Competitive dynamics in a three-dimensional Ising model

J. R. S. Leão, B. C. S. Grandi, and W. Figueiredo*
Departamento de Física, Universidade Federal de Santa Catarina, 88040-900 Florianópolis, SC, Brazil
(Received 28 April 1999)

We consider a three-dimensional ferromagnetic Ising model on a cubic lattice in contact with a heat bath at temperature *T*. The states of the system evolve in time according to two stochastic processes: the one-spin-flip Glauber dynamics where the order parameter is not conserved, and the two-spin-exchange Kawasaki kinetics, which conserves the order parameter. The former process mimics an input of energy into the system. Monte Carlo simulations were employed to determine the phase diagram for the stationary states of the model, and the corresponding critical exponents. Similarly to the observed for the related two-dimensional ferromagnetic Ising model, the phase diagram obtained exhibits the phenomenon of self-organization. Although the stationary states are mainly ferromagnetic at low temperatures, an antiferromagnetic phase appears for extremely high values of the flux of energy. Unlike the ferromagnetic case, the region of the phase diagram occupied by the antiferromagnetic phase is now larger. The determined critical exponents for this nonequilibrium model are in agreement with the well-known accepted values for the three-dimensional equilibrium Ising model. [S1063-651X(99)16111-7]

PACS number(s): 64.60.Ht

In this work we consider a three-dimensional version of a nonequilibrium ferromagnetic Ising model subject to two competing dynamical processes: the one-spin-flip Glauber dynamics [1], with probability *p*, and the two-spin-exchange Kawasaki dynamics [2], with probability $1-p$. While the Glauber dynamics takes account of the relaxation of the spin system in the heat bath at temperature *T*, the Kawasaki one simulates the absorption of energy by the system from an external agency. The role of these two dynamics concerning the symmetries of the system is quite different: the ferromagnetic order parameter is conserved in the Kawasaki kinetics, while it is not conserved in the Glauber one. This model was previously studied in the square lattice by Tomé and de Oliveira [3] using the dynamical pair approximation scheme and by two of us [4] by Monte Carlo simulations. In the pair approximation, the phenomenon of self-organization is observed: the system goes continuously from a ferromagnetic to a paramagnetic state as we increase the flux of energy into the system. By increasing this flux of energy more and more, we pass from the disordered paramagnetic phase to an ordered antiferromagnetic phase. On the other hand, Monte Carlo simulations on this model give a completely different picture, notably at very low temperatures. Although we observe a small antiferromagnetic region in the phase diagram for $p \leq 0.073$, and at very high temperatures, the self-organization phenomenon disappears in the limit of zero temperature. In this limit, we observe that the ferromagnetic phase is stable for all values of the competition parameter *p*.

Our previous analysis is extended now to the three-dimensional ferromagnetic Ising model with competing Glauber and Kawasaki dynamics. We employ Monte Carlo simulations and finite size scaling [5,6] in order to find the phase diagram and the critical exponents of the model. We will show that similarly to the corresponding two-dimensional case, at zero temperature, the ferromagnetic phase is stable for all values of *p*. On the other hand, the antiferromagnetic phase occupies a large area in the phase diagram. In this respect, it is similar to the observed in the pair approximation calculations for the two-dimensional ferromagnetic model [3]. At very high temperatures, the disordered paramagnetic phase is destroyed by a critical value of the flux of energy into the system, and it self-organizes in an antiferromagnetic arrangement of spins.

We consider a ferromagnetic Ising model on a cubic lattice with *N* lattice sites. The energy of the system in the state $\sigma=(\sigma_1,\sigma_2,\ldots,\sigma_N)$, where the spin variable assumes the values $\sigma_i=\pm 1$, is given by

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

In the summation, only spins that are nearest neighbors are considered, and $J>0$. Let $P(\sigma,t)$ be the probability of finding the system in the state σ at time t. The evolution of $P(\sigma,t)$ is given by the following master equation:

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

where $W(\sigma',\sigma)$ gives the probability, per unit time, for the transition from the state σ' to state σ. We assume that the two competing processes can be written as

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

In this equation,

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

*Electronic address: wagner@fisica.ufsc.br

is the single-spin-flip Glauber process, which simulates the relaxation of the system towards the equilibrium states at the temperature T, and

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

is the two-spin-exchange Kawasaki process, which mimics the flux of energy into the system. In the above summation, only pairs of nearest-neighbor spins are considered.

