Numerical method to evaluate the dynamical critical exponent

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A finite-size scaling approach is used to show numerically that dynamical scaling occurs for short and long times independently of the initial conditions. Its main idea is to construct particular quantities scaling as L^0 in the thermodynamic limit $L\to\infty$, L being the linear size of the system. These are the quantities for which the dynamic scaling occurs for short and long times. This approach is applied to obtain the critical dynamical behavior of two- and three-dimensional ferromagnetic Ising models, subjected to Glauber dynamics. [S0163-1829(97)00302-0]

Although the static critical properties of classical spin systems are well described by renormalization group theories (theoretical framework and calculation procedures),[1] the dynamic critical properties[2] are not as well understood. In particular, the value of the dynamic critical exponent z is still an open question even for the two-dimensional Ising model[3–6] when dynamics with local flips of spins are considered. The determination of the exponent z for classical models in different lattice dimensions has been done by using several approaches: field-theoretical dynamical renormalization group methods,[2,7] Monte Carlo simulations,[8–10] renormalization group methods,[11–14] damage spreading,[6,15,16] nonequilibrium relaxation,[17,18] and series expansion.[4,19] For the Ising model the various methods obtain in two dimensions $2.10<z<2.52$ and in three dimensions $1.95<z<2.35$. Usually, some of these methods obtain the z exponent from *long-time behavior*. This limit is hard to be reached because of the critical slowing down that always appears, except for clusters algorithms.[20] Besides, it is also very hard to obtain good statistics in these procedures. Critical slowing down and poor statistics are among the reasons why different calculations produce so many different values for z.

Our objective in this work is to present a finite-size dynamical scaling approach which overcomes the usual difficulties pointed out above. The method is then applied to two- and three-dimensional kinetic Ising models with single spin flips. The method can also be applied to systems with more complex ordering behavior subjected to different dynamics.

Recently, a method has been proposed[21] to evaluate the z exponent from *short-time behavior*. It is based on the scaling relation for the dynamics at early times.[22] In this time regime the magnetization initially grows, characterizing a new universal stage of the relaxation of the magnetization, the so called ''critical initial slip.'' However, it turns out that the initial condition (zero magnetization and very short correlation length) is essential to obtain the dynamical exponent. This happens because the critical initial slip sets right in after a microscopic time scale and eventually crosses over the long-time regime. The characteristic time associated with the critical initial slip is $t_0=m_0^{-z/x}$, where m_0 is the initial magnetization and x is a new exponent. If $m_0=0$, we have that $t_0\to\infty$ and the early time scaling overlaps with the expected long-time scaling.

The short-time behavior obtained by the approach presented in this paper does not depend on the initial condition. It is based on the same ideas developed in a recently proposed renormalization group calculation used to evaluate the static properties of Ising systems.[23] We analyze the relaxation to the equilibrium of well-chosen variables which scales as L^0 (L is the linear size of the system). In order to show that the scaling occurs already for short times independently of the initial conditions, we chose two different initial conditions, both with zero correlation lengths. The first one consists of up and down spins, in such a way that the initial magnetization and a chosen quantity of our schema both have the value zero. In this case the characteristic time scale of the critical initial slip is $t_0\to\infty$. The second initial condition consists of all spins in the up direction. Now, m_0 and the chosen quantity of our approach have their maxima values, namely, 1. In this case the time scale $t_0\sim 1$ is essentially microscopic. The reasons for introducing this finite-size dynamical scaling approach are the following: (i) The weak dependence of the procedure on L implies that the value of z is very good even for the smallest lattices; (ii) the critical temperature and the static exponents are easily obtained with good accuracy; (iii) the chosen variable relaxes exponentially after a transient behavior, thus allowing a good traditional way of calculation of the relaxation time; and (iv) the dynamical scaling occurs for short times independently of the initial condition, hence the evaluation of the z exponent from short-time simulations.

