Monte Carlo investigation of critical dynamics in the three-dimensional Ising model

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We report the results of a Monte Carlo investigation of the (equilibrium) time-displaced correlation functions for the magnetization and energy of a simple cubic Ising model as a function of time, temperature, and lattice size. The simulations were carried out on a CDC CYBER 205 supercomputer employing a high-speed, vectorized multispin coding program and using a total of 5×10^{12} Monte Carlo spin-flip trials. We used $L\times L\times L$ lattices with periodic boundary conditions and L as large as 96. The short-time and long-time behaviors of the correlation functions are analyzed by fits to a sum of exponential decays, and the critical exponent z for the largest relaxation time is extracted using a finite-size-scaling analysis. Our estimate $z=2.04\pm0.03$ resolves an intriguing contradiction in the literature; it satisfies the theoretical lower bound and is in agreement with the prediction obtained by ϵ expansion. We also consider various small systematic errors that typically occur in the analysis of relaxation functions and show how they can lead to spurious results if sufficient care is not exercised.

I. INTRODUCTION

Dynamical properties of spin models are a traditional subject of statistical physics. Although analytical work in this field began some time ago,[1] quantitative verifications of theoretical results and predictions by means of Monte Carlo simulation techniques have been published only recently and are still much less reliable than Monte Carlo results for static properties. An elucidating example is the three-dimensional (3D) Ising model whose static critical exponents are numerically very well known.[2] Within the past few years several attempts employing different Monte Carlo methods have been made to find a reliable numerical estimate[3–7] for the dynamic critical exponent z. The values obtained vary between 2.17 (Ref. 3) and 1.95 (Ref. 6), a region which is much larger than the errors given in the papers. The values tend to become smaller with increasing lattice size and computer time, which suggests that the results may be biased by finite-size effects and/or insufficient statistics. The two most recent values were calculated on a CDC CYBER 205 supercomputer[6] and on the Santa Barbara special purpose computer,[7] on lattices up to $512\times512\times512$ and with Monte Carlo runs with several million Monte Carlo steps. The results were surprising in that both values $z=1.95$ (Ref. 6) and $z=1.99$ (Ref. 7) are smaller than 2 which had been accepted as a lower bound for z for all dimensions d between one and four.[8] This lower bound is the result of an interpolation between second-order ϵ expansions around $d=1$ and 4. The validity of the ϵ expansion results has been conclusively verified by Monte Carlo simulations[9] for $d=2$. (Together with ϵ-expansion results, the previous Monte Carlo results for $d=3$, however, imply that, as a function of d, $z-2$ has zeros between $d=2$ and 3 and between $d=3$ and 4, which is not compatible with the ϵ-expansion result.) An alternative explanation for such small z values might be found in systematic errors in the methods used. Our motivation for this paper is therefore not only to clarify the discussion concerning the numerical value of z, which is even more important as the Santa Barbara results[7] are suspected to be incorrect,[10,11] but to analyze the possible systematic errors which occur in Monte Carlo investigations of dynamical properties. The results of our analysis explain the variety of previous numerical values for z. In our calculation of z we take those systematic errors into account and obtain an improved value for z, which is in good agreement with the ϵ-expansion result.

The paper is organized as follows: In Sec. II we describe our Monte Carlo method and the theoretical background upon which our method is based. In Sec. III we describe our data analysis and present the results. We discuss our results in comparison with other theoretical and numerical work in Sec. IV before summarizing and drawing final conclusions in Sec. V.

II. BACKGROUND

A. Critical dynamics and relaxation functions

The critical dynamics of spin models are typically studied by means of relaxation functions of magnetization, energy, or other observables at or close to the critical temperature. Most of the previously applied Monte Carlo methods for determining the dynamical critical exponent[4–6] z are dynamic Monte Carlo renormalization-group (dynamic MCRG) methods, which are convenient because they do not require the explicit knowledge of the relaxation time τ. These methods are very similar to static MCRG methods; they use dynamic scaling relations between relaxation functions instead of static scaling relation between correlation functions. However, there is one important difference. As opposed to the static case, the limit $L\rightarrow\infty$ (L = lattice size, $T=T_c$) is not sufficient to guarantee the validity of the dynamic scaling relations. An additional condition which must be satisfied is that

relaxation processes in the systems must be governed by a single characteristic relaxation time, i.e., the scaling relations hold only for times sufficiently large that short-time relaxation behavior is irrelevant. For dynamic MCRG methods it is difficult to check whether both conditions are satisfied. We will discuss this point in Sec. IV in more detail. An alternative approach, which we chose, is to estimate τ directly from explicit data for the relaxation functions and determine the critical exponent z from the scaling behavior of τ.

