Nonequilibrium phase transition in the kinetic Ising model: Critical slowing down and the specific-heat singularity

Muktish Acharyya*
Department of Physics, Indian Institute of Science, Bangalore-560012, India
and Condensed Matter Theory Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Bangalore-560064, India
(Received 3 September 1996; revised manuscript received 13 November 1996)

The nonequilibrium dynamic phase transition, in the kinetic Ising model in the presence of an oscillating magnetic field has been studied both by Monte Carlo simulation and by solving numerically the mean-field dynamic equation of motion for the average magnetization. In both cases, the Debye ''relaxation'' behavior of the dynamic order parameter has been observed and the ''relaxation time'' is found to diverge near the dynamic transition point. The Debye relaxation of the dynamic order parameter and the power law divergence of the relaxation time have been obtained from a very approximate solution of the mean-field dynamic equation. The temperature variation of appropriately defined ''specific heat'' is studied by the Monte Carlo simulation near the transition point. The specific heat has been observed to diverge near the dynamic transition point. [S1063-651X(97)02404-5]

PACS number(s): 05.70.Ln, 05.50.+q, 05.30.−d

I. INTRODUCTION

The dynamic response of the Ising system in the presence of an oscillating magnetic field has been studied extensively [1–3] in the last few years. The dynamic hysteresis [1–3] and the nonequilibruim dynamic phase transition [4–6] are two important aspects of the dynamic response of the kinetic Ising model in the presence of an oscillating magnetic field. This kind of phase transition in the Ising model was studied by Tome and Oliviera [4]. 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. They have defined the order parameter as the time averaged magnetization over a full cycle of the oscillating field and showed that depending upon the value of the field and the temperature, the order parameter takes nonzero value from a zero value. Precisely, in the field amplitude and temperature plane, there exists a phase boundary separating dynamic ordered (nonzero value of order parameter) and disordered (order parameter vanishes) phases. They [4] have also observed and located a tricritical point (TCP), [separating the nature (discontinuous-continuous) of the transition] on the phase boundary line (see Fig. 1). However, such a mean-field transition is not truly dynamic in origin and exists even in the static (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.

Lo and Pelcovits [5] first attempted to study the dynamic nature of this phase transition in the kinetic Ising model by the Monte Carlo (MC) simulation. Here, the transition disappears in the zero frequency limit; due to the fluctuations, the magnetization flips to the direction of the magnetic field and the dynamic order parameter (time averaged magnetization) vanishes. However, Lo and Pelcovits [5] have not reported any precise phase boundary. Acharyya and Chakrabarti [6] studied the nonequilibrium dynamic phase transition in the kinetic Ising model in the presence of an oscillating magnetic field by extensive MC simulation. They [6] have also identified that this dynamic phase transition is associated with the breaking of the symmetry of the dynamic hysteresis $(m-h)$ loop. In the dynamically disordered (value of order parameter vanishes) phase the corresponding hysteresis loop is symmetric, and loses its symmetry in the ordered phase (giv-

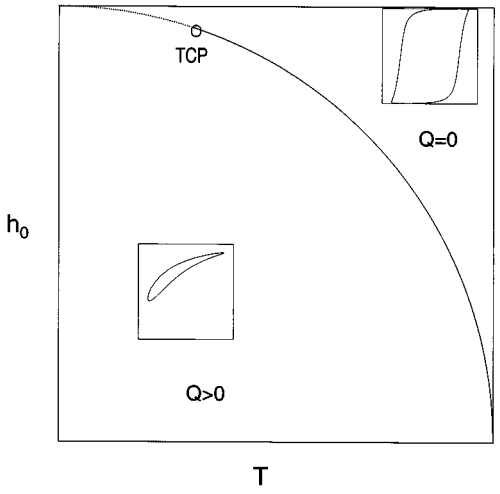

FIG. 1. Schematic diagram of the dynamic phase boundary in the field amplitude (h_0) and temperature (T) plane. The dotted line is the boundary of the discontinuous transition and the solid line represents the boundary of continuous transition. The small circle represents the tricritical point (TCP). Insets demonstrate the breaking of the symmetry of the dynamic hysteresis $(m-h)$ loop due to dynamic transition.

