Stochastic dynamics and the dynamic phase transition in thin ferromagnetic films

Hyunbum Jang,[1] Malcolm J. Grimson,[2] and Thomas B. Woolf[1]
[1]*Department of Physiology, Johns Hopkins University, Baltimore, Maryland 21205, USA*
[2]*Department of Physics, University of Auckland, Auckland, New Zealand*
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The dynamic phase behavior of a classical Heisenberg spin system with a bilinear exchange anisotropy in a planar thin film geometry has been investigated by Monte Carlo simulations using different forms for the stochastic dynamics. In simulations of the dynamic phase transition (DPT) in films subject to a pulsed oscillatory external field with competing surface fields, both Glauber and Metropolis dynamics show a continuous DPT. But while the field amplitude dependence of the DPT is similar in both cases, the transition region for the DPT as a function of temperature is more extended with Metropolis dynamics. The difference arises from a decoupling of the surface and bulk responses of the film near the dynamic phase transition with Metropolis dynamics that is not evident for Glauber dynamics.

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I. INTRODUCTION

In Monte Carlo simulations the algorithm incorporates a stochastic dynamics that provides a rule whereby the system changes from one state to another. There are many different possible types of stochastic dynamics that can involve either single or many particle moves and thereby be either local or nonlocal in character. In equilibrium Monte Carlo simulations a number of different dynamics can lead to the same Boltzmann distribution of states once the simulation has reached equilibrium. The conditions of ergodicity and detailed balance are sufficient to ensure that the equilibrium distribution of states sampled by the algorithm is the correct Boltzmann distribution [1]. Thus one is free to choose any algorithm that obeys ergodicity and detailed balance and one should get the same result in equilibrium Monte Carlo simulations. So the computationally most efficient algorithm is usually selected.

However, the fundamental difficulty that makes nonequilibrium Monte Carlo simulations harder than their equilibrium counterparts is that there is a limited freedom in choosing the dynamics of the Monte Carlo algorithm [1]. The conditions of ergodicity and detailed balance say nothing about the way in which the system comes to equilibrium and different choices for the stochastic dynamics will give rise to different results. Thus the dynamic must be chosen on physical grounds rather than simple computational efficiency and for cluster algorithms the relation of the Monte Carlo process to a realistic dynamical process is unclear [2]. In some cases, when simulating a real material, it is possible to use our understanding of that material to estimate the correct form for the stochastic dynamics. However in other cases the detailed form of the dynamics is not *a priori* clear and macroscopic properties must be used to make some inference as to the form of the stochastic dynamics. Thus it is important to understand the nonequilibrium statistical mechanics of model systems with well-characterized stochastic dynamics.

In recent papers [3–5], Rikvold and Kolesik have shown that the interface structure and velocity in a kinetic Ising ferromagnet driven by an applied field depends strongly on the details of the stochastic dynamics. Here we shall investigate the role of the type of stochastic dynamics on the dynamic phase transition (DPT) observed in a thin ferromagnetic film with competing surface fields where the dynamic variation of the magnetization in the film is the result of interface motion within the film [6–8].

II. MODEL

The system under consideration here is a three-dimensional thin planar film of finite thickness D with competing surface fields subject to a time dependent oscillatory external field $H(t)$ with Hamiltonian

$$\boldsymbol{H}(t) = -J\sum_{\langle i,j\rangle}[(1-\Lambda)(S_i^xS_j^x + S_i^yS_j^y) + S_i^zS_j^z] - h\left(\sum_{i\in\text{surface }1} S_i^z - \sum_{i\in\text{surface }D} S_i^z\right) - H(t)\sum_i S_i^z, \quad (1)$$

where $\mathbf{S}_i=(S_i^x,S_i^y,S_i^z)$ is a unit vector representing the ith spin and the notation $\langle i,j\rangle$ indicates that the sum is restricted to nearest-neighbor pairs of spins. J is a coupling constant characterizing the magnitude of the exchange interaction and Λ characterizes the strength of the bilinear exchange anisotropy. In this paper we have focused on a ferromagnetic ($J>0$) system with a weak bilinear exchange anisotropy of $\Lambda=0.1$, where the system is intermediate in character between the limiting Ising-like ($\Lambda=1$) and Heisenberg ($\Lambda=0$) models [9]. The competing surface fields have a magnitude $h=-0.55$ and the oscillatory driving field $H(t)$ is a square wave of amplitude H_0 and angular frequency ω [7].

