Nonequilibrium antiferromagnetic mixed-spin Ising model

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We studied an antiferromagnetic mixed-spin Ising model on the square lattice subject to two competing stochastic processes. The model system consists of two interpenetrating sublattices of spins $\sigma=1/2$ and $S=1$, and we take only nearest neighbor interactions between pairs of spins. The system is in contact with a heat bath at temperature T, and the exchange of energy with the heat bath occurs via one-spin flip (Glauber dynamics). Besides, the system interacts with an external agency of energy, which supplies energy to it whenever two nearest neighboring spins are simultaneously flipped. By employing Monte Carlo simulations and a dynamical pair approximation, we found the phase diagram for the stationary states of the model in the plane temperature T versus the competition parameter between one- and two-spin flips p. We observed the appearance of three distinct phases, that are separated by continuous transition lines. We also determined the static critical exponents along these lines and we showed that this nonequilibrium model belongs to the universality class of the two-dimensional equilibrium Ising model.

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I. INTRODUCTION

Equilibrium statistical mechanics is a well-known established theory in physics, which provides the tools to understand the thermodynamical properties of a variety of physical systems. In particular, for those systems in what we are able to write a suitable hamiltonian, the equilibrium properties can be found from the appropriate statistical ensemble. On the other hand, there are many interesting problems in physics, chemistry, and biology, for which it is not possible to establish an Hamiltonian function. Sometimes, we know the Hamiltonian, but in contrast, the system can be under the action of time varying external fields. In these cases, typical equilibrium arguments, such as the detailed balance cannot be applied, and a formal theory is not at hand to describe precisely the steady states of the system. One way to handle with these difficulties is to provide an energy function to the model, for instance, one involving short-range couplings in a many particle interacting system, and defining some dynamical processes appropriated to describe its nonequilibrium states. In this work we studied an open system for which we know its energy states and that is under the action of external forces.

The particular model we consider is an antiferromagnetic mixed-spin Ising system on a two-sublattice with spin values $\sigma=1/2$ and $S=1$. While the system is in contact with a heat bath, it is also forced to receive energy from the external environment. The time evolution of the states of the system is then governed by two competing dynamical processes: one simulating the contact of the system with a heat bath at a temperature T, and the other mimicking the input of energy into the system. We choose the Glauber [1] stochastic dynamics to describe the exchange of energy with the heat bath. This can be done by allowing that both σ and S spins relax through one-spin flip. The increase in the energy states of the system is defined in a similar manner, but instead we simultaneously flip a nearest neighbor pair of spins σ and S. Recently, some works [2–4] appeared, focusing their attention on the nature of the phase transitions exhibited by some competing stochastic Ising systems.

The ferrimagnetic materials present a special arrangement of their magnetic moments that can be described by the mixed-spin systems. The existence of a compensation temperature, that is, a temperature below the critical temperature of the material, at which the resultant magnetization is zero, makes the ferrimagnets of great technological interest. Some typical examples of these systems are the two-dimensional organometallic ferrimagnets [5] and the Prussian blue analog [6]. Some calculations concerning the critical properties of the equilibrium mixed-spin systems were performed mainly by using renormalization group methods [7–10], series expansion [11] and Monte Carlo simulations [12].

In an early work, we studied the ferromagnetic version of the mixed-spin Ising model in the framework of the dynamical pair approximation [13] and by Monte Carlo simulations [14]. Its phase diagram, in the plane temperature versus competition parameter between one- and two-spin flips, was determined. We found two continuous transition lines in this plane: one line separating an ordered phase in what the sublattice magnetizations are parallel aligned, from a disordered phase where the sublattice magnetizations are both zero (paramagnetic phase), and other line separating the paramagnetic phase from an ordered phase where the sublattice magnetizations are aligned in opposite directions. Our finite size scaling analysis of the appropriated order parameters showed that the critical exponents along the two continuous lines are the same as those of the equilibrium two-dimensional Ising model.

