Phase transitions in the kinetic Ising model with competing dynamics

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(Received 17 May 2000)

We study the nonequilibrium phase diagram and critical properties of a two-dimensional kinetic Ising model with competing Glauber and Kawasaki dynamics suggested by Tomé and de Oliveira [Phys. Rev. A **40**, 6643 (1989)]. The role of the Kawasaki dynamics, chosen with probability $1-p$, is to simulate a permanent energy flux into the system. The theoretical prediction for the phase diagram is improved significantly by using four- and six-point dynamical mean-field approximations. Monte Carlo simulations support that the ferromagnetic-paramagnetic phase transition changes from second to first order for sufficiently small p. The antiferromagnetic phase is found to be stable for a nonzero value of p even at $T=0$.

PACS number(s): 05.50.+q, 02.70.Lq, 05.70.Ln, 64.60.Cn

Nonequilibrium steady states as a consequence of competing dynamical processes have attracted considerable interest and up to now their understanding is far from complete. There are numerous generalizations of the well-known kinetic Ising model and the resulting steady states exhibit interesting features such as ordering in one dimension [1], the emergence of first-order phase transition [2,3] or the occurence of a novel ordered stationary state not characteristic of the corresponding equilibrium model [4]. An example for the latter case is the dynamical generalization of the Ising model suggested by Tomé and de Oliveira [5] where the competition between a spin-flip Glauber and a spin-exchange Kawasaki dynamics results in a nonequilibrium state. In this model, a modified Kawasaki process is introduced to input energy into the system while the Glauber process ensures the contact with a heat bath at temperature T. In spite of the ferromagnetic interaction, this model can produce an antiferromagnetic ordered state if the energy flux is dominant. Several authors have studied the one-, two-, and three-dimensional versions of this model using dynamical pair approximation and Monte Carlo (MC) simulations [6–10]. A puzzle still remains why MC simulation and dynamical mean-field theory yield different predictions for the phase diagram. This contradiction is rather surprising since the later method was found to yield good qualitative results for several nonequilibrium models [11–15]. In this Brief Report, we revise the MC simulations and present more accurate versions of the dynamical mean-field theory for the two-dimensional model to eliminate the differences between the theoretical predictions and MC simulations.

We consider a two-dimensional square lattice with $L\times L=N$ sites under periodic boundary conditions. The spin variable σ_i at site i takes the values ± 1 and nearest-neighbor ferromagnetic interactions are assumed. The transition from the state represented by $\sigma=\{\sigma_1,\ldots,\sigma_N\}$ to state σ' is determined by two competing process as

$$w(\sigma',\sigma)=pw_G(\sigma',\sigma)+(1-p)w_K(\sigma',\sigma). \tag{1}$$

In this equation, w_G is the usual single-spin-flip Glauber process occurs with probability p. The transition probability of flipping spin i is given by the well-known Metropolis rate $w_i(\sigma)=\min[1,\exp(-\Delta E_i/k_BT)]$, where ΔE_i is the energy change related to the given spin flip. Both the Boltzman's constant and the nearest-neighbor coupling constant are unity as usual. The other competing process, occuring with a probability $1-p$, is the two-spin exchange Kawasaki dynamics characterized by the transition probability of exchanging two nearest-neighbor spins at sites i and j:

$$w_{ij}(\sigma)=\begin{cases}0, & \text{for } \Delta E_{ij}\leqslant 0\\ 1, & \text{for } \Delta E_{ij}>0,\end{cases} \tag{2}$$

where ΔE_{ij} is the energy difference between the final and initial configurations. The definition of these transition rates simulate the contact of the system with the heat bath at temperature T with probability p, and an energy flux into the system with a probability $1-p$. As a consequence of the competing dynamics, there are an ordered ferromagnetic and antiferromagnetic phases separated by a disordered paramagnetic phase in the (p,T) phase diagram [5,7]. It is worth mentioning that the Kawasaki dynamics would mimic an antiferromagnetic Ising model for zero temperature if we modify the Kawasaki rate to allow exchanges of zero energy difference. This provides a better understanding of the existence of the antiferromagnetic ordered state in the low p regime.

