Mixed-spin Ising model with one- and two-spin competing dynamics

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In this work we found the stationary states of a kinetic Ising model, with two different types of spins: $\sigma = 1/2$ and $S = 1$. We divided the spins into two interpenetrating sublattices, and found the time evolution for the probability of the states of the system. We employed two transition rates which compete between themselves: one, associated with the Glauber process, which describes the relaxation of the system through one-spin flips; the other, related to the simultaneous flipping of pairs of neighboring spins, simulates an input of energy into the system. Using the dynamical pair approximation, we determined the equations of motion for the sublattice magnetizations, and also for the correlation function between first neighbors. We found the phase diagram for the stationary states of the model, and we showed that it exhibits two continuous transition lines: one line between the ferrimagnetic and paramagnetic phases, and the other between the paramagnetic and antiferrimagnetic phases.

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I. INTRODUCTION

In this work we studied the nonequilibrium states of a two-sublattice ferromagnetic Ising model with mixed spins $\sigma = 1/2$ and $S = 1$. The time evolution of the states of the system is governed by two competing dynamical process: one simulating the contact of the system with a heat bath at a fixed temperature T, and the other mimicking an input of energy into the system. If a system is subject to an external flux of energy, it can exhibit the self-organization phenomenon. Self-organizing structures are well known in chemical reactions and in fluid dynamics. The book by Nicolis and Prigogine [1] and that by Haken [2] present interesting examples of these phenomena. In our open ferromagnetic spin system, the contact with the heat bath is simulated by the Glauber stochastic process [3], where both σ and S spins relax through single-spin flips. In our model, the flux of energy into the system favors states with the highest energy, generating a competition with the one-spin flip Glauber process. The increase in the energy states is obtained when we simultaneously flip a nearest neighbor pair of spins σ and S. This is not a Kawasaki exchange process [4], as used, for instance, in the work of Tomé and de Oliveira [5] to induce a self-organizing phenomenon in the kinetic Ising model. In their model, the stochastic Kawasaki dynamics conserves the order parameter. Here our particular interest is to investigate the competition between two dynamical processes when the order parameter is not conserved. This is easily achieved with the two-sublattice Ising mixed-spin system, after a simultaneous flipping of a pair of nearest neighbor spins.

We used the dynamical pair approximation [6] to decouple the hierarchy of equations of motion which follow from the application of the master equation approach. We attribute a weight p to the one-spin flip Glauber process, and a weight $(1-p)$ to the two-spin flip process, which increases the energy of the system. We found the stationary states of the model as a function of temperature and of the parameter p, which accounts for the competition between the two dynamical processes. We determined the phase diagram of the model in the plane of temperature T versus competition parameter $(Q = 1-p)$, and we noticed the presence of three different phases: for very small values of Q (small flux of energy), we obtained a ferrimagnetic phase. Increasing the flux of energy, the ferrimagnetic phase becomes unstable, and appears to be a paramagnetic phase. However, when the flux becomes large, we observed a transition from the paramagnetic phase to the ordered antiferrimagnetic phase. In Sec. II, we describe the model and derive the equations of motion for the sublattice magnetizations and the correlation functions of interest. In Sec. III, we apply the pair approximation decoupling scheme to find a closed set of equations of motion. In Sec. IV, we find the stationary states of the system, and exhibit the phase diagram of the model. Finally, in Sec. V, we present our conclusions.

II. MODEL AND EQUATIONS OF MOTION

We consider a ferromagnetic Ising model in a square lattice with mixed spins $\sigma = 1/2$ and $S = 1$, in a bipartite lattice, with the σ spins occupying the sites of one sublattice, and the S spins occupying the sites of the other one, each sublattice containing N sites. A state of the system is represented by $(\sigma,S) \equiv (\sigma_1, \dots, \sigma_l, \dots, \sigma_N; S_1, \dots, S_m, \dots, S_N)$, where the spin variables σ_l can assume the values ± 1 and the spin variables S can assume the values $0, \pm 1$. 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 is taken to be positive. Let us call $p(\sigma,S;t)$ the probability of finding the system in the state (σ,S) at time t. The equation of motion for the probability of the states of the system is given by the gain and loss master equation [7]