*Electronic address: muktish@physics.iisc.ernet.in

 © 1997 The American Physical Society

ing a nonzero value to the dynamic order parameter). They [6] 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 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.

It is worth mentioning here that the statistical distribution of a dynamic order parameter has been studied by Sides *et al.* [7]. The nature of the distribution changes near the dynamic transition point. They have also observed [7] that the fluctuation of the hysteresis loop area becomes considerably large near the dynamic transition point.

In the equilibrium critical phenomena, both the length and time scales diverge at criticality. This gives rise to the singularities in various thermodynamic quantities, such as the specific heat and the relaxation time. Can one expect similar kinds of features in the case of this nonequilibrium dynamic phase transition problem? To be specific, (i) is there any ''relaxation time,'' in this nonequlibrium problem that diverges at the dynamic transition point, and (ii) can there be any appropriately defined ''specific heat,'' that will show singular behavior at the transition point?

The main motivation of this paper is to find some answers to these questions at least numerically. The nonequilibrium dynamic phase transition in the kinetic Ising model in the presence of an oscillating magnetic field has been studied by MC simulation. Also the MF dynamic equation has been solved numerically, to compare the results. The ''relaxation'' behavior (defined in the following section) of the dynamic order parameter [4] and the behavior of specific heat (defined in Sec. III) near the dynamic transition point are studied by MC simulation. It may be mentioned here that the preliminary results of specific-heat singularity near the dynamic transition point were reported briefly in Ref. [8]. More detailed results are reported here. The relaxation behavior has also been studied here by solving numerically the mean-field (MF) dynamic equation of motion of the kinetic Ising model in the presence of an oscillating magnetic field. The MF equation has also been solved exactly in the linearized limit and studied in the relaxation behavior of the dynamic order parameter, near the dynamic transition point. The paper is organized as follows. In Sec. II the relaxation behavior of the order parameter near the dynamic transition point is studied both by the Monte Carlo simulation and by solving the mean-field dynamic equation of motion of the kinetic Ising model. In Sec. III the temperature variation of the specific heat is studied near the transition point only by the Monte Carlo simulation. A brief summary of all the results is given in Sec. IV.

II. RELAXATION BEHAVIOR OF THE DYNAMIC ORDER PARAMETER

A. Monte Carlo study

1. The model and simulation

A ferromagnetically interacting (nearest neighbor) Ising model 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 frequency, respectively, of the oscillating field. The system is in contact with an isothermal heat bath at temperature T. For simplicity all J_{ij} are taken equal to unity and a periodic boundary condition is chosen.

A square lattice of linear size L $(=100)$ has been considered. At any finite temperature T, for a fixed frequency (ω) and amplitude (h_0) of the field, the dynamics of this system has been studied here by Monte Carlo simulation using Glauber single spin-flip dynamics with the Metropolis rate of spin flip. Each lattice site is updated here sequentially and one such full scan over the lattice is defined as the time unit (Monte Carlo step or MCS) here. The initial configuration has been chosen such that all the spins are directed upward. 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.

2. Results

Figure 1 shows the schematic diagram of the dynamic phase boundary in the field amplitude (h_0) and temperature (T) plane. For small values of h_0 and T the dynamic order parameter Q is nonzero and the corresponding dynamic hysteresis loop ($m-h$ loop) is asymmetric, for larger values of h_0 and T, the dynamic order parameter Q vanishes, correspondingly, the $m-h$ loop becomes symmetric (inset of Fig. 1). The dynamic transition temperature (T_d) is a function of field amplitude (h_0). The transition across the dotted line (in Fig. 1) is discontinuous and that across the solid line is continuous. For very small values of h_0 the nature of the dynamic transition is continuous. In this paper, all studies are done in the region where Q always undergoes a continuous transition.