In this section, higher levels of dynamical mean-field approximations are applied to predict a more accurate phase diagram. Following the standard method, (for details see Ref. [11]), the calculation of the temperature (or the probability) dependence of the order parameter makes it possible to identify the phase-transition point. The four-point (six-point) approximation involves finding a hierarchy of evolution equations for the configuration probabilities on $2\times 2(2\times 3)$ clusters [13]. The ferromagnetic-paramagnetic phase transition is described by the variation of the order parameter defined as the stationary value of the total magnetization. It is important to emphasize that the evaluation of the order parameter as a function of control parameter (T or p) is ''capable'' of distinguishing whether the phase transition is continuous or not, in contrast to the linear stability analysis of the paramagnetic solution [5]. Evidently, both methods yield identical results when the transition is continuous. If the transition is discontinuous, the limit of local stability of the disordered phase can also be obtained where the order parameter as a result of an unstable solution becomes zero. Using the more labor-intensive method, a dynamical tricritical be-

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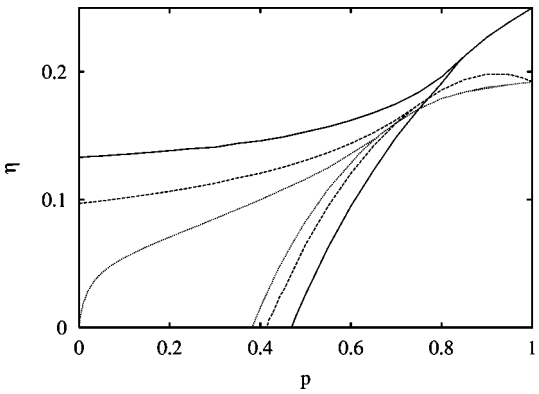

FIG. 1. Critical temperature of ferromagnetic-paramagnetic transition as a function of p. The parameter η is given by $\eta = \exp(-4J/k_BT)$. The prediction of two-point (full curve), four-point (broken curve), and six-point (dotted curve) approximation. The upper (lower) lines show the limits of stability of the ferromagnetic (paramagnetic) phases.

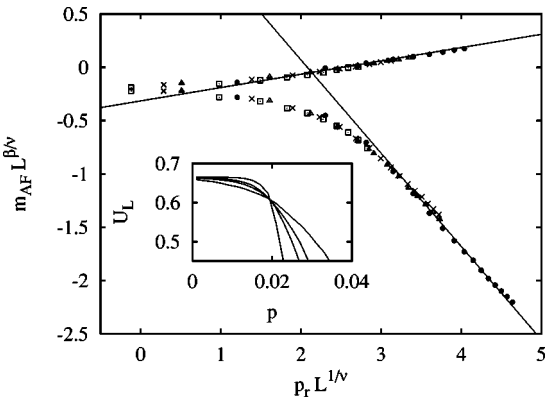

FIG. 2. Finite-size scaling plots of MC data for antiferromagnetic order parameter as a function of reduced p at $T=0$. System sizes are $L=16(\square)$, $24(\times)$, $30(\triangle)$, and $60(\bullet)$. Equilibrium Ising exponents are used with $p_c=0.019$. The slopes of the inserted lines are 1/8 and $-7/8$. The Binder cumulant as a function of p (inset) gives the same critical value of p_c.

havior can be observed. At the level of two-point approximation, the phase transition changes from second to first order if $p<p_t^{(2p)}=0.883$ and the transition temperature is $T_t^{(2p)}=2.546$ at the tricritical point. Improving the accuracy of dynamical mean-field theory, the value of the tricritical point decreases ($p_t^{(4p)}=0.743\, p_t^{(6p)}=0.69$). The corresponding transition temperatures also decrease: $T_t^{(4p)}=2.278$ $T_t^{(6p)}=2.166$. In Fig. 1, the critical temperature is plotted as a function of p where we have adopted the earlier used quantity $\eta=\exp(-4J/k_BT)$ [7]. Here, the limits of local stability of *both* the magnetized (ferromagnetic) and unmagnetized (paramagnetic) steady states are plotted for every calculated level of the dynamical mean-field theory. We believe that the value of the tricritical point will be shifted to a smaller p and the area of the ''hysteresis region'' where both the ordered and the disordered solutions are locally stable will shrink if we apply a higher level of dynamical mean-field approximation. The emergence of first-order transition under the variation of some control parameter has already been observed in other nonequilibrium models [2,16,17]. The mechanism resulting in the first-order transition in our model is similar to those described previously by Dickman [11]: The Kawasaki dynamics is ineffective in a highly magnetized phase where interfaces separating domains with different magnetization are rare but this dynamics can destroy effectively the weakly magnetized state. Finally, we should mention that the four-point approximation predicts a weak maximum of critical temperature as p is varied. A similar observation was suggested in the earlier report of MC simulations [7]. However, the more accurate six-point approximation, which yields the same result in the equilibrium model ($p=1$) as in the four-point approximation, predicts monotonic decrease in T_c.