The motivation to study the model with antiferromagnetic coupling between spins are the results found for the phase diagram of the ferromagnetic [15] and antiferromagnetic [16] nonequilibrium Ising models. In those studies, the system of Ising spins was also subject to two independent competing stochastic dynamics. The one-spin-flip Glauber dynamics

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with probability p and the two-spin-exchange Kawasaki dynamics [17] with probability $(1-p)$. Similarly to the ferromagnetic mixed-spin system, the role of the Glauber dynamics was to describe the relaxation of the spins with the heat bath, while the Kawasaki dynamics accounted for the increase in the energy of the system. While the phase diagram showed the presence of three distinct phases in the ferromagnetic case, only two phases appeared in the corresponding antiferromagnetic case. Then, simply changing the sign of the exchange coupling in these nonequilibrium models does not permit to foreseen unambigously the topology of the phase diagram of the antiferromagnetic model from its ferromagnetic counterpart. The explanation of this behavior is related to the two-spin-exchange Kawasaki dynamics, for which the order parameter does not change. The antiferromagnetic states are more sensitive to this dynamics than the ferromagnetic ones. On the other hand, in the present study of the antiferromagnetic mixed-spin Ising model, the two competing dynamical processes do not conserve the order parameter as in the ferromagnetic case. Here, we want to know if the change on the sign of the exchange coupling will affect the topology of the phase diagram, as happened by using the Kawasaki kinetics in the pure Ising model.

In this work the antiferromagnetic mixed-spin Ising model with competing dynamics is studied within the dynamical pair approximation and through Monte Carlo simulations. As in the previous ferromagnetic model [14] we attributed a weight p to the one-spin flip process, and a weight $(1-p)$ to the two-spin flip process. We determined the phase diagram of the model and we calculated its static critical exponents.

This paper is organized as follows. In the following section we present the model and the equations to describe the time evolution of states. In Sec. III, we find the phase diagram and the critical exponents of the model. Finally, in Sec. IV, we present our conclusions.

II. THE MODEL AND EQUATIONS OF MOTION

The antiferromagnetic mixed-spin Ising model is defined on a square lattice, with spins $\sigma=1/2$ and $S=1$. The lattice is bipartite, with the σ spins occupying the sites of one sublattice, while the S spins occupy the sites of the other sublattice, each sublattice containing N sites. A state of the system is represented by $\{\sigma,S\} \equiv\{\sigma_1,\ldots,\sigma_l,\ldots,\sigma_N;S_1,\ldots,S_m,\ldots,S_N\}$, where the spin variables σ_l can assume the values ±1 and the spin variables S_m can assume the values $0,\pm1$. The energy of the system in the state (σ,S) is given by

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

where the sum is over all nearest neighboring pairs of spins, and $J>0$ is the antiferromagnetic coupling. First of all, we define $p(\sigma,S;t)$ as being the probability of finding the system in the state (σ,S) at time t. The probability states evolve in time according to the master equation

$$\frac{d}{dt}p(\sigma,S;t)=-\sum_{\sigma',S'} W(\sigma,S\rightarrow\sigma',S')p(\sigma,S;t) + \sum_{\sigma',S'} W(\sigma',S'\rightarrow\sigma,S)p(\sigma',S';t), \tag{2}$$

where $W(\sigma,S\rightarrow\sigma',S')$ is the probability, per unit of time, for the transition from the state (σ,S) to the state (σ',S'). As in the ferromagnetic case, the transition rate $W(\sigma,S\rightarrow\sigma',S')$ is written as the sum of two independent stochastic processes with suitable weights. One of these processes is the one-spin flip Glauber kinetics, designed to describe the exchange of energy of the system with a heat bath at temperature T. This can be done through the σ or S spins, and we write in general that

$$W_G(\sigma,S\rightarrow\sigma',S')=W_G(\sigma,S\rightarrow\sigma',S)+W_G(\sigma,S\rightarrow\sigma,S'). \tag{3}$$

