Kinetic Ashkin-Teller model with competing dynamics

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We study a two-dimensional nonequilibrium Ashkin-Teller model based on competing dynamics induced by contact with a heat bath at temperature *T*, and subject to an external source of energy. The dynamics of the system is simulated by two competing stochastic processes: a Glauber dynamics with probability *p*, which simulates the contact with the heat bath; and a Kawasaki dynamics with probability $1-p$, which takes into account the flux 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. The phase diagrams of the model exhibit a self-organization phenomenon for certain values of the fourth coupling interaction strength. On the other hand, from exponent calculations, the equilibrium critical behavior is preserved when nonequilibrium conditions are applied.

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I. INTRODUCTION

In general, nonequilibrium systems display rich and complex behavior such as phase separation, pattern formation, turbulence [1,2], and self-organization as long as nonequilibrium conditions are maintained. These latter structures are called dissipative structures [3], and are found in fluid dynamics and chemical physical reactions [3,4]. Therefore, it is useful first to study simple models of these systems. There exist models of nonequilibrium systems described by stationary distributions that are comparatively easy to study. One example is an open system in contact with a heat bath maintained in a nonequilibrium state by an external source of energy [5]. Another class of nonequilibrium steady state is obtained when the system is closed, and the dynamic is described by a local competition of two dynamics at different temperatures [6]. It is the former type of system that we address in this paper. A typical kinetic Ising model was investigated by allowing only the Glauber single spin-flip dynamics [7], which 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 is a good candidate for a study of self-organization phenomena. It was studied by using the master-equation formalism when the system is governed by two competing processes: the one-spin-flip Glauber dynamics [7] and the two-spin-exchange Kawasaki dynamics [8]. The first dynamic mimics the contact of the system with the heat bath at a fixed temperature *T*, while the second simulates the input of energy into the system. Depending on the competition between the Glauber process with a weight *p* and the Kawasaki process with a weight $1-p$, Tome and Oliveira [5] studied the two-dimensional ferromagnetic Ising model within the dynamical pair approximation (PA). An interesting phase diagram was obtained as a function of the competing parameter *p*. A phase transition from the ferromagnetic to paramagnetic phase occurs as the value $1-p$ is increased. For a further increase of $1-p$, when the Kawasaki process dominates the system self-organizes into an ordered antiferromagnetic phase. By using Monte Carlo (MC) simulations, Grandi and Figueiredo [9] confirmed that this phenomena occurred in the model, but found a phase diagram which is different from the one obtained by the PA [5]. In contrast, in the case of the kinetic antiferromagnetic Ising model both methods, PA [10] and MC [11] yielded only a paramagnetic phase, without any self-organization phenomena, when the Kawasaki dynamics dominated. However, the authors of Ref. [12] showed recently that a self-organization phenomenon may occur if the spin-exchange rate depends on the strength of the exchange between nearest neighbor spins. Another important question is whether critical properties and universality classes of these nonequilibrium systems are the same to the equivalent equilibrium ones. From exponent calculations by MC simulations of the two cited models [9,11], it was shown that the equilibrium critical properties are preserved when nonequilibrium conditions are applied. This confirmed that any nonequilibrium spin-flip dynamics with up-down symmetry belongs to the same universality class of the equilibrium Ising model, as suggested in Ref. [13]. Recently, the antiferromagnetic spin-1 Blume-Capel model was studied, under the effect of these two competing dynamics, by applying finite-size-scaling analysis and MC simulations [14]. It appears in the phase diagrams, for some values of the crystal field, a dynamical tricritical point and a kind of self-organization phenomenon within the disordered phase.

In this paper, we specifically consider the effect of the competing dynamics described above on the two-dimensional ($d=2$) ferromagnetic spin-1/2 Ashkin-Teller (AT) model [15], which is a generalization of the Ising model to a four component system. It may be considered as a superposition of two Ising models, which are described by

