

Phase Transitions and Universality in Nonequilibrium Steady States of Stochastic Ising Models

Jian-Sheng Wang¹ and Joel L. Lebowitz¹

Received January 22, 1988

We present results of direct computer simulations and of Monte Carlo renormalization group (MCRG) studies of the nonequilibrium steady states of a spin system with competing dynamics and of the voter model. The MCRG method, previously used only for equilibrium systems, appears to give useful information also for these nonequilibrium systems. The critical exponents are found to be of Ising type for the competing dynamics model at its second-order phase transitions, and of mean-field type for the voter model (consistent with known results for the latter).

KEY WORDS: Nonequilibrium stationary states; phase transitions; universality; Monte Carlo simulation; Monte Carlo renormalization group; voter model.

1. INTRODUCTION

Equilibrium statistical mechanics has developed many powerful tools for the study of phase transitions and critical phenomena. There is no comparable theory for nonequilibrium phenomena. It is therefore necessary and useful to study simple nonequilibrium systems. This paper concerns phase transitions in nonequilibrium steady states of Ising, equivalently lattice gas, models. The systems evolve according to local stochastic rules. Such systems are often referred to as random or probabilistic cellular automata in the physics literature⁽¹⁾ and as interacting particle systems in the

¹ Department of Mathematics and Physics, Rutgers University, New Brunswick, New Jersey, 08903.

mathematical literature.⁽²⁾ The important point for us is that the steady states of these systems are in general not described by a Gibbs measure with any reasonable Hamiltonian.⁽³⁾

Various models of this type have been studied,⁽⁴⁻⁸⁾ and exact results are known for some of them in certain limits.⁽⁹⁻¹¹⁾ Here we consider a model with competing dynamics of single-spin flips at finite temperature and spin exchanges at infinite temperature. This model was studied recently on the square lattice via computer simulation⁽⁸⁾ and we report results of new simulations that bear out the predictions made in that work. In addition we carried out, for the first time, we believe, a Monte Carlo renormalization group (MCRG) analysis of this model as well as of the "voter model" in three dimensions.⁽²⁾ The voter model is a very popular model in the mathematics literature.

We obtain critical exponents from direct simulations and MCRG approaches consistent with the competing dynamics model being in the same universality class as the Ising model, as predicted in ref. 12. The voter model is exactly soluble and thus provides a check on the MCRG method. The method appears to give correct results, corresponding to classical exponents, despite the pathology of the model.

In the following section, we introduce the competing dynamics model. In Section 3 we present computer simulation results. The MCRG analysis is given in Section 4. The result of MCRG for the voter model is presented in Section 5. The last section contains a discussion of the applicability of the standard MCRG method in nonequilibrium steady-state problems.

2. NONEQUILIBRIUM ISING MODEL WITH COMPETING DYNAMICS

Consider a two-dimensional square lattice of Ising spins $\sigma = \{\sigma(x) \mid x \in Z^2, \sigma(x) = \pm 1\}$. The system evolves according to the following dynamics in a computer simulation⁽⁸⁾: pick a site x at random, perform a Kawasaki spin exchange⁽¹³⁾ with probability p , and attempt a spin flip⁽¹⁴⁾ with probability $1 - p$. The choice is decided by comparing a random number uniformly distributed in $(0, 1)$ with p . If the number is less than p , the Kawasaki spin exchange is performed as if the system is at infinite temperature, i.e., a neighboring site y is chosen at random, and the values of the spins are exchanged without paying attention to their environment. The new configuration σ^{xy} is $\sigma^{xy}(x) = \sigma(y)$, $\sigma^{xy}(y) = \sigma(x)$, and $\sigma^{xy}(x') = \sigma(x')$ for $x' \neq x, y$. If the number is larger than p , a spin flip is considered. The single-spin-flip process is specified by $w(x, \sigma)$, the probability that the spin at site x is flipped when the spin configuration is σ . The choice of $w(x, \sigma)$ is

such that detailed balance is satisfied with respect to a nearest neighbor ferromagnetic Ising model. That is,

$$\frac{w(x, \boldsymbol{\sigma})}{w(x, \boldsymbol{\sigma}^x)} = \exp\{-\beta[H(\boldsymbol{\sigma}^x) - H(\boldsymbol{\sigma})]\} \quad (1)$$

with $H(\boldsymbol{\sigma}) = -J \sum_{|x-y|=1} \sigma(x) \sigma(y)$ and $\beta = 1/k_B T$. Here $\boldsymbol{\sigma}^x$ denotes a configuration of spins that is the same as $\boldsymbol{\sigma}$, except that the spin at site x is flipped, $\sigma^x(x) = -\sigma(x)$.