The other dynamical process considered is a two-spin flip mechanism, which does not depend on temperature and it is used to describe the interaction of the system with an external source of energy. In order to increase the energy of the system, we choose to simultaneously flip a pair of nearest neighbor spins, and we write for this process $W_{GD}(\sigma,S\rightarrow\sigma',S')$. Then, we have the following equation for the total transition probability:

$$W(\sigma,S\rightarrow\sigma',S')=pW_G(\sigma,S\rightarrow\sigma',S')+(1-p)\times W_{GD}(\sigma,S\rightarrow\sigma',S'), \tag{4}$$

where $0\leqslant p\leqslant1$ is the competition parameter between the one-spin flip and two-spin flip processes. The Glauber transition rate is used to describe the one-spin flip changes

$$W_G(\sigma,S\rightarrow\sigma',S')=\sum_{j=1}^{N}\delta_{\sigma_1,\sigma_1'}\delta_{\sigma_2,\sigma_2'}\cdots\delta_{\sigma_j,-\sigma_j'}\cdots\delta_{\sigma_N,\sigma_N'} \times\delta_{S_1,S_1'}\delta_{S_2,S_2'}\cdots\delta_{S_k,S_k'}\cdots\delta_{S_N,S_N'}\omega_j(\sigma') + \sum_{k=1}^{N}\delta_{\sigma_1,\sigma_1'}\delta_{\sigma_2,\sigma_2'}\cdots\delta_{\sigma_j,\sigma_j'}\cdots\delta_{\sigma_N,\sigma_N'} \times\delta_{S_1,S_1'}\delta_{S_2,S_2'}\cdots\delta_{S_k,\tilde{S}_k}\cdots\delta_{S_N,S_N'}\omega_k(\tilde{S}), \tag{5}$$

where $\omega_j(\sigma)$ and $\omega_k(S)$ are the probabilities of flipping the spins σ_j and S_k, respectively. We used the variable $\tilde{S}_k$ to mean the two possible values that a change of the actual spin variable S_k can take. For the one-spin flip transitions, we take

$$\omega_j(\sigma)=\min[1,\exp(-\beta\Delta E_j)], \tag{6}$$

where $\beta=1/k_BT$, and T is the absolute temperature of the heat bath. ΔE_j is the change in energy after flipping spin σ_j at site j. We also assume a similar expression for $\omega_k(S)$. For the two-spin flip we write

$$W_{GD}(\sigma,S\rightarrow\sigma',S') = \sum_{j,k=1}^{N} \delta_{\sigma_1,\sigma_1'}\delta_{\sigma_2,\sigma_2'}\cdots\delta_{\sigma_j,-\sigma_j'}\cdots\delta_{\sigma_N,\sigma_N'} \times \delta_{S_1,S_1'}\delta_{S_2,S_2'}\cdots\delta_{S_k,\tilde{S}_k}\cdots\delta_{S_N,S_N'}\omega_{jk}(\sigma',\tilde{S}), \tag{7}$$

where $\omega_{jk}(\sigma,S)$ is the probability of a simultaneous flipping of the neighboring spins σ_j and S_k. As we want this process favors the increase in the energy of the system, we write

$$\omega_{jk}(\sigma,S)=\begin{cases}0 & \text{if } \Delta E_{jk}\leqslant 0,\\ 1 & \text{if } \Delta E_{jk}>0,\end{cases} \tag{8}$$

where ΔE_{ij} is the change in energy after flipping the spins σ_j and S_k, at the neighboring sites j and k.

From the probability of states $p(\sigma,S;t)$ we can derive expressions for the evolution of the sublattice magnetizations, $\langle\sigma_l\rangle$, $\langle S_m\rangle$, and for the correlation functions, $\langle\sigma_l S_m\rangle$, $\langle S_m^2\rangle$, and $\langle\sigma_l S_m^2\rangle$. The resulting set of equations can be decoupled by using the dynamical pair approximation, and the steady states of the system can be found as a function of T and p. The details of these calculations were presented in our earlier work [13]. In the following section we will present the phase diagram of the model along with the Monte Carlo results.

