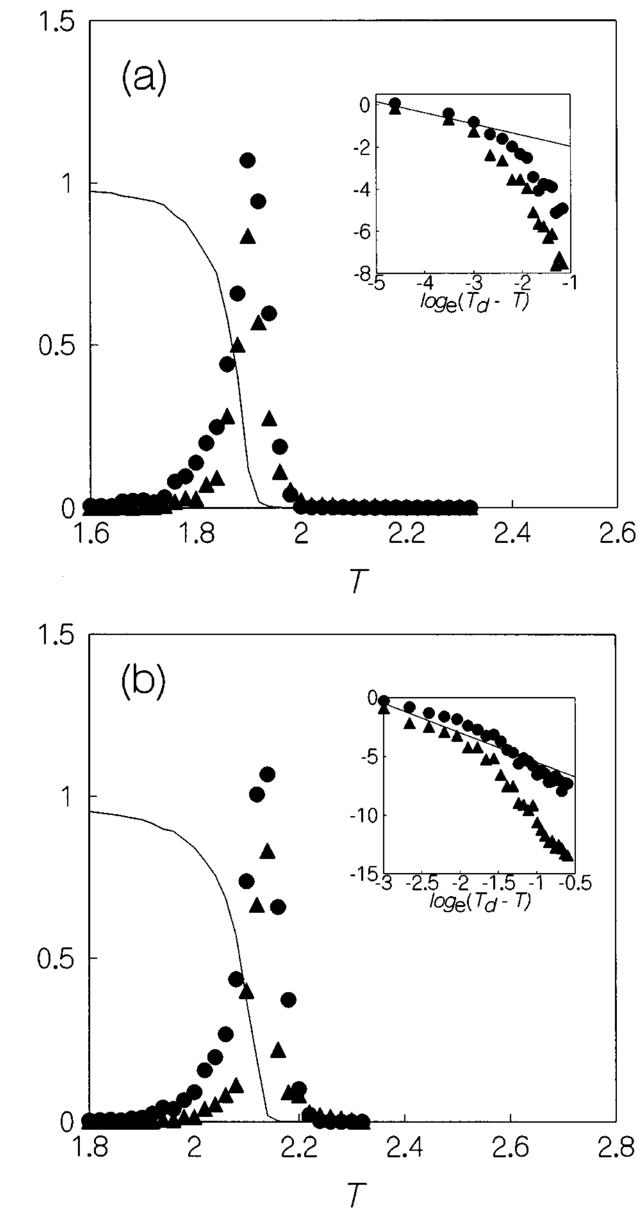

FIG. 1. Temperature variations of $\langle Q \rangle$, χ, and δQ^2 for two different values of field amplitudes h_0: (a) For $h_0 = 0.2$; Q (solid line), χ (circles), and δQ^2 (triangles). (b) For $h_0 = 0.1$; Q (solid line), χ (circles), and δQ^2 (triangles). All the data points are plotted in arbitrary units. Here $\omega = 2\pi\times 0.01$. Corresponding insets show the plots of $\ln_e(\chi)$ (circles) and $\ln_e(\delta Q^2)$ (triangles) against $\ln_e(T_d - T)$. Solid lines represent the linear best fit in a region very close to T_d.

