Monte Carlo study of dynamic universality in two-dimensional Potts models

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We have carried out extensive computer simulations of the dynamic critical behavior of $L \times L$ q-state Potts models for $q=2$, 3, and 4. We fit the equilibrium relaxation functions for energy and order parameter to a sum of exponential decays and use the finite-size dependence at T_c, $\tau \propto L^z$, to extract estimates for z. We find for the longest relaxation time for both energy and for order parameter that $z=2.17\pm0.04$ describes all three values of q. Our results support the dynamic generalization of the "weak universality" hypothesis proposed by Suzuki.

I. INTRODUCTION

Extensive research carried out over the past several decades has led to a fairly complete understanding of static critical phenomena in simple lattice models. The same degree of knowledge does not exist about the time-dependent properties of these models in the vicinity of the critical temperature T_c. Various theoretical approaches[1] have been taken with an emphasis on the determination of a dynamic critical exponent z which describes the critical slowing down. A characteristic relaxation time τ is expected to describe the decay of time-displaced correlations, and as T_c is approached the relaxation time is expected to diverge as

$$\tau \propto a\xi^z , \tag{1}$$

where ξ is the correlation length. If the correlation length diverges as

$$\xi=\xi_0\left|\frac{T-T_c}{T_c}\right|^{-\nu} , \tag{2}$$

then

$$\tau=c\left|\frac{T-T_c}{T_c}\right|^{-\Delta} , \tag{3}$$

where $\Delta=z\nu$. We wish to emphasize that this describes only the linear, or equilibrium, relaxation time. The nonlinear relaxation time which describes the approach to equilibrium diverges with a different exponent $\Delta_{\rm nl}$ which is related to Δ by $\Delta_{\rm nl}^M=\Delta-\beta$ for the order parameter and $\Delta_{\rm nl}^E=\Delta-(1-\alpha)$ for the internal energy.[2] Thus, a precise knowledge of the dynamic exponent z is needed to characterize the dynamic behavior and to allow comparison with theory. The conventional theory of critical slowing down predicts that $z=2-\eta$. In contrast, ϵ-expansion renormalization-group theory combining results in $d=1+\epsilon$ dimensions and $d=4-\epsilon$ dimensions predicts that $z=2.126$ for the two-dimensional Ising model.[3] These two results predict small deviations from 2 but are clearly incompatible with each other. In a more general sense, we are still searching for the criteria which determine not only dynamic exponents for particular systems but also dynamic universality.

The q-state Potts model offers a good opportunity to study dynamic critical behavior in closely related systems with different static critical exponents. Since Potts originally proposed this model[4] in 1952, substantial information about the static properties has been accumulated.[5] In two dimensions, we know that a second-order phase transition occurs for $q=2$, 3, and 4 and that the transition becomes first order for $q>4$. For $q\leq4$, the critical temperatures are known and static exponents assume different values for each q. A broad range of numerical estimates exist for z, from series expansions, Monte Carlo (MC) studies, and Monte Carlo renormalization-group studies, but as shown in Table I, they are scattered and to a large extent incompatible with each other. [A more complete list of numerical estimates prior to 1981 for $q=2$ (the Ising model) is given in Ref. 18.] To further complicate matters, we note that a high-resolution inelastic-neutron-scattering study[19] of the two-dimensional Ising-type antiferromagnet Rb_2CoF_4 yielded a value of $z=1.69\pm0.05$. The variation in the results is particularly pronounced since the deviation from 2 is really the quantity of interest. Due to the lack of accurate estimates for z for the different q values, it is not yet possible to unambiguously answer some fundamental questions such as whether the concept of universality in dynamics has the same importance as in statics; and if so, is there an intrinsic relationship between static and dynamic critical behavior.

In this paper, we present results of an extensive Monte Carlo study of two-, three-, and four-state Potts models carried out at the critical temperature of each model and analyzed using dynamic finite-size scaling. In the next section, we describe the model, simulation, and methods of analysis used. In Sec. III, we present results and analysis, and in Sec. IV, we discuss the implications of this work. We summarize and conclude in Sec. V.