The model film is a simple lattice of size $L\times L\times D$, in units of the lattice spacing. Periodic boundary conditions are applied in the x and y directions. Free boundary conditions are applied in the z direction which is of finite thickness D. A film thickness $D=12$ was used throughout which corresponds to the crossover regime between wall and bulk dominated behavior [10]. The results reported here are for lattices with $L=32$. No significant differences were found for lattices with $L=64$ and 128 at noncritical values of H_0 and T. The full finite-size scaling study required to determine critical

properties of the DPT is beyond the scope of this work.

Monte Carlo simulations were performed using a random spin update scheme. Trial configurations were generated by the rotation of a randomly selected spin through a random angular displacement about one of the x,y,z axes chosen at random [11,12]. A sequence of size $L\times L\times D$ trials comprises one Monte Carlo step per spin (MCSS), the unit of time in these simulations. In all the simulations reported here, the period of the pulsed oscillatory external field was fixed at 240 MCSS and the initial spin configuration was a ferromagnetically ordered state of the spins with $S_i=+1$ for all i.

III. GLAUBER VS METROPOLIS DYNAMICS

Previous studies [6–8] of hysteresis and the dynamic phase transition in anisotropic Heisenberg ferromagnets driven by an oscillatory applied external field have used a dynamic Monte Carlo simulation method with Metropolis dynamics. In Metropolis dynamics the transition probability associated with the trial rotation of the ith spin $S_i\rightarrow S_i'$ is $W_M(S_i\rightarrow S_i')=\min(1,e^{-\beta\Delta E})$ where ΔE is the total energy change. Here, however, we use Glauber dynamics, which is defined by the transition probability $W_G(S_i\rightarrow S_i')=(e^{-\beta\Delta E})/(1+e^{-\beta\Delta E})$. Both Glauber and Metropolis dynamics obey ergodicity and detailed balance [1]. In the Monte Carlo method no physical time is associated with each trial configuration. The unit of time in the simulation is the Monte Carlo step per spin and one MCSS simply corresponds to a series of random modifications of all the degrees of freedom of the system. If the time rate by which a real system can modify all of its degrees of freedom is known by some independent argument, then the number of MCSS can be converted into a real time unit [13,14]. However, in doing this one must be sure that the form of the stochastic dynamics used in the Monte Carlo simulation is appropriate, particularly if the dynamic response of the system depends strongly on the details of the stochastic dynamics. Note that both Glauber and Metropolis dynamics obey ergodicity and detailed balance. Furthermore, if $|\beta\Delta E|\gg 1$ then $W_M\approx W_G$. The only significant difference occurs for $|\beta\Delta E|\ll 1$, when $W_M>W_G$. Thus Metropolis dynamics is always more likely to accept a trial spin rotation that involves a small change in energy.

A. Temperature dependence of the order parameter

The order parameter for the DPT is the period averaged magnetization over a complete cycle of the pulsed field, Q [7]. Figure 1 shows the mean period averaged magnetization $\langle Q\rangle$ as a function of the reduced temperature, $T^*=k_BT/J$, for a pulsed oscillatory field amplitude $H_0=0.3$. The quantity is determined from a sequence of full cycles of the oscillatory field with initial transients discarded. The error bars in the figure correspond to a standard deviation in the measured values and are visible only when they exceed the size of the symbol. Lines joining the symbols in the figure are solely to guide the eye.