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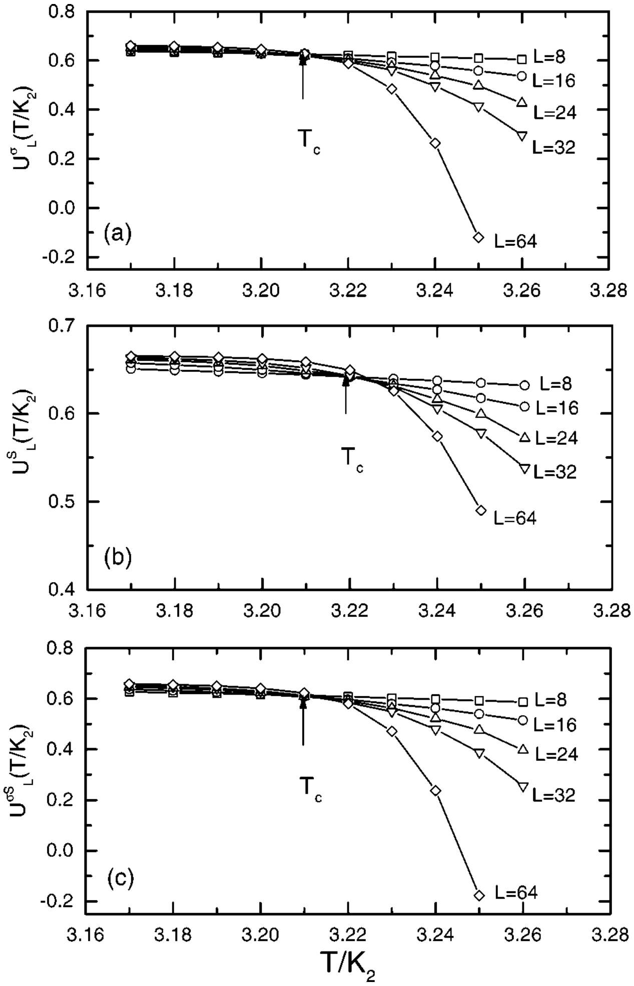

FIG. 1. Plots of the fourth-order cumulants vs the reduced temperature, T/K_2 for $K_4/K_2=1.0$ and $p=0.5$ with various choices of L. The critical temperatures T_c are (a) 3.21 ± 0.01 for $\alpha=\sigma$, (b) 3.22 ± 0.01 for $\alpha=S$, and (c) 3.21 ± 0.01 for $\alpha=\sigma S$ (the lines in all our figures are to guide the eye).

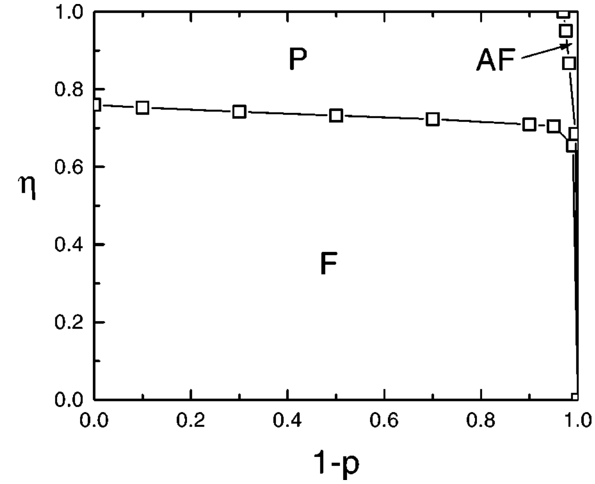

FIG. 2. Phase diagram in the plane $(\eta,1-p)$ for $K_4/K_2=1$ with competing Glauber (probability p) and Kawasaki (probability $1-p$) dynamics. The parameter η is given by $\eta=\exp(-K_2/k_BT)$. The system exhibits paramagnetic (P), ferromagnetic (F), and antiferromagnetic (AF) phases.

variables σ_i and S_i sitting on each of the sites of hypercubic lattice. Within each Ising model, there is two-spin nearest-neighbor interaction with strength K_2. In addition; the different Ising models are coupled by a four-spin interaction with strength K_4. The Hamiltonian of the model is given by

$$H=-K_2\sum_{\langle ij\rangle}(\sigma_i\sigma_j+S_iS_j)-K_4\sum_{\langle ij\rangle}S_iS_j\sigma_i\sigma_j, \qquad (1)$$

where the spins σ_i and S_i are located on sites of a hypercubic lattice, and take the values ±1. The parameters K_2 and K_4 are the two- and four-spin interactions. Different methods, from variational approaches [16,17] to more accurate ones that take into account the effect of fluctuations [16,18–21], have been applied in $d=2$ to study the critical behavior of the equilibrium version of this model. All these methods yielded three different phases: a paramagnetic (P) phase in which neither σ nor S nor anything else is ordered ($\langle\sigma\rangle=\langle S\rangle=\langle\sigma S\rangle=0$); a Baxter phase in which σ and S order independently in a ferromagnetic fashion with $\langle\sigma S\rangle\neq0$; and a partially ordered phase in which σS is ordered ferromagnetically, $\langle\sigma S\rangle\neq0$ but $\langle\sigma\rangle=\langle S\rangle=0$. This latter phase exists only at high temperature, separating the Baxter and the paramagnetic phases. Apart from the variational approaches that give tricritical points, the other accurate methods yield a line of critical points. It connects the Ising critical point at one end ($K_4/K_2=0$) to the four-state Potts critical point at the other end ($K_4/K_2=1$). Along this line the exponents vary continuously [18,20,21].

