Dynamical critical behavior of the three-dimensional Heisenberg model

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We have carried out extensive Monte Carlo simulations of the dynamic critical behavior of $L\times L\times L$ simple-cubic classical Heisenberg models with periodic boundary conditions. The equilibrium relaxation time τ is determined from the long-time exponential decay of the time-displaced correlation function of the magnetization. Using finite-size scaling and corrections to scaling we find that at the critical point $T_c=(0.6929)^{-1}$, τ grows like $\tau\simeq L^z$ with $z=1.96(6)$. In the paramagnetic region we show that the relaxation time is represented by a universal scaling function τL^{-z} vs $(T/T_c-1)L^{1/\nu}$ with $z=1.96(6)$. This estimate is consistent with theoretical predictions and results of experimental studies concerning the dynamical critical behavior of Heisenberg magnets perturbed by order-parameter nonconserving dipolar interactions. We also describe how a simple over-relaxation algorithm of Creutz and of Brown and Woch can be incorporated into the Metropolis sampling method for the classical Heisenberg model, thereby significantly reducing the critical slowing down; the resultant correlation time varies as $\tau\sim(T/T_c-1)^{-0.77}$, which implies $z\simeq 1.10$.

I. INTRODUCTION

The problem of describing the critical dynamics of a simple-cubic classical Heisenberg ferromagnet has been the subject of extensive study for some time.[1–24] Most of the theoretical research applied the mode-coupling[4–9] and renormalization-group[10–24] theories to provide firmly based insight into the nature of spin-correlation functions in the critical region. In particular, the theoretical calculations vindicated the dynamic scaling hypotheses and gave values for the dynamical critical index z, which describes the critical slowing down.

In a system in equilibrium the decay of time-displaced correlations can be described by a characteristic (linear) relaxation time τ which, as the critical temperature T_c is approached, is expected to diverge as[17]

$$\tau\sim\xi^z\ , \tag{1}$$

where ξ is the correlation length. If the correlation length diverges as $\xi\sim(T/T_c-1)^{-\nu}$, then the correlation time varies with temperature as

$$\tau\sim(T/T_c-1)^{-\Delta}\ , \tag{2}$$

where $\Delta\equiv z\nu$. The dependence of the value of the dynamic exponent z on the equation of motion describing the order parameter as well as the conservation laws that apply to the spin system makes the study of the critical dynamics, even for simple systems, considerably more complex than the study of the static behavior. It was found, for example, that for the isotropic Heisenberg ferromagnet with conserved order parameter z is close to $\frac{5}{2}$, whereas in order-parameter nonconserving systems one expects $z\simeq 2$ (Ref. 17).

In this paper we consider "dynamics" introduced through a Markov process, which represents a discretized form of the kinetic evolution of the model described by means of the master equation[25]

$$\frac{\partial P(\{\mathbf{s}\},t)}{\partial t}=\mathcal{L}P(\{\mathbf{s}\},t)\ , \tag{3}$$

where $P(\{\mathbf{s}\},t)$ gives the probability that a spin configuration $\{\mathbf{s}\}$ occurs at time t and $\mathcal{L}$ is the Liouville operator whose explicit form will be given in Sec. IV. The evolution of the system according to the Monte Carlo process is not consistent with its actual physical evolution, although both lead to the same thermal equilibrium distribution.[25] Instead, the Metropolis Monte Carlo technique using a Markovian sampling chain corresponds to the relaxational dynamics, which conserves neither energy nor magnetization ("model A," using the nomenclature of Hohenberg and Halperin, Ref. 17). In this case the conventional theory of critical slowing down predicts[26] $z=2-\eta\simeq 1.97$. Previous theoretical studies[1,12–15] and more recent field-theoretic renormalization-group techniques applied to different versions of the model A in a cubic geometry with periodic boundary conditions[22–24] also yield estimates close to $z=2$. Various experimental investigations[1–3] gave values in the range 1.88–2.09, but, since the experimental errors[2] in the measurement of z are ± 0.05 the agreement between theory and the experiment is still only qualitative.

Our study, the preliminary part of which was published elsewhere[27] (and hereafter is referred to as I), is to the best of our knowledge the first Monte Carlo calculation of the dynamic exponent z for this model. In the next section, we describe the model, methods of simulation and analysis used. In Sec. III, we present results and analysis of the Metropolis Monte Carlo (MC) computations. In Sec. IV we discuss results of simulations with use of the over-relaxed MC algorithm. Our conclusions are found in Sec. V.