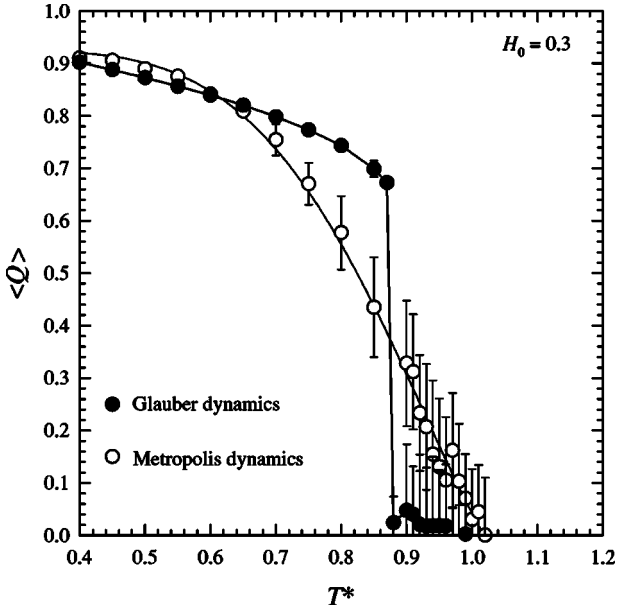

FIG. 1. Mean period averaged magnetization $\langle Q\rangle$ as a function of the temperature T^* with a fixed value of the pulsed oscillatory external field amplitude of $H_0=0.3$ for Glauber (solid circles) and Metropolis (open circles) dynamics.

The figure shows a change in the dynamic order parameter for Glauber (solid circles) and Metropolis (open circles) dynamics as T^* increases. The low temperature state with $\langle Q\rangle\neq 0$ corresponds to a dynamically ordered phase, while at high temperatures a dynamically disordered phase with $\langle Q\rangle=0$ is observed. The results for the two types of stochastic dynamics are the same at low temperatures ($T^*<0.7$) and higher temperatures above the DPT ($T^*>1.0$). However, for intermediate temperatures in the vicinity of the DPT, the form of $\langle Q\rangle$ as a function of T^* for the two types of dynamics is different. The DPT for Metropolis dynamics appears to be continuous with a steady decrease in the dynamic order parameter as the DPT is approached. Note that fluctuations in the dynamic order parameter close to the DPT are large. Furthermore the fluctuations in $\langle Q\rangle$ for the Metropolis dynamics increase steadily with T^* as the DPT is approached. This is in marked contrast to the same system with Glauber dynamics. The fluctuations in $\langle Q\rangle$ for Glauber dynamics remain small with increasing T^* in the dynamically ordered phase, but following the sharp decrease in $\langle Q\rangle$ at $T^*=0.88$, there is a marked increase in the size of the fluctuations in $\langle Q\rangle$. The most striking aspect of the figure is that while the qualitative form of the DPT is markedly different between Glauber and Metropolis dynamics, the locations of the DPT for Glauber and Metropolis dynamics are not so very different.

Large fluctuations in Q close to the DPT arise from competition between the static surface fields and the pulsed oscillatory external field in the system. Further information on the form of the DPT follows from the mean period averaged layer magnetization $\langle Q_n\rangle$ across the film. Figure 2 shows the temperature dependence of the order parameter for the nth layer, Q_n, across the whole film for $H_0=0.3$ with Glauber

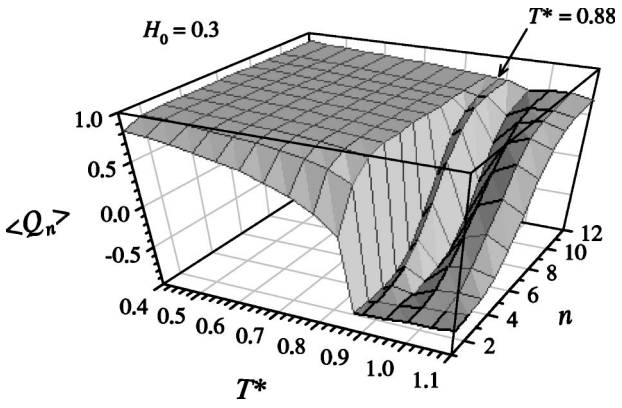

FIG. 2. Mean period averaged magnetizations for the nth layer, $\langle Q_n \rangle$, across the whole film for Glauber dynamics as a function of T^* with a fixed value of the pulsed oscillatory external field amplitude of $H_0 = 0.3$.

dynamics. The figure shows that the DPT in each layer of the film occurs at almost the same temperature. The shape of $\langle Q_n \rangle$ for Glauber dynamics is notably different from the corresponding result for Metropolis dynamics [7] where the critical temperature for the DPT in the surface layers is different from that for the DPT in the bulk of the film. While DPT with Metropolis dynamics is clearly continuous, this is not immediately clear for the system with Glauber dynamics where the DPT is very sharp.