We have performed Monte Carlo simulations, on the square lattice of linear size L, with values of L ranging from $L=16$ to $L=128$, with periodic boundary conditions. We have taken completely random spin configurations as the initial states of our simulations. A new configuration is generated from an old one by the following Markov process: for a given temperature T and a selected value of the competition parameter p, we choose at random a spin of the lattice, and then we generate a random number ξ between zero and unity. If $\xi\leqslant p$ we choose to perform the one-spin flip process, according to the Metropolis prescription given by Eq. (6). If $\xi>p$, then we consider the two-spin flip process. In this case, we randomly select a new spin, which is nearest neighbor of the initial chosen spin, and we apply the prescription given by Eq. (8). At least, the first initial 5×10^4 Monte Carlo steps (MCS) were discarded in order to achieve the stationary regime for all lattice sizes. In order to estimate the quantities of interest, we have considered the next 1×10^6 MCS to calculate the averages for any lattice size. One MCS equals L^2 one-spin flip or two-spin flip trials.

We calculated the sublattice magnetizations per spin, m_1 and m_2, defined as

$$m_1=\frac{1}{N}\left\langle\sum_i S_i\right\rangle \tag{9}$$

and

$$m_2=\frac{1}{N}\left\langle\sum_j \sigma_j\right\rangle. \tag{10}$$

It is also convenient to define the total and the staggered magnetizations, respectively, by

$$m^F=\frac{1}{2}|(m_1+m_2)| \tag{11}$$

and

$$m^{AF}=\frac{1}{2}|(m_1-m_2)|, \tag{12}$$

and their associated reduced fourth-order Binder cumulants [18]

$$U_L(m)=1-\frac{\langle m^4\rangle}{3\langle m^2\rangle^2}. \tag{13}$$

The corresponding susceptibilities are defined by

$$\chi(m)=N\{\langle m^2\rangle-\langle|m|\rangle^2\}, \tag{14}$$

where m can be m^F or m^{AF}.

As will see in following section the model exhibits continuous phase transitions beween ordered and paramagnetic phases. Finite-size scaling relations are used to locate the critical point and to determine the values of the critical exponents. For instance, the finite-size scaling relations for the quantitites define before, in the neighborhood of the stationary critical point p_c, are

$$m_L(p)=L^{-\beta/\nu}m_0(L^{1/\nu}\varepsilon), \tag{15}$$

$$\chi_L(p)=L^{\gamma/\nu}\chi_0(L^{1/\nu}\varepsilon), \tag{16}$$

$$U_L(p)=U_0(L^{1/\nu}\varepsilon), \tag{17}$$

where $\varepsilon=(p-p_c)/p_c$, p_c being the critical competition parameter for each value of T, and ν is the correlation length exponent.

The derivative of Eq. (17) with respect to the competition parameter p give us the following scaling relation:

$$U_L'(p)=L^{1/\nu}\frac{U_0'(L^{1/\nu}\varepsilon)}{p_c}, \tag{18}$$

so that

$$U_L'(p_c)=L^{1/\nu}\frac{U_0'(0)}{p_c}. \tag{19}$$

This last equation gives the critical exponent ν from a log-log plot of $U_L'(p_c)$ versus L.