The finite-size dynamical scaling approach (FSDSA) is based only on the finite-size dynamical scaling hypothesis[2] which, for a thermodynamic quantity P and a finite system of linear dimension L, can be expressed as

$$P(\epsilon',H',t',L')=\ell^{-\phi}P(\epsilon,H,t,L), \tag{1}$$

for arbitrary values of the scaling factor ℓ. We are here adopting the ferromagnetic language where H is the external field, the reduced coupling constant is K, $\epsilon=K-K_c$, where K_c is the critical coupling, $\epsilon'=\ell^{1/\nu}\epsilon$, $H'=\ell^{y}H$, $t'=\ell^{-z}t$, and $L'=\ell^{-1}L$. Here, ν, $1/y$, and z are the correlation length and magnetic and dynamical critical exponents, respectively. Equation (1) has its general validity for $L\to\infty$ and near the

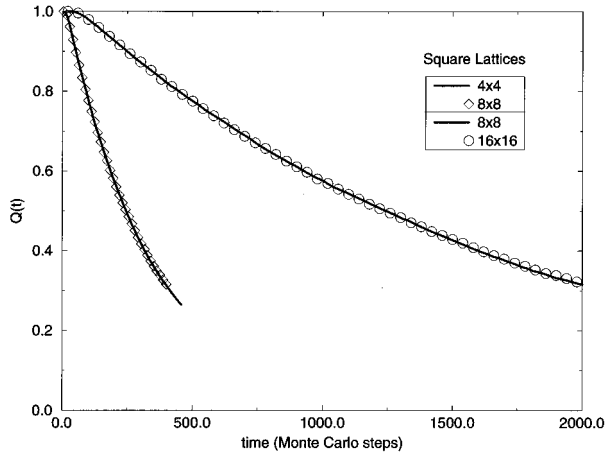

FIG. 1. Long-time behavior of $Q(t)$ for two-dimensional lattices of sizes $L=16,\ 8$ (labelled by the open symbols) together with the corresponding rescaled time of lattices with $L'=L/2$ (represented by solid lines) at the equilibrium fixed points. In the initial condition all spins are in the up direction ($Q=1,\ m_0=1,\ \xi=0$). The statistical errors are smaller than the symbols.

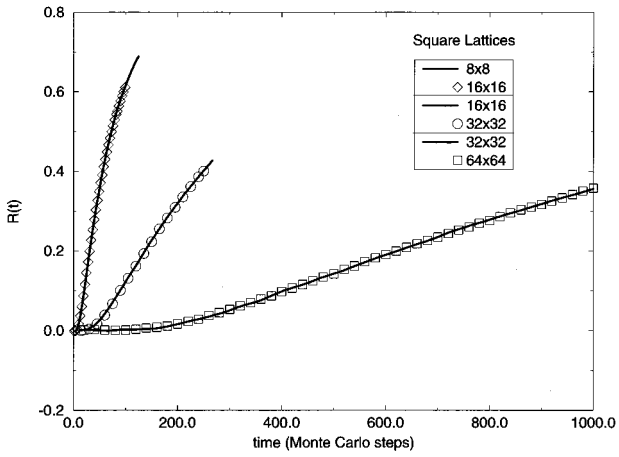

FIG. 2. Short-time behavior of $R(t)$ for two-dimensional lattices of sizes $L=64,\ 32,\ 16$ (labeled by the open symbols) together with the corresponding rescaled time of lattices with $L'=L/2$ (represented by solid lines) at the equilibrium fixed points. The initial condition consists of up and down spins in such a way that $R=0$, $m_0=0$, and $\xi=0$. The statistical errors are smaller than the symbols.

critical point ($\epsilon\approx 0$, $H\approx 0$, and $t\to\infty$). The exponent ϕ defines the critical behavior of the quantity P and is called its anomalous dimension.

