Simple nonequilibrium extension of the Ising model

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(Received 10 May 1996)

We introduce a simple nonequilibrium version of the Ising model, exhibiting an order-disorder phase transition. It corresponds to the competition of two different kinetic processes: one of them ordering the system and the other one disordering it (temperatures zero and infinity, respectively). Owing to the simplicity of the model, it is possible to define a *pseudotemperature* T characterizing the system. By using T we elucidate a striking point recently arisen in the literature, namely, how does the critical region of nonequilibrium systems compare to that of their equilibrium counterparts. Extensive numerical simulations are presented, and the conclusion is made that the model belongs in the equilibrium Ising model universality class confirming a well known conjecture. [S1063-651X(96)12911-1]

PACS number(s): 05.40.+j, 64.60.Cn, 64.60.Ht

I. INTRODUCTION

The Ising model played a central role in the development of the theory of equilibrium phase transitions [1]. Despite the fact that it is defined in a very simple way, it captures the essential properties of a ubiquitous phase transition, namely, that occurring in one component systems with up-down symmetry and no extra symmetries or conservation laws. Extensions of the model to deal with time dependent properties, such as the Kawasaki spin-exchange model for systems with magnetization conservation [2], and the Glauber spin-flip model for systems without extra conservation laws [3], resulted as paradigmatic as their static counterpart. These dynamical Ising models are defined by stochastic master equations, in which the transition rates are such that the associated stationary probability distribution is given by the exponential of minus the Ising Hamiltonian divided by a given temperature and properly normalized, i.e., the well known equilibrium distribution. In this way, these models depict the relaxation to equilibrium.

The possibility of getting exact solutions for $d=1$ and/or $d=2$ [3,4] makes these models an appropriate workbench to study basic properties of systems exhibiting a phase transition.

The following natural extension of the Ising model consists of modifying it somehow in order to study far from equilibrium phase transitions.

This objective can be fulfilled in different ways. One of them, the only one we consider here, is based on the consideration of a system in which different microscopic processes compete with each other. That is, each of the individual processes by itself drives the system to a different stationary state, but the competition between them gives rise to what is called in the literature *dynamical frustration*.

The way to implement this idea in an Ising-like model is by considering a master equation with competing dynamics; i.e., the transition rates are given by a linear superposition of individual, equilibriumlike, transition rates. If only one of the elementary processes was active, then the stationary solution to the corresponding master equation would be an equilibrium one with an associated Ising Hamiltonian and a temperature T_i. The same is true for all the single dynamics, with the only difference being that for each of them the stationary solution is given, by definition, by a different temperature value, $T_1 \neq T_2 \neq T_3 \neq \cdots$ [5]. The stationary states associated with this kind of model do not satisfy, in general, *detailed balance* with respect with any short range effective Hamiltonian, and therefore correspond to nonequilibrium situations. A number of studies and reviews of this sort of model can be found in Refs. [6–8].

In this paper we focus on models with competing spin-flip dynamics at different temperatures (CSF) from those studies in [8–10], that is, we will not consider here processes involving spin exchanges.

These CSF models, from their equilibrium counterparts, may exhibit an order-disorder phase transition. This nonequilibrium transition is what we focus our attention on. There are two different issues that require some attention. The first question is whether these models belong in the same universality class as the equilibrium Ising model, or if their nonequilibrium nature changes the critical behavior. Grinstein, Jayaprakash, and He [11] argued some time ago that, in fact, nonequilibrium models with up-down symmetry and no extra conservation law belong in the Ising universality class. Their argument is based on the observation that the dynamical Ising fixed point is stable under the renormalization group (RG) flow, with respect to the introduction of new terms that preserve the symmetry (even though these may not be derivable from an equilibrium Hamiltonian). That is, the terms responsible for the nonequilibrium nature of these models are irrelevant under RG transformations. So far this expectation has been confirmed numerically for models with competing temperatures [8,10,12].