It has been observed carefully that the dynamic order parameter Q does not acquire the stable value within the first cycle of the oscillating field. It takes several cycles (of the oscillating field) to get stabilized, i.e., it shows relaxation behavior. Starting from the initial (all spins are up) configuration, the Q has been calculated for a various number (say n) of cycles of the oscillating magnetic field and plotted (inset of Fig. 2) against the number of cycles (n). Each value of Q shown here has been obtained by averaging over 100 random Monte Carlo samples. The inset of Fig. 2 shows a typical relaxation behavior of the dynamic order parameter Q. This has been plotted for fixed values of $\omega=2\pi\times 0.04$, $h_0=1.0$, and $T=1.5$. It shows that the dynamic order parameter Q relaxes as time (number of cycles) goes on. The best-fit curves shows that the relaxation is an exponential type. So, one can write $Q\sim Q_0\exp(-n/\Gamma)$, where Γ is the relaxation time which provides the ''time scale'' for this nonequilibrium problem. The physical interpretation of Γ is the number of cycles required so that Q becomes $1/e$ times its initial value (value of Q at starting cycle). From the exponential

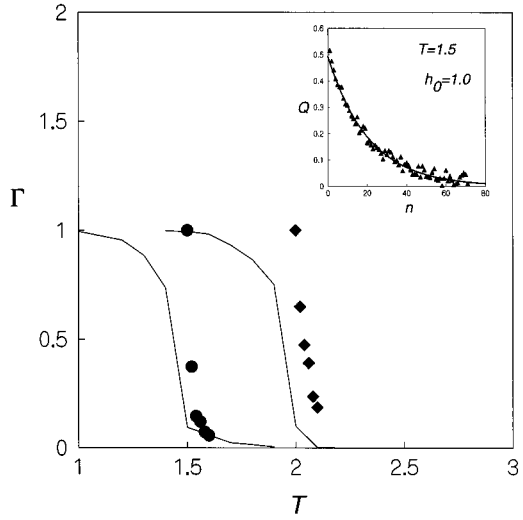

FIG. 2. Monte Carlo results of the temperature (T) variation of relaxation time (Γ) for two different values of field amplitudes (h_0): the bullet represents $h_0=1.0$ and the diamond represents $h_0=0.5$. Solid lines show the temperature (T) variations of dynamic order parameter Q. Inset shows a typical relaxation of Q plotted against the number of cycles n. The solid line is the best-fit exponential form of the data obtained from MC simulation. Here, $L=100$, and $\omega=2\pi\times0.04$.

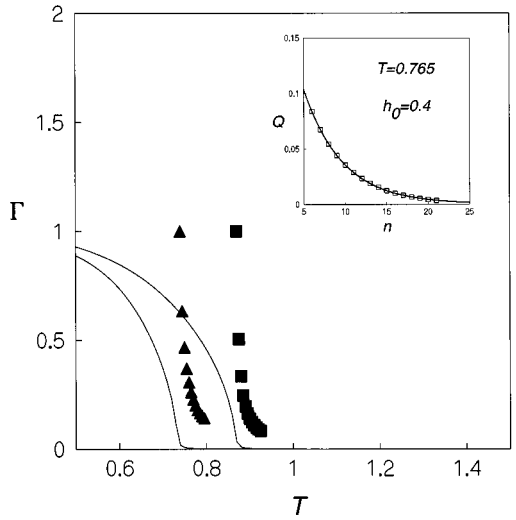

FIG. 3. Mean-field results of the temperature (T) variation of relaxation time (Γ) for two different values of field amplitudes (h_0): the filled triangle represents $h_0=0.4$ and the filled square represents $h_0=0.3$. Solid lines represent the temperature variation of the dynamic order parameter Q. Inset shows a typical relaxation of Q plotted against the number of cycles n. The solid line is the best-fit exponential for the data obtained from the solution of Eq. (2.2). Here, $\omega=2\pi\times0.02$.