We studied the equilibrium time-displaced correlation function $\Phi(t)$ of the magnetization and energy at T_c in an $L\times L\times L$ lattice. In a Monte Carlo run with N successive configurations $\Phi(t)$ is calculated as

$$\Phi_A(t)=\Gamma^{-1}\left[(N-t)^{1}\sum_{t'=1}^{N-t}A(t')A(t'+t) -(N-t)^{-2}\sum_{t'=1}^{N-t}A(t')\sum_{t''=t+1}^{N}A(t'')\right], \quad (1)$$

where $A(t)$ is the magnetization or energy (M and E, respectively) at Monte Carlo step t. Γ is an appropriate normalization factor, $k_BT\chi$ for the magnetization and k_BT^2C for the energy with χ and C denoting susceptibility and specific heat, respectively. The limit for $N\to\infty$ is then

$$\Phi_A(t)\to\frac{\langle A(0)A(t)\rangle-\langle A\rangle^2}{\langle A^2\rangle-\langle A\rangle^2}\ . \quad (2)$$

The time dependence of $\Phi_A(t)$ can be expressed, in general, as[11,12]

$$\Phi_A(t)=\sum_i a_i\exp(-t/\tau_i)\ , \quad (3)$$

where τ_i are the inverse eigenvalues of the Liouville operator of the given kinetic model and the a_i are unknown non-negative coefficients. Since the Liouville operator in a finite system is symmetric, non-negative, and finite,[12,13] the spectrum of eigenvalues is bounded. The smallest eigenvalue governs the long-time behavior of $\Phi_A(t)$, i.e., is the inverse of the relaxation time τ_L which is characteristic for the lattice size considered.

For very short times $\Phi_A(t)$ decays on a time scale given by the initial relaxation time τ^I. Usually τ^I is defined by the derivative of $\Phi_A(t)$ in the limit $t\to0$:

$$\tau^I=\Phi_A(t)\left[-\frac{d\Phi_A(t)}{dt}\right]^{-1},\quad t\to0 =\left[\sum_i\frac{a_i}{\tau_i}\right]^{-1}. \quad (4)$$

It is proportional to the fluctuation of the appropriate observable,[12,13] i.e., proportional to the susceptibility or specific heat for magnetization and energy, respectively. It is not obvious how the limit in Eq. (4) is to be taken for the discrete time scale in a Monte Carlo simulation. We have tried two different methods, namely taking the (numerical) derivative at $t=1,2,\ldots$ and secondly, fitting the derivatives of $\Phi_A(t)$ to the explicit formula of $d\Phi_A(t)/dt$ written as a polynomial in t:

$$-\frac{d\Phi_A(t)}{dt}=1/\tau^I+\sum_{n=1}^{\infty}(-1)^n(1/n!)\sum_i a_i\tau_i^{-n}t^n\ . \quad (5)$$

Whereas the initial relaxation time depends on the method chosen (as it depends on the algorithm used), the critical exponent should be universal if τ^I is determined from the relaxation function at times short compared to the relaxation time τ_L.

In the thermodynamic limit all relaxation times τ_i diverge as

$$\tau_i\propto L^{z(i)} \quad (6)$$

with $z(i)\le z$, the critical exponent of τ_L. For z itself a lower bound is known. Since $a_i\ge0$, a lower bound for τ_L is given by

$$\tau_L\ge\left[\sum_i a_i/\tau_i\right]^{-1}=\tau^I\ . \quad (7)$$

Since τ^I is proportional to the susceptibility in the case of the magnetization,[11] τ diverges with the exponent γ/ν and thus