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

where $W(\sigma,S\to\sigma',S')$ is the probability, per unit of time, for the transition from state (σ,S) to state (σ',S'). In this model, we assume that the transition rate $W(\sigma,S\to\sigma',S')$ is given by the competition between two independent stochastic processes: the one-spin flip Glauber process, intended to describe the relaxation of the σ and S spins in contact with the heat bath at temperature T, is written as

$$W_G(\sigma,S\to\sigma',S') = W_G(\sigma,S\to\sigma',S) + W_G(\sigma,S\to\sigma,S'), \quad (3)$$

and the two-spin flip process, chosen independent of temperature, and intended to increase the energy of the system, is written as $W_{GD}(\sigma,S\to\sigma',S')$. Then we can write the following equation for the total transition probability:

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

where $0\leqslant p\leqslant 1$ is the competition parameter between the one-spin flip and two-spin flip processes. The one-spin flip process is described by the Glauber dynamics, that is,

$$W_G(\sigma',S'\to\sigma,S) = \sum_{j=1}^{N} \delta_{\sigma_1,\sigma'_1}\delta_{\sigma_2,\sigma'_2}\ldots\delta_{\sigma_j,-\sigma'_j}\ldots\delta_{\sigma_N,\sigma'_N} \times \delta_{S_1,S'_1}\delta_{S_2,S'_2}\ldots\delta_{S_k,S'_k}\ldots\delta_{S_N,S'_N}\omega_j(\sigma') + \sum_{k=1}^{N} \delta_{\sigma_1,\sigma'_1}\delta_{\sigma_2,\sigma'_2}\ldots\delta_{\sigma_j,\sigma'_j}\ldots\delta_{\sigma_N,\sigma'_N} \times \delta_{S_1,S'_1}\delta_{S_2,S'_2}\ldots\delta_{S_k,\tilde{S}_k}\ldots\delta_{S_N,S'_N}\omega_k(\tilde{S}), \quad (5)$$

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 state S_k can take. We adopt the Metropolis prescription for these one-spin flip transitions, that is,

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

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 $\omega_k(S)$. The two-spin flip transition rate is written in the form

$$W_{GD}(\sigma',S'\to\sigma,S) = \sum_{j,k=1}^{N} \delta_{\sigma_1,\sigma'_1}\delta_{\sigma_2,\sigma'_2}\ldots\delta_{\sigma_j,-\sigma'_j}\ldots\delta_{\sigma_N,\sigma'_N} \times \delta_{S_1,S'_1}\delta_{S_2,S'_2}\ldots\delta_{S_k,\tilde{S}_k}\ldots\delta_{S_N,S'_N}\omega_{jk}(\sigma',\tilde{S}), \quad (7)$$

where $\omega_{jk}(\sigma,S)$ is the probability of a simultaneous flipping of neighboring spins σ_j and S_k. This process is designed to favor an increase in the energy of the system, and it is written as

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

where ΔE_{jk} is the change in energy after flipping the spins σ_j and S_k, at the neighboring sites j and k. The average value of a function of state $A(\sigma,S)$ is given by

$$\langle A(\sigma,S)\rangle = \sum_{\sigma,S} A(\sigma,S)p(\sigma,S;t), \quad (8)$$

where we sum over all possible configurations of spins σ and S. If, for instance, $A(\sigma,S)=\sigma_l$, we obtain the sublattice magnetization associated with the σ sublattice. On the other hand, if $A(\sigma,S)=S_m$, we obtain the sublattice magnetization related to the S sublattice. In this way, we can write the set of equations:

$$\frac{d}{dt}\langle\sigma_l\rangle = pA_l + (1-p)D_l, \quad (9)$$

$$\frac{d}{dt}\langle S_m\rangle = pB_m + (1-p)E_m, \quad (10)$$

where

$$A_l = -2\langle\sigma_l\omega_l(\sigma)\rangle, \quad (11)$$

$$B_m = \langle(\tilde{S}_m - S_m)\omega_m(S)\rangle, \quad (12)$$

$$D_l = -2\sum_{\substack{k \\ (\text{NN of } l)}} \langle\sigma_l\omega_{lk}(\sigma,S)\rangle, \quad (13)$$

$$E_m = \sum_{\substack{j \\ (\text{NN of } m)}} \langle(\tilde{S}_m - S_m)\omega_{jm}(\sigma,S)\rangle, \quad (14)$$

where (NN of l) means that the sum is performed over all the nearest neighbors of the site l of a given sublattice. For the correlation function between nearest neighbor spins in the sublattices σ and S, $\langle\sigma_lS_m\rangle$, we can write

$$\frac{d}{dt}\langle\sigma_lS_m\rangle = pA_{lm} + (1-p)D_{lm}, \quad (15)$$

where

$$A_{lm} = -2\langle\sigma_lS_m\omega_l(\sigma)\rangle + \langle\sigma_l(\tilde{S}_m - S_m)\omega_m(S)\rangle, \quad (16)$$

$$D_{lm} = -\langle \sigma_l(\tilde{S}_m + S_m)\omega_{lm}(\sigma,S)\rangle + \sum_{\substack{j\neq l \\ (\text{NN of } m)}} \langle \sigma_l(\tilde{S}_m - S_m)\omega_{jm}(\sigma,S)\rangle - 2\sum_{\substack{k\neq m \\ (\text{NN of } l)}} \langle \sigma_l S_m \omega_{lk}(\sigma,S)\rangle. \tag{17}$$