The second interesting point has arisen in a recent paper [9], in which it was shown numerically that the asymptotic region for scaling in CSF models seems to be much wider than its analog in the equilibrium models. A satisfactory ex-

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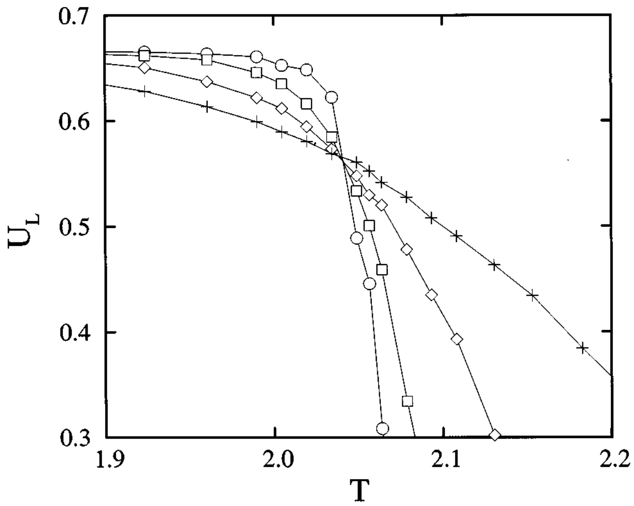

FIG. 1. The normalized fourth order cumulant is plotted for different system sizes as a function of T. ○ are for $L=128$, □ for $L=64$, ◇ for $L=32$, and + for $L=16$. The intersection point corresponds to the critical *pseudotemperature*. The best estimate is $T_{\rm crit}=2.042\pm0.006$.

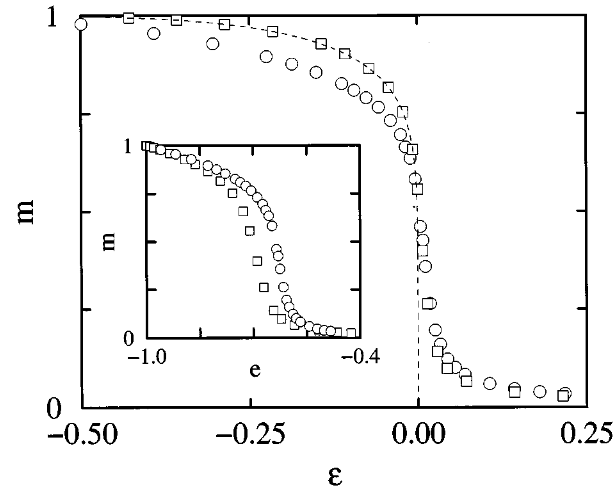

FIG. 2. The magnetization for the Ising model (□), and the nonequilibrium model (○) for $L=128$, as a function of the distance to the critical point ϵ. The dashed line corresponds to the Onsager solution. Inset: magnetization vs energy (pseudoenergy) for the Ising model (□) and the two-temperatures model (○). For a fixed magnetization, the energy is larger in the nonequilibrium case.

planation for that fact is still lacking.

In order to shed some light on the issues of the critical behavior of the model and especially the scaling region size, we introduce the a simple nonequilibrium Ising model with competing dynamics, i.e., a model with only two different spin-flip mechanisms operating at zero and infinite temperature, respectively. The stationary states of this model interpolate between perfect order and complete disorder as a function of a parameter that weighs the probability of each of the two mechanisms to occur; i.e., when the zero temperature mechanism probability is large enough the system is ordered, while when the infinite temperature is dominating the system is disordered. Consequently, a critical point corresponding to the order-disorder transition is expected to separate both regions in the phase diagram.

We present some analytical arguments, as well as extensive Monte Carlo (MC) simulations, paying special attention to the critical behavior, the cluster size distribution, and the asymptotic scaling region extension as compared to their equilibrium counterparts.

Owing to the model simplicity we are able to introduce a *pseudotemperature* that simplifies greatly the problem and allows us to clarify the previously mentioned issue.

II. MODEL DEFINITION

Let us consider a d-dimensional square lattice L, and define a spin variable $s_x=\pm1$ at each site x. The master equation ruling the evolution of the probability $P(\mathbf{s},t)$ of having a configuration $\mathbf{s}=\{s_x, x\in L\}$ at a given time t is

$$\frac{\partial P(\mathbf{s},t)}{\partial t}=\sum_x\,[w(\mathbf{s^x}\rightarrow\mathbf{s})P(\mathbf{s^x},t)-w(\mathbf{s}\rightarrow\mathbf{s^x})P(\mathbf{s},t)], \tag{2.1}$$

where $\mathbf{s^x}$ coincides with $\mathbf{s}$ except for the spin at position x, which is flipped. The transition rates are specified by

$$w(\mathbf{s}\rightarrow\mathbf{s^x})=p+(1-p)\Theta\left(\sum_y\, s_y s_x^x\right) \tag{2.2}$$

where the sum is extended to all the nearest neighbors of x and $\Theta(0)=1$. This correspond to the competition of two Metropolis processes [13]. If $p=1$ all the possible transitions occur with the same probability p, corresponding to a kinetic Ising model at infinite temperature (vanishing magnetization for the stationary state). On the other hand, if $p=0$ the energetically favorable and indifferent transitions occur with probability 1, and the energetically unfavorable processes are forbidden. This correspond to a kinetic Ising model at zero temperature (magnetization, $m=\pm1$ in the stationary state). For $p\in\,]0,1[$, the system is no longer a relaxational equilibrium model.