We have wondered if the interesting AT model, when subjected to the competition between the Glauber and Kawasaki processes, would preserve the picture of self-organization and the equilibrium critical exponents. To better understand and test this equivalence we have used MC simulations and finite-size scaling to explore this rich model, which does not preserve the up-down symmetry for $K_4/K_2\neq0$. The paper is organized as follows: In Sec. II, the dynamics of the model are described. Section III contains the Monte Carlo simulations used to analyze this model. Section IV presents our results and a discussion of our analysis. Finally in Sec. V, we draw our conclusion.

II. DYNAMICS OF THE MODEL

The states of the system evolve in time according to stochastic dynamics. Let $P(r,t)$, $r=(s,S)$, be the probability of state r at time t. The evolution of $P(r,t)$ is given by the master equation [8]

$$\frac{d}{dt}P(r,t)=\sum_{r'}[P(r',t)W(r',r)-P(r,t)W(r,r')], \quad (2)$$

with $r=\sigma, S$ and $r'=\sigma', S'$, and where $W(r',r)$ gives the probability, per unit time, of a transition from state r' to state r, if the system is in state r'. We consider the transition

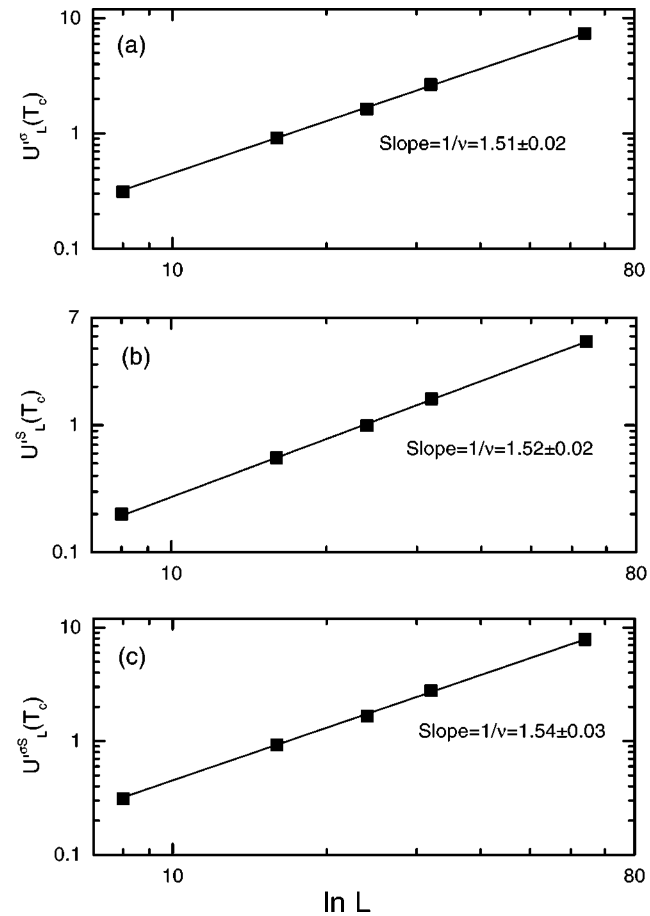

FIG. 3. Finite-size dependence in log-log plots for $U_L'^{(\alpha)}(T_c)$ vs L at the critical point T_c for $K_4/K_2=1.0$ and $p=0.5$. The straight lines are the best fit to the data points. From these slopes we obtain (a) $\nu=0.662\pm0.02$ for $\alpha=\sigma$, (b) $\nu=0.657\pm0.02$ for $\alpha=S$, and (c) $\nu=0.649\pm0.03$ for $\alpha=\sigma S$.