II. MODEL AND METHOD

The Hamiltonian of the Potts model is defined as

$$H(\{\sigma\})=-K\sum_{i,j}\delta_{\sigma_i\sigma_j} , \tag{4}$$

where the spins σ_i and σ_j may have q-different values.

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The inverse temperature factor β is absorbed in K, and the index i,j runs over all nearest-neighbor pairs. We assume $K>0$ so that in the ground state all spins align parallel via a ferromagnetic interaction.

The kinetic evolution of the model is governed by a master equation for the probability function $P(\{\sigma\};t)$ which gives the probability that a spin configuration $\{\sigma\}$ occurs at time t. The master equation can be written as[20]

$$\frac{\partial P(\{\sigma\};t)}{\partial t}=\sum_{\{\sigma\}'}[P(\{\sigma\}';t)W(\{\sigma\}'\rightarrow\{\sigma\}) -P(\{\sigma\};t)W(\{\sigma\}\rightarrow\{\sigma\}')] . \quad (5)$$

Here $W(\{\sigma\}'\rightarrow\{\sigma\})$ is the transition probability per unit time for a spin configuration to transfer from $\{\sigma\}'$ to $\{\sigma\}$.

In our Monte Carlo simulation, the master equation is discretized by a Markovian chain. We have used a "checkerboard"[21] scheme to update a total spin sublattice of a square lattice in order to utilize the vector feature of the CDC Cyber 205 supercomputer. The choice of $W(\{\sigma\}\rightarrow\{\sigma\}')$ is

$$W(\{\sigma\}\rightarrow\{\sigma\}')=\tfrac{1}{2}[1-\tanh(\Delta H)] , \quad (6)$$

where $\Delta H=H(\{\sigma\}')-H(\{\sigma\})$. The transition probability is symmetric and satisfies the condition

$$\frac{W(\{\sigma\}\rightarrow\{\sigma\}')}{W(\{\sigma\}'\rightarrow\{\sigma\})}=e^{-\Delta H} . \quad (7)$$

With this spin-update scheme and the above transition probability, a finite system will decay to a stationary state with the desired Boltzmann distribution no matter what the initial configuration is.[20] If we rewrite Eq. (5) in a matrix form, then

$$\frac{\partial P(\{\sigma\};t)}{\partial t}=\hat{L}P(\{\sigma\};t) , \quad (8)$$

where $\hat{L}$ is the Liouville operator whose matrix elements are given by

$$\hat{L}(\{\sigma\},\{\sigma\})'=\begin{cases} W(\{\sigma\}\rightarrow\{\sigma\}'), & \{\sigma\}\neq\{\sigma\}' \\ -\sum_{\{\sigma\}''}W(\{\sigma\}\rightarrow\{\sigma\}''), & \{\sigma\}=\{\sigma\}' . \end{cases} \quad (9)$$

The fact that $P(\{\sigma\};t)$ decays to an equilibrium distribution P_0 means that all the eigenvalues of $\hat{L}$ are negative except for P_0, which is zero. For a finite system, the spectrum of eigenvalues is discrete and results in exponential decay of time-displaced correlation functions for a finite system even at the critical temperature. Though we did not use the more conventional single spin-flip scheme, we expect that the universal properties, such as the value of the dynamic critical exponent z, will not be affected by different spin-update schemes. Support for this expectation comes from Monte Carlo calculations on the Ising model by Williams.[22] Although the relaxation time τ may actually vary, the change is assumed to happen only in the irrelevant factor which affects the entire time scale.

TABLE I. Survey of estimates for the dynamic exponent z previously made for q-state Potts models.

