Competition between the Glauber and Kawasaki dynamics in the antiferromagnetic Ising model

B. C. S. Grandi and W. Figueiredo
Departamento de Física, Universidade Federal de Santa Catarina, 88040-900 Florianópolis, Santa Catarina, Brazil
(Received 16 May 1994)

We study, within the dynamic-pair approximation, the behavior of the antiferromagnetic Ising model in contact with a heat bath and subject to an external source of energy. The contact with the heat bath is simulated by the Glauber process while the continuous flux of energy into the system is simulated by the Kawasaki process. We find the phase diagram of this model, and we show that, conversely to what happens for the ferromagnetic Ising model, the antiferromagnetic Ising model does not show the phenomenon of self-organization within the dynamic-pair approximation.

I. INTRODUCTION

The self-organization in systems subject to an external flux of energy is an interesting phenomenon studied in the realm of nonequilibrium statistical physics.[1] The self-organization in magnetic systems was considered recently by Tomé and de Oliveira[2] for a ferromagnetic Ising system coupled to a heat bath and subject to an external flux of energy. Their open system is in contact with a heat bath whose stochastic dynamics is simulated by a Glauber process,[3] while the continuous flux of energy is simulated by a stochastic dynamics given by a Kawasaki process,[4] characterized by the exchange of the states of two nearest-neighbor spins. They show that, as the flux of energy is increased, the system goes continuously from the ferromagnetic to the paramagnetic state, and, for a further increase in the flux of energy, it goes continuously to an antiferromagnetic stable state. In this work we investigate the possibility of self-organization for the antiferromagnetic Ising model when we take into account the competition between the Glauber and Kawasaki processes. We show that this model is not symmetric to the ferromagnetic Ising case, since here we only find a transition line between the antiferromagnetic and paramagnetic phases at low flux of energy. If we increase the flux of energy, the only stable states we find are of the paramagnetic type. The equations of motion for the mean values and for the correlation function between nearest-neighboring spins are found from the temporal evolution of the probability to find the system in a given state, through its associated master equation. Then we use the dynamical-pair approximation to solve the coupled system of equations, which permits the determination of the phase diagram of this model.

II. EQUATIONS OF MOTION FOR THE MEAN VALUES

We consider here an antiferromagnetic Ising model on a square lattice with N lattice sites. We represent the state of the system by $\sigma=(\sigma_1,\sigma_2,\ldots,\sigma_N)$, where the spin variable σ_i can take only the values ± 1. The energy of the system in the state σ is given by

$$E(\sigma)=J\sum_{(i,j)}\sigma_i\sigma_j \ , \tag{1}$$

where the summation is only over pairs of nearest-neighbor spins and $J>0$. Following Tomé and de Oliveira[2] we write the evolution of the state σ in time through the master equation. If $P(\sigma,t)$ is the probability of finding the system in the state σ at time t, the associated master equation is written as

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

In this equation, $W(\sigma',\sigma)$ gives the probability, per unit time, for the transition from the state σ' to state σ. In order to take into account the two competing processes we assume that

$$W(\sigma',\sigma)=pW_G(\sigma',\sigma)+(1-p)W_K(\sigma',\sigma) \ , \tag{3}$$

where

$$W_G(\sigma',\sigma)=\sum_{i=1}^{N}\delta_{\sigma_1',\sigma_1}\delta_{\sigma_2',\sigma_2},\ldots,\delta_{\sigma_N',\sigma_N}w_i(\sigma) \tag{4}$$

is the one-spin-flip Glauber process which simulates the contact with the heat bath at temperature T, and

$$W_K(\sigma',\sigma)=\sum_{ij}\delta_{\sigma_1',\sigma_1}\delta_{\sigma_2',\sigma_2},\ldots,\delta_{\sigma_i',\sigma_j},\ldots, \times\delta_{\sigma_j',\sigma_i},\ldots,\delta_{\sigma_N',\sigma_N}w_{ij}(\sigma) \tag{5}$$

is the two-spin-flip Kawasaki process, which simulates the flux of energy into the system. In these two equations $w_i(\sigma)$ is the probability, per unit time, of flipping spin i, while $w_{ij}(\sigma)$ is the probability, per unit time, of exchanging two nearest-neighbor spins i and j. We adopt the following prescriptions for $w_i(\sigma)$ and $w_{ij}(\sigma)$:

