Kinetic phase transition in the antiferromagnetic Ising model with competing dynamics

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The antiferromagnetic Ising model on a square lattice is studied by the dynamic pair approximation, and the competition between the Glauber and Kawasaki dynamics is examined at zero temperature $T=0$. In the phase diagram drawn as a function of the competing parameter p, the important result such as the self-organization is found, and the effects of the spin-exchange strength in the Kawasaki process on the ordered ferromagnetic and antiferromagnetic states are discussed. We find that the exchange in the Kawasaki dynamics favors the ordered ferromagnetic state. [S1063-651X(98)01703-6]

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In recent years there has been much interest in the physics of dynamic or nonequilibrium phase transitions. In particular, the kinetic Ising model was introduced as a simplified model for a variety of biological, chemical, and physical systems [1–7]. The usual kinetic Ising model was investigated by allowing only single spin flips, which were first introduced by Glauber [8]. As is well known, however, the Glauber kinetic Ising model is a special case of more general spin-flip models that admit multiple spin flips. The kinetic Ising model in the presence of multiple spin flips serves for the study of self-organization phenomena in many different problems concerning the phase transitions of the magnetic systems. The emergence of the phenomena of self-organization in the kinetic Ising spin system has been studied by using the master-equation formalism when the system is governed by two competing processes: the one-spin-flip Glauber dynamics [8] and the two-spin-flip Kawasaki dynamics [7]. For the Glauber process, the system is characterized by single spin flips due to its contact with the heat bath at fixed temperature T. On the other hand, the Kawasaki dynamics is characterized by the exchange of the states of two nearest-neighbor spins. Depending on the competition between the Glauber process with a weight p and the Kawasaki process with a weight $(1-p)$, one can determine an interesting phase diagram as a function of the competing parameter p, which shows ferromagnetic, antiferromagnetic, and paramagnetic phases. For a two-dimensional ferromagnetic Ising system, Tome and de Oliveira [9] showed that within the dynamical pair approximation, the system undergoes a phase transition from the ferromagnetic to the paramagnetic phase as the value $(1-p)$ is increased, and for a further increase of $(1-p)$ the Kawasaki process dominates, and the system self-organizes into an ordered antiferromagnetic phase. In contrast, when the interactions between spins are of the antiferromagnetic type, Grandi and Figueiredo [10] found that the self-organization phenomenon does not appear when the Kawasaki dynamics dominates, and the only stable phase that remains is the paramagnetic one. Despite this theoretical progress, some important effects on the phase transition of such systems have not been addressed, because the Kawasaki dynamics has been simplified to be independent of the strength of exchange between spins when the change in energy is less than zero [9,10]. In this paper, we apply the dynamical pair approximation to examine the competition between the Glauber and the Kawasaki dynamics in the two-dimensional Ising antiferromagnetic system at zero temperature. We will be interested in particular in the Kawasaki two-spin exchange process. We think that the exchange probability between spins is dependent on the strength of exchange between spins. Our goal is to determine whether the competition between this modified Kawasaki dynamics and the spin-flip Glauber one causes the self-organization behavior. The result is novel: the system will self-organize from the paramagnetic phase into the ordered ferromagnetic phase when the Kawasaki dynamics is the dominant one. For the vanishing of the spin-exchange strength, our result reduces to that obtained by Grandi and Figueiredo [10] where the ordered ferromagnetic phase does not exist.

We consider an antiferromagnetic Ising model on a square lattice with N lattice sites. The state of the system is represented by $\sigma=(\sigma_1,\sigma_2,\ldots,\sigma_i,\ldots\sigma_N)$, where σ_i is the spin variable at site i, taking the value $+1$ or -1. The energy of the system in state σ is given by

$$E=J\sum_{\langle i,j\rangle}\sigma_i\sigma_j, \tag{1}$$

where $J>0$ for antiferromagnetism, and $\langle i,j\rangle$ runs over nearest neighbors. Following Tome and de Oliveira [9], we