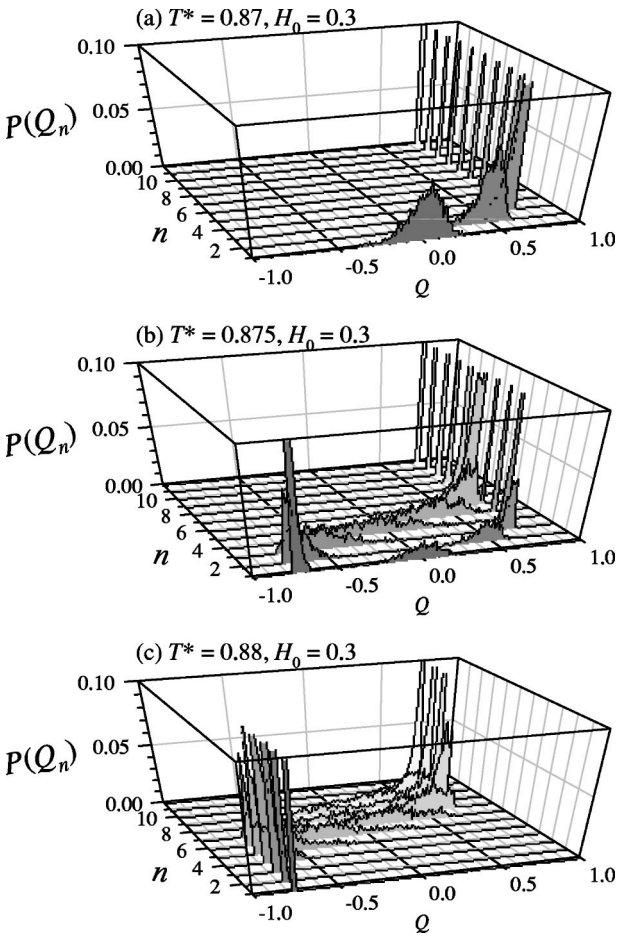

FIG. 3. Distributions of the layer order parameter $P(Q_n)$ for Glauber dynamics with a fixed value of the pulsed oscillatory external field amplitude of $H_0 = 0.3$ at temperatures T^*=(a) 0.87, (b) 0.875, and (c) 0.88.

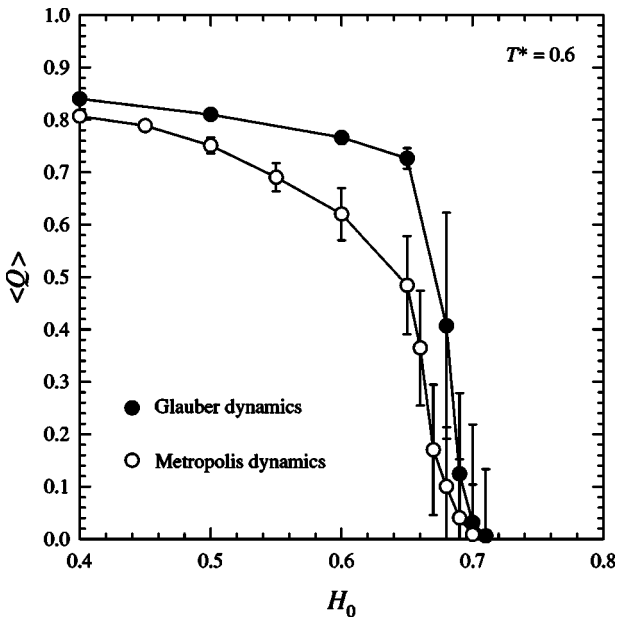

FIG. 4. Mean period averaged magnetization $\langle Q \rangle$ as a function of the pulsed oscillatory external field amplitude H_0 at a fixed value of the temperature of $T^* = 0.6$ for Glauber (solid circles) and Metropolis (open circles) dynamics.