The equations of motion for the sublattice magnetizations $\langle\sigma_l\rangle$ and $\langle S_m\rangle$, and for the correlation function $\langle\sigma_l S_m\rangle$ are exact. Unfortunately, we do not know an exact expression for the probability distribution of the states. We need to employ some approximation scheme in order to decouple the set of equations. Here we appeal to the pair approximation, which is the simplest approximation beyond the mean field one.

III. PAIR APPROXIMATION

Considering the application of the pair approximation to this dynamical mixed-spin problem, a set of self-consistent equations is not immediately obtained, because there also appear the correlations $\langle S_m^2\rangle$ and $\langle \sigma_l S_m^2\rangle$. To see this, let us consider a single pair of spins σ and S. We can write the following identity for the joint probability of the spins σ and S:

$$p(\sigma,S;t) = \sum_{\sigma',S'} \delta_{\sigma,\sigma'}\delta_{S,S'} p(\sigma',S';t), \tag{18}$$

where

$$\delta_{\sigma,\sigma'} = \frac{1}{2}(1+\sigma\sigma'), \tag{19}$$

and

$$\delta_{S,S'} = 1 - (S^2 + S'^2) + \frac{1}{2}SS' + \frac{3}{2}(SS')^2. \tag{20}$$

Then the probability for the pair (σ,S), at time t, can be written as

$$p(\sigma,S;t) = \frac{1}{2}\Big[1 + \sigma\langle\sigma(t)\rangle + \frac{1}{2}S\langle S(t)\rangle - S^2 - \langle S^2(t)\rangle + \frac{3}{2}S^2\langle S^2(t)\rangle + \frac{1}{2}\sigma S\langle\sigma(t)S(t)\rangle - \sigma S^2\langle\sigma(t)\rangle - \sigma\langle\sigma(t)S^2(t)\rangle + \frac{3}{2}\sigma S^2\langle\sigma(t)S^2(t)\rangle\Big]. \tag{21}$$

Before proceeding with the calculations, let us write the equations of motion for the correlations $\langle S_m^2\rangle$ and $\langle\sigma_l S_m^2\rangle$:

$$\frac{d}{dt}\langle S_m^2\rangle = pC_m + (1-p)F_m, \tag{22}$$

$$\frac{d}{dt}\langle \sigma_l S_m^2\rangle = pB_{lm} + (1-p)E_{lm}, \tag{23}$$

where

$$C_m = \langle(\tilde{S}_m^2 - S_m^2)\omega_m(S)\rangle, \tag{24}$$

$$F_m = \sum_{\substack{j \\ (\text{NN of } m)}} \langle(\tilde{S}_m^2 - S_m^2)\omega_{jm}(\sigma,S)\rangle, \tag{25}$$

$$B_{lm} = -2\langle\sigma_l S_m^2\omega_l(\sigma)\rangle + \langle\sigma_l(\tilde{S}_m^2 - S_m^2)\omega_m(S)\rangle, \tag{26}$$

$$E_{lm} = -\langle\sigma_l(\tilde{S}_m^2 + S_m^2)\omega_{lm}(\sigma,S)\rangle + \sum_{\substack{j\neq l \\ (\text{NN of } m)}} \langle\sigma_l(\tilde{S}_m^2 - S_m^2)\omega_{jm}(\sigma,S)\rangle - 2\sum_{\substack{k\neq m \\ (\text{NN of } l)}} \langle\sigma_l S_m^2\omega_{lk}(\sigma,S)\rangle. \tag{27}$$