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write the evolution of the state σ in time through the master equation. Let $P(\sigma,t)$ be the probability of state σ at time t. The evolution of $P(\sigma,t)$ is given by the master equation

$$\frac{dP(\sigma,t)}{dt}=\sum_{\sigma'}\left[P(\sigma',t)\omega(\sigma',\sigma)-P(\sigma,t)\omega(\sigma,\sigma')\right], \tag{2}$$

where $\omega(\sigma',\sigma)$ gives the probability, per unit time, of the transition from state σ' to state σ, if the system is state σ'. In order to take into account the two competing Glauber and Kawasaki dynamics, we assume that

$$\omega(\sigma',\sigma)=p\,\omega_G(\sigma',\sigma)+(1-p)\,\omega_K(\sigma',\sigma), \tag{3}$$

where p measures a weight for the Glauber process and $(1-p)$ for the Kawasaki one. And $\omega_G(\sigma',\sigma)$ is associated to the Glauber process and $\omega_K(\sigma',\sigma)$ to the Kawasaki process, respectively. The Glauber process is simulated by the one-spin flip dynamics [8], so that

$$\omega_G(\sigma',\sigma)=\sum_{i=1}^{N}\delta_{\sigma_1'\sigma_1}\delta_{\sigma_2'\sigma_2}\cdots\delta_{\sigma_i'-\sigma_i}\cdots\delta_{\sigma_N'\sigma_N}\omega_i(\sigma), \tag{4}$$

where $\omega_i(\sigma)$ is the probability of flipping spin i. The contact with the heat bath at temperature $T=0$ follows the Metropolis prescription

$$\omega_i(\sigma)=\begin{cases}1, & \text{if} \quad \Delta E_i\leqslant 0\\ 0, & \text{if} \quad \Delta E_i>0,\end{cases} \tag{5}$$

where ΔE_i is the change in energy obtained after flipping spin i. On the other hand, the Kawasaki process is simulated by the two-spin exchange dynamics [7], that is,

$$\omega_K(\sigma',\sigma)=\sum_{\langle i,j\rangle}^{N}\delta_{\sigma_1'\sigma_1}\cdots\delta_{\sigma_i'\sigma_j}\cdots\delta_{\sigma_j'\sigma_i}\cdots\delta_{\sigma_N'\sigma_N}\omega_{ij}(\sigma), \tag{6}$$

where $\omega_{ij}(\sigma)$ is the probability of exchange between the nearest-neighbor spin i and j. If the change in energy after exchanging the neighboring spins i and j is positive, then the new configuration is automatically accepted; if, however, it is negative, the new configuration is accepted with probability, depending on the strength of the exchange between spins. We take

$$\omega_{ij}(\sigma)=\begin{cases}\exp(\Delta E_{ij}/D), & \text{if} \quad \Delta E_{ij}<0\\ 1, & \text{if} \quad \Delta E_{ij}\geqslant 0,\end{cases} \tag{7}$$

where ΔE_{ij} is the change in energy obtained after exchange of spins i and j. D is the strength of exchange between two nearest-neighbor spins i and j. In the vanishing of the two-spin exchange strength $D=0$, Eq. (7) reduces to the case considered by Grandi and Figueiredo [10]. On the other hand, for very large values of D, Eq. (7) shows that the system favors the full exchange between spins, independent of the energy change of exchange between spins. Let us denote by $\langle f(\sigma)\rangle$ the average of the state function $f(\sigma)$, that is,

$$\langle f(\sigma)\rangle=\sum_{\sigma} f(\sigma)P(\sigma,t). \tag{8}$$

Combining the master equation (2) with Eq. (8), the equation for the magnetization $\langle\sigma_i\rangle$ of spin i and for the correlation $\langle\sigma_j\sigma_k\rangle$ of the nearest-neighbor spin j and k can be derived to yield

$$\frac{d\langle\sigma_i\rangle}{dt}=pA_i+(1-p)B_i, \tag{9}$$

$$\frac{d\langle\sigma_j\sigma_k\rangle}{dt}=pA_{jk}+(1-p)B_{jk}, \tag{10}$$

with

$$A_i=-2\langle\sigma_i\omega_i(\sigma)\rangle, \tag{11}$$

$$A_{jk}=-2\langle\sigma_j\sigma_k\omega_j(\sigma)\rangle-2\langle\sigma_j\sigma_k\omega_k(\sigma)\rangle, \tag{12}$$

$$B_i=\sum_{\substack{l\\(\text{NN of } i)}}\langle(\sigma_l-\sigma_i)\omega_{li}(\sigma)\rangle, \tag{13}$$