II. THEORETICAL BACKGROUND AND SIMULATION METHOD

The Hamiltonian of the simple-cubic classical Heisenberg model is defined as

$$H=-J\sum_{\langle ij\rangle}\mathbf{s}_i\cdot\mathbf{s}_j\ , \tag{4}$$

where $\langle ij\rangle$ denotes all nearest-neighbor pairs of classical three component spins $\mathbf{s}_i$ and $\mathbf{s}_j$ on the simple-cubic lattice. (In the following we adopt units in which $J/k_B=1$.) The kinetic Heisenberg model is defined by the master equation[25] [compare Eq. (3)]

$$\begin{aligned}\frac{\partial P(\{\mathbf{s}\},t)}{\partial t}&=\mathcal{L}P(\{\mathbf{s}\},t)\\&=-\sum_{\{\mathbf{s}'\}}w(\{\mathbf{s}\}\rightarrow\{\mathbf{s}'\})P(\{\mathbf{s}\},t)\\&\quad+\sum_{\{\mathbf{s}'\}}w(\{\mathbf{s}'\}\rightarrow\{\mathbf{s}\})P(\{\mathbf{s}'\},t)\ ,\end{aligned} \tag{5}$$

where $w(\{\mathbf{s}\}\rightarrow\{\mathbf{s}'\})$ is the transition probability per unit time for a spin configuration to transfer from $\{\mathbf{s}\}$ to $\{\mathbf{s}'\}$. In our Monte Carlo study, the master equation is discretized by a Markov chain. We have used a checkerboard lattice decomposition and a conventional Metropolis spin-flip scheme to update a total spin sublattice of the simple-cubic lattice. This means that each new spin direction $\mathbf{s}'$ on a given sublattice is chosen with a probability, which is distributed uniformly on the unit sphere, whereas the transition rate $w(\{\mathbf{s}\}\rightarrow\{\mathbf{s}'\})$ is given by

$$w(\{\mathbf{s}\}\rightarrow\{\mathbf{s}'\})=\min[1,\exp(-\Delta E)]\ , \tag{6}$$

with $\Delta E=H(\{\mathbf{s}'\})-H(\{\mathbf{s}\})$. The eigenvalues $\{\lambda_i\}$ $(\lambda_0>\lambda_1>\cdots)$ of the Liouville operator $\mathcal{L}$ give the relaxation times $\{\tau_i\}$ of the system

$$\tau_i=-\frac{1}{\lambda_i}\ , \tag{7}$$

so that the relaxation of the magnetization of the kinetic Heisenberg model may be regarded as an eigenvalue problem of the operator $\mathcal{L}$. The eigenvalue λ_0 $(=0)$ corresponds to equilibrium and the second largest one $(=-1/\tau)$ gives the slowest (linear) relaxation time describing the magnetization.

We have considered $L\times L\times L$ systems with periodic boundary conditions. According to the dynamic finite size scaling ansatz,[28] in the dynamic critical region the relaxation time τ scales as

$$\tau(\xi,L,t)=L^z g(\xi/L,tL^{-z})\ , \tag{8}$$

where ξ is the correlation length and $g(x,y)$ is the scaling function. At T_c the characteristic length scale is set by the lattice size itself, implying that the relaxation time is given by

$$\tau\sim L^z\ , \tag{9}$$

for asymptotically large L. We determine z using the relations in Eqs. (2) and (9). The difficulty of this approach is, however, that the correlation time cannot be measured directly and must be extracted from other quantities. We used the magnetization data for this purpose. The magnetization, or order parameter, is defined[25] as the root mean square of the spontaneous magnetization vector $\mathbf{M}$, i.e.,

$$M=(M_x^2+M_y^2+M_z^2)^{1/2}\ , \tag{10}$$

where $M_{x,y,z}=(1/N)\sum_i s_i^{x,y,z}$ and N is the number of spins. From the magnetization, its time-displaced correlation function

$$\phi(t)=\frac{\langle\mathbf{M}(0)\cdot\mathbf{M}(t)\rangle-\langle\mathbf{M}(0)\rangle\cdot\langle\mathbf{M}(0)\rangle}{\langle\mathbf{M}(0)\cdot\mathbf{M}(0)\rangle-\langle\mathbf{M}(0)\rangle\cdot\langle\mathbf{M}(0)\rangle}\ , \tag{11}$$

is calculated. [Here $\mathbf{M}(t)$ denotes the spontaneous magnetization at time t.] $\phi(t)$ can be written, in general, as[29]

$$\phi(t)=\sum_i A_i\exp(-t/\tau_i)\ , \tag{12}$$

where the A_i are some unknown coefficients. Using a standard nonlinear least-squares-fitting routine one can, in principle, extract from $\phi(t)$ the entire set of τ_i's, the largest of which is singled out as the relaxation time τ. However, the quality of the data was only good enough to warrant a two-exponential fit

$$\phi(t)=A_1e^{-t/\tau_1}+A_2e^{-t/\tau_2}\ , \tag{13}$$

which was used over intervals of up to $t=3000$ MC steps (MCS's) in order to approximate the "long-time" behavior of $\phi(t)$. For comparison we also applied a single-exponent fit, $\sim Ae^{-t/\tau}$ over restricted regions of time displacement: at long times a single-exponential fit yielded a relaxation time, which was a few percent smaller than the value obtained from a two exponential matching procedure.