There is a lot of freedom in the choice of $w(x, \boldsymbol{\sigma})$. We will consider the original Glauber rate,⁽¹⁴⁾

$$w(x, \boldsymbol{\sigma}) = \frac{1}{8} \sum_{s=\pm 1} [1 - s\sigma(x)] \prod_{i=1}^2 \{1 + \frac{1}{2}s\gamma[\sigma(x + e_i) + \sigma(x - e_i)]\} \quad (2)$$

and the Metropolis rate,⁽¹⁵⁾

$$w(x, \boldsymbol{\sigma}) = \min\{1, \exp[-\beta \Delta H(\boldsymbol{\sigma})]\} \quad (3)$$

$$\Delta H(\boldsymbol{\sigma}) = H(\boldsymbol{\sigma}^x) - H(\boldsymbol{\sigma}) = 2J\sigma(x) \sum_{i=1}^2 [\sigma(x + e_i) + \sigma(x - e_i)] \quad (4)$$

where $\gamma = \tanh 2\beta J$, and e_i is unit lattice vector in i direction.

In the absence of spin exchanges ($p=0$), the steady state is just the Gibbs state of the nearest neighbor Ising model at temperature β^{-1} independent of the choice of flip rates. However, for $p \neq 0$ we have a non-equilibrium situation. The steady state is not described by a Gibbs measure and depends on the form of $w(x, \boldsymbol{\sigma})$.⁽⁸⁾

Exact results of the competing dynamics model are known⁽⁸⁾ in the "scaling limit" $p \rightarrow 1$ when time and space are scaled by $(1-p)^{-1}$ and $(1-p)^{-1/2}$, respectively. In that limit, the system is described by a continuous magnetization density $m(\mathbf{r}, t)$, which evolves according to a nonlinear partial differential equation of the diffusion-reaction type⁽⁹⁾

$$\frac{\partial m(\mathbf{r}, t)}{\partial t} = \frac{1}{2} \nabla^2 m(\mathbf{r}, t) - \frac{\partial V(m)}{\partial m} \quad (5)$$

where $V(m)$ is a polynomial in m which depends on the choice of $w(x, \boldsymbol{\sigma})$.

In the previous computer simulation⁽⁸⁾ with the Metropolis rate, it was found that the stationary state of this system undergoes a second-order transition as a function of βJ for small p and a first-order one for large p . This is interpreted in ref. 8 as a change from the standard second-order equilibrium phase transition at $p=0$ to a first-order, mean-field-type transition found in the bifurcations of (5) about the $m=0$ solution. It is

found that for the Glauber $w(x, \sigma)$ the bifurcations in (5) give a second-order transition. Therefore, if the analysis in ref. 8 is right, there should be no change from a second-order transition in the Glauber case.

Dickman⁽¹⁶⁾ studied the same model using a mean-field-type approximation with the Metropolis rate. The equations he obtains agree, when $p \rightarrow 1$, with the scaling limit results. We give here the results of this approximation for the Glauber rate.

3. COMPUTER SIMULATION OF THE COMPETING DYNAMICS

We carried out more detailed simulations of the competing dynamics using both the Glauber rate (2) and the Metropolis rate (3). Systems of sizes $L \times L$ ($L=8, 16, 32, 64, 128$) and runs up to 10^5 Monte Carlo steps per spin were investigated. The transition temperatures are estimated in several ways: (1) From peaks of the "susceptibility" defined by magnetization fluctuations in the usual way,

$$\chi = \frac{\beta}{L^2} \left\{ \left\langle \left[\sum_x \sigma(x) \right]^2 \right\rangle - \left\langle \sum_x \sigma(x) \right\rangle^2 \right\} \quad (6)$$

(2) By looking directly at the distribution of the magnetization

$$P(m) = \left\langle \delta \left(m - \frac{1}{L^2} \sum_x \sigma(x) \right) \right\rangle \quad (7)$$

The function $P(m)$ has a single peak above the transition temperature at $m=0$, and develops double peaks at $\pm m^* \neq 0$ for ordered phases. (3) By a Monte Carlo renormalization group (MCRG) method, looking at the flow of correlation functions under renormalization group transformations. The transition temperatures estimated by different methods agree with each other within a few percent.