In these equations, $w_i(\sigma)$ is the transition probability of flipping spin i, while $w_{ij}(\sigma)$ is the transition probability of exchanging two nearest-neighbor spins i and j. We use the following prescriptions for $w_i(\sigma)$ and $w_{ij}(\sigma)$:

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

which is the Metropolis [7] transition rate, and

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

where ΔE_i is the change in energy when spin i is flipped and ΔE_{ij} is the change in energy after exchanging the nearest-neighbor spins i and j.

We have performed Monte Carlo simulations on a simple cubic lattice with $N = L^3$ sites, with values of L ranging from $L = 5$ up to $L = 23$. We have used in all of our simulations helicoidal boundary conditions. We have started the simulations employing different initial states (ferromagnetic, antiferromagnetic, and paramagnetic) to guarantee that the final stationary states we obtain are the same for a given pair of values of p and T, independently of the initial configuration. For a given temperature T and a selected value of the probability p, we choose at random a spin at site i, from a given initial configuration. Then, we generate a random number ξ_1 between zero and unity. If $\xi_1 \leqslant p$, we choose to perform the Glauber process: we determine the value of ΔE_i and the corresponding w_i according to the prescription of Eq. (6). Then, we generate another random number ξ_2 between zero and unity: if $\xi_2 \leqslant w_i$, we flip the spin at site i, otherwise we do not. If $\xi_1 > p$, we go over the Kawasaki process: we again generate another random number ξ_3, between zero and unity, in order to select one of the six nearest neighbors of the spin at site i, say, spin at j. Then we find the value of ΔE_{ij} and the corresponding transition rate w_{ij}: we exchange the selected spins only if $w_{ij} = 1$. We have discarded the first $10^4 \times N$ Monte Carlo steps in order to achieve the stationary regime for all lattice sizes we consider. One Monte Carlo step equals N single-spin flips or exchange of spin trials. To estimate the quantities of interest, we used 5×10^4 Monte Carlo steps to calculate the averages for any lattice size.

The steady phase diagram of the model and its associated critical exponents can be evaluated by using the finite-size scaling concepts [5] applied to some thermodynamic properties of the system. For a system with linear dimension L, we define, at the stationary states, the magnetization M_L, the susceptibility χ_L, and the reduced fourth-order cumulant [6] U_L by the following expressions:

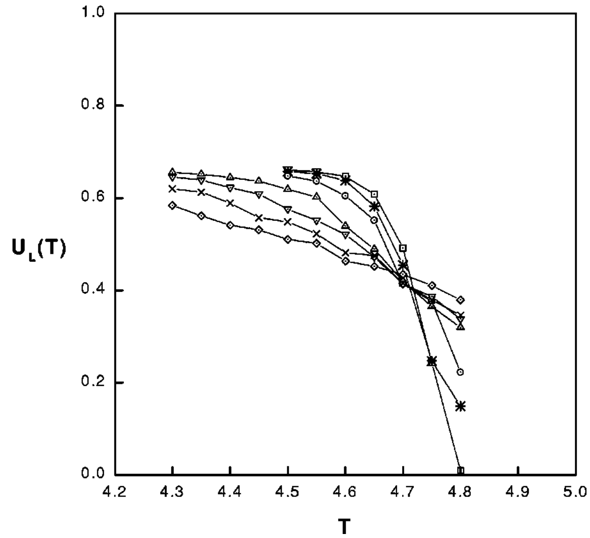

FIG. 1. Reduced fourth-order cumulant $U_L(T)$, for $p = 0.5$, as a function of temperature T for several values of the lattice size L. Diamonds correspond to $L = 5$, crosses to $L = 7$, down triangles to $L = 9$, up triangles to $L = 11$, circles to $L = 15$, stars to $L = 19$, and squares to $L = 23$. We join the data points of each lattice size by a broken line to guide the eye. The critical temperature is $T_c = 4.69 \pm 0.01$ in units of J/k_B.

$$M_L = \langle |m| \rangle, \tag{8}$$

$$\chi_L = N\{\langle m^2 \rangle - \langle |m| \rangle^2\}, \tag{9}$$

$$U_L = 1 - \frac{\langle m^4 \rangle}{3\langle m^2 \rangle^2}, \tag{10}$$

where $m = (1/N)\sum_{i=1}^{N} \sigma_i$.