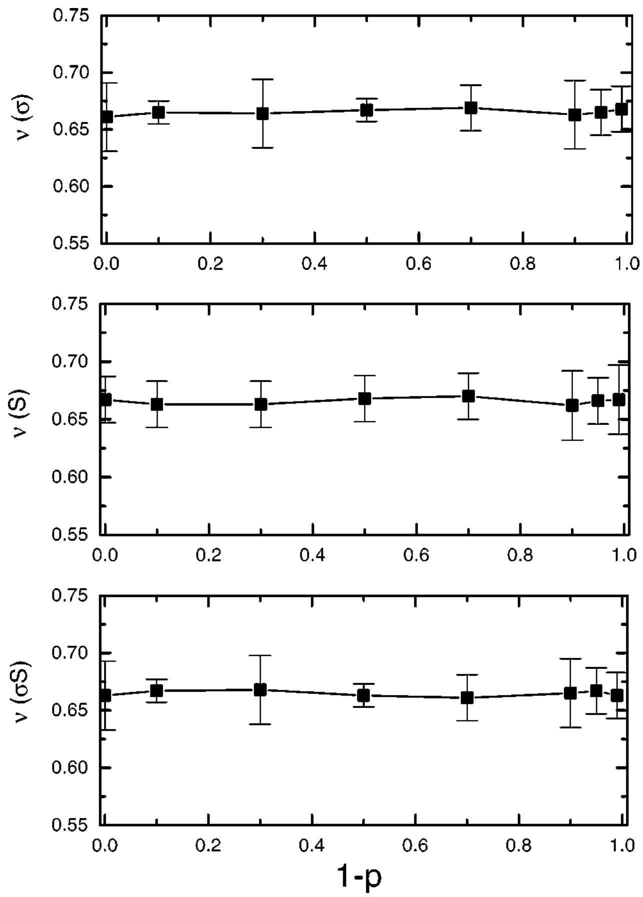

FIG. 4. Critical exponent $\nu(\alpha)$ (where α denotes the phases σ, S, and σS, respectively) as a function of $1-p$ at the critical line represented in Fig. 2. The error bars give the accuracy of our Monte Carlo data points. The estimated values of ν are around the corresponding equilibrium four state Potts value $\nu=\frac{2}{3}$.

probability $W(r',r)$, which is constructed in order to take into account two competing processes, such as

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

where

$$W_G(r',r)=\sum_{i=1}^{N}\ \delta_{r_1'r_1}\delta_{r_2'r_2}\ldots\delta_{r_i'r_i}\ldots\delta_{r_N'r_N}w_i(r), \tag{4}$$

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

$$W_K(r',r)=\sum_{i=1}^{N}\ \delta_{r_1'r_1},\ldots.\delta_{r_i'r_j}\ldots\delta_{r_j'r_i},\ldots,\delta_{r_N'r_N}w_{ij}(r) \tag{5}$$

is the two-spin exchange Kawasaki process, which simulates the flux of energy into the system. In these equations $w_i(r)$ and $w_{ij}(r)$ are the probability per unit time of flipping spin i and the exchange of two nearest-neighboring spins i and j. The contact with the heat bath at temperature T is given by

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

where ΔE_i is the change in energy when spin i is flipped, and k_B is the Boltzmann factor.

For the two-spin exchange Kawasaki dynamics $w_{ij}(r)$, we also take the prescription

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

where ΔE_{ij} is the energy difference between the states after and before the exchange of the neighboring spins i and j.

III. MONTE CARLO SIMULATIONS

We have performed MC simulations on a square lattice with $L\times L=N$ sites ($2N$ spins), with periodic boundary conditions. We often start from different initial configurations to check if the final state (steady state) obtained is the right one. The simulation procedure used is similar to that of Ref. [11], and is resumed in the following: For given parameters of the model $(p,T/K_2,K_4/K_2)$, a lattice site i, containing the two

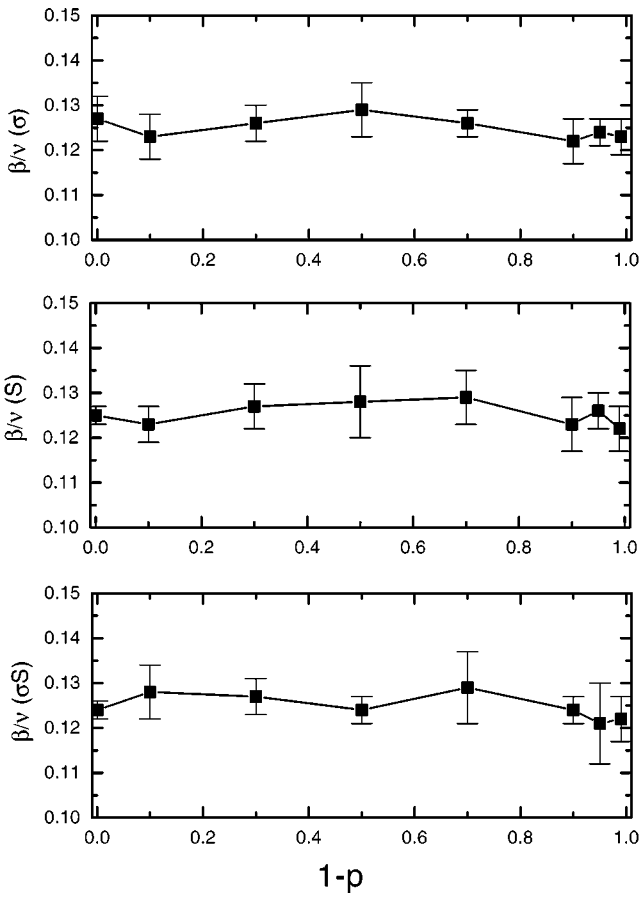

FIG. 5. Ratio β/ν (α) as a function of $1-p$ at the critical line represented in Fig. 2. The estimated values of this ratio are around the corresponding equilibrium four state Potts value $\frac{1}{8}$.