III. NONEXISTENCE OF AN EFFECTIVE HAMILTONIAN

The idea of effective Hamiltonians was introduced by Garrido and Marro [14] some years ago. Since then it has proven to be a useful tool. Under a set of specified circumstances it can be shown that certain nonequilibrium models with competing dynamics can be mapped onto equilibrium models with effective parameters. Next, we try to find an effective Hamiltonian for our model. For that purpose we assume that an effective kinetic equilibrium Ising model with Metropolis dynamics exist. The transition rates can then be written as

$$w(\mathbf{s}\rightarrow\mathbf{s^x})=\min\left(1,\exp\left(\frac{1}{T_{\rm eff}}\sum_y\, s_y s_x^x\right)\right). \tag{3.1}$$

In order to determine $T_{\rm eff}$ we have to consider the different values of s_x and its nearest neighbors. Notice that only the energetically unfavorable transitions depend on $T_{\rm eff}$ (for the rest we have just 1). There are two different kinds of increas-

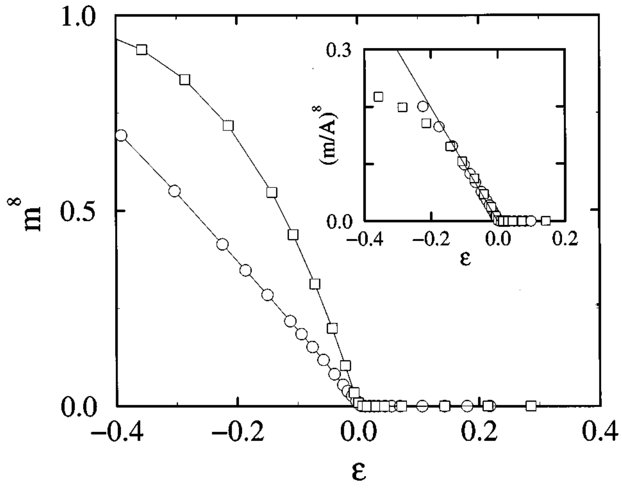

FIG. 3. Plot of m^8 vs ϵ for $L=128$. ○ are for the nonequilibrium case and □ for the Ising model. The linear behavior around the critical point implies that $\beta=1/8$. In the inset, $(m/A)^8$ vs ϵ for both the equilibrium and the nonequilibrium case. A is the thermodynamic amplitude.

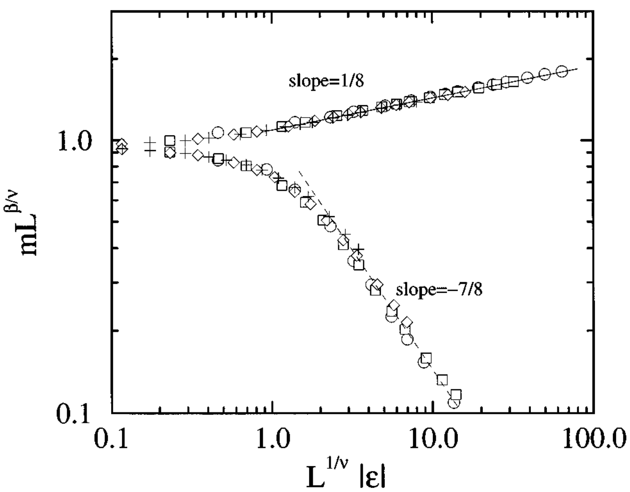

FIG. 4. Log-log plot of $mL^{\beta/\nu}$ vs $\epsilon L^{1/\nu}$ for the nonequilibrium case and for different system sizes (we use the same symbols as in Fig. 1). Data collapse is observed for $\nu=1$ and $\beta=1/8$.