In the neighborhood of the steady critical point T_c, we can write the following finite-size scaling relations:

$$M_L(T) = L^{-\beta/\nu} M_0(L^{1/\nu}\epsilon), \tag{11}$$

$$\chi_L(T) = L^{\gamma/\nu} \chi_0(L^{1/\nu}\epsilon), \tag{12}$$

$$U_L(T) = U_0(L^{1/\nu}\epsilon), \tag{13}$$

where $\epsilon = (T - T_c)/T_c$, T_c being the critical temperature for each value of p.

The derivative of Eq. (13) with respect to the temperature T give us the following scaling relation:

$$U_L'(T) = L^{1/\nu} U_0'(L^{1/\nu}\epsilon), \tag{14}$$

so that $U_L'(T_c) = L^{1/\nu} U_0'(0)$. Then, we can find the critical exponent ν from the log-log plot of $U_L'(T_c)$ versus L.

In order to locate the critical temperature T_c of the model, we have plotted in Fig. 1, for $p = 0.5$, the reduced fourth-order cumulant $U_L(T)$, defined by Eq. (10), as a function of temperature T, for several values of L, as indicated in the figure. The scaling relation for the fourth-order cumulant shows that, at the critical temperature, all curves of $U_L(T)$ must intercept themselves at T_c for whatever value of L. For

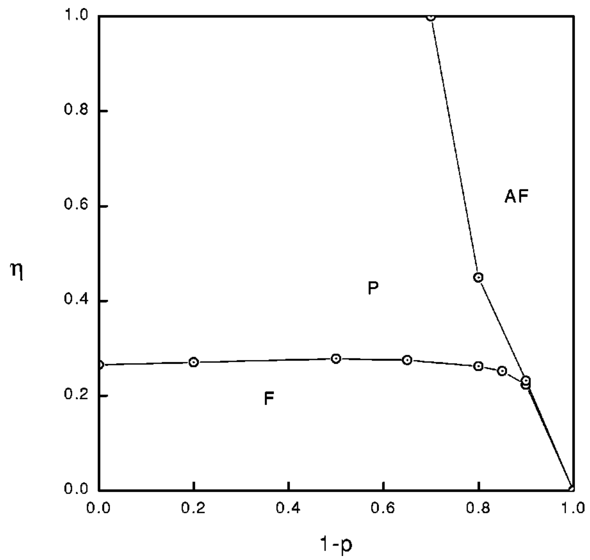

FIG. 2. Phase diagram of three-dimensional competing ferromagnetic Ising model. $\eta = \exp[-(J/k_BT)]$ and $1-p$ is related to the flux of energy. F, P, and AF refer to the ferromagnetic, paramagnetic, and antiferromagnetic phases, respectively.

this particular value of p, we have found $T_c = 4.69 \pm 0.01$, in units of (J/k_B), for the transition between the ferromagnetic and the paramagnetic phases. We have followed the same procedure for other values of p in order to determine the complete phase diagram of the model. We exhibit in Fig. 2 the phase diagram we found in the plane $\eta = \exp[-(J/k_BT)]$ versus $(1-p)$. As we can see, the antiferromagnetic phase occupies a large region of the phase diagram when compared with that observed for the corresponding two-dimensional ferromagnetic Ising model [4]. We also note that for $T=0$, the ferromagnetic phase is stable for all values of p. This is different from the pair approximation calculation [3] in two dimensions where, at $T=0$, the ferromagnetic, the paramagnetic and the antiferromagnetic phases are present. For very high values of temperature, the critical value for the paramagnetic to the antiferromagnetic transition is $p=0.3$. We remember that the pair approximation gives for this transition, in two dimensions, the value $p=0.35$, while our Monte Carlo simulations gave the value $p=0.075$.