$$z\ge\gamma/\nu=1.96\ . \quad (8)$$

There is another inequality which can be easily derived. Since $\Phi_A(t=0)=1$, the sum of all coefficients in Eq. (3) must be unity. It follows then for the smallest relaxation time $\tau_{\min}$,

$$\tau_{\min}=\sum_i a_i\tau_{\min}\le\sum_i a_i\tau_i=\tau^I\ . \quad (9)$$

So far we have briefly summarized some exactly known properties of $\Phi_A(t)$ as a function of t and lattice size. In a Monte Carlo simulation there is another parameter which may influence $\Phi_A(t)$ and thus the estimate of z drastically, namely the length of the computer simulation itself. As the two terms of Eq. (1) are taken from the same data set, the calculated relaxation function is systematically small. This effect has been mentioned by several authors[14,15] but has never been studied quantitatively. It can be described as follows: Consider a Monte Carlo run with N successive configurations cut into M pieces of P successive configurations, i.e., $N=MP$. Φ_A can then be split into contributions from relaxation functions Φ_{jA} within the jth piece ($j=1$ to M) and a coarse-grained relaxation function $\Phi_{\mathrm{cg},A}$ describing the relaxation of the average values of A from piece to piece. Using the short notations $n(j)=(j-1)P+1$ and $m(j)=jP$ for the first and last time step, respectively, of the jth piece, Φ_{jA} and $\Phi_{\mathrm{cg},A}$ are given by

$$\Phi_{j,A}(t)=\Gamma^{-1}\left[(P-t)^{-1}\sum_{t'=n(j)}^{m(j)-t}A(t')(t')A(t'+t)-(P-t)^{-2}\sum_{t'=n(j)}^{m(j)-t}A(t')\sum_{t''=n(j)+t}^{m(j)}A(t'')\right], \quad (10a)$$

$$\Phi_{\mathrm{cg},A}(t)=\Gamma^{-1}\left[(P-t)^{-2}\sum_{j=1}^{M}\sum_{t'=n(j)}^{m(j)-t}A(t')\sum_{t''=n(j)+t}^{m(j)}A(t'')-M^{-2}(P-t)^{-2}\sum_{i=1}^{M}\sum_{j=1}^{M}\sum_{t'=n(i)}^{m(i)-t}A(t')\sum_{t''=n(j)+t}^{m(j)}a(t'')\right] . \tag{10b}$$

Using these expressions, Eq. (1) then becomes equivalent to

$$\Phi_A(t)=M^{-1}\sum_{j=1}^{M}\Phi_{j,A}(t)+\Phi_{\mathrm{cg},A}(t) . \tag{11}$$

In the limit $M\to\infty$, $N\to\infty$, $P=N/M=$const the left-hand side of Eq. (11) converges to the expression for $\Phi_A(t)$ at infinite N, Eq. (2). The first term of the right-hand side of Eq. (11) becomes the statistical expectation value of $\Phi_A(t)$ calculated in a time-limited Monte Carlo simulation of P configurations. The coarse-grained relaxation function is for $t\ll P$ approximately equal to the variance of the average of A over P successive Monte Carlo steps, i.e., according to the central limit theorem for Markov processes[16] proportional to $1/P$. Thus, by replacing N for P we get, for our original problem, namely the dependence of $\Phi_A(t)$ of the number of configurations in the Monte Carlo simulation N, the relation

$$\Phi_A(t)\approx\frac{\langle A(0)A(t)\rangle-\langle A\rangle^2}{\langle A^2\rangle-\langle A\rangle^2}-\mathrm{const}/N \quad N\to\infty . \tag{12}$$

The $\approx$ sign in Eq. (12) means that $\Phi_A(t)$ is a random variable with statistical fluctuations. Equation (12) is exact for the expectation value of $\Phi_A(t)$.