fitting, the relaxation time (Γ) has been measured. The temperature (T) variation, for fixed values of ω and h_0, of this relaxation time Γ has been studied (in the disordered region of dynamic transition) and displayed in Fig. 2. The temperature (T) variations of Γ are shown (Fig. 2) for two different values of $h_0(=0.5$ and $1.0)$ and for a fixed value of $\omega=2\pi\times0.04$ here. From the figure (Fig. 2) it is clear that the relaxation time Γ diverges near the dynamic transition point (where Q vanishes) in the both cases ($h_0=0.5$ and 1.0).

B. Mean-field study

1. Mean-field equation of motion and numerical solution

Although as mentioned earlier the mean-field system does not undergo a true dynamic transition (as the transition exists even in the static limit), the mean-field case has been considered here as a pathological one.

The time evolution of the average magnetization (under mean-field approximation) in the presence of an oscillating magnetic field can be described by the equation

$$\tau\frac{dm}{dt}=-m+\tanh\left(\frac{m(t)+h(t)}{T}\right), \tag{2.2}$$

where $m(t)$ is the instantaneous magnetization, $h(t)=h_0\cos(\omega t)$ is a sinusoidally oscillating magnetic field, T is the temperature, and τ is a constant.

This equation has been solved by fourth order Runge-Kutta method taking $\tau=2\pi\times0.01$ and $dt=0.01$. The initial boundary condition is $m(0)=1.0$. From the numerical solution for the instantaneous magnetization $m(t)$, the dynamic order parameter Q $[=(\omega/2\pi)\oint m(t)dt]$ has been calculated.

2. Results

The inset of Fig. 3 shows a typical relaxation of the dynamic order parameter Q for $\omega=2\pi\times0.02$, $h_0=0.4$, and $T=0.765$. Here, also the exponential type of relaxation is observed and the relaxation time has been measured in the same way, discussed earlier (in the MC case). Figure 3 shows the temperature variation of the relaxation time Γ for $\omega=2\pi\times0.02$ and two different values of h_0 $(=0.3$ and $0.4)$. Here, also from the figure, (Fig. 3) it is clear that the typical time scale or the relaxation time Γ for this nonequilibrium problem diverges for both the cases ($h_0=0.3$ and 0.4) near the dynamic transition point (where Q vanishes).

3. An approximate solution of the MF equation

In the limit of $h_0\to0$ and $T>1$, Eq. (2.2) can be linearized (i.e., linearizing the tanh term) as

$$\tau\frac{dm}{dt}=-\epsilon m+\frac{h_0\cos(\omega t)}{T},$$

where $\epsilon=1-1/T$. The solution of the above equation is

$$m(t)=\exp(-\epsilon t/\tau)+m_0\cos(\omega t-\phi),$$

where m_0 and ϕ are two constants. The value of the dynamic order parameter Q at the nth cycle of the oscillating field is

$$Q=\frac{\omega}{2\pi}\oint m(t)dt=\frac{\omega}{2\pi}\int_{t_{n-1}}^{t_n}m(t)dt,$$