In this paper we present a complete account of the simulations of the three-dimensional cubic Heisenberg ferromagnet on a series of $L\times L\times L$ lattices $(6\le L\le 24)$ with periodic boundary conditions, including new data and additional analysis, which were not presented in I. As before, we used a vectorized, checkerboard Metropolis algorithm and made multiple runs for each lattice size investigated. For each simulation we discarded 2×10^4 MCS's, which was more than 12 times the largest calculated correlation time, and then retained up to 10^6 MCS's to determine the averages. The total number of Monte Carlo sweeps per lattice site was between 5.6 and 12 million configurations for all lattice sizes. On the CYBER 205 vector processor, which was used in our calculations, we obtained the speed of 4.5 μs per update, which was essential to obtain accurate results. We shall also present results obtained using a vectorized Monte Carlo algorithm, which combined Metropolis sweeps with updates produced by a vectorized over-relaxation method.

III. RESULTS FROM METROPOLIS MC SIMULATIONS

We begin our investigation of the dynamical critical behavior in the classical Heisenberg ferromagnet by studying the linear relaxation time τ at the critical tem-

perature T_c. Following Ref. 30, we initially used the estimate for the critical coupling of $K_c \equiv J/k_B T = 0.6916$. Preliminary results of this study (described in I) suggested us, however, that a more accurate value of the inverse critical temperature is a fraction of a percent higher: $K_c = 0.6929(1)$. We arrived at this new estimate after carrying out a comprehensive analysis of the static critical behavior in the model, the results of which are presented elsewhere[31] (and hereafter are referred to as II.) This evaluation was obtained by employing high-precision data for the magnetization probability density, calculating its higher moments, and using finite-size scaling and the optimized Monte Carlo data analysis suggested by Ferrenberg and Swendsen.[32] (For further details about techniques applied the reader is referred to II.) As a consistency check of the result we made a finite-size-scaling analysis of various thermodynamical quantities that one can obtain from the probability distribution for magnetization M at the critical point K_c. For example, the equilibrium magnetization M is expected to satisfy the scaling relation

$$M \sim L^{-\beta/\nu} . \tag{14}$$

Figure 1 shows results of finite-size-scaling analysis for the order parameter M. Since the accuracy of our simulation was very high (please note that the error bars are smaller than the size of the points) it was possible to observe that the asymptotic finite-size-scaling regime was already reached for $L = 10$ or perhaps even for $L = 8$. From the plot of $\log_{10} M$ vs $\log_{10} L$ we determined that $\beta/\nu = 0.516(3)$, which is almost identical to the renormalization-group estimate[23–35] 0.517(6). The value of the ratio β/ν found in I was significantly larger [0.550(7)], since in that case the magnetization was evaluated at $K = 0.6916$, which was lower than the critical coupling $K_c = 0.6929$. A similar finite-size analysis of the susceptibility data gave us $\gamma/\nu = 1.969(7)$, which, again, is very close to the ϵ-expansion estimate[28] 1.966(14). Finally, the value of the correlation length exponent obtained in II, $\nu = 0.706(9)$, matches almost exactly the theoretical value 0.705(3). These results clearly support the correctness of our final estimate of K_c. (Note that more recent higher precision studies of the static critical behavior[36] also verified our results in II.)

Figure 2 displays the typical picture obtained after the two-exponential data-fitting procedure for $\phi(t)$ on a lattice with $L = 14$. The fitting quality is very good for times t smaller than the correlation time τ, i.e., until $\phi(t)$ approaches e^{-1}. Moreover, the curve calculated from parameters derived from the first magnetization relaxation data region [i.e., for $t \leq \bar{t}$ such that $\phi(\bar{t}) \simeq e^{-1}$] matches the data reasonably well in an interval, which extends up to $t = 3000$ [$\cong 4.9 \times \tau$ for $L = 14$; $\phi(3000) \simeq 0.01$]. If we fit the data by a single exponential, however, we obtain a correlation time that is about 3% smaller than that for a two-exponential fit. This means that more than one τ_i gives a non-negligible contribution to the fast decay region of the correlation function in the vicinity of $t = 0$. The second relaxation time τ_2 was about 15 times smaller than τ_1 whereas the amplitude ratio A_2/A_1 about 0.01. We have also found similar results for other lattice sizes.

