Phase transitions in a nonequilibrium Potts model: A Monte Carlo study of critical behavior

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(Received 6 December 1993)

The nonequilibrium steady states of the three-state Potts model, coupled to two thermal reservoirs at different temperatures, are studied by Monte Carlo simulations using Glauber dynamics. In addition to the quartic cumulant, we measure another invariant, cubic in the magnetization. The second-order phase transition in the equilibrium model is shown to persist for the nonequilibrium cases. The critical properties of all models are found to belong to the same universality class.

PACS number(s): 64.60.Cn, 05.70.Jk, 64.60.Fr, 75.10.Hk

Over the past decade, much has been learned about the statistical mechanics of nonequilibrium steady states which clearly lie outside the regime of linear-response theories. A large party of the research to date focused on the uniformly driven Ising lattice gas, first introduced [1,2] as a model for superionic conductors [3]. Among the many phenomena which display distinctly nonequilibrium characteristics, the critical behavior of this "standard model" is shown to belong in the universality class of a non-Hamiltonian fixed point [4,5]. Similarly, when the lattice gas is driven by random uniaxial fields or by an appropriate coupling to two thermal baths at different temperatures, critical singularities are found to be in yet another non-Ising class [6,7]. In stark contrast, when a particle *nonconserving* dynamics is imposed on the same Ising model and driven into nonequilibrium steady states, the critical properties are controlled by the Wilson-Fisher fixed point; i.e., they fall into the *equilibrium* class [8]. Derived with field-theoretic renormalization-group techniques, this result is confirmed in Monte Carlo studies with a variety of drive [9,10].

Much less is known about driven systems with more than two states per site. In particular, only a few three-state systems have been studied so far [11]. All the models considered, motivated by different reasons, have had dynamics that are asymmetric between the three states. No one explored the effects of drive on the second-order phase transition in the symmetric case, i.e., the Potts model [12] in two dimensions ($d=2$). In this Brief Report, we present simulation results of a symmetric three-state ($q=3$) model evolving with spin-flip or Glauber dynamics [13], and driven far from equilibrium by coupling to two thermal baths at unequal temperatures. Unlike the Ising case, the cubic invariant [14] in the $q=3$ and 4 Potts Hamiltonian prevents a successful application of the field-theoretic renormalization-group treatment of the *equilibrium critical* behavior. Lacking a reliably systematic approach [15], we cannot follow [8], so that there is no theoretical basis for believing that the universality class remains unchanged when nonequilibrium, Glauber-type dynamics is introduced. Thus we are left with only an intuitive argument; i.e., that coarse graining should smear out the distinction between the local temperature differences so that these systems should behave as if they are set at a single, intermediate effective temperature. Against this background, it is important to carry out simulation studies and see if this intuitive picture is correct.

Our model consists of a periodic square lattice of L^2 sites, labeled by i. On each site is assigned a two-dimensional spin variable $\mathbf{m}_i$. Each $\mathbf{m}_i$ has unit length and makes an angle of $2\pi l/3$ with the x axis, where $l=0$ and ± 1. The energy of a configuration is $E(\{\mathbf{m}_i\})=-J\sum_{\langle ij\rangle}\delta_{\mathbf{m}_i\mathbf{m}_j}$, where $\delta_{\mathbf{m}_i\mathbf{m}_j}$ is the Kroniker delta, and the sum runs over all nearest-neighbor pairs $\langle ij\rangle$. We consider only the $J>0$ case (ferromagnetic interactions), and set $J=1$; i.e., our inverse temperatures will be quoted in units of $1/J$. The dynamics is defined by the moves and acceptance rates of our simulation. A Monte Carlo sweep (MCS) consists of L^2 moves. In a move, the spin at a randomly chosen site is changed to one of its two other possibilities, with probability given by the Metropolis rates [16]: $\mathcal{P}(\mathbf{m}_i\to\mathbf{m}_i')=\min\{1,\exp[\beta_i(E'-E)]\}$, where the inverse temperature β_i takes one of two values $\alpha\beta$ and β, depending on whether the sum of the x and y coordinates of i is even or odd, and E and E' are the energy of the configurations before and after the move, respectively. When $\alpha=1$, the model is simply the equilibrium three-state Potts model, but when $\alpha>1$ there is a constant flux of energy from the even sites, through the system, into the odd sites, and the characteristics of the steady state are, in general, distinctly nonequilibrium.

Simulations of the system were performed with temperature ratios α of 1, 2, and ∞. The $\alpha=1$ equilibrium case was included as a check on our methods, since β_c and the critical exponents are known exactly [12,17], and for a direct comparison with the nonequilibrium results. For the "$\alpha=\infty$" cases, we actually set $\beta_{\text{odd}}=10$, which excludes all energy-increasing spin flips. In all cases, we sweep in β and present our data as functions thereof.