$$w_i(\sigma)=\min\left[1,\exp\left[-\frac{\Delta E_i}{k_BT}\right]\right] , \tag{6}$$

and

$$w_{ij}=\begin{cases}0 & \text{for } \Delta E_{ij}\le 0 \ ,\\ 1 & \text{for } \Delta E_{ij}>0 \ ,\end{cases} \tag{7}$$

where ΔE_i is the change in energy after flipping spin i, and ΔE_{ij} is the change in energy after exchanging spins i and j. It is easy to show that the temporal evolution for the magnetization $\langle \sigma_i \rangle$ and for the correlation function between nearest-neighbor spins $\langle \sigma_j \sigma_k \rangle$ is given, respectively, by

$$\frac{d\langle \sigma_i \rangle}{dt} = pA_i + (1-p)B_i \ , \tag{8}$$

$$\frac{d\langle \sigma_j \sigma_k \rangle}{dt} = pA_{jk} + (1-p)B_{jk} \ , \tag{9}$$

where

$$A_i = -2\langle \sigma_i w_i(\sigma) \rangle \ , \tag{10}$$

$$A_{jk} = -2\langle \sigma_j \sigma_k w_j(\sigma) \rangle - 2\langle \sigma_j \sigma_k w_k(\sigma) \rangle \ , \tag{11}$$

$$B_i = \sum_{\substack{l \\ (\text{NN of } i)}} \langle (\sigma_l - \sigma_i) w_{li}(\sigma) \rangle \ , \tag{12}$$

$$B_{jk} = \sum_{\substack{l \neq k \\ (\text{NN of } j)}} \langle (\sigma_l \sigma_k - \sigma_j \sigma_k) w_{jl}(\sigma) \rangle + \sum_{\substack{l \neq j \\ (\text{NN of } k)}} \langle (\sigma_j \sigma_l - \sigma_j \sigma_k) w_{kl}(\sigma) \rangle \ , \tag{13}$$

and (NN of i) indicates that the summation is over the nearest neighbors of site i. Although the set of equations (8)–(13) is exact, the mean values of the right-hand sides of these equations cannot be calculated because we do not know the exact full expression for the probability $P(\sigma,t)$. Then we need to consider an approximate expression for $P(\sigma,t)$. We employ here the pair approximation[5,6] to evaluate the mean values on the right-hand sides of Eqs. (10)–(13). First of all, we divide our lattice into two sublattices, so that first-neighbor sites belong to different sublattices, and look for solutions such that $\langle \sigma_1 \rangle = m_1$ for any spin belonging to sublattice 1, and $\langle \sigma_2 \rangle = m_2$ for any spin of sublattice 2. The correlation function between spins σ_1 and σ_2 is written as $\langle \sigma_1 \sigma_2 \rangle = r$. If we then perform these calculations within the pair approximation we easily obtain the expressions for the evolution of m_1, m_2, and r. We then can write the following expressions:

$$A_1(m_1,m_2,r) = -\frac{2}{x_1^3}(z^4 + 4z^3v_1 + 6z^2v_1^2 + 4\eta z v_1^3 + \eta^2 v_1^4) + \frac{2}{y_1^3}(w^4 + 4w^3v_2 + 6w^2v_2^2 + 4\eta w v_2^3 + \eta^2 v_2^4) \ , \tag{14}$$

$$A_2(m_1,m_2,r) = A_1(m_2,m_1,r) \ , \tag{15}$$

$$\begin{aligned} A_{12}(m_1,m_2,r) = {} & \frac{1}{x_1^3}(-2z^4 - 4z^3v_1 + 4\eta z v_1^3 + 2\eta^2 v_1^4) + \frac{1}{y_1^3}(-2w^4 - 4w^3v_2 + 4\eta w v_2^3 + 2\eta^2 v_2^4) \\ & + \frac{1}{x_2^3}(-2z^4 - 4z^3v_2 + 4\eta z v_2^3 + 2\eta^2 v_2^4) + \frac{1}{y_2^3}(-2w^4 - 4w^3v_1 + 4\eta w v_1^3 + 2\eta^2 v_1^4) \ , \end{aligned} \tag{16}$$