Using the above procedure we arrived at estimates for τ ($= \tau_1$) for all lattice sizes L. We show a $\log_{10}\tau$ vs $\log_{10} L$ plot in Fig. 3. As expected from Eq. (9), we notice that the plot is indeed linear for all lattices. The size of the error bars, however, does not allow us to determine the limits of the asymptotic scaling and whether it is the same size as for the equilibrium magnetization. Our best fit gave the estimate $z = 1.91(6)$. Moreover, if we exclude the two smallest lattice sizes from the fitting procedure, the estimate for the exponent z becomes even smaller: $z = 1.90(6)$. This result is slightly smaller than the value obtained on lattices with $6 \leq L \leq 20$ (with about two times lesser statistics), which we previously reported in I. It is also smaller than the lower bound $\gamma/\nu = 2 - \eta = 1.966(14)$, in contrast to the conventional theory of critical slowing down.[17] This discrepancy can be accounted for through the inclusion of the corrections to scaling (see below). We have also tried to determine whether our result is affected by the value of K_c we chose. We therefore performed some additional runs at $K_c = 0.6929$ for $L = 18$, 20, and 24, with 6, 4.9, and 4 million additional configurations, respectively (which took

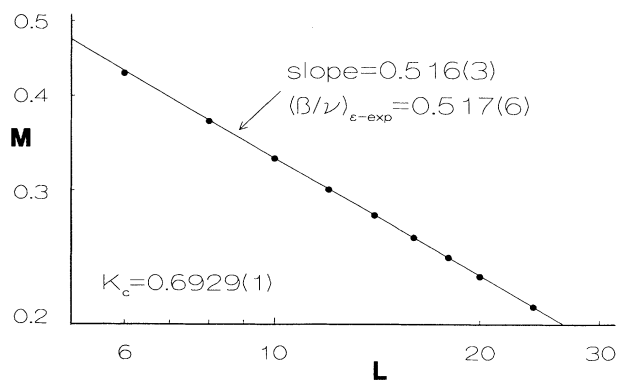

FIG. 1. Log-log plot of the magnetization M vs the lattice size L. The plotted values of M have been calculated by optimized reweighting (see text) at $K_c = 0.6929$.

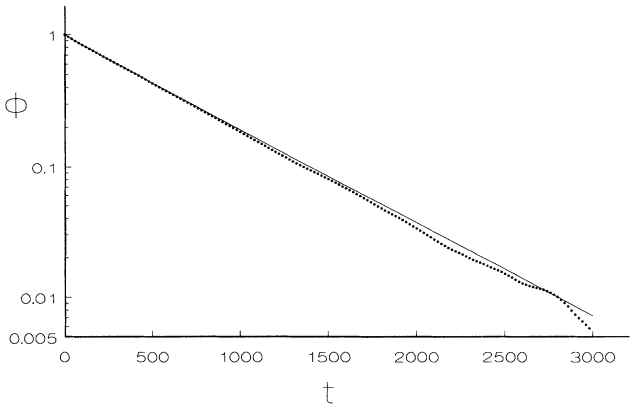

FIG. 2. Log-log plot of the magnetization correlation functions $\phi(t)$ for a $14 \times 14 \times 14$ lattice. The bold curve shows the data and the thin line is the result of a two-exponent fit routine.

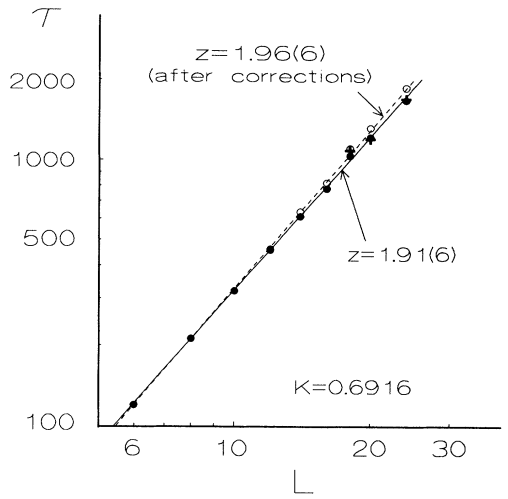

FIG. 3. Log-log plot of the longest relaxation time τ for the magnetization vs the lattice size L obtained with the assumption that $K_c=0.6916$. The solid line represents the best linear fit to the data. The three crosses indicate data collected at $K_c=0.6929$. Open circles represent the relaxation times after accounting for additional corrections to scaling (see text). The broken line represents the best linear fit to these points. The error bars are smaller than the size of the points.