We started with some relatively short runs to determine the order of the transition and to estimate the transition temperature. Those simulations were performed on systems with $L=4$, 8, 16, 32, and 64. The runs were $\sim 10^6$ MCS's in length, and data were taken every 20 MCS's. Typically a few thousand MCS's were discarded before taking data, to allow the system to reach a steady state. To study the critical properties, we measured a

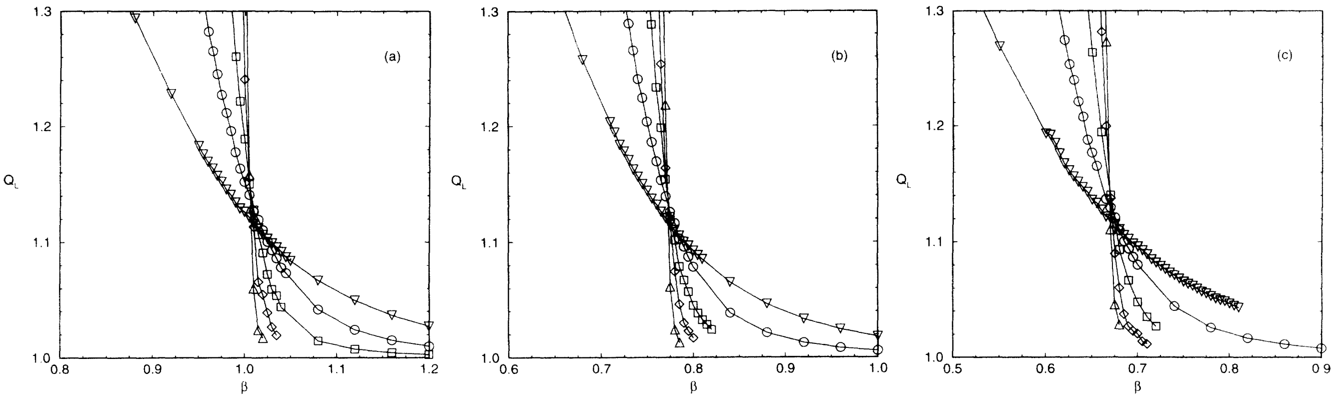


FIG. 1. Q_L as a function of β for $\alpha=1$ (a), $\alpha=2$ (b), and $\alpha=\infty$ (c). The data shown are for $L=4$ (∇), 8 ($\bigcirc$), 16 ($\square$), 32 ($\Diamond$), and 64 ($\triangle$).

number of different quantities including the total magnetization $\mathbf{M}\equiv\sum_i \mathbf{m}_i$ and the total energy E of the configurations. With $\mathbf{M}$, we construct the following two ratios:

$$Q_L=\frac{\langle(\mathbf{M}^2)^2\rangle}{\langle\mathbf{M}^2\rangle^2} \quad\text{and}\quad F_L=\frac{\langle M_x^3-3M_xM_y^2\rangle}{\langle\mathbf{M}^2\rangle^{3/2}} . \tag{1}$$

The former was introduced by Binder [18] as an efficient method to locate T_c. In the $L\to\infty$ limit, it is a universal quantity [19] in the equilibrium Ising model and was used in several nonequilibrium cases successfully [10]. Anticipating the same behavior for the equilibrium Potts model, we consider Q_L, which turns out to be the *only* quartic invariant for $q=3$ [14]. Generalizing to the case for the cubic invariant, we introduce the later. Like Q_L, F_L is a step function in the thermodynamic limit. It vanishes above T_c and becomes unity below criticality. Though there is no field-theoretic basis that F_∞ at T_c should be universal, we believe that it is so and exploit it in this study.

Qualitatively all of the quantities measured behave similarly for all three values of α, thus indicating that the second-order transition of the equilibrium model persists when $\alpha>1$. The results for Q_L are shown in Fig. 1. Curves corresponding to the different system sizes cross. Crossings associated with successive pairs of L's converge to a point, the abscissa of which is identified as the critical β_c. We see that the data for the $\alpha=1$ case converge, from above, to the exact equilibrium critical value 1.005 [12]. For the other two cases, similar well-behaved convergence allows us to locate β_c with some confidence. As in the two-temperature Ising model [10], the phase transition is still present even if one of the temperatures is set at zero, in contrast to the anisotropic equilibrium model in which setting one coupling at infinity automatically leads to ordered states. Next, by examining the values of Q_L at the crossings, we see that they appear to be the same for all three cases. Since $Q_\infty(\beta_c)$ is a universal quantity, this behavior suggests that we remain in one universality class as we move away from equilibrium.