Now we search for solutions such that $m_1 = \langle\sigma_l\rangle$, for any spin belonging to the σ sublattice, and $m_2 = \langle S_m\rangle$, for any spin belonging to the S sublattice. We also define the correlation functions $r = \langle\sigma_l S_m\rangle$, $q = \langle S_m^2\rangle$ and $q_1 = \langle\sigma_l S_m^2\rangle$. In this way, we can write the following expressions for the one- and two-spin probabilities:

$$P_1(\sigma_1) = \frac{1}{2}(1+\sigma_1 m_1), \tag{28}$$

$$P_2(S_2) = 1 + \frac{1}{2}S_2 m_2 - S_2^2 - \left(1 - \frac{3}{2}S_2^2\right)q, \tag{29}$$

$$P_{12}(\sigma_1,S_2) = \frac{1}{2}\Big[1 + \sigma_1 m_1 + \frac{1}{2}S_2 m_2 - S_2^2 - \left(1-\frac{3}{2}S_2^2\right)q + \frac{1}{2}\sigma_1 S_2 r - \sigma_1 S_2^2 m_1 - \sigma_1\left(1-\frac{3}{2}S_2^2\right)q_1\Big], \tag{30}$$

where σ_1 and S_2 are nearest neighboring spins belonging to the σ and S sublattices, respectively. To find the mean values of interest, we need to consider three different types of clusters: For the square lattice, the A cluster is composed of a spin σ_1 of the σ sublattice, surrounded by four spins S_i of the S sublattice. The probability of this cluster is

$$P_A = P_1(\sigma_1)\prod_{\substack{i \\ (\text{NN of } 1)}} \frac{P_{12}(\sigma_1,S_i)}{P_1(\sigma_1)}. \tag{31}$$

The second cluster we consider, the B cluster, is composed of a spin S_2 of the S sublattice, surrounded by four spins σ_l of the σ sublattice. The probability of this cluster is given by

$$P_B = P_2(S_2)\prod_{\substack{l \\ (\text{NN of } 2)}} \frac{P_{12}(\sigma_l,S_2)}{P_2(S_2)}. \tag{32}$$

The third cluster, the C cluster, is made up of a pair of nearest neighbor spins σ_1, belonging to the σ sublattice; S_2

belonging to the S sublattice; and their nearest neighbors. In this pair approximation, the probability of this cluster is given by

$$P_C = P_{12}(\sigma_1, S_2) \prod_{\substack{i\neq 2 \\ (\text{NN of } 1)}} \frac{P_{12}(\sigma_1, S_i)}{P_1(\sigma_1)} \prod_{\substack{l\neq 1 \\ (\text{NN of } 2)}} \frac{P_{12}(\sigma_l, S_2)}{P_2(S_2)}. \tag{33}$$

After straightforward, but tedious, algebraic manipulations, we finally arrive at the following set of equations for the time evolution of the sublattice magnetizations and correlation functions:

$$\frac{d}{dt} m_1 = pA_1(m_1, m_2, r, q, q_1) + (1-p) D_1(m_1, m_2, r, q, q_1), \tag{34}$$

$$\frac{d}{dt} m_2 = pB_2(m_1, m_2, r, q, q_1) + (1-p) E_2(m_1, m_2, r, q, q_1), \tag{35}$$

$$\frac{d}{dt} q = pC_2(m_1, m_2, r, q, q_1) + (1-p) F_2(m_1, m_2, r, q, q_1), \tag{36}$$

$$\frac{d}{dt} r = pA_{12}(m_1, m_2, r, q, q_1) + (1-p) D_{12}(m_1, m_2, r, q, q_1), \tag{37}$$

$$\frac{d}{dt} q_1 = pB_{12}(m_1, m_2, r, q, q_1) + (1-p) E_{12}(m_1, m_2, r, q, q_1). \tag{38}$$

The expressions which appear on the right-hand sides of Eqs. (34)–(38) are too lengthy to present here. In Sec. IV we will obtain the numerical solutions of the above system of equations.

IV. STATIONARY STATES AND PHASE DIAGRAM

The steady state solutions of the system of equations (34)–(38) are obtained by employing the fourth-order Runge-Kutta method. For selected values of p and T, we find three different types of magnetic ordering: a ferrimagnetic state, with $m_1 \neq m_2$, and $m_1 > 0$, $m_2 > 0$; a paramagnetic state, with $m_1 = m_2 = 0$; and an antiferrimagnetic state, where $m_1 \neq m_2$, and $m_1 < 0$, $m_2 > 0$. In Fig. 1, we exhibit the phase diagram of the model in the plane $\eta = \exp(-1/2\theta)$, versus $Q = 1-p$, where $\theta = k_B T/2zJ$ is the reduced temperature, and z is the number of nearest neighbors ($z=4$ for the square lattice). It displays three different phases, separated by two continuous transition lines: one between the ferrimagnetic (F) and paramagnetic (P) phases, and the other between the paramagnetic (P) and antiferrimagnetic (AF) phases. For the particular case $Q=0$, where only one-spin flips are permitted, the stationary state coincides with the thermodynamic equilibrium state, because there is no flux of energy into the system. In this pair approximation, we found the value $\theta_c = 0.3068$ for the transition temperature between the ferrimagnetic and paramagnetic phases. The mean field value for this critical temperature is $\theta_c = 0.408$. Other known estimates