where $t_n=2\pi n/\omega$. The value of Q, at the nth cycle, can be written as

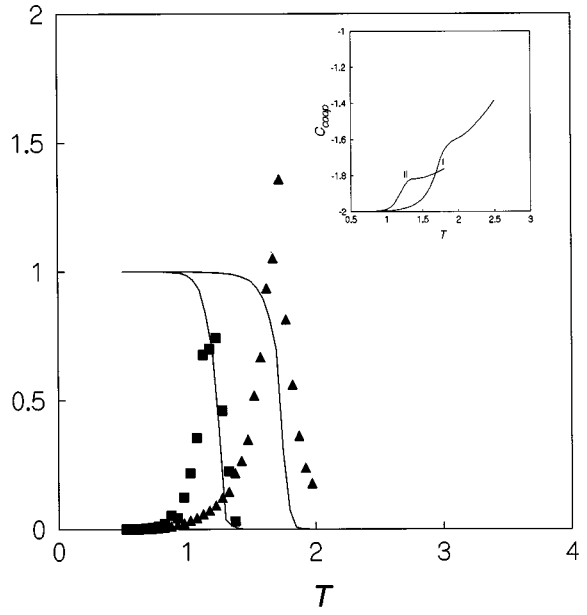

FIG. 4. Monte Carlo results of the temperature variations of C_{coop} for two different values of h_0: the filled square represents $h_0=0.8$ and the filled triangle represents $h_0=0.4$. Solid lines represent the temperature variations of Q. Inset shows the temperature variations of E_{coop} for two different values of h_0: (I) $h_0=0.8$ and (II) $h_0=0.4$. Here, $L=100$ and $\omega=2\pi\times0.01$.

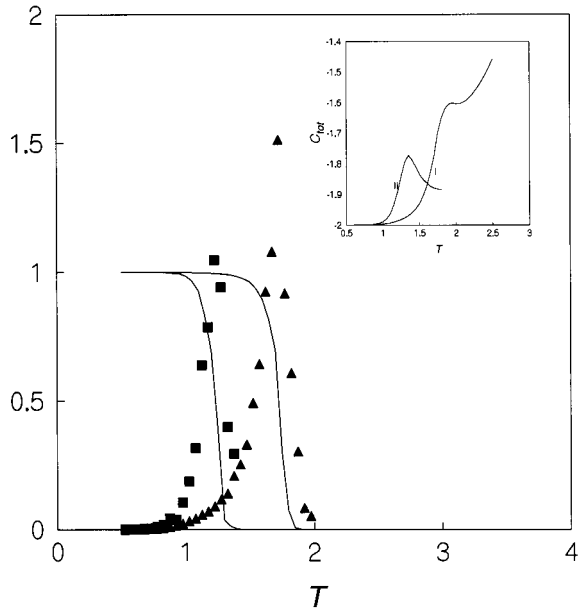

FIG. 5. Monte Carlo results of the temperature variations of C_{tot} for two different values of h_0: the filled square represents $h_0=0.8$ and the filled triangle represents $h_0 = 0.4$. Solid lines represent the temperature variations of Q. Inset shows the temperature variations of E_{tot} for two different values of h_0: (I) $h_0=0.8$ and (II) $h_0=0.4$. Here, $L=100$ and $\omega=2\pi\times0.01$.

$$Q=Q_0\exp\left(-\frac{2\pi n\epsilon}{\tau\omega}\right)=Q_0\exp(-n/\Gamma),$$

where Q_0 is a constant independent of n. The above form shows that Q relaxes exponentially with the number of cycles n of the oscillating field. The relaxation time Γ is equal to $(\tau\omega/2\pi)\epsilon^{-1}$. It should be noted here that the dynamic transition occurs at $T=1$ in the limit $h_0\to0$ [4]. So, for $h_0\to0$ near the dynamic transition point (where the linearization holds well) the behavior of relaxation time is

$$\Gamma\sim\epsilon^{-1}\sim[T-T_d(h_0\to0)]^{-1},$$

which shows the power law (exponent is unity) divergence of the relaxation time at the dynamic transition point.

III. BEHAVIOR OF SPECIFIC HEAT NEAR THE TRANSITION POINT

The time averaged (over a full cycle) cooperative energy of the system may be defined as

$$E_{\text{coop}}=-(\omega/2\pi L^2)\oint\left(\sum_{\langle ij\rangle}s_i^z s_j^z\right)dt,$$

and the time averaged (over a full cycle) total energy (including both cooperative and field part) of the system can be written as

$$E_{\text{tot}}=-(\omega/2\pi L^2)\oint\left(\sum_{\langle ij\rangle}s_i^z s_j^z+h(t)\sum_i s_i^z\right)dt.$$

The temperature variations of E_{tot} and E_{coop} have been studied. The specific heats are defined as $C_{\text{tot}}=dE_{\text{tot}}/dT$ and $C_{\text{coop}}=dE_{\text{coop}}/dT$. The temperature variations of the specific heats have also been studied and have prominent divergent behavior near the dynamic transition point (where Q vanishes).