	Q		
Ref.	2	3	4
6		2.2	
7	2.2		
8	2.13		
9	2.0	2.8	4.0
10		2.7	
11	1.90	2.28	2.85
12	2.24		
13	1.819	1.922	2.0
14	2.0		
15	2.125		
16	1.90		
17	2.0		
This work "best estimates"	2.13	2.17	2.19

The magnetization, or order parameter, is defined as[11]

$$M=\max\left[\frac{qN_{\rm sub}-N}{N(q-1)}\right] , \quad (10)$$

where q is the number of substates ($q=2,3,4$), N is the number of spins, and $N_{\rm sub}$ is the number of spins in a substate. Note that in this definition, the magnetization is always non-negative. All our simulations are performed at the critical temperature of an infinite system, but this temperature is a little below the temperature where the specific heat shows a peak for the finite system, so in fact our finite system is under its "critical" temperature. Because we deal with a finite system in extremely long simulations, eventually the system will shift from one free-energy minimum, where a substate dominates, to another free-energy minimum (minima) where another substate dominates. Of course it is just an alternative statement to saying that there is no true symmetry breaking in a finite system. By defining magnetization according to Eq. (10), we sample the relaxation time of the magnetic fluctuation rather than calculate the time characteristic for the free-energy-minimum–shifting process mentioned above.

From the magnetization, its time-displaced correlation function

$$\phi(t)=\frac{1}{t_{\rm max}-t}\sum_{t'=0}^{t_{\rm max}-t}\frac{M(t+t')M(t')-\langle M\rangle^2}{\langle M^2\rangle-\langle M\rangle^2} \quad (11)$$

is calculated. In practice, we take two sets A,B of MC sequences of the magnetization data from the same simulation. A and B have the same number of data, but while the MC sequence of set A starts from a time assigned as zero, the MC sequence of set B begins at time which is t in the time reference frame of set A. So every entry of set B is corresponding to an entry of set A through a retarded time t. Then $\phi(t)$ is given by standard definition of correlation between two data sets,

$$\phi(t)=\frac{N'\sum_{i=1}^{N'}a_ib_i-\left[\sum_{i=1}^{N'}a_i\right]\left[\sum_{i=1}^{N'}b_i\right]}{\left[N'\sum_{i=1}^{N'}a_i^2-\left[\sum_{i=1}^{N'}a_i\right]^2\right]^{1/2}\left[N'\sum_{i=1}^{N'}b_i^2-\left[\sum_{i=1}^{N'}b_i\right]^2\right]^{1/2}}, \tag{12}$$

where N is the number of total data in set A or B. $\phi(t)$ is assumed to have a form used by Kretschmer *et al.*[23] for a Glauber model with nonconserved order parameters,

$$\phi(t)=\sum_{i=1}^{N}A_ie^{-t/\tau_i}\quad(\tau_1>\tau_2>\cdots>\tau_n>0)\ , \tag{13}$$

where the τ_i are determined by the eigenvalues of the Liouville operator. The largest τ is singled out as the relaxation time which is used to determine z. A corresponding process may be carried out for the internal energy.

We have considered $L\times L$ systems with periodic boundary conditions. According to the hypothesis of dynamic finite-size scaling, in the dynamic critical region the time-dependent magnetization is scaled as[24]

$$M(\epsilon,L,t)=L^{-\beta/\nu}g(\epsilon L^{-1/\nu},tL^{-z})\ , \tag{14}$$

where $\epsilon=|T-T_c|/T_c$. This implies that at T_c the relaxation time is given by

$$\tau=\tilde{a}L^z \tag{15}$$

for sufficiently large L.

The general features which we found for $\phi(t)$ are shown in Fig. 1. There apparently are three time regions where the behavior of $\phi(t)$ is different. The first region (region I) starts from $\phi(t)=1$ and ends at about $\phi(t)\approx e^{-0.5}$. In this region we see a fast decay of $\phi(t)$. More than one τ gives non-negligible contributions to this fast decay so the data analysis is a little complicated in this short-time region. The second region (region II) extends from $\phi(t)\approx e^{-0.5}$ to $\phi(t)\approx e^{-1.5}$, where an exponential function $Ae^{-t/\tau}$ gives an acceptable fit. Beyond the second region, the quality of statistics is deteriorated by the weaker correlation of magnetization when the time displacement is longer than the characteristic relaxation time. The MC data begin oscillating and meaningful information is difficult to extract from them. The values of $\phi(t)$ which mark the boundaries to these regions are valid only for these models; in other models the regions may be distributed differently.