III. PHASE DIAGRAM

In this section we present the results we have obtained for the phase diagram of the antiferromagnetic mixed-spin Ising model, as well as its critical exponents. Figure 1 is the phase diagram in the plane temperature T versus competition parameter p. The dashed lines represent the results of the pair approximation calculations, while the data points are the re-

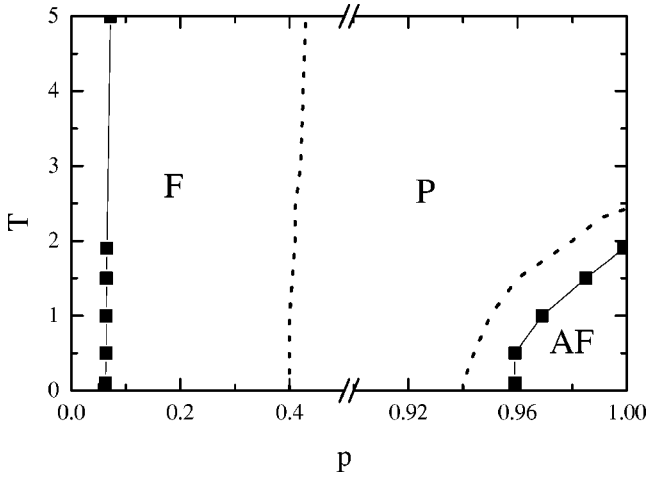

FIG. 1. Phase diagram of the antiferromagnetic mixed-spin Ising model in the plane temperature T versus competition parameter p. The letters denote the F and AF ordered phases and P the paramagnetic phase. The dashed lines represent the pair approximation calculations and the squares are the data from Monte Carlo simulations. The lines joining the squares are only a guide to the eye. The temperature is measured in units of J/k_B and p is a dimensionless parameter.

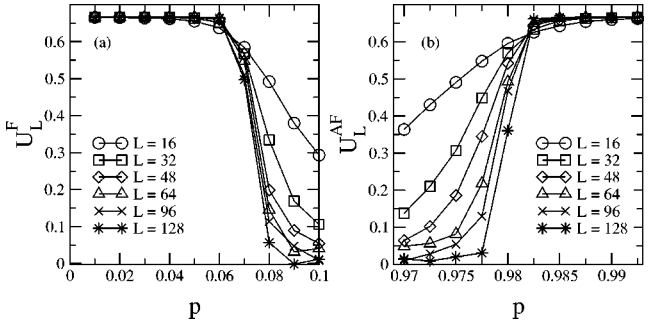

FIG. 2. Reduced fourth-order cumulant for various lattice sizes as indicated in the figures. (a) U_L^F is the cumulant near the critical point of the F-P transition, and (b) U_L^{AF} is the cumulant near the critical point of the AF-P transition. The temperature is fixed at the value $T=1.5$.

sults found from simulations. The phase diagram exhibits three different phases, separated by two continuous transition lines: one line separating an ordered phase (AF), where one sublattice magnetization is positive and the other negative, from a disordered paramagnetic phase (P), where both sublattice magnetizations are zero. The other line separates the paramagnetic phase from an ordered ferromagnetic phase (F), where the sublattice magnetizations are positive. Although the coupling is of the antiferromagnetic type, the antiferromagnetic phase occupies only a small region of the phase diagram. As we increase the flux of energy into the system, which in the present model corresponds to decrease the value of p, the AF phase disappears. However, for a very intense flux of energy, a ferromagnetic phase appears. The basic difference between the pair approximation and Monte Carlo calculations is the size of the region occupied by the disordered phase. This region is very large in Monte Carlo simulations. The calculations based on the pair approximation differ slightly for the ferromagnetic and antiferromagnetic couplings. For instance, at very small temperatures, the transition point in the antiferromagnetic case deviates to lower values of p compared to the ferromagnetic case.

However, the topology of the ferromagnetic and antiferromagnetic phase diagrams are essentially the same: changing the sign of the interaction coupling is equivalent to exchange the places of the F and AF phases in both diagrams. Then, the two-spin flip dynamics in this mixed-spin model does not prevent the formation of another phase at very large values of the flux of energy. This is different from that we have seen in the pure antiferromagnetic Ising model [16], when the exchange of two nearest neighbor spins (Kawasaki kinetics) conserves the order parameter. The simple two-spin flip does not conserve the order parameter within the mixed-spin Ising model. Indeed, even when two nearest neighbor spins are parallel, we can flip them, changing the order parameter and increasing the energy of the system. On the other hand, in the pure Ising case, the exchange of a pair of parallel spins does not add more energy to the system because its state remains the same.