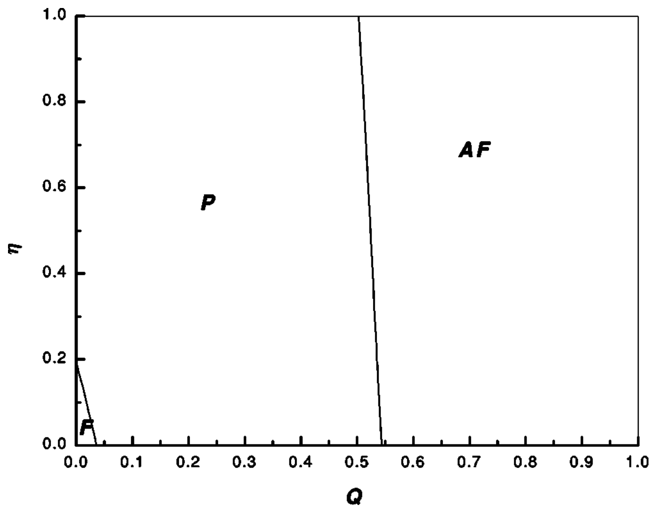

FIG. 1. Phase diagram of the mixed-spin ferromagnetic Ising model in the plane η vs Q. $\eta = \exp(-1/2\theta)$, where $\theta = k_B T/2zJ$ is the reduced temperature, and $Q = 1-p$ is the competition parameter between the one- and two-spin flip processes. F, P, and AF, denote the ferrimagnetic, paramagnetic, and antiferrimagnetic phases, respectively.

for this critical temperature are $\theta_c = 0.182$ from real space renormalization [8], $\theta_c = 0.244$ from series expansion calculations [9], $\theta_c = 0.24$ from Monte Carlo simulations [10], and $\theta_c = 0.322$ from mean field renormalization group calculations [11].

We point up that the competition between the one- and two-spin flip already appears for small values of Q. For $\theta < \theta_c$, and for very small values of Q, the one-spin flip process is the dominant one, and the ferrimagnetic phase is stable below a critical value of the competition parameter Q. However, the two-spin flip process, which simulates an input of energy into the system, easily destroys the ferrimagnetic phase. For instance, the critical value at $\theta = 0$ is $Q_c = 0.04$. Above this critical value, we enter into the paramagnetic phase, where the sublattice magnetizations m_1 and m_2 vanish. Increasing the flux of energy, we reach another critical value of Q, where the paramagnetic phase becomes unstable, and an antiferrimagnetic phase appears. The transition between the paramagnetic and antiferrimagnetic phases is continuous, and the transition line is almost independent of temperature. This stresses the dominant character of the two-spin flip over the one-spin flip, because the former was chosen to be independent of temperature. In Fig. 2 we show the plot of the sublattice magnetization m_1 as a function of the competition parameter Q for two selected values of the reduced temperature: one value below the critical temperature θ_c, and the other one above it. In both cases, we notice that there is a critical value of Q, almost independent of temperature, where the sublattice magnetization m_1 is nonanalytic. This marks the dynamical phase transition between the paramagnetic and antiferrimagnetic phases. The same behavior is also observed for the other sublattice magnetization m_2. In Fig. 3, we also exhibit the plot of $q = \langle S^2 \rangle$ versus the competition parameter Q for the same two temperatures of Fig. 2. At the paramagnetic-antiferrimagnetic transition, we find a similar nonanalytical behavior for q, as already seen for m_1 and m_2.