Assuming a single exponential decay for $\Phi_A(t)$, one can easily derive a relation for the corresponding relaxation time $\tau_{L,N}$ estimated from a time-limited Monte Carlo simulation with N configurations:

$$\begin{aligned}&\tau_{L,N}\to\tau_L, \quad N\to\infty ,\\ &1/\tau_{L,N}\approx 1/\tau_L+c/N, \quad N\to\infty ,\end{aligned} \tag{13}$$

c is a dimensionless, and therefore L-independent, constant. Thus, Eq. (13) can be written in a scaled version:

$$\tau_{L,N}/\tau_L=f(N^{-1}\tau_L)\approx 1-c(N/\tau_L)^{-1}, \quad N/\tau_L\to\infty . \tag{14}$$

B. Dynamic finite-size scaling

For temperatures away from T_c there are two characteristic length scales in the system, namely besides the lattice size L, the (finite) correlation length. All preceding formulas remain valid except Eq. (6) which has to be replaced by the finite-size-scaling expression[17,18]

$$\tau(\epsilon,L)=L^z f(\epsilon L^{1/\nu}), \quad \epsilon=(T-T_c)/T_c \tag{15a}$$

with

$$f(x)\propto x^{-z\nu}, \quad x\to\infty . \tag{15b}$$

From Eq. (3) it is obvious that the relaxation function itself can be written in a simple scaling form like Eq. (15) only for sufficiently long times when all exponential terms besides one can be neglected. This scaling form then follows in a trivial way from Eq. (15) for $\tau=\tau_L$.

A finite-size-scaling analysis of equilibrium relaxation functions for $T\neq T_c$ is an alternative to our method of determining the dynamical critical exponent z. As has become clear from the preceding considerations, it is dangerous to assume a simple scaling form for the relaxation functions themselves. The finite-size-scaling analysis rather should be applied to the relaxation times determined by a direct examination of the relaxation functions. As there do not exist published data for finite-size-scaling analyses for $T\neq T_c$ within equilibrium (for an analysis of nonlinear relaxation see Ref. 3), we present our data here, although they are of less accuracy than our data at T_c and do not improve our estimate of z taken from the analysis at T_c.

C. Monte Carlo method

The Monte Carlo simulations were carried out with a highly optimized multispin coding program[19] on the CDC CYBER 205 vector computer at the University of Georgia. It simulates the Ising model in the canonical ensemble generating a new random number for each spin update. The boundary conditions are periodic and the kinetic model is defined by the symmetric transition probability. As reported by other authors recently, the multispin-updating procedure[20] does not affect the kinetics for long times. This conclusion coincides with our experience that the number of sublattices used in the implementation on a vector computer does not influence the relaxation times. However, relaxation times do depend on the specific choice of the transition probability,[21,22] i.e., on the kinetic model chosen, but without affecting the results for critical exponents. Thus, our results for z are universal (for local spin-flip algorithms) whereas the relaxation times themselves are not. The maximum speed of this program is 18 000 000 updates per sec (38 000 000 updates per second in an updated version[23]). The simulations were performed at the estimated critical temperature[2] $J/kT_c=0.221\,654$.

In our Monte Carlo investigation of the long-time behavior of $\Phi_A(t)$, we calculated $\Phi_M(t)$ and $\Phi_E(t)$ for lattices with $L=8$, 12, 16, 24, 32, 48, 64, and 96. The number of Monte Carlo sweeps per lattice size were 3 000 000 except for $L=16$ where 20 000 000 Monte Carlo configurations were generated in order to study systematic errors intensively. The total number of single spin flips invested in this investigation is about 5×10^{12}. An appropriate number of configurations in the beginning of the simulation (typically about 20 times the relaxation time itself) was discarded in order to ensure that the system was in equilibrium. The remaining number of sweeps

corresponds to the number N in the preceding formulas. The magnetization and energy were calculated after every tenth sweep. As the relaxation times are at least of the order of 100 for the lattice sizes simulated and more than 10^5 data points remained, the loss of information was marginal. For our simulations with $T \neq T_c$ we used lattice sizes $L=16$, 24, 32, and 48, the number of Monte Carlo steps used was between 1 000 000 and 500 000 with a smaller number for the larger lattices.

To study the short-time behavior of $\Phi_A(t)$ at $T=T_c$ we made separate Monte Carlo runs with a calculation of magnetization and energy after every sweep but with less accuracy. The number of sweeps varied between 1 000 000 and 80 000 depending on the lattice size. The simulations were only done for $L=16$, 24, 32, and 48.