Our Metropolis-rate transition temperatures agree with those of ref. 8. For the Glauber rate the results are new. We find first that, unlike the Metropolis case, here the transition temperature increases as p increases. We plot the inverse transition temperatures as a function of p for the two rates in Fig. 1. The solid line is a mean-field result using Dickman's method.⁽¹⁶⁾ The mean-field and simulation results approach each other for large p . The values $\beta_c J = 0.282 \pm 0.002$ at $p = 0.95$ and $\beta_c J = 0.275 \pm 0.004$ at $p = 0.975$ for size $L=128$ are in good agreement with the value $\beta_c J = 0.2747$ ($\tanh 2\beta_c J = 1/2$)⁽⁸⁾ in the scaling limit.

Figure 2 is a plot of the second moment of magnetization distribution $\langle m^2 \rangle$ versus inverse temperature β at $p = 0.95$ for the Glauber rate. The

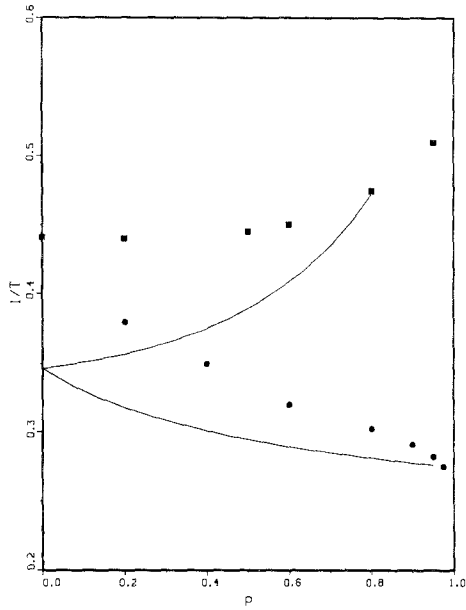


Fig. 1. Inverse transition temperature β_c of the competing dynamics model in two dimensions as a function of spin-exchange rate p for the Glauber rate (circles) and the Metropolis rate (squares). The solid line is a mean-field result.

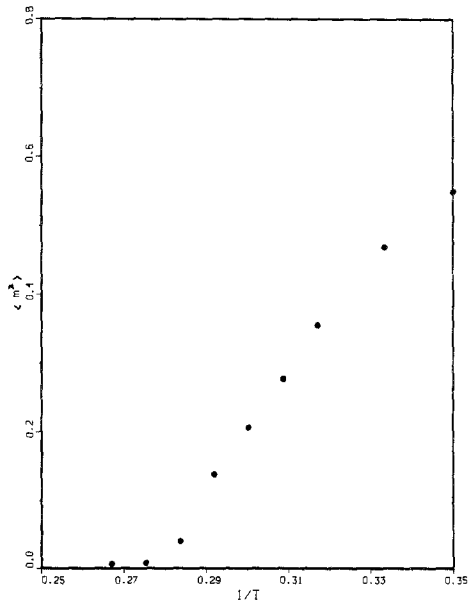


Fig. 2. Second moment $\langle m^2 \rangle$ versus inverse temperature β at spin-exchange rate $p = 0.95$ for the Glauber rate with size $L = 64$.

finite-size effect is rather weak in the Glauber case. The data indicate that the phase transition for the Glauber rate is "second order" with no noticeable discontinuity in the magnetization (and energy) as a function of β . There is a range of temperatures where $\langle m^2 \rangle$ behaves linearly in β , which is an indication of a crossover to the mean-field behavior expected in the limit $p \rightarrow 1$.⁽⁸⁾ On the other hand, finite-size effects are very pronounced for the Metropolis rate, and magnetization as a function of β appears to develop a discontinuity in the infinite-size limit at large p . Figure 3 is a plot of $\langle m^2 \rangle^{1/2}$ as a function of β for $L = 128$, $p = 0.95$. The transition temperature and jump in magnetization are in agreement with the $p \rightarrow 1$ limit values, $\beta_c J = 0.515$, $\Delta m = 0.925$.⁽⁸⁾ The "specific heat," calculated from the fluctuation of energy, seems not to diverge at the transition for the Glauber rate. This is in contrast to the Metropolis case, where the "specific heat" has a very sharp, δ -function-like divergence, reflecting a discontinuity of nearest neighbor correlation.