The basic idea of the FSDSA is to look for quantities having zero anomalous dimension ($\phi=0$). Here we study the spin-1/2 Ising model defined by the reduced Hamiltonian

$$-\beta\mathcal{H}=K\sum_{\langle i,j\rangle}\sigma_i\sigma_j+H\sum_i\sigma_i,\quad \sigma_i=\pm 1, \tag{2}$$

where $\beta=1/k_BT$, T is the temperature, and k_B the Boltzmann constant. The time evolution is driven by the Glauber dynamics,[24] which is defined by transition rate of flipping the ith spin,

$$w_i(\sigma_i)=\frac{\alpha}{2}[1-\tanh(E_i\sigma_i)], \tag{3}$$

where $E_i=K\Sigma_j\sigma_j$, j are the neighbors of i and $1/\alpha$ is the time scale. One of the quantities having $\phi=0$ is given by

$$Q(t)=\left\langle \operatorname{sgn}\left(\frac{1}{N}\sum_{i=1}^{N}\sigma_i\right)\right\rangle, \tag{4}$$

where $\langle\cdots\rangle$ means the nonequilibrium average and $\operatorname{sgn}(x)=-1(x<0),\ 0(x=0),\ +1(x>0)$.

Let us analyze the quantity $Q(t=\infty)=\langle q\rangle$ first introduced in Ref. 23. For the usual order parameter, the magnetization $m=\langle\mu\rangle$, the probability distribution $\mathcal{P}(\mu)$ in the limit $N\to\infty$, $T<T_c$, $H\to 0^+$, reduces to a single δ function centered at $\mu=m_p$. Here m_p depends on the temperature. The probability distribution $\mathcal{P}(q)$ related to the quantity q also reduces to a single δ function centered at $q_0=1$ in the same limit. However, differently from the magnetization $q_0=1$ for $T<T_c$ independently of the value of T. In other words, Q is constant for $T<T_c$. According to the finite-size scaling hypothesis, the anomalous dimension is given by $\phi=-(\text{critical exponent})/\nu$, which for the magnetization $m\sim\epsilon^{\beta}$ is $\phi=-\beta/\nu$. In the present formalism, as we argued $Q\sim\epsilon^0$, and so $\phi=0$. These properties are extended to the study of the dynamics.

In general, the variables with $\phi=0$ are identified from the physical order parameter of the system. For instance, for the Potts model, which has many states, one chooses a privileged state among r possible spin orientations. For a given lattice spin configuration determine whether the majority of the spins are in this privileged state (set the counter equal to 1) or in any other state [set the counter equal to $-1/(r-1)$]. Define Q as the average of this counter.[25] In a similar fashion the same procedure can be applied to other models, such as the Blume-Emery-Griffiths model (for $S=1$, there are three states).

The other quantity having $\phi=0$ is given by

$$R(t)=\left\langle \operatorname{sgn}\left(\frac{1}{M}\sum_{\text{top}}\sigma_i\right)\operatorname{sgn}\left(\frac{1}{M}\sum_{\text{bottom}}\sigma_i\right)\right\rangle. \tag{5}$$

For a finite system consisting of a hypercube one has $N=L^d$ spins and $M=L^{d-1}$ spins on its top and bottom hypersurfaces. By considering further periodic boundary conditions, due to this extra symmetry, the ''top'' and ''bottom'' hypersurfaces in Eq. (5) can be considered those located at the positions r and $r+L/2$, respectively, with L even. Then, the two independent equations

$$Q_{L'}(K',H',t')=Q_L(K,H,t), \tag{6}$$

$$R_{L'}(K',H',t')=R_L(K,H,t), \tag{7}$$

define the FSDSA. In order to study the dynamical critical properties, we first evaluate the equilibrium fixed point for each pair of lattices ($K'=K=K_c$, $H'=H=0$). Then we look for the time evolution of these variables at the equilibrium fixed point: (i) the Q variable from an initial nonequilibrium state ($Q=1$) to the equilibrium value ($Q_{\text{eq}}=0$), (ii) the R variable from an initial state with $R=1$, and (iii) the

