Nonequilibrium Phase Transition and 'Specific-heat' singularity in the kinetic Ising model: A Monte Carlo Study

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Abstract:

The nonequilibrium phase transition has been studied by Monte Carlo simulation in a ferromagnetically interacting (nearest neighbour) kinetic Ising model in presence of a sinusoidally oscillating magnetic field. The ('specific-heat') temperature derivative of energies (averaged over a full cycle of the oscillating field) diverge near the dynamic transition point.

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I. Introduction

The dynamics of Ising system in presence of an oscillating magnetic field has been studied extensively [1,3] in the last few years. The dynamic hysteretic response [1,3] and the nonequilibrium dynamic phase transition [2,3] became an interesting and important part of these studies. The nonequilibrium dynamic phase transition in the kinetic Ising model in presence of a sinusoidally oscillating magnetic field has been studied first by Tome and Oliviera [2]. They have solved the dynamic mean field equation of motion for the average magnetisation of the kinetic Ising model in presence of a sinusoidally oscillating magnetic field. Defining the dynamic order parameter as the time averaged magnetisation over a full cycle of the oscillating field, they showed that in the field amplitude and temperature plane there exists a phase boundary separating dynamic ordered and disordered phase. Precisely, below the phase boundary the value of the order parameter is nonzero and it gets zero value above the boundary. There exists a tricritical point on the phase boundary line separating the nature (discontinuous/continuous) of the dynamic transition.

Later, Acharyya and Chakrabarti [3] studied this nonequilibrium phase transition in the kinetic Ising model by extensive Monte Carlo simulations. They have also studied [3] the temperature variations of the AC susceptibility components. Their important observation was that the imaginary (real) part of AC susceptibility gives a peak (dip) at the dynamic transition point, indicating the thermodynamic nature of this type of nonequilibrium dynamic phase transition.

Here, in this paper the time averaged (over a full cycle of the oscillating field) cooperative energy and total energy of the system have been calculated by Monte Carlo simulation and studied the temperature variation of the temperature derivatives (‘specific-heat’) of those energies. These ‘specific-heat’ like quantities are observed to diverge very near the dynamic transition point (where the dynamic order parameter vanishes). The paper is organised as follows: in section II the model and the simulation scheme are discussed very briefly, the results are reported in section III and the paper ends with
some concluding remarks in section IV.

II. Model and Simulation

A ferromagnetically interacting (nearest neighbour) Ising system in presence of an oscillating magnetic field can be represented by the Hamiltonian,

$$ H = - \sum_{<ij>} J_{ij} s_i^z s_j^z - h(t) \sum_i s_i^z. $$

Here, $s_i^z (\pm 1)$ represents Ising spin variable and, $h(t) = h_0 \cos(\omega t)$ is the externally applied oscillating magnetic field. $h_0$ and $\omega$ are the amplitude and frequency of the field. For simplicity all $J_{ij} (> 0)$’s are taken here equal to unity and boundary condition is periodic.

Here, a square lattice of linear size $L (= 100)$ has been considered. At any finite temperature $T$ and for a fixed frequency ($\omega$) 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. Each lattice site is updated here sequentially and one such full scan over the lattice is defined as the time unit here.

The following quantities are calculated, for a fixed values of $T$, $\omega$ and $h_0$:

(i) The dynamic order parameter, $Q = (\omega/2\pi) \oint m(t) dt$, where $m(t)$ is the instantaneous magnetisation. This is essentially the time $(t)$ averaged magnetisation over a full cycle of the oscillating magnetic field.

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

$$ E_{coop} = -(\omega/2\pi L^2) \oint \left( \sum_{<ij>} s_i^z s_j^z \right) dt. $$

(iii) The time averaged (over a full cycle) total energy of the system

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

Each data point has been obtained by averaging over 50 different random Monte Carlo samples.
III. Results

The temperature derivatives of $E_{coop}$ and $E_{tot}$ can be called 'specific-heat' for this nonequilibrium problem. The temperature variations of $Q$, $C_{coop} = \delta E_{coop}/\delta T$ and $C_{tot} = \delta E_{tot}/\delta T$ have been studied. For a fixed values of the field amplitude $h_0$, the dynamic order parameter $Q$ shows a continuous (depending upon the value of $h_0$) phase transition at temperature $T_d(h_0)$ [3]. 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 $Q$, $C_{coop}$ and $C_{tot}$ have been shown in Fig. 1. In this case the frequency ($\omega$) of the field is kept fixed ($\omega = 0.0628$). From the figure it is clear that the 'specific-heat' s $C_{coop}$ and $C_{tot}$ diverge near the dynamic phase transition point. $C_{tot}$ shows more prominent divergence than that showed by $C_{coop}$. Some of the results have been checked for larger sizes ($L = 200$) and no significant deviation was observed. The CPU time used here, to generate the whole set of data in IBM workstation, is approximately 16 hours.

IV. Concluding remarks

In conclusion, the nonequilibrium phase transition in the kinetic Ising model has been studied by Monte Carlo simulation. The 'specific-heat' shows divergence near the dynamic transition point. The divergence of 'specific-heat' near the dynamic transition point is a distinct signal of phase transition and an indication of the thermodynamic nature of this class of nonequilibrium phase transition. The indication of the thermodynamic nature of this type of nonequilibrium transition was first observed by Acharyya and Chakrabarti [3] in their study of the temperature variation of AC susceptibility. This observation of 'specific-heat' divergence near the transition point re-confirms, by another independent way, the thermodynamic nature of dynamic phase transition. A lot of computational effort is required to establish precisely the divergence of 'specific-heat' near the transition point. The work is in progress in this front and the details will be reported elsewhere.

It would be quite interesting to know how the dynamic order parameter goes to zero and specific heat diverges as one approaches the transition point. The universality
class of this type of nonequilibrium transition, is not yet known.

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Figure Caption

Fig.1. Temperature variation of $Q$ (solid line), $C_{coop}$ (circle) and $C_{tot}$ (triangle) for fixed $\omega (= 0.0628)$ and two different values of the field amplitude ($h_0$): (I) $h_0 = 0.4$ and (II) $h_0 = 0.8$. $L = 100$ here.