ing energy processes: those in which the four s_x nearest neighbors (nn) are equal to s_x, and those for which only three NN are equal to s_x. For these, equating Eqs. (2.2) and (3.1), we have

$$T_{\rm eff}^{(4)}=-\frac{4}{\ln(1-p)} \tag{3.2}$$

and

$$T_{\rm eff}^{(8)}=-\frac{8}{\ln(1-p)}, \tag{3.3}$$

respectively. This means that all the possible stochastic processes can be represented by an effective equilibrium transition rate, but the effective parameters depend upon the kind of process under consideration. Therefore the effective temperature cannot be defined in a unique way and there is no effective Hamiltonian casting this system. Therefore, the model cannot be mapped into a kinetic Ising model with effective parameters. Nevertheless, it is useful to define a *pseudotemperature* $T\equiv T_{\rm eff}^{(4)}$ [15]. Notice that at the critical point the inequality $T_{\rm eff}^{(4)}<T_{\rm Onsager}<T_{\rm eff}^{(8)}$ has to hold. The inability to find an effective Hamiltonian leaves us with the only possibility of using mean field type of approximations or numerical schemes to get insight into the system behavior.

IV. MONTE CARLO SIMULATION

In this section we present the results of intensive MC simulations we have performed. We concentrate on the determination of the critical point, critical exponents, and some qualitative properties of the critical region. We have studied the model on a two-dimensional square lattice, $N=L\times L$, and considered different system sizes, $L=16,32,64$, and 128, providing enough data to perform a finite size scaling analysis. We take data after letting the systems evolve long enough (typically between 10^5 and 3×10^5 MC steps per particle), so it is guaranteed that it has reached its stationary state. The stationary regime involves typically between 10^6 and 2×10^6 MC steps with data collected every 200 MC steps. We have performed similar simulations for the two-dimensional Ising model in order to compare our results with the equilibrium case. An accurate estimate of the critical value of p, i.e., p_c, is important for reliable determination of critical exponents. We get it from a finite size analysis of the normalized fourth-order cumulant of the stationary distribution, defined as [16,17]

$$U_L=1-\frac{\langle m^4\rangle_L}{3\langle m^2\rangle_L^2}, \tag{4.1}$$

where m is the magnetization $m=1/N\langle\Sigma_{\mathbf{x}}s_{\mathbf{x}}\rangle$ and $\langle\rangle_L$ stands for the average over configurations for the system size L. U_L has the useful property of growing with the system size in the ordered phase, and decreasing in the disordered one. Owing to that property, one may determine the critical point (see Fig. 1). Our best estimate is $p_c=0.859\pm0.001$, which, using the pseudotemperature introduced in the previous section, corresponds to $T_{\rm crit}=2.042\pm0.006$. From now on we express the results in terms of

$$\epsilon\equiv\frac{T-T_{\rm crit}}{T_{\rm crit}}. \tag{4.2}$$

In which follows we compute three different critical exponents β,ν, and γ associated to the magnetization, correlation length, and susceptibility, respectively [18]; other exponents can be calculated from them using well known scaling relations [1].

In Fig. 2 we present data for the magnetization as a function of ϵ for $L=128$. Data for the equilibrium Ising model simulation are presented too. In Fig. 3 we plot m^8 versus ϵ for both the equilibrium and the nonequilibrium cases; from the linear behavior below the critical point we conclude that $m\simeq A\epsilon^{1/8}$; therefore $\beta=1/8$ as in the equilibrium Ising model. Note, however, that the thermodynamic amplitudes, which are nonuniversal, are different. Using this exponent value and the scaling law $m\sim\epsilon^{\beta}f(\epsilon L^{1/\nu})$, where f is a universal function and β and ν are defined in the standard way [17], we can adjust ν so that we have the same function