To ensure the accuracy of the analysis of data, we used both a two-exponent fit

$$f(t)=A_1e^{-t/\tau_1}+A_2e^{-t/\tau_2} \tag{16}$$

to approximate the "long-time" behavior of $\phi(t)$ as well as a single-exponent fit ($\sim Ae^{-t/\tau}$) and compare the results. The use of Eq. (16) allows us to extend the range of t over which accurate information can be obtained to smaller t and, most importantly, to provide a first-order correction to the estimate of the longest relaxation time τ_1. The two methods yielded results which only differed slightly from each other.

We performed Monte Carlo simulations[25] on a series of $L\times L$ lattices with periodic boundary conditions with L ranging from 12 to 64. For every lattice size, multiple simulations were performed, and for each individual MC simulation, 10^5 Monte Carlo steps/site (MCS) were first discarded and then 3.8×10^5 MCS were retained for determining $\phi(t)$. For smaller lattice sizes, such as $L=12$ and 16, we performed 4–6 MC simulations; for larger lattice size, $L=50$ or 64, we carried out 10 MC simulations to average out increased fluctuations. We then calculated the time-displaced correlation function of magnetization and extracted the relaxation time τ using a standard nonlinear least-squares-fitting method.[26] Finally, we made a log-log plot of τ versus L to find the value of z.

III. RESULTS

As one check of our Monte Carlo approach for the dynamic problem, we calculated static critical exponents from our data. The equilibrium magnetization is expected to satisfy the scaling relation[27]

$$M=bL^{-\beta/\nu}\ . \tag{17}$$

In Fig. 2 we show a log-log plot of magnetization versus

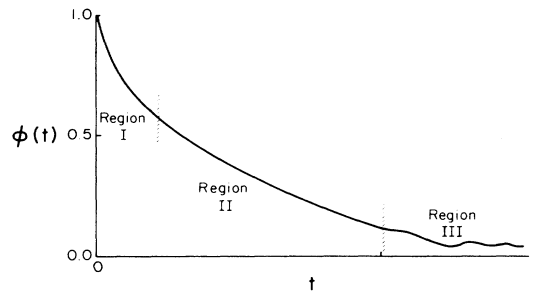

FIG. 1. Characteristic behavior of the time-displaced correlation function $\phi(t)$.

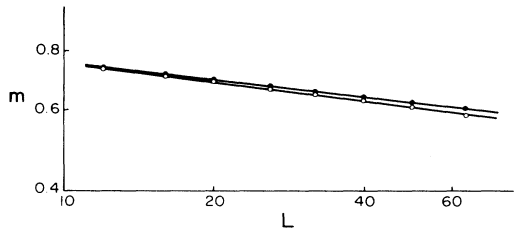

FIG. 2. Log-log plot of the magnetization M vs lattice size L for q-state Potts models at their respective values of T_c. Data for $q=2$ and 4 are essentially identical and are shown by closed circles. Data for $q=3$ are shown by open circles. The solid lines have the known asymptotic slopes equal to β/ν.

lattice size L. As we can see, the accuracy of our Monte Carlo data is very high regarding the static behavior of all three Potts models. In addition, Fig. 2 shows that within the accuracy of our data, the asymptotic finite-size scaling regime is reached for the lattice sizes studied. (Of course, this does not guarantee that we have the same quality of data or that the asymptotic size regime has been reached for the dynamic behavior.)

Figures 3 and 4 display typical pictures resulting from the data-fitting procedure for $q=4$ on a lattice with $L=64$. Figure 3 is for a two-exponent fit of the magnetization relaxation data in region I. Note that though the parameters of the fitting function are derived from region I, the curve calculated from those parameters fits the data quite well in part of region II, until $\phi(t)$ approaches about $e^{-1.5}$. (In a smaller lattice, the fit is even better.) The same MC data are shown in Fig. 4, but this time the fitted curve is the result of one-exponent fit in region II. The difference in the estimates for the longest relaxation time τ_1 is less than 2%.