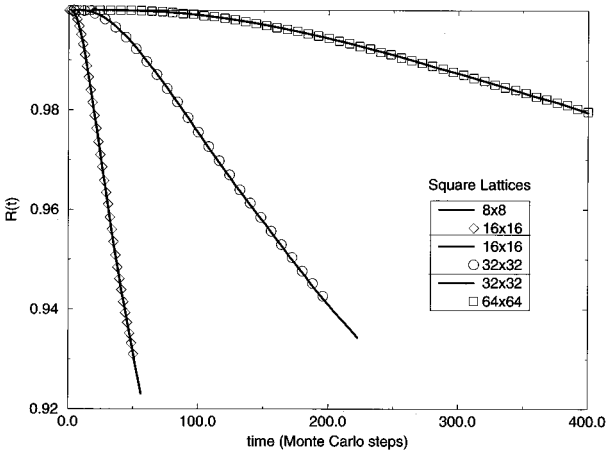

FIG. 3. Short-time behavior of $R(t)$ for two-dimensional lattices of sizes $L=64,\ 32,\ 16$ (labeled by the open symbols) together with the corresponding rescaled time of lattices with $L'=L/2$ (represented by solid lines) at the equilibrium fixed points. The initial condition is given by $R=m_0=1$. The statistical errors are smaller than the symbols.

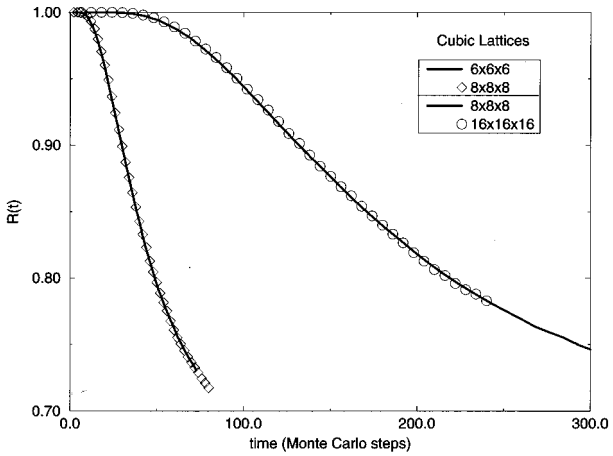

FIG. 4. Short-time behavior of $R(t)$ for three-dimensional lattices of sizes $L=16,\ 8$ (labeled by the open symbols) together with the corresponding rescaled time of lattices with $L'=8,\ 6$ (represented by solid lines) at the equilibrium fixed points. The initial condition is given by $R=m_0=1$. The statistical errors are smaller than the symbols.

R variable from an initial state with $R=0$ and zero correlation length. Differently from methods which obtain short-time scaling only for certain initial condition (such as zero magnetization), we will show that the short time behavior of the quantities Q and R is independent of the initial condition.

By Monte Carlo simulations we have analyzed two-dimensional lattices of sizes $L=4$ up to $L=64$. The equilibrium values and their errors, for each lattice, were obtained by 20 independent runs. In each run, after reaching equilibrium, we have considered 10 000 configurations entering into the average of R. Two sequential configurations were separated by τ Monte Carlo steps, where τ is the relaxation time of R near the criticality. The critical value K_c and an estimate of the correlation length exponent ν for two lattices were obtained by collapsing the two corresponding curves $R_L(K)\times\{K_c+\epsilon^{1/\nu}(K-K_c)\}$.

The decay of $Q(t)$ to the equilibrium at the critical value K_c and $H=0$ was evaluated with 100 000 samples. In Fig. 1 the time behavior of Q for a square lattice with linear size $L=8$ and the rescaled time for a lattice with linear size $L'=4$ and similarly for $L=16$ and $L'=8$ are shown. Note that the long-time behavior is reached since Q is approaching its equilibrium value $Q=0$. The collapse of the two curves is very good in the beginning of the decay as well in the asymptotic regime. This indicates that scaling occurs for both short and long times and it is characterized by the same z exponent. In Fig. 2 the short-time behavior of the correlation function R at the equilibrium fixed point is shown. The system is prepared with a sequence of spin up and down such that $R(t=0)=0$, $m_0=0$, and the correlation length is zero. This is the same initial condition used in Ref. 22 in order to have the early-time scaling extended. We present in this figure the results of collapsed curves for the lattices (64×32), (32×16), and (16×8). In Fig. 3 we present the short-time behavior of the correlation function for the same lattices described above with a different initial condition. Here we prepare the system with all spins up such that $R(t=0)=1$ and $m_0=1$. The results presented in Figs. 2 and 3 were obtained with 300 000 samples for lattices smaller than $L=32$ and for the lattices $L=32$ and $L=64$ we use 200 000 and 60 000 samples, respectively. It is worth mentioning that short-time scaling occurs for both initial conditions. We have also checked the long-time behavior of the correlation function