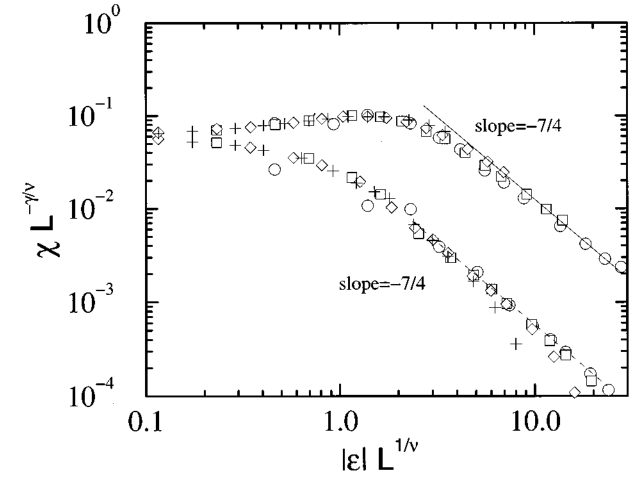

FIG. 5. Log-log plot of $\chi L^{-\gamma/\nu}$ vs $\epsilon L^{1/\nu}$ for the nonequilibrium case and for different system sizes (we use the same symbols as in Fig. 1). Data collapse is observed for $\nu=1$ and $\gamma=7/4$.

$f(\epsilon L^{1/\nu})$ for the different system sizes. Using the fact that near the critical point $\epsilon \sim L^{-1/\nu}$, it is possible to conclude that $mL^{\beta/\nu}$ has to be a universal function of $\epsilon L^{1/\nu}$ independent of L. In Fig. 4 the collapse of the curves for different system sizes is shown when $\nu=1$, i.e., the equilibrium value.

Analogously, in Fig. 5, based on the scaling relation $\chi \sim \epsilon^{\gamma} g(\epsilon L^{1/\nu})$, where χ is the magnetic susceptibility (that is, the derivative of the magnetization with respect to T), and γ its associated critical exponent [17,18], we observe data collapse for $\gamma=7/4$.

Using scaling relations the remaining critical exponents can be computed, and the conclusion is made that the system belongs in the two-dimensional Ising model universality class confirming once again the conjecture in [11].

In order to further explore analogies and differences between the equilibrium and nonequilibrium problems, we determine numerically the asymptotic behavior of the cluster distribution around the critical point. Following the ideas originally proposed by Fisher [19] and later developed by Cambier and Nauenberg [20] we compute the following two magnitudes: $P(l)$ and $S(l)$ defined as the total number of clusters of size l taken from a given number of independent configurations and the mean value of the surface. Here l represents the number of spins aligned in a given direction that have at least another nearest neighbor aligned spin, and S is the number of NN broken bonds associated with the boundary of the cluster averaged for each value of l. In the critical region we have that [20]

$$P(l) \sim l^{-\tau} g(\epsilon l^{y}) \tag{4.3}$$

and

$$S(l) \sim l^{\sigma} h(\epsilon l^{y}), \tag{4.4}$$

where g and h are universal functions and τ, σ, and y are critical exponents. These exponents have been computed for the equilibrium Ising model by Cambier and Nauenberg [20], giving $\tau \approx 2.05$, $\sigma \approx 0.68$, and $y \approx 0.44$, respectively. In Fig. 6 we show the results of our numerical simulations for $P(l)$; values are obtained from 5000 independent configurations in the stationary state.

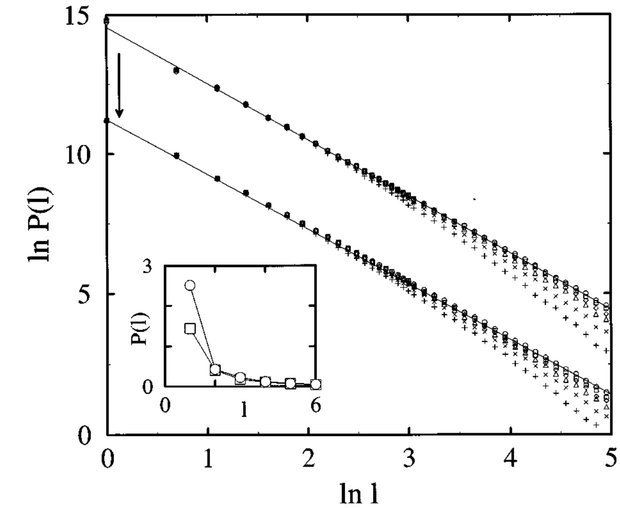

FIG. 6. Log-log plot of $P(l)$ defined as the average number of the clusters of a given size l, for different system sizes. The upper (lower) curve corresponds to the nonequilibrium (equilibrium) situation. The lower curve is displaced three units in the vertical direction for a better data visualization. In the upper curve: ○, $\epsilon=0.0.0036$; □, $\epsilon=0.0109$; ◇, $\epsilon=0.0181$; △, $\epsilon=0.0254$; x, $\epsilon=0.0398$; $+$, $\epsilon=0.0579$. In the lower one ○, $\epsilon=0.0071$; □, $\epsilon=0.0129$; ◇, $\epsilon=0.0173$; △, $\epsilon=0.0217$; ×, $\epsilon=0.0428$; $+$, $\epsilon=0.0525$. In both cases the best fit gives $\tau \approx 2.054$. Inset: linear plot of $P(l)/10^6$. For small cluster sizes there is a difference between the equilibrium and the nonequilibrium curves.