Using this procedure we obtained estimates for τ_1 and τ_2 for all lattice sizes for all three q values. We show a log-log plot of τ_1 versus lattice size L in Fig. 5. Within the accuracy of our data, we find that a single power law [see Eq. (15)] describes the results for all lattice sizes. The slopes of linear fits to the data give estimates for z which are 2.14 ± 0.05 for $q=2$, 2.18 ± 0.05 for $q=3$, and 2.21 ± 0.06 for $q=4$. The value of the amplitude $\tilde{a}$ increases monotonically for increasing q.

As shown in Fig. 6, the second relaxation times for the magnetization are usually about 10% of the corresponding longest relaxation time. Their error bars are too large to give a truly accurate estimate of scaling exponent associated with τ_2; however, it appears that the exponent is close to z, and larger than γ/ν. The value of γ/ν is the scaling exponent of the initial (short-time) relaxation time τ_s characteristic of the dynamics of small domains whose size is much less than the correlation length[28]. In this time regime, the conventional dynamic theory holds;[1] therefore, γ/ν is a lower bound for the dynamic critical exponent.

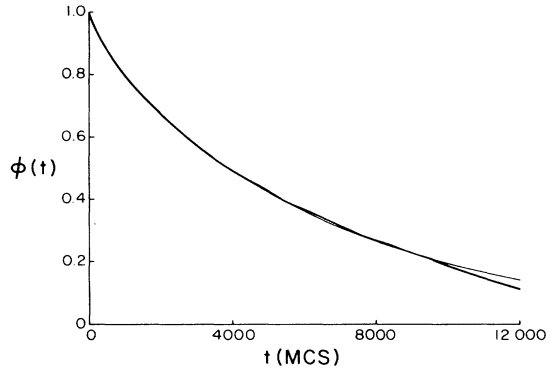

FIG. 3. Two-exponent fit to the magnetization correlation function $\phi(t)$ for the four-state Potts model on an $L=64$ lattice. The bold curve shows the data and the light curve is the result of the fit routine. Data were fitted from $t=100$ to 2600 MCS.

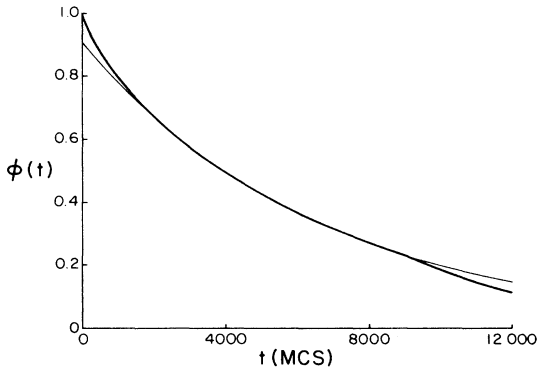

FIG. 4. One-exponent fit for the four-state Potts-model data shown in Fig. 3. The bold curve shows the data and the light curve is the result of the fit routine. Data are fitted from $t=2600$ to 9000 MCS.

Though it is also straightforward to obtain energy data from MC simulations, and the energy data are supposed to yield the same dynamic critical exponent z as given by magnetization data, we found that extracting z in this way is difficult. The energy time-displaced correlation decays much faster than the magnetization time-displaced correlation as shown in Fig. 7. The dynamics of small clusters, which have a larger ratio of surface to volume, may not significantly affect the decay of magnetization correlation, but they are the reason for the faster short-time decay of energy correlations. If we write the energy time-displaced correlation in the form of Eq. (13), it means that the amplitude A_i for the shorter relaxation times may be comparable to A_1, the amplitude for the longest relaxation time.