Here again, a square lattice of linear size L $(=100)$ has been considered. Both E_{coop} and E_{tot} are calculated using MC simulation. Each data point has been obtained by averaging over 100 different MC samples.

A. Results

The temperature derivatives of E_{coop} and E_{tot} can be defined as the specific heats for this nonequilibrium problem. The temperature variations of Q, $C_{\text{coop}}(=dE_{\text{coop}}/dT)$, and $C_{\text{tot}}(=dE_{\text{tot}}/dT)$ have been studied. The values of h_0 $(=0.4$ and $0.8)$ are chosen here in such a way that Q always undergoes a continuous transition. The temperature variations of Q, C_{coop}, are shown in Fig. 4. The inset shows the variation of total cooperative energy E_{coop} (per spin) with temperature (T). In this case the frequency (ω) of the field is kept fixed $(\omega=0.0628)$. Figure 5 shows the temperature variation (for the same values of ω, h_0, and T) of C_{tot} and the inset shows the temperature variation of the total (cooperative + field) energy (per spin). From the figure it is clear that the appropriately defined specific heats C_{coop} and C_{tot} diverge near the dynamic phase transition point.

IV. SUMMARY

The nonequlibrium dynamic phase transition, in the kinetic Ising model in the presence of an oscillating magnetic field, is studied both by Monte Carlo simulation and by solving the mean-field dynamic equation of motion.

Acharyya and Chakrabarti [6] observed that the complex susceptibility components have peaks (or dips) at the dynamic transition point. Sides *et al.* [7] observed that the fluctuation in the hysteresis loop area grows (seems to diverge) near the dynamic transition point.

In this study it is observed that the relaxation time and the appropriately defined specific heat diverge near the dynamic transition point. All the results are obtained here numerically. No attempts were made to extract any exponent values from the numerical studies.

It should be mentioned that recent experiments [9] on ultrathin ferromagnetic Fe/Au(001) films have been performed to investigate the frequency dependence of hysteresis loop areas. Recently, attempts have been made [10] to measure the dynamic order parameter Q experimentally, in the same material, by extending their previous study [9]. The dynamic phase transitions have been studied from the observed variation of Q. However, the detailed study of the dynamic phase transitions by measuring variations of associated response functions (such as the ac susceptibility, specific heat, correlations, relaxations, etc.) have not been done experimentally.

ACKNOWLEDGMENTS

The author is grateful to the Jawaharlal Nehru Center for Advanced Scientific Research, Bangalore for financial support and computational facilities. The author thanks B. K. Chakrabarti for a critical reading of the manuscript and for helpful discussions.

[1] lM. Rao, H. R. Krishnamurthy, and R. Pandit, Phys. Rev. B **42**, 856 (1990).
[2] P. B. Thomas and D. Dhar, J. Phys. A **26**, 3973 (1993).
[3] S. Sengupta, Y. Marathe, and S. Puri, Phys. Rev. B **45**, 4251 (1990).
[4] T. Tome and M. J. de Oliviera, Phys. Rev. A **41**, 4251 (1990).
[5] W. S. Lo and R. A. Pelcovits, Phys. Rev. A **42**, 7471 (1990).
[6] M. Acharyya and B. K. Chakrabarti, Phys. Rev. B **52**, 6550 (1995).
[7] S. W. Sides, R. A. Ramos, P. A. Rikvold, and M. A. Novotny (unpublished); see also J. Appl. Phys. **79**, 6482 (1996).
[8] M. Acharyya, Physica A **235**, 469 (1997).
[9] Y. L. He and G. C. Wang, Phys. Rev. Lett. **70**, 2336 (1993).
[10] G. C. Wang *et al.* (unpublished).