$$B_{jk}=\sum_{\substack{l(\neq k)\\(\text{NN of } j)}}\langle\sigma_k(\sigma_l-\sigma_j)\omega_{jl}(\sigma)\rangle+\sum_{\substack{l(\neq j)\\(\text{NN of } k)}}\langle\sigma_j(\sigma_l-\sigma_k)\omega_{kl}(\sigma)\rangle, \tag{14}$$

where (NN of i) means that the summation is over the nearest neighbors of site i. Although the set of equations (11)–(14) is exact, the mean values of these equations cannot be calculated because we do not know the exact full expression for the probability $P(\sigma,t)$. Here, we apply the pair approximation method [9,11] to calculate the average value in Eqs. (11)–(14). In the pair approximation, the system is described by a central spin with its nearest neighbors and a pair of nearest-neighbor spins surrounded by its nearest-neighbor spins to estimate the quantities A_i, A_{jk} and B_i, B_{jk}, respectively. The probability of the various environments of a given spin or pair of spins is written in terms of the probability of a pair of spins [9,11,12], which, in turn, is obtained from the values of $\langle\sigma_i\rangle$ and $\langle\sigma_j\sigma_k\rangle$. Thus a set of self-consistent equations for the time evolution of $\langle\sigma_i\rangle$ and $\langle\sigma_j\sigma_k\rangle$ are obtained by averaging over the probability of clusters of spins considered. We assume that the lattice is bipartite and divided into 1 and 2 sublattices, with respective magnetizations m_1 and m_2. Then, we look for solutions such that $\langle\sigma_i\rangle=m_1$ for any spin belonging to sublattice 1, $\langle\sigma_j\rangle=m_2$ for any spin belonging to sublattice 2, and $\langle\sigma_i\sigma_j\rangle=r$ for any pair of nearest-neighbor spins i and j. By using the pair approximation and taking into account the transition probability given by Eqs. (3)–(7), after straightforward calculation on Eqs. (11)–(14) we obtain the self-consistent equations for the evolution of the quantities m_1, m_2, and r,

$$\frac{dm_1}{dt}=pA_1(m_1,m_2,r)+(1-p)B_1(m_1,m_2,r), \tag{15}$$

$$\frac{dm_2}{dt}=pA_2(m_1,m_2,r)+(1-p)B_2(m_1,m_2,r), \quad (16)$$

$$\frac{dr}{dt}=pA_{12}(m_1,m_2,r)+(1-p)B_{12}(m_1,m_2,r), \quad (17)$$

where A_1, A_2, A_{12}, B_1, B_2, and B_{12} are given by

$$A_1(m_1,m_2,r)=-\frac{2}{x_1^3}(z^4+4z^3v_1+6z^2v_1^2)+\frac{2}{y_1^3}(w^4+4w^3v_2+6w^2v_2^2), \quad (18)$$

$$A_2(m_1,m_2,r)=A_1(m_2,m_1,r), \quad (19)$$

$$A_{12}(m_1,m_2,r)=-\frac{1}{x_1^3}(2z^4+4z^3v_1)-\frac{1}{y_1^3}(2w^4+4w^3v_2)-\frac{1}{x_2^3}(2z^4+4z^3v_2)-\frac{1}{y_2^3}(2w^4+4w^3v_1), \quad (20)$$

$$\begin{aligned}B_1(m_1,m_2,r)=&-\frac{8}{x_1^3y_2^3}[z^3v_1^4+3z^2v_1^5+3zv_1^6+v_1^7\\&+3\eta z^3wv_1^3+9z^2wv_1^4+9zwv_1^5+3wv_1^6\\&+3\eta^2z^3w^2v_1^2+9\eta z^2w^2v_1^3+9zw^2v_1^4\\&+3w^2v_1^5+\eta^3z^3w^3v_1+3\eta^2z^2w^3v_1^2\\&+3\eta zw^3v_1^3+w^3v_1^4]+\frac{8}{x_2^3y_1^3}[z^3v_2^4+3z^2v_2^5\\&+3zv_2^6+v_2^7+3\eta z^3wv_2^3+9z^2wv_2^4+9zwv_2^5\\&+3wv_2^6+3\eta^2z^3w^2v_2^2+9\eta z^2w^2v_2^3\\&+9zw^2v_2^4+3w^2v_2^5+\eta^3z^3w^3v_2\\&+3\eta^2z^2w^3v_2^2+3\eta zw^3v_2^3+w^3v_2^4], \quad (21)\end{aligned}$$