A few remarks follow. The first one for $P(l)$ is that the scaled curves for different values of p near the critical point collapse within good agreement. The second one is that in the log-log plot we have the same slope for both the equilibrium and the nonequilibrium cases, the best estimate being $\tau=2.054$. This shows, once again, that both are in the same universality class. The last remark is that for very small clusters (i.e., sizes $l=1$) there is a clear difference between the equilibrium and nonequilibrium curves: in the nonequilibrium case the number of clusters with one particle is larger than expected (see inset in Fig. 6). This has a simple explanation in terms of the *pseudotemperature* that we previously introduced. As in the nonequilibrium model, $T_{\rm eff}^{(8)} = 2T_{\rm eff}^{(4)}$ it is more likely to flip a spin completely surrounded by aligned spins than one with only three aligned neighbors. Consequently, it is more likely to have fluctuations in the clusters interior than in the borders. This increases the number of one spin clusters. For larger cluster this effect is much smaller, and for $l=5$, is unobservable; in particular the asymptotic behavior, for large clusters, is unaffected by this effect. In Fig. 7 we show two different configurations: for the Ising model and the two-temperatures model. In both cases, the magnetization is chosen to be the same, but it is clear that one spin cluster is favored in the nonequilibrium case. The effect of this can also be observed in some physical magnitudes. For example, in Fig. 2 (see inset) we represent the magnetization as a function of the energy (or *pseudoenergy* in the nonequilibrium case) defined as $e \equiv -(2N)^{-1}\Sigma_{(x,y)} s_{\mathbf{x}} s_{\mathbf{y}}$ where $(\mathbf{x},\mathbf{y})$ are nearest neighbors pairs. For a fixed magnetization, the energy is larger in the nonequilibrium model, corresponding to the fact that there are more isolated one-spin clusters.

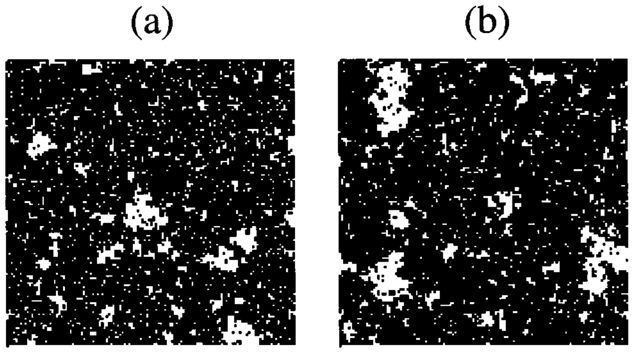

FIG. 7. (a) A configuration with magnetization, $m \approx 0.67$ for the two-temperatures model. Black dots represent up spins. (b) A configuration for the equilibrium Ising model with the same value of the magnetization. The number of one-particle clusters is larger in the nonequilibrium model.

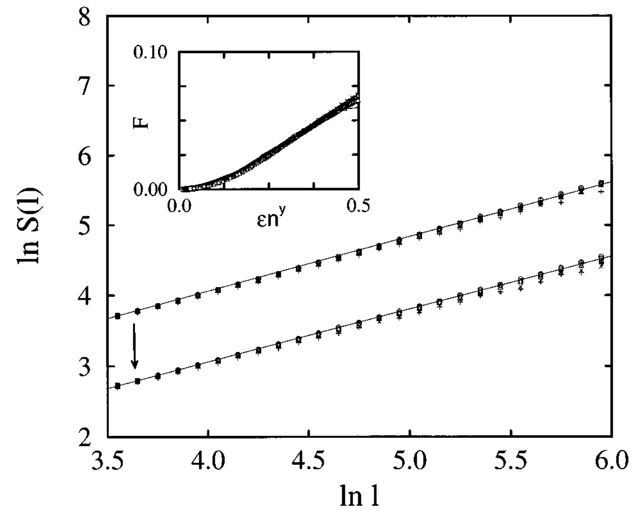

FIG. 8. Log-log plot of $S(l)$ defined as the average surface of the clusters of size l for $20<l<300$ for different system sizes (the symbols are the same as in Fig. 6). The lower (upper) curve correspond to the equilibrium (nonequilibrium) model. The nonequilibrium curve is displaced two units in the vertical direction. In both cases the best fit gives $\sigma \approx 0.68$. Inset: scaling function F in the nonequilibrium case. See text for further explanations.