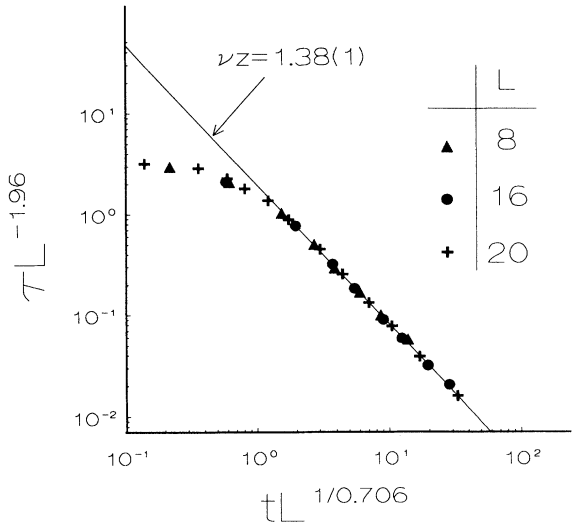

FIG. 4. Finite-size-scaling log-log plot of the relaxation time τ vs the reduced temperature for lattices with $L=8$, 16, and 20 in the paramagnetic region; $K_c=0.6929$. The value of the slope of the fitted straight line is $\nu z=1.38(1)$.

us about 230 h of CPU time). Unfortunately, even these long runs were insufficient to accurately estimate new correlation times (for these lattices) or an improved value of the critical index z. The new data points lie within the error bars of the data points corresponding to $K=0.6916$, although somewhat higher (see Fig. 3).

As mentioned earlier in the text, one can also determine the dynamical exponent z from the temperature dependence of τ in the vicinity of T_c with use of Eq. (2). For three lattices with $L=8$, 16, and 20 and nine different temperatures in the paramagnetic part of the critical region ($1.46\le T\le 3.00$), we generated two runs, each 8×10^5 MCS's long. Then we calculated the correlation function $\phi(t)$ and used single- and double-exponential fits to obtain an estimate for τ. Repeating this procedure for each lattice size we arrived at the finite-size scaling log-log plot of τL^{-z} vs $(T/T_c-1)L^{-1/\nu}$, with $T_c^{-1}=K_c=0.6929$ and $\nu=0.706$, shown in Fig. 4. The best fit was obtained for $z=1.96(5)$. The error in z was determined by considering the quality of the fit upon deviating from the best fit result. The upper plateau of the graph (i.e., the region $x\simeq0$, $y\simeq B$) represents $\tau\simeq BL^z$ behavior, whereas the linear part of the curve corresponds to the bulklike behavior $\tau\sim t^{-\nu z}$. Moreover, the renormalization-group estimate[33–35] $\nu z=1.38(5)$ matches exactly the value of the linear slope found with use of a least-square-fitting routine, $\nu z=1.38(1)$.

Now we turn to a simple analysis of the correction to scaling to account for the fact that the simulation temperature used for calculation of the exponent z according to the finite-size-scaling formula, Eq. (9), was slightly different than the infinite lattice value,[31] $K_c=0.6929$. First, we estimate the value of the constant $B=y(x=0)$ entering the finite-size-scaling function. The results of simulations for the three largest lattice sizes ($L=18$, 20, and 24) carried out at $K_c=0.6929$ can be employed to deduce the value of parameters $B_L\equiv\tau(L)=L^{-z}$, which leads to the estimate $B\cong(B_{18}+B_{20}+B_{24})/3\cong3.478$. Moreover, for the six largest lattices with $12\le L\le24$ the measurements carried out at $K=0.6916$ correspond to the scaling variable $x_L\equiv(K_c/K-1)L^{1/\nu}$, with a typical value $x_{20}\simeq0.132$. Employing a linear approximation to the finite-size dynamical scaling curve (y vs x) in the neighborhood of $x\simeq0$ one estimates the value $y_L\equiv y(x_L)$, e.g., $y(x_{20})\simeq3.192$. Finally, we obtain the finite-size-scaling corrections to the correlation time: $\Delta\tau_L\equiv(B-y_L)L^z$, ($\Delta\tau_{20}\simeq101$, i.e., $\Delta\tau_{20}/\tau_{20}\simeq8.3\%$). After accounting for the changes in the correlation times for this range of the lattice sizes (compare Fig. 3) we arrived at the new value of the slope on the linear plot of $\log_{10}\tau$ vs $\log_{10}L$, from which we deduced the corrected value of the dynamical exponent $z=1.96(4)$. Our final estimate for the dynamical exponent z, obtained with use of this self-consistent quantitative method of analysis, is $z=1.96(6)$. (Note, that the scaling function itself contains the information about the dynamic exponent.) As a final comment on the above result, we would like to point out that even a small uncertainty ΔK_c in the value of the critical temperature ($\Delta K_c/K_c\simeq2\times10^{-3}$) can produce more than an order of magnitude larger change in the value of the static (e.g., $\Delta\beta/\beta\sim7\times10^{-2}$) or dynamical ($\Delta z/z\sim3\times10^{-2}$) critical exponents. (These estimate are obtained using the values of the exponents β and z calculated at $K=0.6916$ and $K_c=0.6929$).