$$B_2(m_1,m_2,r)=-B_1(m_1,m_2,r), \quad (22)$$

$$\begin{aligned}B_{12}(m_1,m_2,r)=&\frac{12}{x_1^3y_2^3}[z^2v_1^5+2zv_1^6+3wzv_1^5+v_1^7+2wv_1^6\\&+w^2v_1^5-\eta wz^3v_1^3-2\eta^2w^2z^3v_1^2\\&-3\eta w^2z^2v_1^3-\eta^3z^3w^3v_1-\eta w^3zv_1^3\\&-2\eta^2z^3w^2v_1^2]+\frac{12}{x_2^3y_1^3}[z^2v_2^5+2zv_2^6\\&+3wzv_2^5+v_2^7+2wv_2^6+w^2v_2^5-\eta wz^3v_2^3\\&-2\eta^2w^2z^3v_2^2-3\eta w^2z^2v_2^3-\eta^3z^3w^3v_2\\&-\eta w^3zv_2^3-2\eta^2z^3w^2v_2^2], \quad (23)\end{aligned}$$

where

$$x_1=\tfrac{1}{2}(1+m_1),\quad y_1=\tfrac{1}{2}(1-m_1),$$

$$x_2=\tfrac{1}{2}(1+m_2),\quad y_2=\tfrac{1}{2}(1-m_2),$$

$$z=\tfrac{1}{4}(1+m_1+m_2+r),\quad v_1=\tfrac{1}{4}(1+m_1-m_2-r),$$

$$v_2=\tfrac{1}{4}(1-m_1+m_2-r),\quad w=\tfrac{1}{4}(1-m_1-m_2+r),$$

$$\eta=\exp(-4J/D).$$

Depending on the parameters m_1 and m_2, there are the following three types of stationary states: the paramagnetic $m_1=m_2=0$, the ferromagnetic $m_1=m_2\neq 0$, and the antiferromagnetic state $m_1=-m_2\neq 0$. The paramagnetic state corresponds to the trivial solutions of Eqs. (15)–(17). Setting $m_1=m_2=0$, we get the equation describing the paramagnetic stable state,

$$p(z^4+2z^3v)-24(1-p)(5z^2v^5+4zv^6+v^7-\eta^3z^6v-4\eta^2z^5v^2-5\eta z^4v^3)=0, \quad (24)$$

where $z=(1+r^*)/4$, $v=(1-r^*)/4$, $\eta=\exp(-4J/D)$, and $r=r^*$ is the solution of $pA_{12}(0,0r^*)+(1-p)B_{12}(0,0r^*)=0$. On the other hand, we can distinguish the ferromagnetic state from the antiferromagnetic state by defining the quantities $m_A=(m_1-m_2)/2$ and $m_F=(m_1+m_2)/2$, respectively. To derive the transition lines for the disordered paramagnetic and ordered phases, we can expand the right-hand side of Eqs. (15)–(17) up to linear terms in m_1 and m_2 and obtain

$$\frac{dm_A}{dt}=\lambda_A m_A, \quad (25)$$

$$\frac{dm_F}{dt}=\lambda_F m_F, \quad (26)$$

where

$$\begin{aligned}\lambda_A=&16p(6z^4+24z^3v+36z^2v^2-4z^3-12z^2v)\\&+512(1-p)[15z^2(12v^5-5v^4)\\&+6z(12v^6-6v^5)+(12v^7-7v^6)+20z^3(12v^4-4v^3)\\&+15\eta z^4(12v^3-3v^2)+12\eta^2z^5(6v^2-v)\\&+\eta^3z^6(12v-1)],\end{aligned}$$

$$\lambda_F=16p[12(3z^2-z)v^2+12(2z^3-z^2)v-4z^3+6z^4].$$

The boundary between the ferromagnetic (antiferromagnetic) and paramagnetic phases is given by the simultaneous solution of Eq. (24) and $\lambda_F=0$ ($\lambda_A=0$). The resulting phase diagram is shown in Fig. 1. As is seen from this figure, the stable antiferromagnetic region is very small near $p=1$ even at zero temperature $T=0$, and is easily destroyed by a small ratio $(1-p)/p$ where the Glauber process still dominates. Increasing the ratio $(1-p)/p$, the equilibrium ordered antiferromagnetic state quickly disappears, giving place to the disordered paramagnetic state. With a further increase of the ratio $(1-p)/p$, the Kawasaki process starts to dominate. A most interesting finding is that for nonzero exchange strength