Proceeding to F_L, we first note that these differ from Q_L in two significant ways: (a) F_L is not monotonic in β, so that F_∞ is a step function with an "overshoot" at the discontinuity; and (b) there are two crossings for each pair of curves (Fig. 2). At this point, it is difficult to explain such novel behavior theoretically, especially considering that even a Landau-Ginzburg-like theory for the second-order transition does not exist. Using the $\alpha=1$ case as a guide, we see that the two crossings lie on either side of the critical point. This feature may be exploited to provide a *lower bound* for β_c. We remark that, for each pair of L's, the crossing in Q_L lies within these bounds. As $L\to\infty$, these bounds appear to converge,

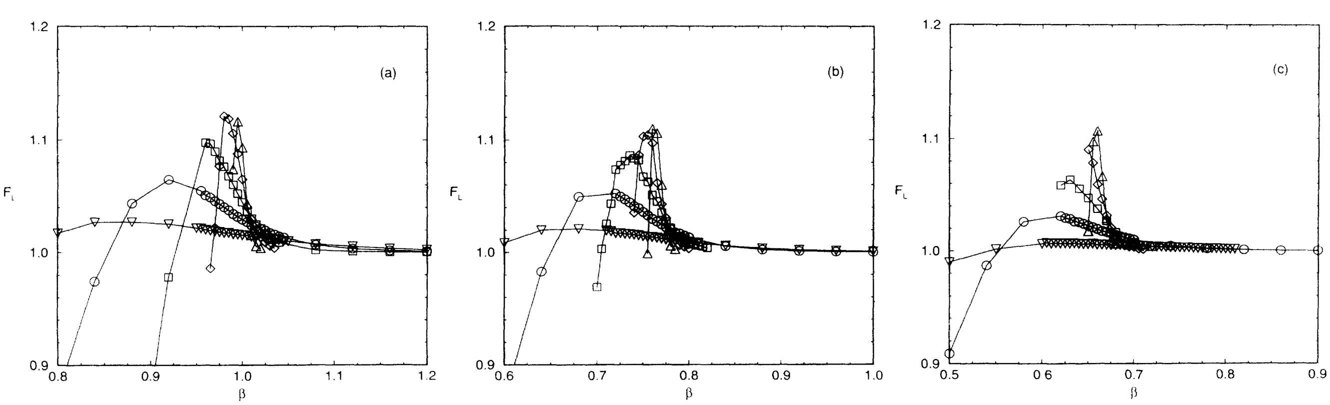


FIG. 2. F_L as a function of β for $\alpha=1$ (a), $\alpha=2$ (b), $\alpha=\infty$ (c). The data shown are for $L=4$ (∇), 8 ($\bigcirc$), 16 ($\square$), 32 ($\Diamond$), and 64 ($\triangle$).

giving us further confidence in our estimate for β_c in the nonequilibrium cases. In Table I, we summarize our results for $\beta_c(\alpha)$. It is remarkable that both $\beta_c(2)/\beta_c(1)$ and $\beta_c(\infty)/\beta_c(1)$ are essentially identical to those in the Ising case [10]. Following [10], we can give an estimate using mean-field "theory," also arriving at $\beta_c(\alpha)=1/\sqrt{\alpha}$. While this is qualitatively correct for $\alpha=2$, it is entirely inadequate for large α. To continue, we see that the behavior of $F_L(\beta)$, as L increases, is essentially the same for the three α's. Though it is unknown if $F_\infty(\beta_c)$ is also universal, we argue that this behavior supports our conjecture that the equilibrium fixed point controls the critical singularities of all $\alpha\neq 1$ models.

To further check this conjecture, we preformed some longer runs at the estimated critical temperatures, with $L=8$, 16, 32, and 64. The length of these runs were, respectively, 10^6, 4×10^6, 10^7, and 2×10^6 MCS's, while data were taken every 10, 40, 100, and 20 MCS's. During these runs, we measured the fluctuations in the energy $C_L\equiv\beta^2(\langle E^2\rangle-\langle E\rangle^2)/L^2$ and magnetization $\chi_L\equiv(\langle \mathbf{M}^2\rangle-\langle \mathbf{M}\rangle^2)/L^2$. For an equilibrium system, C_L and χ_L are the specific heat and susceptibility, respectively. For nonequilibrium systems, the fluctuation dissipation theorem does not hold and the connection fails in general. Nevertheless, we expect these quantities to scale at T_c as a power of L. The results are displayed in log-log plots [Figs. 3(a) and 3(b)], with the error bars estimated by binning the data. It is clear that driving our system into nonequilibrium steady states does not drive these critical properties out of the equilibrium class. To determine the exponents quantitatively, we fit the data to the following functional forms:

$$C_L\approx C_0+aL^{2y_t-2} \quad\text{and}\quad \chi_L\approx\chi_0+bL^{2y_h-2}, \tag{2}$$

where C_0, a, χ_0, and b are unknown parameters. The lines through the data in Fig. 3 are the results of a nonlinear least-squares fitting procedure. In Table I, we give the numerical values for the exponents, showing that they do not differ significantly for the various α's and that they are close to the exact values of the equilibrium model [12]. The slight systematic deviations away from the exact values is likely due to finite-size effects, which we have not included in our analysis. These results confirm our conjecture that the fixed point of the equilibrium model is stable against this type of nonequilibrium dynamics.