The critical points found in the phase diagram of the Fig. 1, were determined by the crossing of the fourth-order cumulants for different lattice sizes at the critical point [18]. In order to find the critical parameter, we fixed the temperature, which is measured in units of J/k_B, and we have plotted $U_L(p)$ versus the competition parameter p, for all the lattice sizes L as shown in Figs. 2(a) and 2(b) for the particular temperature $T=1.5$. Our estimate for the critical competition parameter, at the transition line between the ordered AF and paramagnetic P phases is $p_c=0.9812\pm0.0001$, while its value at the other transition line ($F-P$ transition line) is $p_c=0.065\pm0.001$.

It is also easy to determine the critical exponents of the model from the Monte Carlo data. For instance, log-log plots of the Eqs. (15), (16), and (19), respectively, for the magnetization, susceptibility and derivative of the cumulants, at the critical point p_c, give us the critical exponents from the slope of the corresponding straight lines. This can be seen in Fig. 3, for the transition between the AF and P phases at $T=1.5$. From the best fit to the data points we found $\nu=1.04\pm0.05$, $\beta/\nu=0.13\pm0.01$, and $\gamma/\nu=1.69\pm0.07$. The same procedure was used to find the critical exponents for

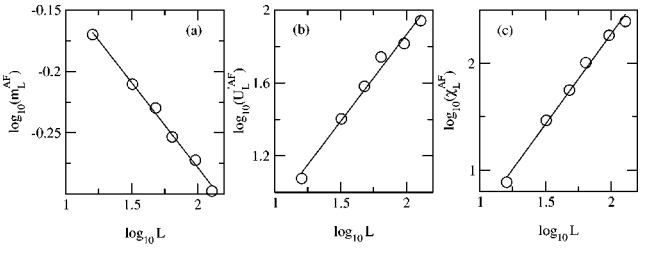

FIG. 3. Log-log plots of (a) the order parameter, (b) the derivative of the cumulant, and (c) the susceptibility as a function of the lattice size, at the critical point of the AF-P transition and $T=1.5$. The straight lines are the best fit to the data points. The sizes of the circles are chosen so that the error bars are inside them.

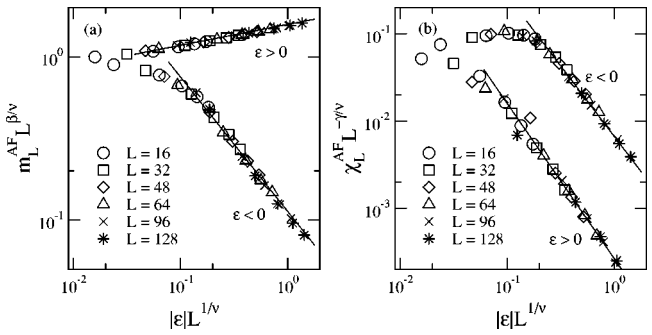

FIG. 4. Finite-size scaling (full data collapse) near the critical point of the AF-P transition for (a) the order parameter m_L^{AF}, and (b) susceptibility χ_L^{AF}, for different values of L as indicated in the figures. The parameter ε is defined by $\varepsilon=(p-p_c)/p_c$. The straight lines represent the asymptotic behavior of the scaling functions. The temperature is $T=1.5$, and the optimal values of the critical exponents are $\nu=1.01\pm0.01$, $\beta=0.125\pm0.001$, and $\gamma=1.74\pm0.01$.

other values of temperature, and at the $P-F$ boundary.