III. RESULTS AND ANALYSIS

A. The long-time behavior of Φ_A at T_c and the determination of z

In Monte Carlo work on critical dynamics, the long-time behavior of $\Phi_A(t)$ is usually assumed to be exponential with one relaxation time τ_L. Our analysis shows that this assumption is dangerous because it might be valid only at times where Monte Carlo data for the relaxation function cannot be analyzed, as we will show later on. According to Eq. (3) the true time dependence is determined by a finite, but very large, set of relaxation times. In an analysis of numerical data for $\Phi_A(t)$ this can only be taken into account by a fit of the data to a function of the form of Eq. (3), i.e., to a sum of exponential decay functions. The feasibility of this procedure is limited by (a) the quality of the data (and of the nonlinear least-squares fitting method), and (b) the width of the interval in which the different relaxation times are spread.

The first restriction is obvious. A fit procedure is reasonable only if the number of exponential terms is small. The analysis of the relaxation function must therefore be extended to large times where the corrections to the dominant exponential term are small. Typically, the data become worse with larger time displacements due to statistical fluctuations, and fits to an exponential decay become almost impossible if the data oscillate with increasing time. The importance of the second point becomes clear in a comparison between the relaxation functions for magnetization and energy, respectively. Although the critical exponent for the largest relaxation time is the same for both (≈ 2.0), the initial relaxation times diverge with $\gamma/\nu=1.96$ for the magnetization and as $\alpha/\nu=0.18$ for the energy. Equation (9) then indicates that the difference between τ_L and the smallest relaxation time $\tau_{\min}$ is much greater for the energy than for the magnetization. The broader the range of different relaxation times, the more terms, i.e., the more fit parameters, must be considered. More fit parameters means less significance in the results at a given accuracy of the data. Thus, for a given Monte Carlo simulation the analysis of Φ_M yields a better estimate for the dominant relaxation time than that of Φ_E.

Figure 1 shows data and fits of Φ_M and Φ_E for $L=32$. We were able to fit two exponential terms for Φ_M and three for Φ_E. The fit interval was taken from $t=10$ up to the largest relaxation time itself. For $L=16$ we could extend the interval up to four times the relaxation time without changing the fit parameters significantly. We tested whether the number of exponential terms in the fit function was sufficient by checking if the sum of the coefficients a_i was unity. This is always satisfied for Φ_M, but for Φ_E the sum is smaller than one, i.e., three terms are not sufficient to describe the relaxation function properly. However, Fig. 1 shows that the fit function and data coincide well over the whole fit interval indicating that the fit function is insufficient only for very early times (smaller than 10). This fitting procedure has been used effectively in the examination of relaxation in two-dimensional Potts models.[9]

The importance of considering more than one relaxation time is demonstrated in Fig. 2(a). It shows Φ_E for

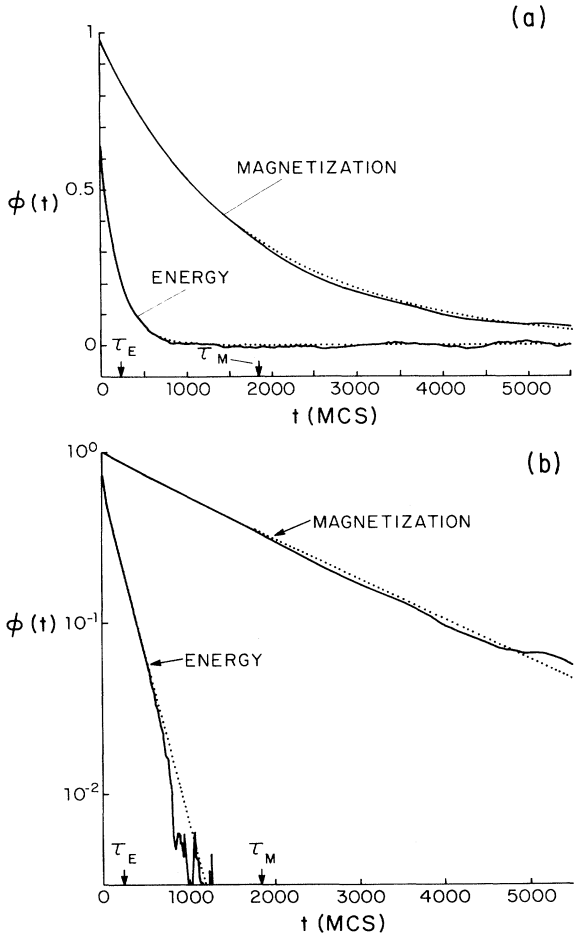

FIG. 1. Time-displaced correlation functions for magnetization and energy for $L=32$ at $T=T_c$. The dotted curves represent the functions fitted to the data in a fit interval $[10,\tau_M]$ and $[10,\tau_E]$, respectively. τ_M and τ_E denote the largest relaxation time for magnetization and energy, respectively.