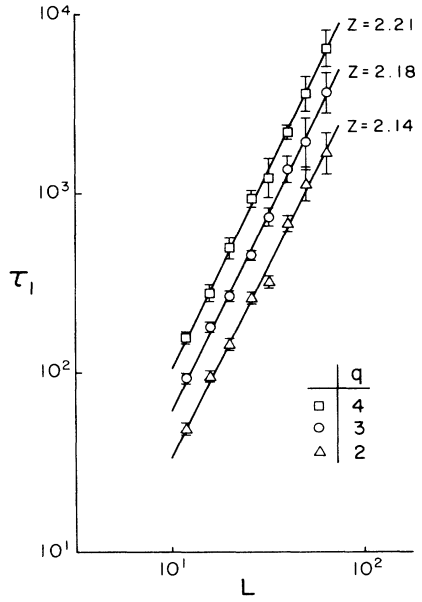

FIG. 5. Log-log plot of the longest relaxation time τ_1 for the magnetization vs lattice size L.

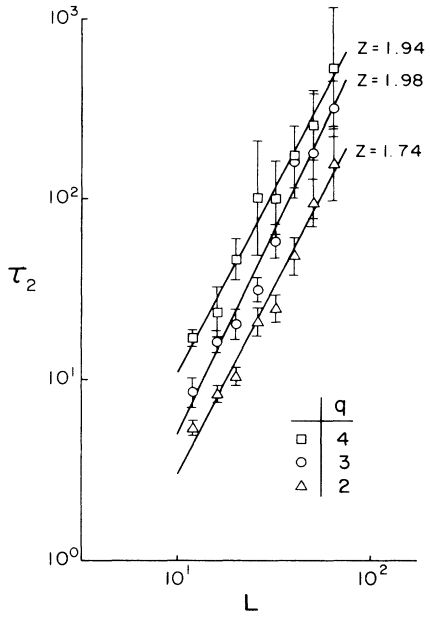

FIG. 6. Log-log plot of the second longest relaxation time τ_2 vs lattice size L. Note the difference in vertical scale as compared to Fig. 5.

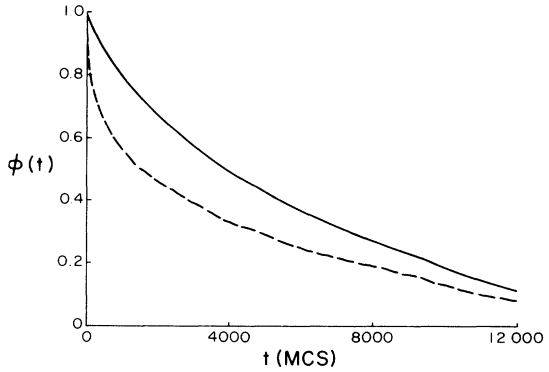

FIG. 7. Comparison of the time-displaced correlation function for the magnetization (——) and the internal energy (— — —) for the four-state Potts model on an $L=64$ lattice.

This effect becomes more pronounced when the lattice size gets larger because the larger lattice can contain more small clusters. Using a two-parameter fit for the energy time-displaced correlation, we find A_1 is about 0.5 and A_2 is about 0.3; whereas, in the magnetization case, A_1 is at least 0.9 and A_2 is close to 0.1 for all the lattice sizes we used. Thus, for the energy time-displaced correlation data, in the short-time region, to get a reasonable data fit, one has to use a sum of many exponential terms. If we fit the data from $\phi(t)=1$ to $e^{-1.5}$ by the two-exponent method, the fitting quality is displayed in Fig. 8. Although the fit seems quite reasonable, when we look carefully at short times (see the inset), we see systematic deviations from the data. This difference is attributable to the truncation of Eq. (13). In contrast, the magnetization data are well described by a two-exponential fit almost to $t=0$. We therefore carried out two-exponent fits beginning with $\phi(t)\sim 0.6$ and then extending to smaller values (longer times). The longest relaxation times and exponent z derived from energy data are presented in Fig. 9. Within the errors, the relaxation times are the same as for the magnetization and yield the same value of z. The second relaxation time for the energy is imprecise, see Fig. 10, but suggests a value of z which is less than 2.