$$\begin{aligned} B_1(m_1,m_2,r) = {} & -\frac{8}{x_1^3 y_2^3}(3z^2v_1^5 + 3zv_1^6 + 3w^2v_1^5 + 3wv_1^6 + 9zwv_1^5 + v_1^7) \\ & + \frac{8}{x_2^3 y_1^3}(3z^2v_2^5 + 3zv_2^6 + 3w^2v_2^5 + 3wv_2^6 + 9zwv_2^5 + v_2^7) \ , \end{aligned} \tag{17}$$

$$B_2(m_1,m_2,r) = -B_1(m_1,m_2,r) \ , \tag{18}$$

$$\begin{aligned} B_{12}(m_1,m_2,r) = {} & \frac{6}{x_1^3 y_2^3}(3z^3v_1^3w + 3z^3v_1^2w^2 + 3z^2v_1^3w^2 + z^3w^3v_1 \\ & + z^2v_1^2w^3 - zv_1^3w^3 - z^2v_1^5 + zv_1^6 + v_1^7 + 3zwv_1^5 + 3wv_1^6 + 3w^2v_1^5) \\ & + \frac{6}{x_2^3 y_1^3}(3zw^3v_2^3 + 3z^2w^3v_2^2 + 3z^2w^2v_2^3 + z^3w^3v_2 + z^3w^2v_2^2 \\ & - z^3wv_2^3 - w^2v_2^5 + wv_2^6 + v_2^7 + 3zwv_2^5 + 3zv_2^6 + 3z^2v_2^5) \ , \end{aligned} \tag{19}$$

where

$$x_{1,2} = \tfrac{1}{2}(1 + m_{1,2}) \ , \tag{20}$$

$$y_{1,2} = \tfrac{1}{2}(1 - m_{1,2}) \ , \tag{21}$$

$$z = \tfrac{1}{4}(1 + m_1 + m_2 + r) \ , \tag{22}$$

$$v_{1,2} = \tfrac{1}{4}(1 + m_{1,2} - m_{2,1} - r) \ , \tag{23}$$

$$w = \tfrac{1}{4}(1 - m_1 - m_2 + r) \ , \tag{24}$$

$$\eta = \exp\left[-\frac{4J}{k_B T}\right] . \tag{25}$$

III. RESULTS

We look for the stationary solutions of Eqs. (8) and (9). We try solutions of the following types: $m_1 = -m_2 \neq 0$, antiferromagnetic stable states, $m_1 = m_2 \neq 0$, ferromagnetic stable solutions, and $m_1 = m_2 = 0$, corresponding to the paramagnetic stable states. Then, the paramagnetic stationary state is given by the following expression:

$$p(-z^4-2z^3v+2\eta zv^3+\eta^2v^4)+12(1-p)\times(z^6v+4z^5v^2+5z^4v^3+5z^2v^5+4zv^6+v^7)=0\ , \quad (26)$$

where $z=(1+r^*)/4$, $v=(1-r^*)/4$, $\eta=\exp(-4J/k_BT)$, and r^* is the stationary solution of Eq. (9) where we have taken $m_1=m_2=0$. We can find the phase diagram for this antiferromagnetic model by considering the stationary solutions for m_1 and m_2 from Eq. (8). If we write the order parameter for the ferromagnetic phase in the form $m_F=(m_1+m_2)/2$, and the antiferromagnetic phase as $m_A=(m_1-m_2)/2$, and we expand the right-hand side of Eq. (8) up to linear terms in m_1 and m_2, we obtain

$$\frac{dm_A}{dt}=\lambda_A m_A\ , \quad (27)$$

$$\frac{dm_F}{dt}=\lambda_F m_F\ , \quad (28)$$

where

$$\lambda_A=32p[\eta^2(3v^4-2v^3)+3\eta(4v^3-2v^2)z+6(3v^2-v)z^2+2(6v-1)z^3+3z^4]+512(1-p)[15(12v^5-5v^4)z^2+6(12v^6-6v^5)z-7v^6]\ , \quad (29)$$

$$\lambda_F=32p[3\eta^2v^4+2\eta(6z-1)v^3+6(3z^2-z)v^2+6(2z^3-z^2)v-2z^3+3z^4]\ , \quad (30)$$