The susceptibility defined by Eq. (6) diverges at the transition temperatures. Assuming a form of power-law divergence $\chi \sim |\beta - \beta_c(p)|^{-\gamma}$, we found $\gamma = 1.76 \pm 0.10$ at $p = 0.25$ for the Glauber rate, which is consistent with the Ising exponent $\gamma = 7/4$.

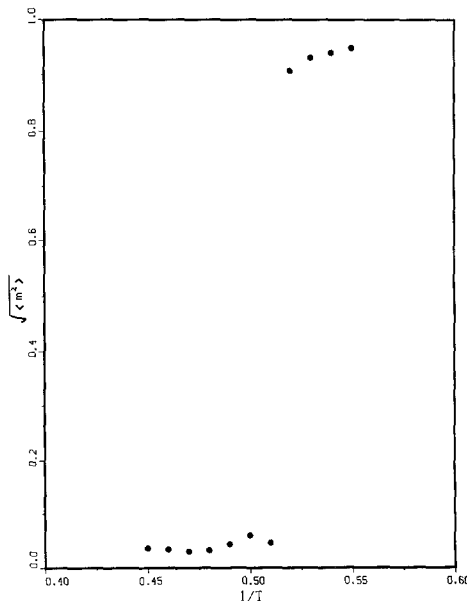


Fig. 3. Magnetization $\langle m^2 \rangle^{1/2}$ as a function of β at $p = 0.95$ for the Metropolis rate with a linear size $L = 128$.

4. MONTE CARLO RENORMALIZATION GROUP ANALYSIS

The Monte Carlo renormalization group (MCRG) method⁽¹⁷⁻¹⁹⁾ has been used successfully for equilibrium systems to determine critical temperatures and critical exponents accurately. We apply the same procedure to nonequilibrium steady states. For each "typical configuration" $\sigma^{(0)}$ generated by computer simulation, successive renormalization transformations $\sigma^{(n)} \rightarrow \sigma^{(n+1)}$ are carried out as follows.⁽¹⁷⁾ The lattice sites are divided into 2×2 blocks of four spins and the transformed configuration is obtained by representing a group of four spins in a block by a single block (Ising) spin. The new block spin is determined by a majority rule, that is, the block spin will take the value $+1$ (-1) if the majority of the spins in the block are $+1$ (-1). If there is no majority, it is chosen $+1$ or -1 with equal probability. Each time a transformation is carried out, the (linear) lattice size L shrinks by a factor 2. This transformation procedure is carried out several times, until the lattice size becomes very small and finite-size effects become severe. The central idea of the renormalization group is that the transformation will bring the system to a fixed point if the system is at criticality (infinite correlation length). We *assume* that such a fixed point exists for nonequilibrium steady states.

Let us define

$$C_{\alpha\beta}^{(n,m)} = \langle S_{\alpha}^{(n)} S_{\beta}^{(m)} \rangle - \langle S_{\alpha}^{(n)} \rangle \langle S_{\beta}^{(m)} \rangle \quad (8)$$










where $S_{\alpha}^{(n)}$ is an α -type operator on $\sigma^{(n)}$. For example, $S_h^{(n)} = \sum_x \sigma^{(n)}(x)$ is the total magnetization, and $S_e^{(n)} = \sum_{|x-y|=1} \sigma^{(n)}(x) \sigma^{(n)}(y)$ is nearest neighbor coupling. Table I is a list of operators considered in this work. As in equilibrium MCRG, the linearized renormalization group transformation matrix $T_{\alpha\beta}^{(n)}$ is given by

$$T^{(n)} = [C^{(n,n)}]^{-1} C^{(n,n-1)} \quad (9)$$

The matrix $T_{\alpha\beta}^{(n)}$ is block diagonal among odd and even operators with respect to inversion [$\sigma'(x) = -\sigma(x)$] in $S_{\alpha}^{(n)}$. The largest odd eigenvalue is an estimate of b^{y_H} and the largest even eigenvalue is for b^{y_T} . If the system is at criticality, these eigenvalues should be stationary with respect to n . This gives a good method of locating the transition temperature.