From our Monte Carlo simulations, we can also evaluate the critical exponents of the model. From Eq. (14), we see that, at the critical temperature T_c, $U_L'(T_c)$ scales as $L^{1/\nu}$. Then, from the log-log plot of $U_L'(T_c)$ versus L, as can be seen in Fig. 3, for $p=0.5$, the best fit to the Monte Carlo data gives us $\nu = 0.67 \pm 0.04$. By constructing the similar log-log plots for the magnetization, $M_L(T_c)$, and for the susceptibility, $\chi_L(T_c)$, we can find the values of the ratios β/ν and γ/ν. For the value $p=0.5$, we found the values $\beta/\nu = 0.53 \pm 0.01$ and $\gamma/\nu = 1.93 \pm 0.03$. Finally, we show in Figs. 4–6, the plots we have obtained for the exponent ν, and for the ratios β/ν and γ/ν, respectively, for other values of the competition parameter at the stationary critical line for the ferromagnetic to paramagnetic transition. We would like to stress that the values we have obtained for these critical exponents compare very well with the analogous static exponents of the corresponding three-dimensional equilibrium Ising model.

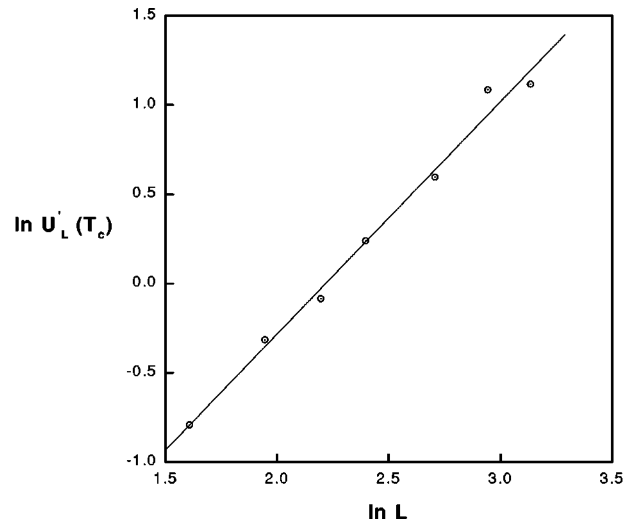

FIG. 3. Log-log plot of $U_L'(T_c)$ versus L for $p=0.5$. The straight line is the best fit to the data, which gives $\nu = 0.67 \pm 0.04$.

For instance, the numerical investigations in equilibrium by Ferrenberg and Landau [8] yield $\nu = 0.6289$ and $\beta/\nu = 0.518$. As our nonequilibrium model preserves the up-down symmetry, it is expected that it belongs to the same universality class of the equilibrium Ising model [9].

In summary, we have determined the phase diagram and studied the stationary critical properties of a nonequilibrium ferromagnetic Ising model in a simple cubic lattice, when the system is in contact with a heat bath at temperature T, and subject to an external flux of energy. The exchange of energy with the heat reservoir is assumed to be represented by the stochastic Glauber process, while the flux of energy into the system is simulated by a kind of Kawasaki diffusive process. The phase diagram of the model was obtained through Monte Carlo simulations and is similar to the one found for the two-dimensional ferromagnetic Ising model with the same competing stochastic processes. At zero temperature we have only a steady ferromagnetic state for any value of

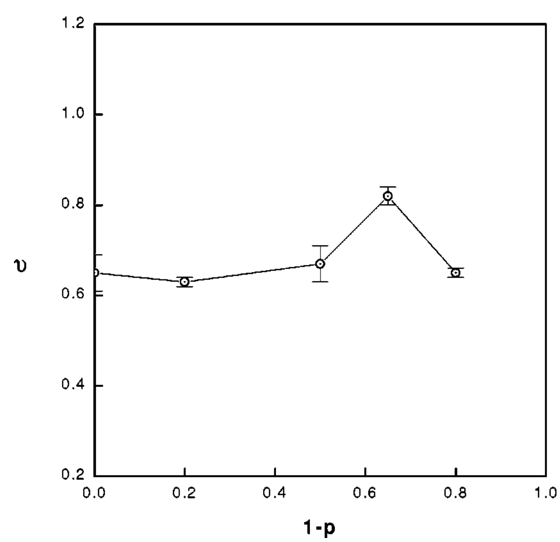

FIG. 4. Critical exponent ν as a function of the parameter $1-p$ at the ferromagnetic-paramagnetic transition line of Fig. 2. The error bars give the accuracy of our Monte Carlo data points.