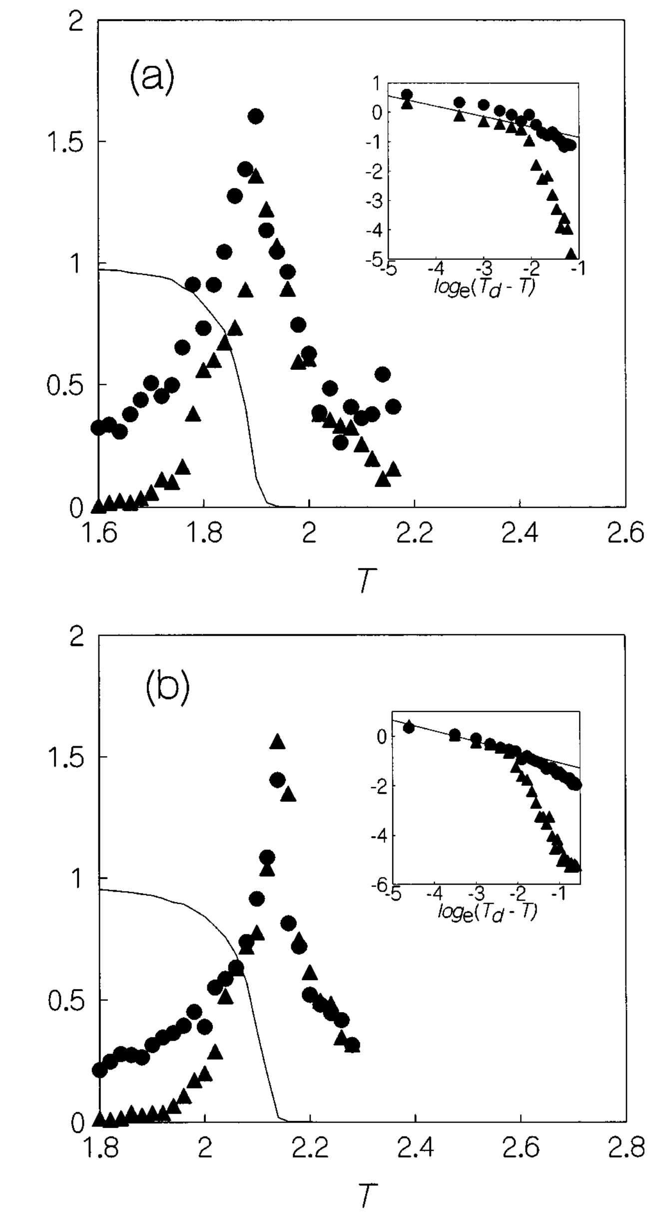

FIG. 2. Temperature variations of $\langle Q \rangle$, C, and δE^2 for two different values of field amplitudes h_0: (a) For $h_0 = 0.2$; Q (solid line), C (circles), and δE^2 (triangles). (b) For $h_0 = 0.1$; Q (solid line), C (circles), and δE^2 (triangles). All the data points are plotted in arbitrary units. Here $\omega = 2\pi\times 0.01$. Corresponding insets show the plots of $\ln_e(C)$ (circles) and $\ln_e(\delta E^2)$ (triangles) against $\ln_e(T_d - T)$. Solid lines represent the linear best fit in the region very close to T_d.

$$C = \frac{d\langle E \rangle}{dT}.$$

Here, also a square lattice of linear size L (=100) was considered. $\langle E^2 \rangle$ and $\langle E \rangle$ are calculated using MC simulation. The averaging was done over 100 different (uncorrelated) MC samples.

The temperature variation of the specific heat was studied [11], and prominent divergent behavior was found near the dynamic transition point (where $\langle Q \rangle$ vanishes). The temperature variation of the fluctuation of energy $(\delta E)^2$ was studied, and is plotted in Fig. 2. From the figure it is clear that the mean square fluctuation of energy (δE^2) and the specific heat (C) both diverge near the dynamic transition point (where the dynamic order parameter Q vanishes)

This was studied for two different values of field amplitude h_0 [Fig. 2(a) is for $h_0 = 0.2$ and Fig. 2(b) is for $h_0 = 0.1$]. Here also (like the earlier case) the specific heat C and δE^2 are observed to diverge at temperatures T_d. The temperatures $T_d(h_0)$, at which C and δE^2 diverge, are 1.91 ± 0.01 for $h_0 = 0.2$ [Fig. 2(a)] and 2.15$\pm$0.01 for $h_0 = 0.1$

[Fig. 2(b)]. These values also agree with the phase diagram estimated from vanishing of Q. The $\ln_e(C)$ vs $\ln_e(T_d-T)$ and $\ln_e(\delta E^2)$ vs $\ln_e(T_d-T)$ plots show (insets of Fig. 2) that $C \sim (T_d-T)^{-\gamma}$ and $\delta E^2 \sim (T_d-T)^{-\gamma}$. For $h_0 = 0.2$, $\gamma \sim 0.35$ [inset of Fig. 2(a)] and for $h_0 = 0.1$, $\gamma \sim 0.43$ [inset of Fig. 2(b)]. Like the earlier case, here also the results show that both χ and δQ^2 diverge near T_d as a power law with the same exponent α, though there is a crossover region (where the effective exponent values are different).

IV. SUMMARY

The nonequilibrium dynamic phase transition in the kinetic Ising model, in the presence of an oscillating magnetic field, is studied by Monte Carlo simulation. Acharyya and Chakrabarti [7] observed that the complex susceptibility components have peaks (or dips) at the dynamic transition point. Sides *et al.* [8] observed that the fluctuation in the hysteresis loop area grows (seems to diverge) near the dynamic transition point. It has been observed [11] that the relaxation time and the appropriately defined specific heat diverge near the dynamic transition point.

The mean square fluctuation of dynamic order parameter and the susceptibility are studied as a function of temperature, near the dynamic transition point. Both show the power law variation with respect to the reduced temperature near the dynamic transition point with the same exponent values. Similar, observation has been made for the case of mean square fluctuation of the energy and specific heat. It appears that although the effective exponent values for the fluctuation and the appropriate linear response differ considerably, away from the dynamic transition point T_d they eventually converge and give identical value as the temperature interval $|T_d-T|$ decreases and falls within a narrow crossover region. These numerical observations indicate that the fluctuation-dissipation relation [1] holds well in this case of the nonequilibrium phase transition in the kinetic Ising model. However, at this stage, to our knowledge, there is no analytic support of the FDT in this case.

Finally, it should be mentioned, in this context, that experiments [9] on ultrathin ferromagnetic Fe/Au(001) films were performed to study the frequency dependence of hysteresis loop areas. Recently, attempts were made [10] to measure the dynamic order parameter Q experimentally, in the same material, by extending their previous study [9]. The dynamic phase transition was studied from the observed temperature variation of Q. However, a detailed investigation of the dynamic phase transitions by measuring variations of associated response functions (like the ac susceptibility, specific heat, correlations, relaxations, etc.) has not yet been performed experimentally, to our knowledge.

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