In Fig. 8 we show the results for the numerical measure of $S(l)$. The scaling now is better than in Fig. 6. The exponent is again the same as in equilibrium. In the inset we represent the function $F(x)$ defined by

$$F(\epsilon n^y) \equiv \epsilon^{1/y} \sum_{l=1}^{n} l^{\tau} P(l,\epsilon). \tag{4.5}$$

We observe curve collapse for $\tau = 2.054 \pm 0.004$ and $y = 0.44 \pm 0.01$, which, again, coincide with the equilibrium values within the accuracy limits.

V. CRITICAL REGION SIZE

In this section we address the problem of the critical region size. It was argued in [9] that the two-temperatures Ising model has a much broader region in which the critical scaling holds than the equilibrium Ising model [see, for example, Fig. 1(b) in [9]]. In particular the scaling region for the magnetization is one order of magnitude larger than its equilibrium counterpart. The question arose as to what the essential physical difference between the equilibrium and nonequilibrium Ising models is.

In what follows, we present evidence that, in fact, there is no essential difference and find a simple explanation for the divergences observed in [9].

First of all, let us revisit Fig. 3. It seems that the linear approximation around the critical point is valid for a wider interval than it is in equilibrium. Imagine now that we represent m^8 as a function of $\epsilon_p \equiv (p - p_c)/p_c$ in analogy to what is done in [9]. As can be easily shown

$$\epsilon = \frac{T - T_{\mathrm{crit}}}{T_{\mathrm{crit}}} \approx \frac{p - p_{\mathrm{crit}}}{p_{\mathrm{crit}}} \frac{p_{\mathrm{crit}}}{p_{\mathrm{crit}} - 1} = \frac{\epsilon_p}{6.092\cdots}, \tag{5.1}$$

that is, there is a factor larger than 6, between ϵ and ϵ_p. Therefore, expressing the results in terms of ϵ_p results in a broadening of the critical region by a factor of about 6. This factor gets rid of the huge difference between critical domains observed in [9].

The introduction of the *pseudotemperature*, for our particularly simple model, allows us to define an ϵ parameter that permits a more suitable comparison with equilibrium results. But, even representing all the physical magnitudes in terms of ϵ, there is still a significantly larger scaling region for the nonequilibrium model as can be observed in Fig. 3. This could suggest that for a given fixed magnetization the correlation length is larger for the nonequilibrium case, so it is somehow nearer to the critical point. In order to avoid completely any effect associated with the ϵ definition, we have plotted the correlation length versus magnetization for both the equilibrium and the nonequilibrium cases. There is a very good agreement between the two curves showing that in fact there is no fundamental physical difference between the equilibrium and nonequilibrium cases. Only the thermodynamic amplitude A, which is not a universal quantity, is different in both cases. To further corroborate this conclusion, we have replotted $(m/A)^8$ versus ϵ. In that new plot, it is checked that the scaling regions are essentially indistinguishable in both cases (see Fig. 3, inset) confirming that the apparent difference in the critical region sizes is due to the different definition of the relative distance to the critical point, ϵ.

VI. CONCLUSIONS

We have introduced a simple nonequilibrium extension of the Ising model. We show that it cannot be represented by an effective equilibrium Hamiltonian, therefore the standard equilibrium techniques are not available to study the model. Nevertheless, it is possible to define a *pseudotemperature* which allows us to make a more suitable comparison of the model with the equilibrium Ising model than those performed in previous papers. In particular, it is shown that the model belongs in the Ising universality class, and that there is no essential physical difference giving rise to a much broader critical region as was recently proposed.

ACKNOWLEDGMENTS

We are grateful to P. L. Garrido, J. Marro, and G. Grinstein for helpful comments, and D. Martínez and Yuhai Tu for a critical reading of the manuscript. This work has been partially supported by NATO through a grant to M.A.M, and by DGICYT through Grant No. PB91-0709. J.J.A. is grateful for a postdoctoral grant from DGICYT (Spain).

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