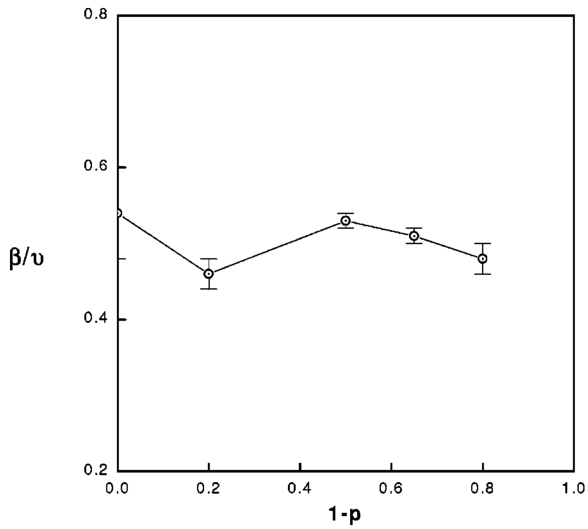

FIG. 5. Ratio β/ν as a function of the parameter $1-p$ at the ferromagnetic-paramagnetic transition line of Fig. 2. The error bars give the accuracy of our Monte Carlo data points.

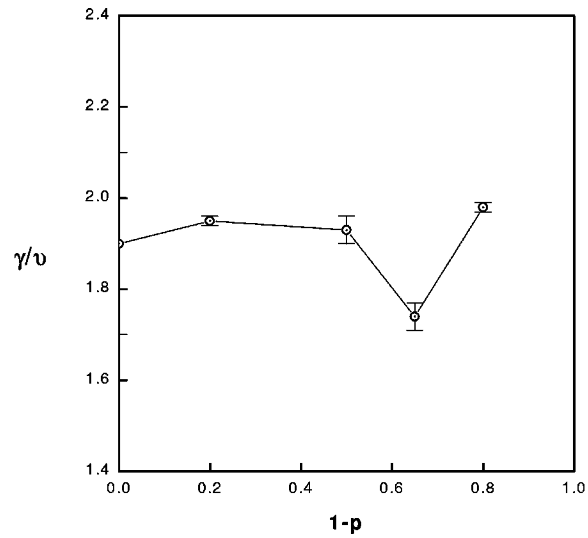

FIG. 6. Ratio γ/ν as a function of the parameter $1-p$ at the ferromagnetic-paramagnetic transition line of Fig. 2. The error bars give the accuracy of our Monte Carlo data points.

the competition parameter. The area of phase diagram covered by the antiferromagnetic phase is larger than the corresponding two-dimensional version of the model. We have also calculated the critical exponents of this model, and we have found that its values are in accordance with those expected for the equilibrium Ising model in three dimensions.

This work was partially supported by the Brazilian agencies CNPq and FINEP.

[1] R. J. Glauber, J. Math. Phys. **4**, 294 (1963).
[2] K. Kawasaki, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, London, 1972), Vol. 4.
[3] T. Tomé and M. J. de Oliveira, Phys. Rev. A **40**, 6643 (1989).
[4] B. C. S. Grandi and W. Figueiredo, Phys. Rev. E **53**, 5484 (1996).
[5] V. Privman, *Finite-Size Scaling and Numerical Simulation of Statistical Systems* (World Scientific, Singapore, 1990).
[6] K. Binder, Z. Phys. B **43**, 119 (1981).
[7] N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. **21**, 1087 (1953).
[8] A. M. Ferrenberg and D. P. Landau, Phys. Rev. B **44**, 5081 (1991).
[9] K. E. Bassler and B. Schmittmann, Phys. Rev. Lett. **73**, 3343 (1994).