We calculated $T_{\alpha\beta}^{(n)}$ for lattice sizes up to $L = 128$ at $p = 0.25, 0.50$ for the Metropolis rate. The estimates of exponents from eigenvalues of $T_{\alpha\beta}^{(n)}$ are listed in Table II. The dependence of the estimated exponents on the number of operators included is weak. This means that only the first few short-distance interactions are important. There is a finite-size effect on the apparent transition temperatures. The exponent y_H is estimated to be

Table I. Types of Operators Used in Monte Carlo Renormalization Group Analysis

α	S_x	Description
1		Magnetization
2		Triplet spins, right angle
3		Triplet spins, straight line
4		Nearest neighbor
5		Next nearest neighbor
6		Four spins on a plaquette
7		Two spins distance 2 apart
8		Two spins, (1, 2) position
9		Four pins on a rectangle

1.82 ± 0.03 at $p = 0.50$. The exponent $y_T = 1/\nu$ converges slowly to 1.00 ± 0.05 after two or three renormalization transformations. We interpret our results as consistent with the equilibrium Ising model exponents $y_H = 1.875$ and $y_T = 1$.⁽²⁰⁾

In the case of the Glauber rate we considered $p = 0.25, 0.50,$ and 0.95 . The exponent y_T is 1.0 ± 0.1 , consistent with the equilibrium Ising model exponent $y_T = 1$. However, the value y_H at $p = 0.95$ is lower than the equilibrium Ising value, but increases slowly with renormalization group transformation. We expect that it finally flows to the Ising value. The difficulty with large p , we think, is due to a crossover to a mean-field behavior at $p \rightarrow 1$.

These calculations indicate that the critical exponents for the non-equilibrium second-order phase transition of the competing dynamics are consistent with the equilibrium Ising exponents, which suggest universality for the dynamics, in agreement with ref. 12.

Table II. Estimated Critical Exponents by MCRG for the Competing Dynamics Model at $\rho = 0.5$ with Metropolis Flip Rate^a

RG step	Number of interactions	$1/T_c = 0.453,$ $L = 128$	$1/T_c = 0.450,$ $L = 64$	$1/T_c = 0.448,$ $L = 32$
Exponent Y_H				
1	1	1.822	1.815	1.812
	2	1.814	1.810	1.806
	3	1.814	1.810	1.806
2	1	1.840	1.829	1.819
	2	1.840	1.829	1.818
	3	1.840	1.829	1.818
3	1	1.840	1.820	1.800
	2	1.840	1.821	1.800
	3	1.839	1.821	1.800
4	1	1.839	1.811	
	2	1.839	1.815	
	3	1.839	1.815	
5	1	1.844		
	2	1.847		
	3	1.847		
Exponent Y_T				
1	1	1.492	1.434	1.422
	2	1.488	1.437	1.435
	3	1.485	1.438	1.432
	4	1.465	1.430	1.425
	5	1.460	1.427	1.423
	6	1.459	1.424	1.420
2	1	1.321	1.244	1.234
	2	1.325	1.265	1.258
	3	1.326	1.266	1.258
	4	1.324	1.270	1.261
	5	1.324	1.273	1.264
	6	1.324	1.272	1.262
3	1	1.122	1.020	0.975
	2	1.148	1.068	1.030
	3	1.152	1.069	1.030
	4	1.151	1.081	1.038
	5	1.154	1.094	1.055
	6	1.152	1.101	1.059
4	1	1.043	0.920	
	2	1.084	0.984	
	3	1.078	0.985	
	4	1.088	0.985	
	5	1.084	1.015	
	6	1.078	1.020	
5	1	0.972		
	2	1.003		
	3	0.990		
	4	1.012		
	5	0.939		
	6	0.955		

The data are from runs with 10^4 Monte Carlo steps.