To study the antiferromagnetic order-disorder phase transition, the lattice points are divided into two interpenetrating sublattices. The ordered state is described by the average sublattice magnetization where the order parameter (m_{AF}) is the difference of the sublattice magnetizations. As well as for the ferromagnetic-paramagnetic phase transition, the transition point is extracted from the $m_{AF}(p,T)$ functions [18,19]. At the level of two-point approximation, our calculations have reproduced the result published previously [5]. Namely, there is a negligible dependence of critical p from the temperature when the parameter p is varied at fixed T. As an example, the antiferromagnetic phase is stable even at $T=0$ if $p<p_c^{(2p)}(T=0)=0.323$. Employing more accurate approximations, the qualitative feature of this phase transition remains unchanged, however, the shift in critical p is significant: $p_c^{(4p)}(T=0)=0.095$ $p_c^{(6p)}(T=0)=0.047$. The decrease of p_c as we employ more accurate approximations can be understood since the lower level of approximation (such as two-point level) truncates the correlations beyond a shorter distance. Therefore, this level requires a more intensive influence of the Glauber process to destroy the antiferromagnetic order. Although the area of the ordered phase shrinks if we increase the level of approximation, the antiferromagnetic ordered phase remains stable even at $T=0$ for small value of p.

Motivated by the above results of the theoretical predictions, we have revised the MC simulations for this model. In the case of antiferromagnetic order-disorder transition, the main discrepancy is that previous simulations suggest a stable ferromagnetic phase for *all* values of p at $T=0$ [7]. Obviously, the completely ordered ferromagnetic state cannot be destroyed by a Kawasaki dynamics. However, if the

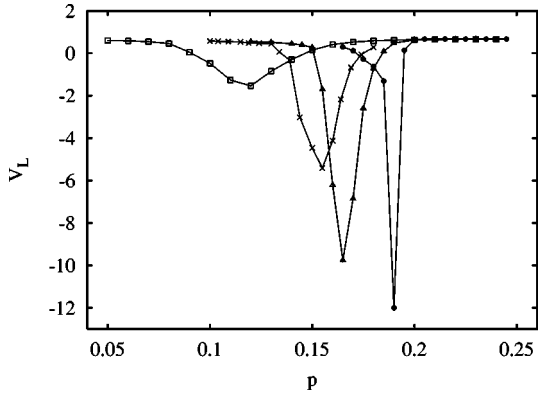

FIG. 3. Reduced fourth-order cumulant V_L, for $T=1.0$, as a function of p for system size $L=16(\square)$, $24(\times)$, $30(\triangle)$, and $60(\bullet)$.

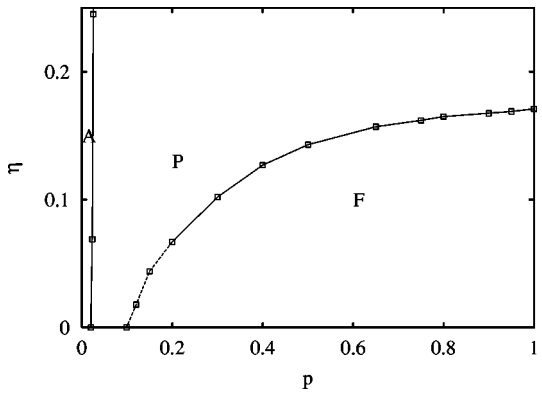

FIG. 4. Monte Carlo results (□) for the phase diagram. The solid curves are for continuous phase transitions while the broken curve represents discontinuous transition. The antiferromagnetic (A), paramagnetic (P), and ferromagnetic (F) phases are indicated. The tricritical point is at $p_t^{(MC)}=0.2$ and $T_t^{(MC)}=1.49$, while the six-point approximation predicts $p_t^{(6p)}=0.69$ and $T_t^{(6p)}=2.166$.

initial state is disordered, the system evolves to the antiferromagnetic ordered state having maximal energy at a small value of p. Furthermore, even the ferromagnetic state containing some defects may decay if the system size is large enough. Finite-size effects are especially serious at low temperatures because a small system may evolve to the completely ordered ferromagnetic state with considerable probability and can become trapped.