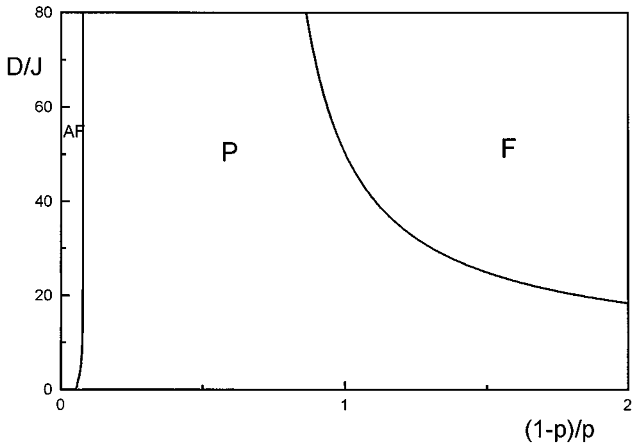

FIG. 1. Phase diagram of the antiferromagnetic Ising system with competing Glauber (probability p) and Kawasaki (probability $1-p$) dynamics. D measures the strength of exchange between two nearest-neighbor spins when ΔE_{ij} is less than zero. As the ratio $(1-p)/p$ increases, the system goes continuously from the antiferromagnetic (AF) to the paramagnetic (P) state, and self-organizes into an ordered ferromagnetic (F) stable state.

$D\neq 0$ the system will self-organize into a new stationary phase, which is identified with the ordered ferromagnetic phase. In the $D\rightarrow 0$ limit, the paramagnetic-ferromagnetic phase boundary does not appear and there exist only two stationary antiferromagnetic and paramagnetic states. This is agreement with the conclusion of Grandi and Figueiredo [10]. On the other hand, the transition line between the antiferromagnetic and paramagnetic phases, which occurs at large values of the competition parameter p where the Glauber process dominates, is affected only slightly by the strength of exchange D. In contrast, the paramagnetic-ferromagnetic phase transition appearing at large values of $(1-p)$ for any exchange rate $D\neq 0$ where the Kawasaki process dominates, is affected largely by the strength of exchange D. We find that the region of the ferromagnetic phase is enlarged by increasing the magnitude of the spin-exchange strength D in the Kawasaki process when the change in spin-exchange energy is less than zero. This indicates that the two-spin exchange strength favors the ferromagnetic ordering, like phase separation problem in chemically reactive binary mixtures [6].

In conclusion, the antiferromagnetic Ising model with competing Glauber and Kawasaki dynamics has been investigated by combining the master-equation formalism with the dynamic pair approximation. We have discussed aspects of the self-organization phenomenon of the system at $T=0$, and demonstrated the existence of the transition from the disordered paramagnetic into the ferromagnetic phases as the ratio $(1-p)/p$ increases. The region of the ferromagnetic phase decreases with a decrease of the spin-exchange strength D, and when the strength of exchange $D=0$, our results reduce to that of Grandi and Figueiredo, where the ordered ferromagnetic state disappears.

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[1] J. Marro and R. Dickman, *Nonequilibrium Phase transitions* (Cambridge University Press, Cambridge, 1997).
[2] J. L. Skinner, J. Chem. Phys. **79**, 1955 (1983).
[3] T. Vojta, Phys. Rev. E **55**, 5157 (1997).
[4] Z. F. Huang and B. L. Gu, Phys. Rev. E **55**, R4841 (1997).
[5] E. P. Gueuvoghlanian and T. Tome, Int. J. Mod. Phys. B **10**, 1245 (1997).
[6] S. C. Glotzer, P. Stauffer, and N. Jan, Phys. Rev. Lett. **72**, 4109 (1994).
[7] K. Kawasaki, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, London, 1972), Vol. 2, p. 443.
[8] R. J. Glauber, J. Math. Phys. **4**, 294 (1963).
[9] T. Tome and M. J. de Oliveira, Phys. Rev. A **40**, 6643 (1989).
[10] B. C. S. Grandi and W. Figueiredo, Phys. Rev. B **50**, 12 595 (1994).
[11] H. Mamada and F. Takano, J. Phys. Soc. Jpn. **25**, 675 (1968).
[12] R. Dickman, Phys. Lett. A **122**, 463 (1987).