5. MCRG ON THE VOTER MODEL

The voter model⁽²⁾ is a single-spin-flip dynamical model given by the flip rate

$$w_v(x, \sigma) = \frac{1}{2} \left[1 - \frac{1}{2d} \sigma(x) \sum_{|x-y|=1} \sigma(y) \right] \quad (10)$$

This dynamics models the situation in which each lattice site is occupied by a voter who has to decide between voting yes or no [$\sigma(x) = 1$ or -1] on a certain issue. The voter does this by looking at one of his or her $2d$ neighbors (chosen at random) and adopting its position on the issue.

For a system of finite size with periodic boundary conditions, it is clear that the only stationary states are that of a consensus $\sigma(x) = +1$ or $\sigma(x) = -1$ for all x , everybody up or everybody down. What about the infinite system? For $d = 1, 2$ there are only consensus states. For $d \geq 3$, on the other hand, there are unique steady states for every value of $m = \langle \sigma(x) \rangle$. The pair correlation function in these states behaves like r^{2-d} ($d \geq 3$).⁽²⁾

For the sake of convenience of computer simulations, which are always done on a finite lattice, a random spin-flip process is added to (10).⁽²¹⁾ In terms of flip rate we let

$$w(x, \sigma) = (1 - \lambda) w_v(x, \sigma) + \frac{1}{2} \lambda [1 + (1 - 2p) \sigma(x)] \quad (11)$$

where $0 \leq p, \lambda \leq 1$ and w_v is given in (10).

The time evolution of the correlation functions can be obtained with the help of the master equation

$$\frac{\partial P(\sigma, t)}{\partial t} = \sum_x w(x, \sigma^x) P(\sigma^x, t) - \sum_x w(x, \sigma) P(\sigma, t) \quad (12)$$

One can easily see that in the steady state the correlation functions satisfy simple linear equations,

$$\langle \sigma(x) \rangle - \frac{1 - \lambda}{2d} \sum_{|x-y|=1} \langle \sigma(y) \rangle + \lambda(1 - 2p) = 0 \quad (13)$$

$$G(x) - \frac{1 - \lambda}{2d} \sum_{|x-y|=1} G(y) + \lambda(1 - 2p) \langle \sigma(0) \rangle = 0 \quad (14)$$

where $G(x) = \langle \sigma(0) \sigma(x) \rangle$. We consider solutions for $p = 1/2$ in three dimensions. From Eq. (13) we have $\langle \sigma(x) \rangle = 0$. Using Fourier transfor-

mation, Eq. (14) is solved on an $L \times L \times L$ lattice with periodic boundary conditions,

$$G_{L,\lambda}(x_1, x_2, x_3) = c \sum_{1 \leq l_1, l_2, l_3 \leq L} \frac{\cos(2\pi/L)(x_1 l_1 + x_2 l_2 + x_3 l_3)}{1/(1-\lambda) - \frac{1}{3}[\cos(2\pi l_1/L) + \cos(2\pi l_2/L) + \cos(2\pi l_3/L)]} \quad (15)$$

where c is a normalization constant determined by $G_{L,\lambda}(0, 0, 0) = 1$, and l_1, l_2, l_3 and x_1, x_2, x_3 take integer values. The pair correlation function has the property

$$G_{L,\lambda}(x_1, x_2, x_3) \rightarrow 1 \quad \text{as } \lambda \rightarrow 0, \quad \text{for fixed } L \quad (16)$$

and

$$G_{L,\lambda}(x_1, x_2, x_3) \rightarrow e^{-r/\xi}/r \quad \text{as } L \rightarrow \infty, \quad \text{for fixed } \lambda \quad (17)$$

where $r = (x_1^2 + x_2^2 + x_3^2)^{1/2}$ and $\xi = [(1-\lambda)/\lambda]^{1/2}$. The order of the limits $\lambda \rightarrow 0$ and $L \rightarrow \infty$ cannot be interchanged. For an infinite system, as $\lambda \rightarrow 0$, the correlations become long-ranged and the system becomes critical. Comparing (17) with the standard Ising form $r^{2-d-\eta}$, we have $\eta = 0$. If we identify λ with $T - T_c$, the correlation length diverges as $\xi \sim \lambda^{-\nu}$ with $\nu = 1/2$. These exponents clearly have mean-field values. It is also known⁽²²⁾ that for $\lambda = 0$ the magnetization in a volume of side D divided by $D^{5/2}$, $\sum \sigma(x)/D^{5/2}$, goes to a Gaussian random variable as $D \rightarrow \infty$.