$L=48$ together with the leading term of the fit function, the sum of the two most dominant terms and, finally, the complete fit function including three exponential decay terms. It is obvious, that corrections to the dominant term are negligible only in the region where the data are bad and a reasonable fit is not possible at all. That means using more than one exponential decay term is necessary in order to accurately analyze the data in the time region where they are best. Additionally, it seems clear that the common method of estimating relaxation times by integrating over all data can be considerably biased by contributions from short-time relaxations which lead to an anomalously small value for τ_L. As discussed before, the situation is much less pronounced for Φ_M. Figure 2(b) shows the data for $L=48$ together with the dominant term of the fit function and the complete fit function consisting of two terms.

The largest relaxation time obtained by the fit procedure corresponds to $\tau_{L,N}$ of Eqs. (13) and (14). It depends not only on the lattice size but additionally on the length of the Monte Carlo simulation denoted by N. According to Eq. (12), this dependence can be canceled out by a linear extrapolation to $N\to\infty$ in a plot of $1/\tau_{L,N}$ against N^{-1}. Moreover, one can improve the reliability of the estimate for τ_L by using Eq. (14) as a finite-size scaling formula. Similar to a standard finite-size scaling analysis, we analyzed the data for different lattice sizes for 15 different values of N and plotted the data according to Eq. (14) for two lattice sizes into one plot. If the estimates for τ_L are correct, the data for the different lattice sizes should collapse onto one curve. We took the data for $L=16$ as reference data because of their extremely good statistics, i.e., the relaxation times of all lattice sizes were estimated by varying τ_L in Eq. (14) and plotting the data for the considered lattice size together with those for $L=16$. For $L=24$ this procedure is shown in Fig. 3. The shift in $\tau_{L,N}$ with respect to τ_L is $\sim 1\%$ when N is 100 times the relaxation time. Thus about 10 000 000 sweeps are necessary in order to get a practically unbiased estimate for the relaxation time of a $96\times 96\times 96$ lattice; 10 000 000 sweeps would require more than 100 h CPU time on a CDC CYBER 205 using the most sophisticated CDC programs. The results of this analysis are shown in Fig. 4. The errors were calculated as follows: The set of Monte Carlo data were cut into six pieces and each of them analyzed separately. An error estimate for τ_L was then obtained by a standard error analysis with the sample of six relaxation times. Independently, an error was estimated in the finite-size-scaling analysis according to Eq. (14). The greater error was taken as the final error estimate.

The values for τ_L are plotted against L with logarithmic scales in Fig. 4. According to Eq. (6), they should follow a straight line for asymptotically large L, and indeed within the accuracy of our data we cannot see any finite-size corrections for lattice sizes $L\geq 12$. An error-weighted least-squares fit to the points obtained from the analysis of Φ_M for $L\geq 12$ yields a value for the critical