In order to verify the continuous nature of the DPT for Glauber dynamics as a function of T^*, the order parameter distributions for the nth layer, $P(Q_n)$, across the whole film are obtained. Figure 3 shows $P(Q_n)$ for $H_0 = 0.3$ at (a) $T^* = 0.87$, (b) $T^* = 0.875$, and (c) $T^* = 0.88$. In both the dynamically ordered phase at $T^* = 0.87$ and the dynamically disordered phase at $T^* = 0.88$, the order parameter distributions for each layer $P(Q_n)$ display a single peak structure. Close to the transition at $T^* = 0.875$, $P(Q_n)$ has a double peak structure in some layers. This shows that the DPT is continuous. None of the layers in the figure shows evidence of a three-peak structure with peaks at $\pm Q$ and $Q = 0$ that would indicate a discontinuous DPT. All the layers of the film show the one- or two-peak structure consistent with a continuous DPT, the single peak being a result of the surface fields hindering magnetization reversal.

B. Field amplitude dependence of the order parameter

Figure 4 shows the mean period averaged magnetization $\langle Q \rangle$ as a function of the pulsed oscillatory external field amplitude H_0 at a fixed temperature of $T^* = 0.6$. It is immediately apparent from the figure that the qualitative form of $\langle Q \rangle$ for Glauber dynamics (solid circles) is very similar to that for Metropolis dynamics (open circles) as a function of H_0. For both types of dynamics at a fixed temperature the DPT is clearly continuous and $\langle Q \rangle$ vanishes at a value of $H_0 \approx 0.71$.

IV. CONCLUSION

The different forms for the dynamic phase transition for the system with Glauber and Metropolis dynamics result

from the different values for the transition probabilities of the two dynamics in trial spin rotations that involve only small changes in the total energy. In Metropolis dynamics, any trial single spin rotation that results in a reduction of the total energy is accepted. But for Glauber dynamics there is a (small) probability that a lower energy trial configuration will be rejected. Thus high energy reverse magnetization states can persist to higher temperatures in the film with Glauber dynamics than with Metropolis dynamics. As a result, dynamically ordered states can persist to higher temperatures in systems with Glauber dynamics.

For a given H_0, the apparent sudden change in the dynamic order parameter for the film at the DPT with Glauber dynamics is a result of the change in the layer dynamic order parameter occurring at the same temperature for all the layers of the film. In contrast, for Metropolis dynamics [7] the system shows a DPT in the surface layers of the film that occurs at a lower temperature to the DPT in the bulk of the film. This decoupling of the surface and bulk responses of the film to the applied oscillatory field gives rise to a mixed state of the film in which dynamically ordered surfaces coexist with a dynamically disordered bulk. This mixed state of the film persists over a range of temperature and gives rise to an extended region of large fluctuations of the dynamic order parameter for the film. However, while the DPT for the film is much sharper for Glauber dynamics than with Metropolis dynamics, the DPT is continuous in both cases. There is evidence for a discontinuous DPT as a function of the exchange anisotropy in the Hamiltonian, but for fixed Λ the DPT is continuous [8].

The choice of the transition probability for Glauber dynamics has a physical origin in the interaction of the spin with a heat bath, whereas, in Metropolis dynamics the transition probability has a mathematical origin, being generated simply from the Metropolis criterion for equilibrium Monte Carlo simulations. This work shows that while both types of dynamics give continuous DPTs at similar locations, the mixed state that is observed over an extended temperature range near the DPT with Metropolis dynamics is not observed for Glauber dynamics. Thus caution is required in choosing the form of the stochastic dynamics in nonequilibrium Monte Carlo simulations to ensure that the physics of the system is being correctly modeled.

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