TABLE I. The values of the dynamical critical exponent z obtained from $Q(t)$ with $Q(0)=1$ and $R(t)$ with $R(0)=1$ and $R(0)=0$ for several two-dimensional lattices. Also shown the reduced critical coupling K_c and the critical exponent ν obtained in equilibrium. The equilibrium exact values are $K_c=0.4407$ and $\nu=1$.

	Exponent z				
Lattices	$Q(t)$	$R(t)[R(0)=1]$	$R(t)[R(0)=0]$	K_c	ν
6, 4	2.105	1.960	1.930	0.4346	0.984
8, 4	2.110	1.990	1.980	0.4361	0.993
8, 6	2.115	2.020	2.050	0.4375	0.983
16, 8	2.130	2.110	2.105	0.4400	1.007
32, 16	2.160	2.150	2.155	0.4407	1.000
64, 32	2.165	2.165	2.165	0.4407	1.000

TABLE II. The values of the dynamical critical exponent z obtained from $Q(t)$ with $Q(0)=1$ and $R(t)$ with $R(0)=1$ and $R(0)=0$ for three-dimensional lattices. Also shown the reduced critical coupling K_c and the critical exponent ν obtained in equilibrium. The equilibrium expected values are $K_c=0.222$ and $\nu=0.63$.

	Exponent z				
Lattices	$Q(t)$	$R(t)[R(0)=1]$	$R(t)[R(0)=0]$	K_c	ν
8, 6	2.07	2.08	2.04	0.2214	0.656
16, 8	2.09	2.11	2.04	0.2220	0.630

for the smallest lattices and the results for the z exponent are the same as the ones obtained from the short time behavior.

In Fig. 4 we show the short-time behavior of the correlation function R with the initial condition $R(t=0)=1$ for the three-dimensional lattices ($L=16$ and $L'=8$) and ($L=8$ and $L'=6$) at the equilibrium fixed points. Here we use 300 000 samples for lattices smaller than $L=16$ and 50 000 samples for the lattice with $L=16$. The short-time scaling shows up from lattices larger than $L=6$ for $Q(t)$ and $R(t)$ with two different initial conditions.

Table I presents the reduced critical coupling, the static critical exponent ν, and the dynamical critical exponent z for the two-dimensional lattices. The errors were estimated by the standard deviation of five independent runs and they affect the last digit of the numbers of the table. The results are quite good even for the smallest lattices. Our best result is $z=2.16\pm0.03$ for the lattices with $L=64$ and $L'=32$.

Table II shows the results for the three-dimensional lattices. In this case the values for the exponent z obtained using different initial conditions have not yet reached a common value as in the two-dimensional case. This is because the lattice sizes used in the three-dimensional problem are small and the surface effects are still relevant. We believe that an increase of the lattice sizes, which is beyond our present computation power, will eventually lead to a common result.

In conclusion, we have presented a method showing scaling for short-times and leading to the evaluation of the dynamical exponent even for small lattices. This method can easily be applied to others systems with more complex critical behavior. For example, by using similar variables Q and R, the tricritical and tetracritical equilibrium behaviors of the Blume-Capel model for spin $S=1$ and $S=3/2$, respectively, have been studied.[26] The dynamics of this system can be as well implemented straightforwardly following the same prescription used here. Similar statements can be made for the Potts model.[25] Moreover, dynamics other than Glauber's can as well be implemented. In particular, the nonequilibrium Ising model with competitive Glauber and Kawasaki dynamics[27,28] can be studied by the present method.

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