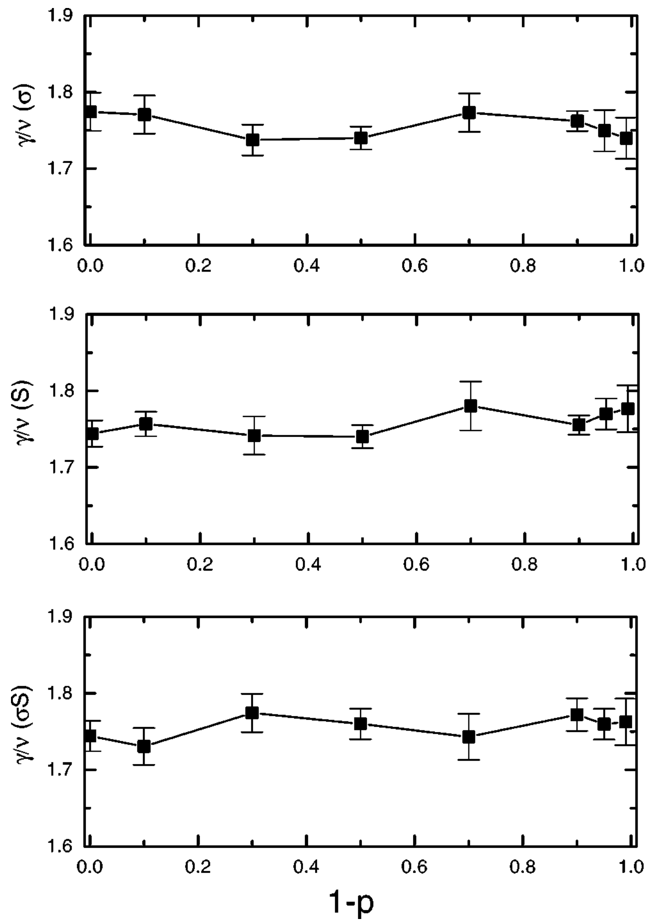

FIG. 6. Ratio γ/ν (α) as function of $1-p$ at the critical line represented in Fig. 2. The estimated values of this ratio are around the corresponding equilibrium four state Potts value $\frac{7}{4}$.

spins σ and S, is first randomly chosen. At each site we first consider the σ spin and then the S spin as the reference spin. Then one chooses a random number η_l between 0 and 1. If $\eta_l \leqslant p$, a spin-flip process is attempted. Otherwise, if $\eta_l > p$, a spin exchange of site i is attempted with a randomly selected neighboring site j.

The physical quantities of use are the magnetizations $M_\alpha(\alpha=\sigma, S, \sigma S)$. Their associated fluctuations (susceptibilities) and fourth-order cumulants are given, respectively, by

$$M_\alpha = \langle |M_\alpha| \rangle = \frac{1}{NV} \sum_c \sum_i \alpha_i(c) \quad \text{with} \quad \alpha = \sigma, S, \sigma S,$$

$$\chi_\alpha = \frac{N}{k_B T} (\langle M_\alpha^2 \rangle - \langle M_\alpha \rangle^2) \quad \text{with} \quad \alpha = \sigma, S, \sigma S, \qquad (8)$$

$$U_L = 1 - \frac{\langle M_\alpha^4 \rangle}{3 \langle M_\alpha^2 \rangle^2} \quad \text{with} \quad \alpha = \sigma, S, \sigma S,$$

where i runs over the lattice sites. c runs over the configurations obtained to update the lattice over one sweep of the entire N sites [one Monte Carlo step (MCS)]. They are counted after the system reaches thermal equilibrium. V is the number of MCS [10].

Finally, we will use finite size scaling theory [11,22] to analyze our results. Following this approach, in the neighborhood of the infinite critical point T_c and by using the scaled variable $x = tL^{l/v}$ $(t = |1 - T/T_c|)$, the above quantities, for sufficiently large L, obey

$$M_L(T) = L^{-\beta/v} f(x),$$

$$\chi_L(T) = L^{\gamma/v} g(x), \qquad (9)$$

$$U_L(T) = U_0(x),$$

where $f(x) \rightarrow Bx^\beta$, and $g(x) \rightarrow Cx^\gamma$ in the limit of $t \rightarrow 0$ and $x \rightarrow \infty$, so that the infinite lattice critical behavior is recovered. If we derive the third of Eqs. (9) with respect to the temperature T, we obtain the scaling relation