We applied the Monte Carlo renormalization group method to the voter model and observed the following features (Fig. 4). For fixed $\lambda > 0$, where the system is not at criticality, the renormalization group transformation brings the system to a more disordered state. As λ approaches zero, but keeping $\xi < L$, the system behaves essentially as an infinite system. The exponents estimated from the first-step renormalization group transformation are consistent with the mean-field values, $y_H = 5/2$ and $y_T = 2$. Convergence of the exponents with iterations of renormalization group transformation is poor because of finite-size effects, which become severe as $\xi \rightarrow L$. The consensus state with all spins up (or all spins down) gives $y_H = 3$. Even though the voter model has this pathological behavior, our results are consistent with mean-field values for the exponents in the infinite-size, small- λ limit.

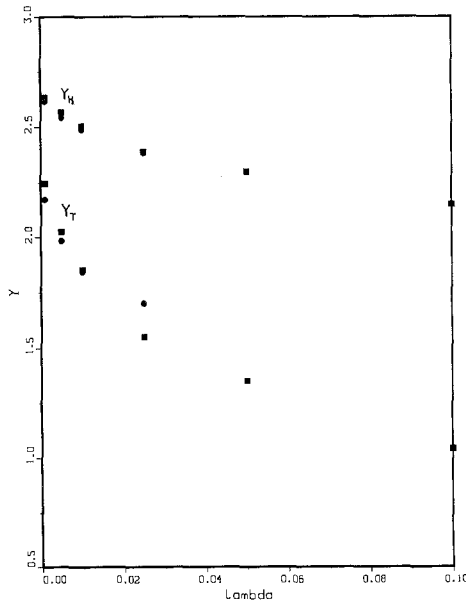


Fig. 4. The exponents y_H and y_T of the voter model in three dimensions, calculated from first-step renormalization group transformation, as a function of parameter λ for various sizes: squares, $L = 16$; circles, $L = 32$.

6. DISCUSSIONS

The relations between eigenvalues of the renormalization group transformation matrix and critical exponents are $\nu = 1/y_T$ and $\eta = d + 2 - 2y_H$, where ν and η are defined through the correlation length $\xi \sim |T - T_c|^{-\nu}$ and correlation function $G(r) \sim r^{2-d-\eta}$. Derivations of those relations are in refs. 18, 19, and 23. They are based on the existence of a flow on a space of Hamiltonians that specify the measures under successive renormalizations. Values of y_T and y_H for Ising and mean-field models are found from these relations.

As already mentioned, the models studied in this paper have stationary measures that are not Gibbsian with any Hamiltonian. (This can be proven rigorously for the voter model⁽²⁴⁾ and is almost certainly the case for the competing dynamics.) Yet, as we saw, a blind application of the renormalization group gave values of y_T and y_H consistent with expectations and with direct measurement of critical exponents. Why this should be so is not entirely clear. Most likely the success of MCRG in these systems is due to the fact that the successive distributions under RG transformations are described, at least approximately, by Gibbs measures with

short-range interactions which flow, at criticality, toward the same fixed point in the space of measures as do the corresponding Ising and mean-field models. This is in fact what is argued by Grinstein *et al.*⁽¹²⁾ should happen for general kinetic Ising models and our results on the competing dynamics model appears to confirm their analysis. The voter model, on the other hand, is clearly in a different universality class. The results of Presutti and Spohn⁽²²⁾ in fact show rigorously that under the proper block renormalization the measure flows to the Gaussian fixed point and our results are consistent with this.

We conclude with the hope that there will be further applications of the MCRG method to nonequilibrium problems. A study near the "tricritical" point is also of considerable interest.

ACKNOWLEDGMENTS

This research was supported in part by National Science Foundation grant DMR-86-12369, and, for work done at the Institute for Theoretical Physics, Santa Barbara, by the National Science Foundation under grant PHY82-17853, supplemented by funds from the National Aeronautics and Space Administration. In addition, J.-S. W. was supported by a Rutgers Supercomputer Postdoctoral Fellowship.

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