As we mentioned in Sec. I, several authors in the past successfully investigated the critical dynamics of purely dissipative models, which do not conserve either the energy or the order parameter.[1,12–15] While the con-

ventional theory of the critical slowing down predicts[12,17] $z=2-\eta$ in this case, different formulations of the renormalization-group approach consistently gave a slightly higher value[1,12-15]

$$z=2+c\eta\ ,\ c=6\ln(4/3)-1\ , \tag{15}$$

i.e., $z\simeq 2.024$. Quite a long time ago Suzuki demonstrated[13] that the critical dynamical behavior of a system described by a master equation, Eq. (3), with the Hamiltonian of the Ginzberg-Landau type,[12,17] is the same as this obtained in the (purely) dissipative time-dependent Ginzburg-Landau (TDGL) model with nonconserved order parameter.[12,17] Consequently, he obtained the same dynamic critical exponent z as for this version of the TDGL model. Since the dynamic universality class of the three-dimensional version of this model is believed to be the same as of the simple-cubic (i.e., isotropic) Heisenberg ferromagnet,[12,17] we would expect that our estimate of the exponent z will be consistent with the value given by Eq. (4). The observed difference between our results, $z=1.96(7)$ and $z\simeq 2.02$ may be related to some systematic bias resulting from, e.g., a relatively narrow range of the lattice sizes, which we studied. Although the statistical accuracy of our simulations was very high, we could not determine more accurate values of the correlation times, which would allow us to carry out a meaningful analysis of the corrections to finite-size scaling and to improve the value of the dynamical exponent z. Another source of systematic error may arise from the finite length of the Monte Carlo simulation; this was found to be non-negligible in a recent simulation of the $d=3$ Ising model with very high statistics.[37] However, we did not carefully pursue any systematic error analysis in this direction.

A direct comparison of our results for the dynamic properties of the model with experimental results is somewhat difficult, since, as was already mentioned, the artificial stochastic dynamics of the Monte Carlo process yields purely relaxational behavior of a real-cubic Heisenberg ferromagnets.[25] However, recent experimental studies of the critical behavior of isotropic ferromagnets (as, e.g., insulating compounds EuO, EuS) revealed that the breakdown of dynamical scaling and crossover from $z\simeq 2.5$ (observed in inelastic critical neutron scattering at wave vectors $q\geq q_D$ in the spectral linewidth ω of EuS) to $z\simeq 2.0$ (at wave vectors smaller than a dipolar wave vector q_D) can be attributed to presence of the spin nonconserving dipolar forces.[1-3,38] Recently, Frey and Schwabl[9] succeeded in calculating the dynamic effects of dipolar interactions by a mode-coupling method and demonstrated that at $T=T_c$ the demagnetization (i.e., dipolar) effects become dominant only for $q\leq q_D/5$. This result explained the observation,[1-3,38] that the expected crossover from isotropic to dipolar critical behavior, accompanied by a change of the dynamical critical index z from $\frac{5}{2}$ to 2, has not been detected by neutron-scattering experiments in a canonical Heisenberg ferromagnet, EuO, over the entire measured range of q (0.015–0.3 Å^{-1}; for EuO $q_D\simeq 0.15$ Å^{-1}, whereas for EuS $q_D\simeq 0.27$ Å^{-1}).

IV. OVER-RELAXED METROPOLIS MONTE CARLO SIMULATIONS

In the previous sections we demonstrated that the critical slowing down occurring at the second-order phase transition in the classical simple-cubic Heisenberg ferromagnet means that long simulations are needed to extract static quantities. Typically, the computational effort needed to obtain one statistically independent sample for this system grows at the critical point as $L^{3+z}\simeq L^{5}$.[39] One way out is to choose another dynamical evolution of the system (described by a different master equation) which leads, in turn, to a smaller value of the dynamical exponent z.