$$U_L'(T) = L^{1/v} U_0'(x). \qquad (10)$$

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

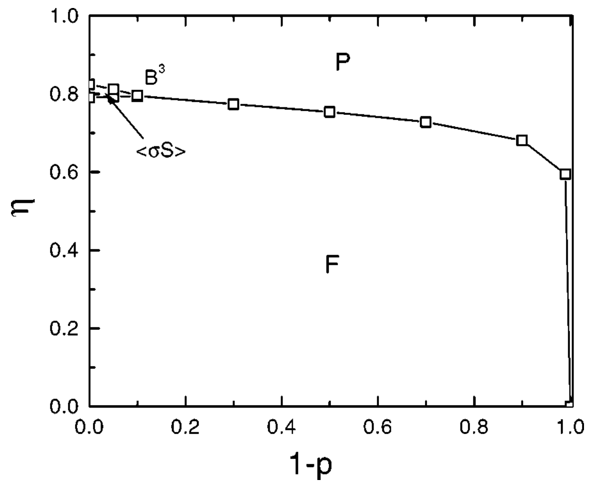

FIG. 7. Phase diagram in the plane (η,$1-p$) for $K_4/K_2=2$. The system exhibits paramagnetic (P), ferromagnetic (F), and partially ordered (PO) phases. B^3 denotes a multicritical point.

IV. PHASE DIAGRAMS AND CRITICAL EXPONENTS

Our phase diagrams are obtained from MC simulations for different sizes ranging from $L=8$, 16, 24, 32, and 64. The number of Monte Carlo steps needed to reach the steady state depends on the model parameters and the system size considered. Very long MCS's are used, typically from 5×10^5 to 10^6 MCS's for thermal equilibration and 6×10^6 MCS's for all system sizes, to calculate the quantities of interest. We have plotted the phase diagrams in the plane $[\eta=\exp(-K_2/k_BT), 1-p]$ for certain values of K_4/K_2. We note that, in our program, the ferromagnetic and antiferromagnetic order parameters associated with σ, S, and σS, as well as their associated susceptibilities and cumulants, are computed.

In the absence of the fourth coupling interaction, $K_4/K_2=0$, the AT model is reduced to two decoupled Ising models. Consequently the phase diagram and the critical exponents (figures not shown) are similar to those obtained by Grandi and Figueiredo [9], namely, a self-organization phenomena, which occurs when the Kawasaki process dominates, and the preservation of the equilibrium Ising critical exponents.

For weak K_4/K_2,$K_4/K_2=1$, the AT model has the symmetry of the four-state Potts model [16–21] in the equilibrium case. The critical temperature for every value of p is better located by using the standard cumulant intersection method (for σ, S, and σS) for several lattice sizes [9,22]. We can see in Fig. 1 that all the fourth-order cumulants associated with the magnetizations $\langle\sigma\rangle$, $\langle S\rangle$, and $\langle\sigma S\rangle$ intersect at nearly the same critical temperature T_c for whatever value of L within statistical errors. Using this method, we have determined the phase diagram when the Kawasaki process is applied. It is shown in Fig. 2 that we have two phases: a paramagnetic (P) phase where $\langle\sigma\rangle=\langle S\rangle=\langle\sigma S\rangle=0$, and a ferromagnetic ($F$) phase where $\langle\sigma\rangle$ and $\langle S\rangle$ are ordered ferromagnetically and $\langle\sigma S\rangle\neq0$. A critical line separates these two phases. For very high values of the flux of energy into the system, in the neighborhood of $p=0$, a self-organization phenomena occurs in the phase diagram where an antiferromagnetic phase emerges from the disordered paramagnetic phase. For the pure Kawasaki case, $p=0$, the evolution of the system is the same for whatever temperature; then we always go to a state of maximum energy compatible with a given initial magnetization.