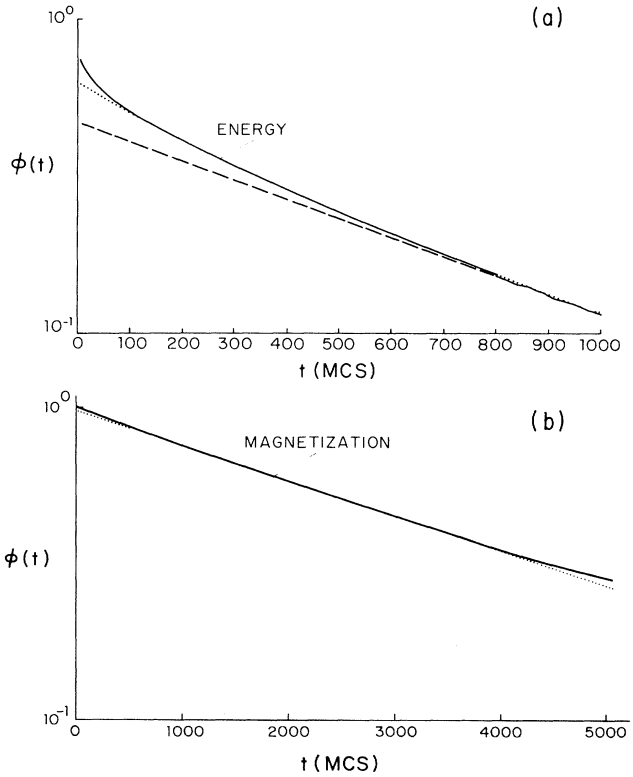

FIG. 2. (a) Energy-energy time-displaced correlation function for $L=48$. The time axes coincide roughly with the fit interval. In addition to the complete three-exponential-fit function, the dominant term and the dominant plus the second dominant term are shown. (b) The magnetization-magnetization time-displaced correlation function for $L=48$. Here the fit function consists of two terms only.

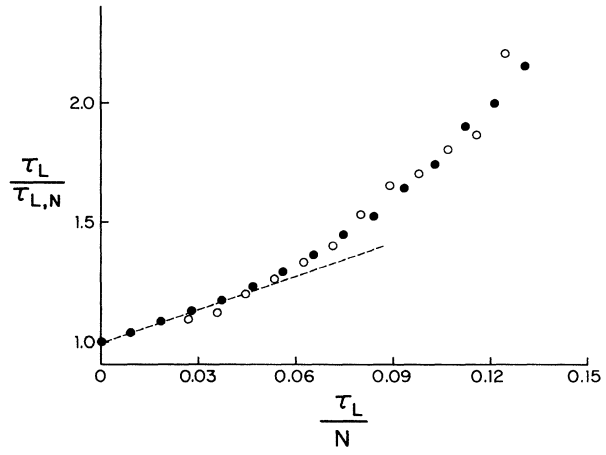

FIG. 3. Plot of scaled inverse relaxation times vs scaled inverse number of configurations of the Monte Carlo experiment according to Eq. (14) with different values for τ_L. The lattice sizes are 16 and 24.

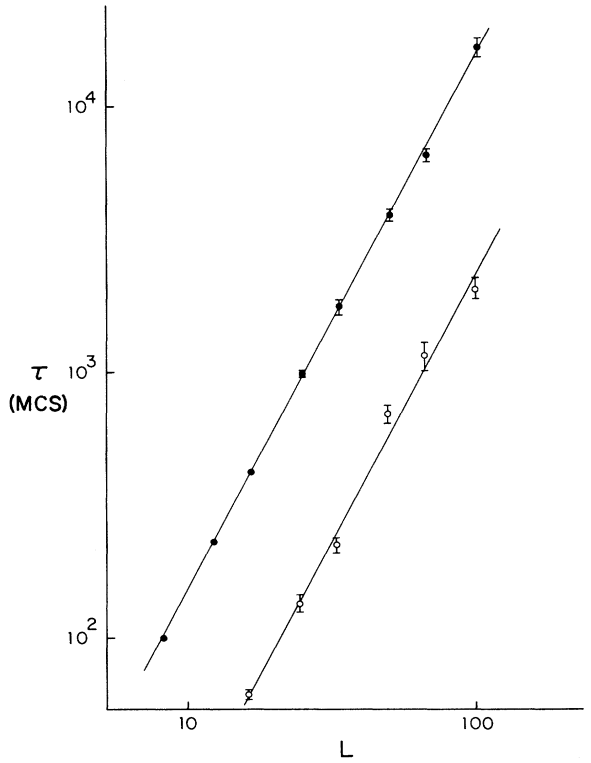

FIG. 4. Plot of the relaxation times for energy and magnetization vs lattice size. The critical exponent z is given by the slope of the straight line fitted to the data points.

exponent z of 2.04 ± 0.03 in agreement with the ϵ-expansion result[8] $z=2.02$. The data points obtained from the analysis of Φ_E are much less accurate but still yield an estimate $z=2.03\pm0.10$ which is consistent with the value obtained from Φ_M. With such large errors we cannot make a strong statement about the universality of z but we can say that the exponents obtained from Φ_M and Φ_E are consistent with a single value.