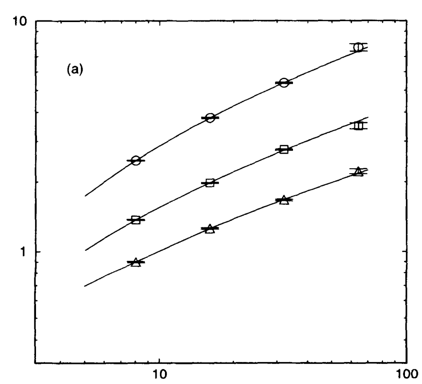
TABLE I. Numerical results for estimated critical point and the fitted values of the thermal and magnetic exponents y_t and y_h. β_c is given in units $1/J$, with estimated errors at less than 0.1%. For the exponents, the error bars (in parentheses) correspond to 95% confidence bounds. The exact values of the equilibrium exponents are $y_t=\frac{6}{5}$ and $y_h=\frac{28}{15}$.

α	β_c	y_t	y_h
1	1.005	1.15 (5)	1.872 (18)
2	0.772	1.15 (4)	1.886 (17)
∞	0.668	1.16 (7)	1.872 (59)

We have also attempted scaling plots for Q_L, F_L, and C_L, in an effort to find universal scaling functions. However, we refrain from drawing a conclusion since only the $L=32$ and 64 sets of data collapsed. Work is in progress involving larger L's and toward a systematic study of finite-size effects.

In summary, we have performed Monte Carlo simulations on a two-temperature three-state Potts model with Glauber dynamics. In addition to the cumulant ratio usually exploited to locate T_c for the Ising model, we proposed another ratio, based on the cubic invariant of the Potts model. Equilibrium critical properties are found to agree well with exact values. For nonequilibrium cases, our results suggest that the second-order transition persists at all temperature ratios and that the universality class remains unchanged. These findings, being remarkably similar to those in the case of two-temperature Ising models with Glauber dynamics, support an appealing and intuitive picture that the long-wavelength, low-frequency properties of such systems are well described by a model effectively in equilibrium at a single, intermediate temperature.

We conclude by discussing some open questions and possibilities for future work. One is to measure various macroscopic quantities in this model, away from T_c, in



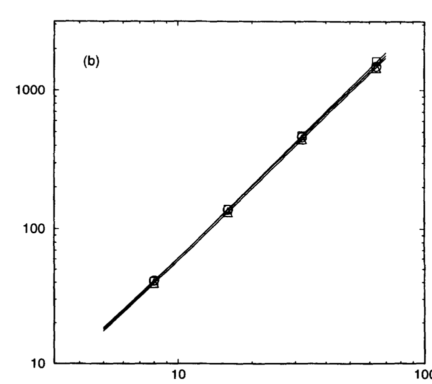


FIG. 3. Results for y_t (a) and y_h (b), from long simulations performed at the critical points for $\alpha=1$ (○), 2 (□), and ∞ (△). The error bars, suppressed in (b) for clarity, indicate one standard deviation. The solid lines show the results of curve fitting.

order to test the validity of the intuitive picture. Venturing slightly further, it would be interesting to explore the critical properties of $q=3$ Potts models with *other* types of nonequilibrium dynamics, such as the various kinds of particle conserving dynamics imposed on driven Ising lattice gases. Since these systems display critical phenomena drastically different from their equilibrium counterpart, we suspect that the same holds true of the three-state Potts model. Work is in progress to determine these new critical properties. Progressing to $q>3$ cases, there is a subtle transition in the $q=4$, $d=2$ equilibrium Potts model [12], which readily presents itself as a natural extension of this study. Of course, a central question in the broader perspective is the following. When a system in a *nonequilibrium* steady state undergoes a second-order phase transition, how do we identify the essential ingredients which produce non-Hamiltonian critical behavior? At present, having only examples and models, we are far from a systematic classification. Finally, beyond critical phenomena, it is undoubtedly important to explore the effects of nonequilibrium dynamics on a first-order transition, which is the hallmark of most Potts models.

We thank Z. Rácz and B. Schmittmann for stimulating discussions. This research is supported in part by grants from the National Science Foundation through the Division of Materials Research and the Jeffress Memorial Trust.

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