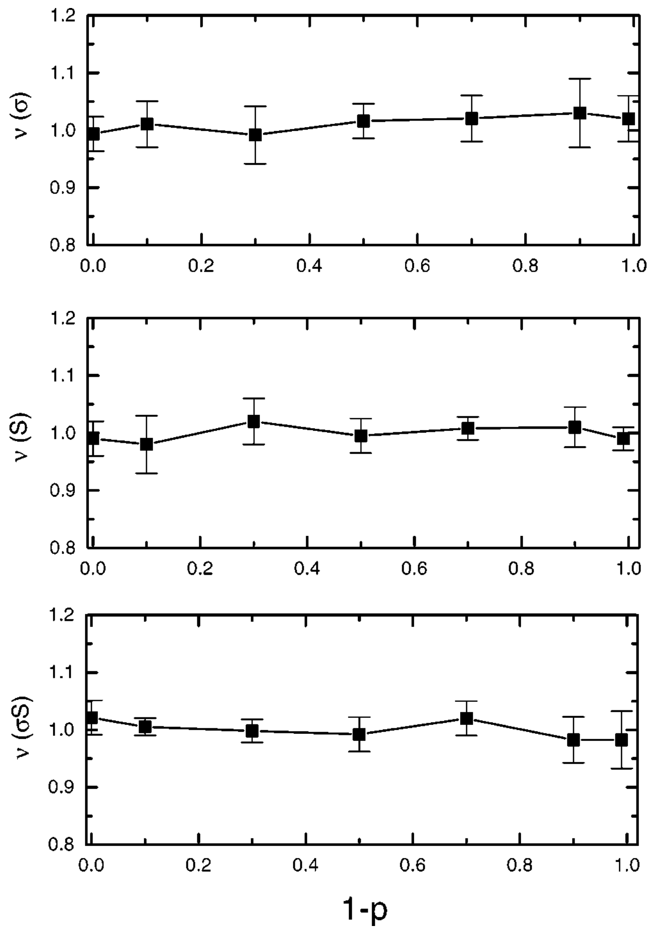

FIG. 8. Critical exponent ν (α) (where α denotes the phases σ, S, and σS, respectively), as a function of $(1-p)$ at the critical line represented in Fig. 7. The error bars give the accuracy of our Monte Carlo data points. The estimated values of ν are around the corresponding equilibrium Ising value $\nu=1$.

On the other hand, we have also extracted the associated critical exponents from our data by using finite size scaling relations [Eqs. (9) and (10)]. Thus with T_c determined, we have calculated the exponents v, β, and γ from the log-log plots of the derivative of the cumulants, the magnetizations and the susceptibilities, respectively, as functions of L [11,22]. For every log-log plot we have calculated the values of U_L, M_L, and χ_L at the critical temperature $T_c(p)$ obtained from Fig. 2. Another way to find the critical exponent v is to use the location of the susceptibility peak at the finite lattice critical temperature $T_c(L)$, namely, $T_c(L)-T_c\approx L^{-1/v}$ (figures not shown). Both methods yield, within statistical errors, values of v that are nearly consistent to each other [22] (see Fig. 3). As we can see from Figs. 4–6, our estimates of v, β/v, and γ/v as functions of $1-p$ are in agreement with the corresponding equilibrium four-state

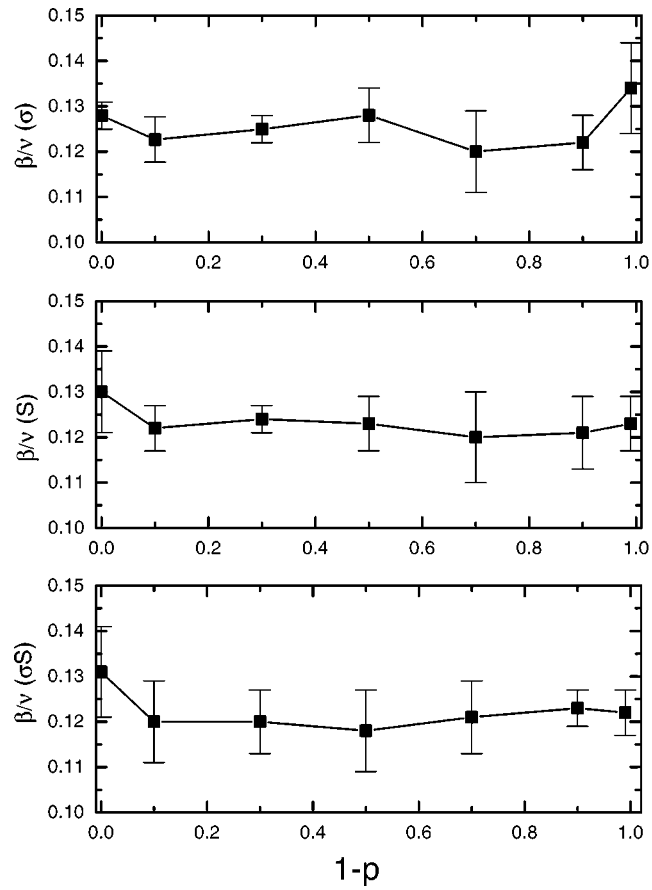

FIG. 9. Ratio β/ν (α) as a function of $1-p$ at the critical line represented in Fig. 7. The estimated values of this ratio are around the corresponding equilibrium Ising value $\frac{1}{8}$.