with $z=(1+r^*)/4$ and $v=(1-r^*)/4$. The transition between the antiferromagnetic and paramagnetic phases can be obtained by solving simultaneously Eqs. (26) and (29) with $\lambda_A=0$. This defines the continuous paramagnetic-antiferromagnetic transition line as we can see in Fig. 1. If $p=1$, we find that the Néel temperature is given by $k_BT=2.885J$, which is the equilibrium critical temperature in the Bethe-Peierls approximation. It is interesting to note that the stable antiferromagnetic region is very small when compared with the corresponding region obtained for the ferromagnetic Ising model.[2] The antiferromagnetic phase is destroyed by a small input of energy into the system. If we try to solve simultaneously Eqs. (26) and (30) with $\lambda_F=0$, we do not find any solution for p in the range $0<p\leq 1$. That is, the paramagnetic-ferromagnetic transition line is absent in this antiferromagnetic model. Therefore, the self-organization phenomenon, observed for the ferromagnetic Ising model with competing Glauber and Kawasaki dynamics,[2] has no counterpart for the antiferromagnetic Ising model with the same two competing dynamics for any finite value of the parameter $(1-p)/p$.

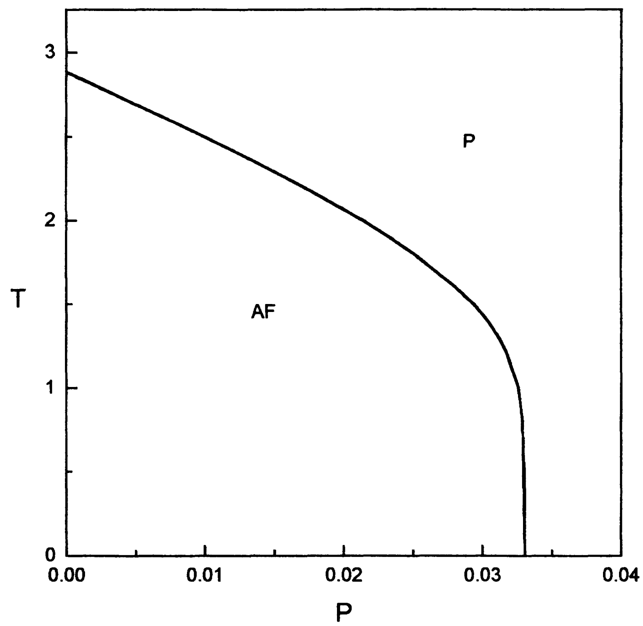

FIG. 1. Phase diagram of the kinetic antiferromagnetic Ising model in two dimensions. T is the heat-bath temperature and $P=(1-p)/p$ is related to the flux of energy. The system exhibits only the antiferromagnetic (AF) and paramagnetic (P) phases, separated by a line of continuous nonequilibrium transitions.

IV. CONCLUSIONS

We have studied the behavior of an antiferromagnetic Ising model in two dimensions, which is in contact with a heat bath and subject to a continuous flux of energy from an external source. By employing the dynamical-pair approximation we have found only two stationary states: the antiferromagnetic and paramagnetic states. For finite values of the energy input, which is simulated by the Kawasaki dynamics, the ferromagnetic state is never attained. Moreover, the antiferromagnetic region occupies only a small area in the phase diagram. That is, the nonequilibrium antiferromagnetic state is easily destroyed with a small flux of energy into the system. As expected, the flux of energy into the system breaks the symmetry between the ferromagnetic and antiferromagnetic Ising models observed in equilibrium. While the ferromagnetic Ising model subject to two competing dynamics exhibits the self-organization phenomenon, the antiferromagnetic Ising model displays only a paramagnetic-antiferromagnetic transition line in its phase diagram.

ACKNOWLEDGMENTS

We wish to thank Mario José de Oliveira and Tânia Tomé for many suggestions, and Jürgen F. Stilck for a critical reading of the manuscript. We also acknowledge the Brazilian agency CNPq for financial support.

[1]G. Nicolis and I. Prigogine, *Self-Organization in Non-Equilibrium Systems* (Wiley, New York, 1977).
[2]T. Tomé and M. J. de Oliveira, Phys. Rev. A **21**, 6643 (1989).
[3]R. J. Glauber, J. Math. Phys. **4**, 294 (1963).
[4]K. Kawasaki, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, London, 1972), Vol. 2.
[5]H. Mamada and F. Takano, J. Phys. Soc. Jpn. **25**, 675 (1968).
[6]R. Dickman, Phys. Lett. A **122**, 463 (1987).