For the purely local updating occurring in the Metropolis MC scheme, the slow modes are the long-wavelength ones, and a natural method to speed up those modes is to choose a collective-mode updating. An example of such a method is the Swendsen-Wang algorithm,[40] which significantly reduces the value of the dynamical critical exponent; e.g., for the $d=2$ Ising model one obtains[40] $z\simeq 0.35$ instead of[41] $z\simeq 2.125$ expected for a standard Metropolis algorithm. Recently, a simple variation of the scheme of Metropolis *et al.* for the Monte Carlo simulation of statistical systems was proposed by Creutz[42] (and independently, by Brown and Woch).[43] Their approach was motivated by over-relaxation ideas (used to speed up convergence of matrix inversion algorithms) that have been recently generalized to stochastic processes.[44] The basic idea behind the method is to choose a trial position for a given variable in a phase space region which is as far as possible from the old value, while keeping the energy constant. A natural realization of this idea is to find the locus of minimum energy for a given variable, and then make a trial move on the "opposite" side of the old value.[32] For the Heisenberg model on a simple-cubic lattice the trial choice consists of reflecting (i.e., rotating by 180°) the spin at a given site about the $\mathbf{S}_{\mathrm{NN}}$, where $\mathbf{S}_{\mathrm{NN}}$ is the sum of the nearest-neighbor spins.

The update of spins is done with a combination of over-relaxed and Metropolis algorithms. Each configuration represents N_{or} sweeps through the lattice followed by N_{Met} Metropolis steps. Although the implementation of the overrelaxed scheme is microcanonical, the Metropolis "hits" make the whole algorithm ergodic. Surprisingly, this purely local algorithm succeeded, in some cases, in achieving strong collective effects.[42-51] Recent theoretical analysis and numerical measurements by several groups appear to confirm[45-51] that with use of this method one can reduce critical slowing down to $z=1$. In practice, however, the observed improvement is rather researcher dependent; for example, in a recent study[52] of the phase transitions in the $d=2$ XY model the over-relaxation algorithm was demonstrated to decorrelate as $\tau\sim\xi^{1.2}$.

We applied the over-relaxed scheme to study the dynamical critical behavior in the simple-cubic classical Heisenberg ferromagnet by updating spins with a succession of N_{or} over-relaxed and N_{Met} Metropolis sweeps. We made measurements of observables after each lattice update. Simulations were carried out on a $16\times 16\times 16$

lattice and seven temperatures in the paramagnetic phase ($1.5 \leq T \leq 2.5$). Again, after discarding 2×10^4 conventional Metropolis configurations we created over-relaxed Metropolis data for combinations $N_{\rm Met}=2$ and $N_{\rm or}=1$, 8, or 198, with the constraint that the total number of configurations was 8×10^5. Then we followed the procedure described above to compute the correlation function $\phi(t)$. We used a simple-exponential fit to calculate the correlation time τ (which is given in units of Monte Carlo time, i.e., the interval between two MC sweeps through the lattice). Repeating this scheme for each ratio $N_{\rm or}/N_{\rm Met}$, we arrived at the log-log plot of τ vs T/T_c-1, shown in Fig. 5. It is easy to see that the data collected for $N_{\rm or}/N_{\rm Met}=1/2$, 8/2, 198/2, can be fitted with good precision to straight lines of slopes $\Delta=1.24, 1.02, 0.77$, respectively. Accepting the ϵ-expansion value of the correlation exponent $\nu\simeq0.705$, we estimated that

$$z\simeq1.76(6) \quad (N_{\rm or}/N_{\rm Met}=1/2)\,, \tag{16a}$$

$$z\simeq1.44(7) \quad (N_{\rm or}/N_{\rm Met}=8/2)\,, \tag{16b}$$

$$z\simeq1.10(6) \quad (N_{\rm or}/N_{\rm Met}=198/2)\,. \tag{16c}$$

It is quite possible that by varying the relative number of $N_{\rm or}$ and $N_{\rm Met}$ one can reduce critical slowing down even further, i.e., to its lower limit[45,46] $z=1$. Since spin updating via the over-relaxation mechanism is essentially a microcanonical procedure, and one is usually interested in canonical expectation values of the thermodynamic quantities, it is imperative that a substantial number of conventional Metropolis hits be made together with energy-conserving updates. This sets an upper bound on the value of the ratio of $N_{\rm or}/N_{\rm Met}$ one might want to use in a given simulation; we estimate that the optimal choice is $N_{\rm or}/N_{\rm Met}\simeq10$.