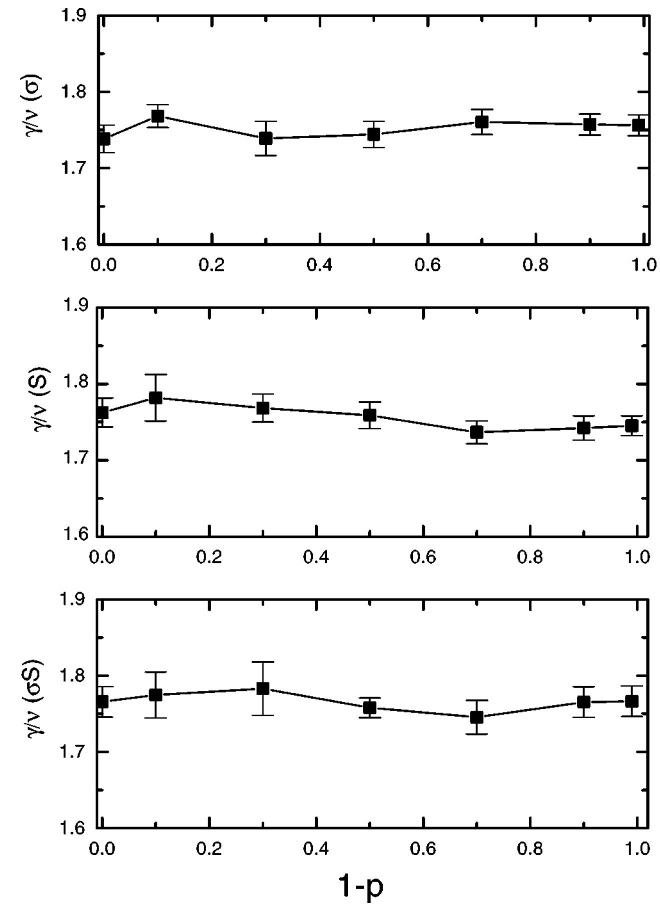

FIG. 10. Ratio γ/ν (α) as function of $1-p$ at the critical line represented in Fig. 7. The estimated values of this ratio are around the corresponding equilibrium Ising value $\frac{7}{4}$.

Potts exponents ($v=\frac{2}{3}$, $\beta/v=\frac{1}{8}$, and $\gamma/v=\frac{7}{4}$) [19,20], and show that the argument of Ref. [13] also holds for this model. Although we do not present detailed calculations concerning the continuous transition between the paramagnetic and antiferromagnetic phases, the critical temperature and the critical exponents can be obtained in a similar manner as the ferromagnetic-paramagnetic transition. For instance, for $p=0.005$ we have found the following values: $T_c=6.08\pm0.02$, $v=0.68\pm0.03$, $\beta/v=0.14\pm0.02$, and $\gamma/v=1.73\pm0.05$.

When K_4/K_2 is increased, $K_4/K_2>1$, a different topology appears. Our results from MC data are plotted in Fig. 7 for $K_4/K_2=2$. We have obtained three phases: a paramagnetic phase, a ferromagnetic phase and a partially ordered (PO) phase at high temperatures. They are all separated by critical lines of second order. The latter PO phase ($\langle\sigma S\rangle\neq0$ but $\langle\sigma\rangle=\langle S\rangle=0$), which exists at equilibrium ($p=1$), persists for small values of the flux of energy (i.e., when the Glauber process still dominates the dynamics) and separates the ferromagnetic phase from the paramagnetic one. By increasing the flux of energy, the PO phase disappears, and we have only a critical line, which separates the ferromagnetic and paramagnetic phases. It is a decreasing function of *p*. Since the dominant dynamic is the Kawasaki process, we did not observe within our simulations, for any value of *p* and for all values of temperature T/K_2, any self-organization phenomenon in the system. The only stationary state is the disordered one whatever the initial starting configuration (ferromagnetic, antiferromagnetic, or disordered phases).

The critical exponents associated with this phase diagram have been calculated. However, we point out that in the equilibrium case ($p=1$), the transitions ferro↔PO and PO↔parra both belong to the Ising universality class with well known exponents ($v=1$, $\beta/v=1/8$, and $\gamma/v=7/4$) [20,21]. By using the same analysis as described above, in Figs. 8–10 we show our estimates of the stationary exponents v, β/v, and γ/v as functions of $1-p$. They all compare in a good way with the corresponding equilibrium $2d$ Ising critical exponents. Thus the argument of Ref. [13] is also preserved for this value of the fourth coupling interaction.

V. CONCLUSION

We have determined the phase diagram and studied the stationary critical properties of a nonequilibrium Ashkin-Teller model in a square lattice, where the system is in contact with a heat bath at temperature *T* and subject to an external flux of energy. The phase diagrams of the model we have obtained through Monte Carlo simulations exhibit, for small values of K_4/K_2, a self-organization phenomena which disappears for stronger ones.

Finally, with the use of finite size scaling ideas, the critical exponents have been calculated. Our results show that for $K_4/K_2=1$, we have a line of critical points that belong to the four-state Potts model. When the coupling K_4/K_2 becomes stronger, $K_4/K_2=2$, the exponent calculations show that both the critical lines F-PO, PO-P, and F-P, which separate the different phases of the system, belong to the Ising universality class.

ACKNOWLEDGMENT

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