This model system exhibits a self-organization phenom-

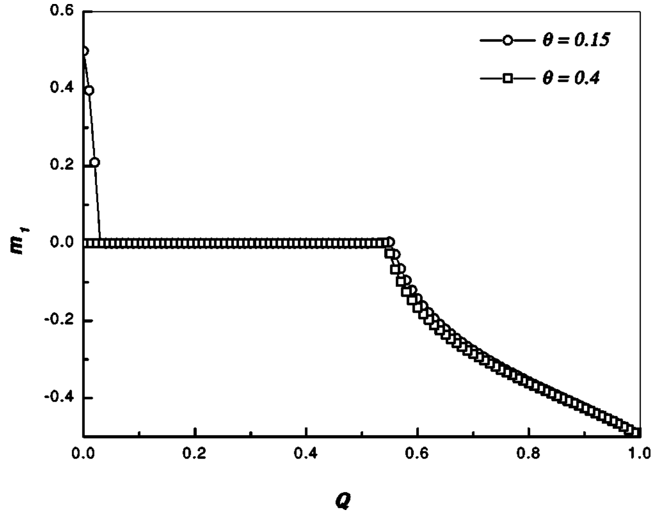

FIG. 2. Magnetization m_1 as a function of the competition parameter Q, for two different temperatures, as indicated in the figure.

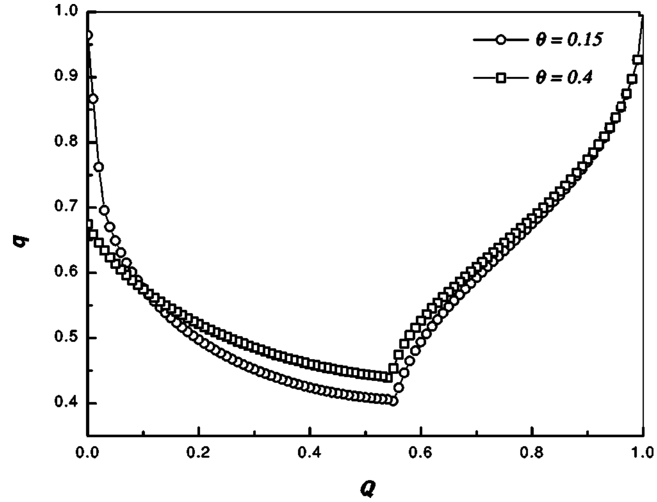

FIG. 3. Autocorrelation function $q=\langle S^2\rangle$ as a function of the competition parameter Q, for two selected values of temperature, as indicated in the figure.

enon: when the flux of energy is not present, we have a well defined equilibrium ferrimagnetic phase for all values of the reduced temperature, such that $\theta<\theta_c$. However, when the system is submitted to a small flux of energy, the ferrimagnetic state can become unstable due to the simultaneous flipping of pairs of neighboring spins. The system will enter into a paramagnetic phase, after a critical value of the parameter Q, which measures the competition between one- and two-spin flips, is attained. If we still increase the flux of energy, the paramagnetic phase will become unstable, and finally we will reach an ordered antiferromagnetic phase, at a higher value of the competition parameter. We would like to stress that we could reverse the whole process, decreasing the flux of energy from an ordered antiferrimagnetic steady state and finally arriving at a ferrimagnetic state, after crossing a paramagnetic region. We would like to point out that the inclusion of a magnetic field in our model system will change the phase diagram we have obtained. The ferrimagnetic to paramagnetic transition at $Q=0$ will disappear, and the transition lines between the ferrimagnetic and paramagnetic phases, and between the paramagnetic and antiferrimagnetic phases, will move to the right in our Fig. 1, i.e., in the direction of high values of Q. The main effect of a magnetic field is ultimately to destroy the antiferrimagnetic phase at large values of the field. We intend, in the future, to include the detailed effects of the field and of single-ion anisotropy in this two-sublattice mixed-spin Ising model.

V. CONCLUSIONS

In this work we have considered a nonequilibrium mixed-spin ferromagnetic Ising model in a square lattice. The dynamical states of the system evolve in time following two competing dynamical processes: a one-spin flip of a spin of either $\sigma=1/2$ or $S=1$ sublattice, which accounts for the relaxation of the system in the heat bath, and a simultaneous flipping of two neighboring σ and S spins, which is assumed to be independent of temperature, and that simulates a flux of energy into the system. The equations of motion were decoupled by the dynamical pair approximation, and we found three different possible steady states. The phase diagram exhibits, at a very low flux of energy, a ferrimagnetic phase, which becomes unstable at a critical value of the competition parameter between the two dynamical processes. Above this critical value, the spin system settles into a paramagnetic phase, and a new critical value of the competition parameter is attained. If the flux of energy is sufficiently high, the system will organize itself into an antiferrimagnetic arrangement of spins. The ferrimagnetic to paramagnetic and paramagnetic to antiferrimagnetic transitions are both continuous phase transitions.

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