IV. DISCUSSION

If we combine the exponent estimates for magnetization and energy, we obtain "best estimates" of 2.13 for $q=2$, 2.17 for $q=3$, and 2.19 for $q=4$, with an error of ~ 3–4% on each. The value for $q=2$ agrees quite well with the recent large-scale Monte Carlo renormalization-group study of Williams.[8] Although these estimates increase slightly as q becomes larger, the variation is well within the error bars. We therefore believe that our results strongly suggest that the dynamic exponent z which governs the long-time relaxation is the same for all three values of q. This finding is in contrast with the static behavior of these models which shows distinctly different critical exponents for each q value. Suzuki's idea[29] of "weak universality" places $q=2$ and 4 in the same class since "reduced" critical exponents $(2-\alpha)/\nu$, γ/ν, etc (or equivalently the exponent δ) are the same, but the $q=3$ model has slightly different reduced exponents, e.g., $\gamma/\nu=1.733$ instead of 1.750. However, the dynamic exponent z is already a reduced exponent since $z=\Delta/\nu$; thus, the idea of weak universality appears to be stronger for dynamics than for statics. A second extension of weak universality would be to assume that δ determines the dynamic class. In this case, we would expect that $q=2$ and 4 would have the same value of z, but that for $q=3$ the value would be about 7% smaller (i.e., $\delta=14$ for $q=3$ and $\delta=15$ for $q=2,4$). The data do not seem to support this scenario.

According to Kretschmer *et al.*,[23] there should be an

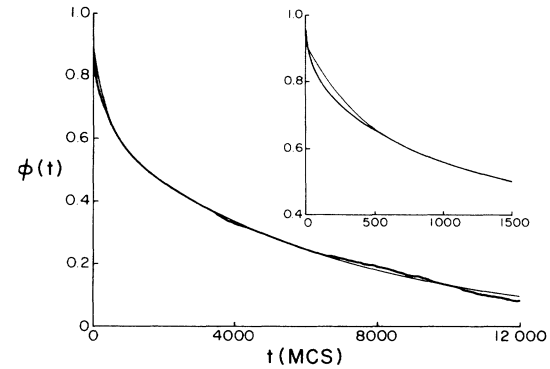

FIG. 8. Two-exponent fit to the time-displaced correlation function for the internal energy for the four-state Potts model and an $L=64$ lattice. The bold curve shows the data and the light curve is the result of the fit routine. The inset shows a magnified view of the short-time behavior.

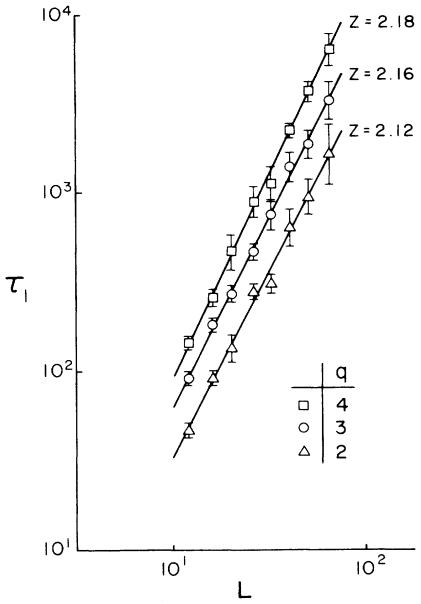

FIG. 9. Log-log plot of the longest relaxation time τ, for the internal energy vs lattice size.