We can improve the values found for the critical exponents, by collapsing the data points. For instance, we exhibit in Figs. 4 (a) and 4(b) the data collapse for the order parameter m_L^{AF} and for the susceptibility χ_L^{AF}, respectively. The Eqs. (15) and (16) can be written as

$$m_L(p)=L^{-\beta/\nu}m_0^{\mp}(L^{1/\nu}|\varepsilon|), \tag{20}$$

$$\chi_L(p)=L^{\gamma/\nu}\chi_0^{\mp}(L^{1/\nu}|\varepsilon|), \tag{21}$$

where the two branches, $\varepsilon<0$ (paramagnetic phase) and $\varepsilon>0$ (antiferromagnetic phase) are considered, and $\varepsilon=(p-p_c)/p_c$. For the infinite lattice size we have $m(p)\sim(p-p_c)^{\beta}$ and $\chi(p)\sim|p-p_c|^{-\gamma}$. Then, for large values of $L^{1/\nu}|\varepsilon|$ and $\varepsilon>0$, the slopes of curves in the Figs. 4(a) and 4(b) give us directly the values of the exponents β and $-\gamma$, respectively. On the other hand, for large values of $L^{1/\nu}|\varepsilon|$ and $\varepsilon<0$, the slopes of the curves in Figs. 4(a) and 4(b) furnish the values of $\beta-\nu$ and $-\gamma$, respectively. At this point, we call attention that the abscissas in the Figs. 8 and 9 of our earlier paper [14] must be replaced by $|\varepsilon|L^{1/\nu}$, and the signs of ε in Figs. 8(a) and 8(b) must be exchanged.

The optimal values we have found for the critical exponents employing this procedure are: at the $AF-P$ transition line (Fig. 4) $\nu=1.01\pm0.01$, $\beta=0.125\pm0.001$, and $\gamma=1.74\pm0.01$ and at the $F-P$ transition line, whose plots are not shown, $\nu=1.01\pm0.02$, $\beta=0.124\pm0.002$, and $\gamma=1.74\pm0.02$. Although we have exhibited the results only for the temperature $T=1.5$, we have repeated the whole process outlined above for other points along the critical lines. The bulk of our results clearly indicates that the nonequilibrium antiferromagnetic mixed-spin Ising model is in the same class of universality of the two-dimensional equilibrium Ising model. The choice of the two-spin flip dynamical process that is used to simulate the absorption of energy by the system, does not affect the static critical exponents of the model.

IV. CONCLUSIONS

The phase diagram of a nonequilibrium mixed-spin Ising model was determined through Monte Carlo simulations and pair approximation calculations. The spins $\sigma=1/2$ and $S=1$ occupy the sites of a square lattice and the nearest neighbors of any spin σ are the S spins, and vice versa. The coupling between spins σ and S is antiferromagnetic. The system was in contact with a heat bath at fixed temperature and, at the same time, subjected to an external flux of energy. The contact with the heat bath was simulated by the one-spin flip Glauber process with probability p, while the flux of energy was simulated by a process involving a simultaneous flipping of a pair of nearest neighbor spins, with probability $(1-p)$. Both dynamical processes do not preserve the order parameter. We have shown that the phase diagram contains three phases separated by two continuous transition lines. When the flux of energy is very small the system is antiferromagnetically ordered, while for large values of the flux of energy, the system stays in a ferromagnetic phase. For intermediate values of the flux of energy the system remains in a paramagnetic state. The phase diagram is similar that found for the ferromagnetic case. Changing the sign of the magnetic coupling is equivalent to change in the phase diagram the places of the ferromagnetic and antiferromagnetic phases. This symmetry is not observed for the pure Ising model when we change the sign of the magnetic coupling and the two-spin flip mechanism is of the Kawasaki type. The preserving order parameter Kawasaki kinetics destroys this symmetry.

We have also determined the critical exponents ν, β, and γ for the antiferromagnetic mixed-spin Ising model at the transition lines. The values we found for the static critical exponents of this nonequilibrium model leave it in the same universality class of the equilibrium Ising model in two dimensions.

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