Our extensive MC simulations support the prediction of dynamic mean-field theory, namely, the antiferromagnetic ordered phase exists even at zero temperature for a small value of p. The location of the critical point (p_c) at zero temperature was first estimated from the finite-size scaling of the cumulants of order parameter $U_L=1-\langle m_{AF}^4\rangle_L/3\langle m_{AF}^2\rangle_L^2$ [20]. As shown in the inset of Fig. 2, the plot of the reduced fourth-order cumulant for the different system size indicates clearly the nonzero value of critical probability. An alternating estimate was produced from the scaling plots of $m_{AF}L^{\beta/\nu}$ versus $L^{1/\nu}|p-p_c|/p_c$. Assuming that the universality class of the transition is that of the equilibrium Ising class [21], the fitting parameter p_c was determined by observing the collapse of data. Both methods yield the same result: $p_c(T=0)=0.019\pm0.0005$. For comparison, the corresponding value of the dynamical mean-field six-point approximation is $p_c^{(6p)}=0.047$.

It is also interesting to discuss the saturation of the order parameter $m_{AF}\to 1$ when $p\to 0$ at a fixed value of T. A typical value of the order parameter at $p=0.005$ is $m_{AF}(0.005)\approx 0.75$. If we start from a completely ordered antiferromagnetic state at a small value of p, only a Glauber process can generate a point defect with probability p. The Kawasaki process leaves this point defect unchanged because the single-point defect is surrounded by (1,1) or $(-1,-1)$ pairs. The defect can only be repaired by a subsequent Glauber process that is energetically unfavorable. In other words, the large concentration of long-lived point defects results in the unusual decrease in the order parameter. Based on this simple picture, a master equation for the defects can be constructed to estimate the order parameter at small p. This calculation yields

$$m_{AF}(p)=[1+p\exp(8J/k_BT)]^{-1}. \tag{3}$$

As a result, the saturation of the order parameter can only be observed if $p<\exp(-8J/k_BT)$.

In the case of ferromagnetic order-disorder transition, the crucial question is to decide whether computer simulations exhibit the emergence of first-order transition. For this purpose, we determine the fourth-order cumulant of energy ($V_L=1-\langle E^4\rangle_L/3\langle E^2\rangle_L^2$) as a function of the control parameter for different system sizes [22]. Simulations unambiguously have justified that the transition turns to be first-order if $p<p_t^{(MC)}\approx 0.2; T<T_t^{(MC)}\approx 1.49$. (The six-point approximation predicts $p_t^{(6p)}=0.69$ and $T_t^{(6p)}=2.166$.) The discontinuous transition has been detected if the temperature or the parameter p is varied below the tricitical values. Figure 3 illustrates the first-order transition where the values of V_L are averaged over 2×10^6 MC steps (for $L=16$) and 5×10^7 MC steps (for $L=60$). It is important to emphasize that very long MC runs are necessary to get the correct behavior. As an example, at $p=0.15$ and $L=30$ the ergodic time is about 5×10^6 MC steps but a clear hysteresis is observed in the order parameter as a function of temperature if the observation time is about 10^5 MC steps. The ferromagnetic-paramagnetic phase transition was also detected at zero temperature ($p_c^{(MC)}(T=0)=0.10(5)$) in agreement with the above prediction of dynamic mean-field theories. Our simulations have also supported that the critical temperature decreases monotonously if we decrease the competing parameter p. Our results are summarized in a phase diagram shown in Fig. 4 where the size of the boxes indicates the statistical error.

In summary, we have shown that starting from the equilibrium ferromagnetic state, all of the three possible stationary states can be reached even at zero temperature by increasing the energy flux. The ferromagnetic-paramagnetic phase transition changes from second to first order for sufficiently small p. These behaviors are supported by both more accurate dynamical mean-field approximations and MC simulations. The qualitative prediction of the mean-field approximations for the nonequilibrium phase diagram is satisfactory while the numerical differences between the approximations and MC simulations are still significant. The emergence of the dynamical tricritical point is in agreement with earlier observations in similar nonequilibrium models.

The author thanks György Szabó for stimulating discussions. He also thanks the HAS for financial support. This research was also supported by the Hungarian National Research Fund (OTKA) under Grant No. F-30449.

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