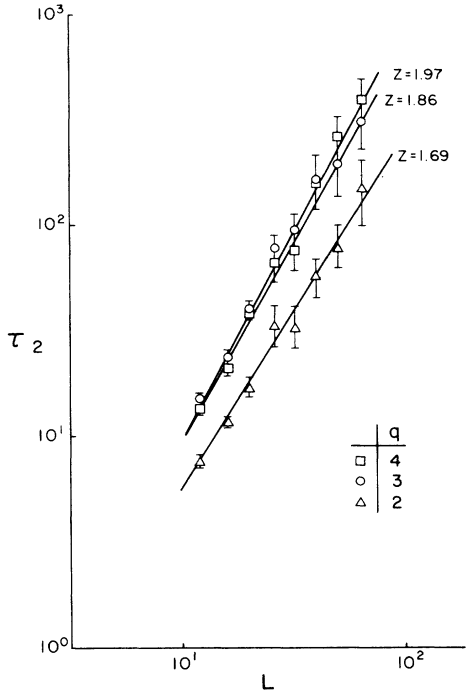

FIG. 10. Log-log plot of the second longest relaxation time τ_2 for the internal energy vs lattice size L. Note the difference in vertical scale as compared to Fig. 9.

entire spectrum of relaxation times τ_i, but all of them should scale with the same exponent. In contrast, we find a second "effective" relaxation time τ_2 which seems to be described by an exponent $z' < z$. The errors in our estimates are sufficiently large that we cannot be certain if z' is the same for all q values.

Our results of the value of z are quite far from those predicted by Domany (see Table I), who proposed a scaling relation[9]

$$z=(2+\alpha)/\nu \ , \tag{18}$$

which implies that z is 2, 2.8, and 4 for two-, three-, and four-state Potts models, respectively. Our results give much smaller values of z, and although we cannot ensure that we have calculated the exact relaxation time, we do not believe that the values of z could be consistent with Eq. (18).

If we look at the master equation [Eqs. (5) and (8)], we realize that the spectrum of the Liouville operator[12] is nearly continuous. For the 4-state Potts model on an $L=64$ lattice, the operator is a $4^{4096}\times 4^{4096}$ matrix, and it is very difficult to single out a particular eigenvalue. From intuitive physical grounds, we can argue that due to the finiteness of the system, there may be a cutoff in the spectrum of eigenvalues, which limits the dynamics of the domains commensurate to the correlation length in size. The cutoff value of λ^{-1} should scale as L^z, and the tail which characterizes the dynamics of small clusters should scale as $L^{\gamma/\nu}$. All other λ are assumed scale by an exponent less than z but larger than γ/ν. A more appropriate form of $\phi(t)$ than Eq. (13) would be

$$\phi(t)=\int_0^\infty e^{-\lambda D t} P(\lambda)\phi_\lambda \overline{A}_\lambda d\lambda \ , \tag{19}$$

where D is a factor relevant to the dimension of a cluster's volume (for magnetization) or surface (for energy), $1/D\lambda$ is the actual relaxation time we calculated, ϕ_λ is a function related to probability function $P_\lambda(\{\sigma\})$, which is an eigenvalue of the Liouville operator, and $\overline{A}_\lambda$ is an average over the coefficients of the eigenvector $P_\lambda(\{\sigma\})$ obtained by decomposing the initial probability function $P(\{\sigma\}_i t)$ with respect to the eigenvector set of the Liouville operator. By carrying out an inverse Laplacian transformation on $\phi(t)$, we could obtain the product $P(\lambda)\phi_\lambda \overline{A}_\lambda$, and see how it is scaled with respect to lattice size L. Our procedure simply uses two "effective" relaxation times to describe the behavior given by Eq. (19).

V. CONCLUSION

Using large-scale Monte Carlo simulations of the linear (equilibrium) relaxation, we find that more than one exponential decay term is needed to accurately describe the relaxation function out to rather long times. We obtain essentially the same value for z for energy and magnetization for all three q values. This result suggests that an extension of weak universality applies to dynamic critical behavior.

Note added in proof. We have just learned of two recent simulation studies of the nonlinear relaxation of these models. O. F. de Alcantara Bonfim (unpublished) used dynamic scaling arguments together with Monte Carlo data and obtained estimates for z which are quite close to ours. L. de Arcangelis and N. Jan [J. Phys. A **19**, L1179 (1986)] found much larger values using a dynamic Monte Carlo renormalization-group method.

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