Our results remain in very good agreement with recent measurements[52] of over-relaxed Metropolis decorrelations in the planar rotator ($d=2$ XY) model, where it was found that for the configuration $N_{\rm or}=8$, $N_{\rm Met}=2$ the autocorrelation time diverges like $\tau=0.15\xi^{1.48}$, whereas the combination $N_{\rm or}=15$, $N_{\rm Met}=2$ corresponds to $\tau=0.15\xi^{1.2}$. This can be regarded as another "empirical evidence" in favor of the over-relaxation even for a three-dimensional classical spin system.[47] Nevertheless, our preliminary results did not answer some important questions regarding the algorithm and its implementation. It was recently conjectured by Neuberger[46,47] that the over-relaxation may be represented by a new dynamical renormalization-group universality class.[17] The version of the algorithm the workers studied included a free over-relaxation parameter[43] ω, which was tuned to allow the system to reach the "critical damping"[46,47] with the optimal relaxation rate corresponding to $\omega_{\rm opt}<2$ and leading to the dynamical critical exponent z equal to 1. The version of the algorithm we used,[42,52] however, is composed of alternations of the extremely over-relaxed iterations (given by $\omega=2$) with a number of the Metropolis sweeps. It is not clear to us, whether a purely microcanonical (extremely over-relaxed) version of the algorithm has the same (if any) universality class as the version studied by Heller and Neuberger.[46–48] If the answer is positive (i.e., if $z=1$ even for $\omega=2$), then the "effective" dynamic exponent $z_{\rm eff}$ calculated in the simulation scheme with use of a mixture of two different (as far as conservation laws and universality classes are concerned) algorithms, should cross over from 2 to 1 as the ratio $N_{\rm or}/N_{\rm Met}$ varies between 0 and ∞. The results of our simulations presented above seem to support this general picture.

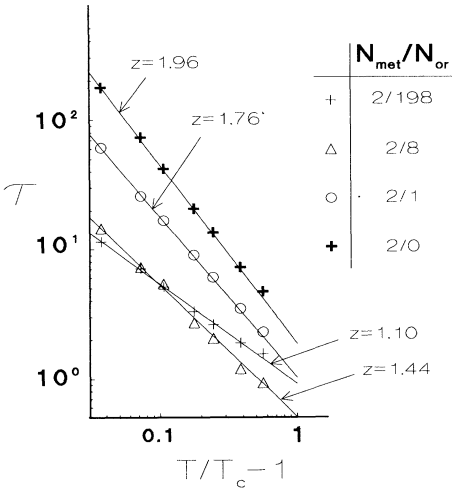

FIG. 5. Log-log plot of the relaxation time τ vs the reduced temperature for a $16\times16\times16$ lattice in the paramagnetic region for different values of $N_{\rm or}/N_{\rm Met}$; $K_c=0.6929$. The lines represent the best linear fits to the data in the scaling regime.

V. SUMMARY AND CONCLUSIONS

Using large-scale Monte Carlo simulations we have described the dynamic critical behavior of the three-dimensional simple-cubic Heisenberg model by investigating the temperature and size dependence of the equilibrium (linear) relaxation time τ in the vicinity of the critical point. Both methods discussed in the text gave us, after making additional finite-size corrections to scaling, about the same value of the dynamical exponent $z=1.96(7)$. This result is consistent with that obtained within the framework of the renormalization-group theory[12–15] $z\simeq2.02$ and with current experimental estimates.[1] It would be desirable, however, to improve the accuracy of our result using simulations for larger system sizes. For example, in the recent study of the critical dynamics in the $d=3$ Ising model the workers used lattices with $L\leq96$ (and runs with 3×10^6 MCS's/site) and obtained an estimate $z=2.04(3)$. [The purely relaxational Ising model is believed to belong to the same dynamical universality class—model A of Halperin and Hohenberg—as the purely dissipative Heisenberg system. Hence, the dynamic critical exponent z is also given by Eq. (15) but with the static exponent $\eta\simeq0.031$ that of the $d=3$ Ising model. This means that the dynamical exponents for the Ising and Heisenberg models are *approximately* equal: $z_{3d}^{\rm Heis}\simeq z_{3d}^{\rm Ising}\simeq2.0$.] Since creation of

12×10^6 MCS's on a $24\times24\times24$ lattice took us about 240 h of CPU time, equally accurate calculations performed on a lattice with $L=48$ would call for the equivalent of about 7600 h of Cyber 205 times which is, by any measure, an enormous computational demand. It might be more sensible to improve the precision of calculations of the dynamical exponent z with use of longer Monte Carlo runs, obtaining more accurate values of the correlation times so that an additional analysis of finite-size corrections to scaling could be meaningfully employed.

We have also demonstrated that the over-relaxed Metropolis algorithm can be successfully employed to produce faster decorrelations in a classical cubic spin system (which was recently seriously questioned).[46] We found that for an appropriate combination of over-relaxed and Metropolis MC steps, the dynamical critical exponent is reduced from $z\simeq2.0$ to 1.1. This study demonstrates that one can add over-relaxation to existing Monte Carlo programs with very little effort and significantly increases the efficiency of Monte Carlo calculations.

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