B. The short-time behavior of Φ_A

The determination of an initial relaxation time which corresponds to that defined for a continuous time scale requires a fit of the numerical derivatives of the relaxation functions to the polynomial given in Eq. (5). Whether such a fit can be carried out is mainly influenced by the width of the interval in which the different relaxation times are spread. The absolute value of the nth coefficient of this polynomial [see Eq. (5)] is given by

$$(1/n!)\sum_i a_i \tau_i^{-n} \geq (1/n!)\tau_L^{-n} . \tag{16}$$

When the relaxation times τ_i are grouped in a very small range close to τ_L, then the coefficients drop with increasing n approximately like the right-hand side of the above inequality. For a wider range of different relaxation times, the coefficients decrease slower and more terms must be considered in the fit procedure. This difference appears very pronounced when comparing our data for Φ_M with those of Φ_E. Whereas for Φ_M a fit to a polynomial of second order in t was sufficient for the first 20 time steps, a fit for Φ_E was not possible at all with a reasonable number of terms ($n<6$). Instead, we took the negative inverse of the numerical derivatives of Φ_E for very short times ($t=1$, 2, 4, 8) as an estimate for the initial relaxation time. The results of both procedures are plotted in Fig. 5. For Φ_M the divergence of τ^I with L

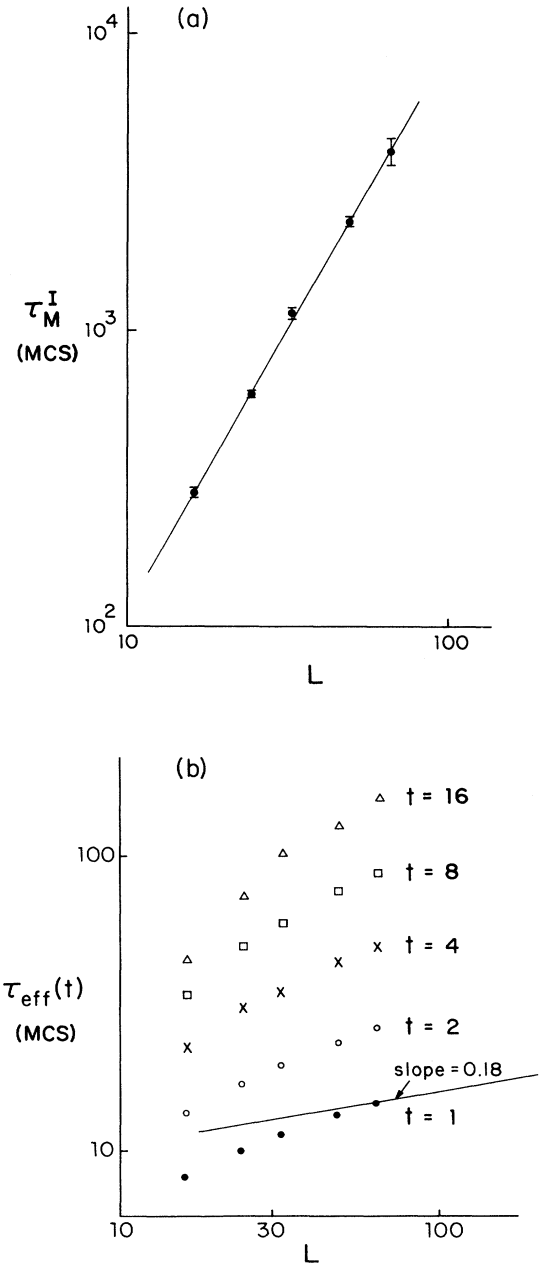

FIG. 5. Scaling plot of the initial relaxation time for the magnetization vs lattice size: (a) magnetization, (b) energy.

agrees with the expected theoretical value γ/ν for the critical exponent. For Φ_E this is true only for $L \geq 32$ because our method of determining the initial relaxation time induces a strong correction to scaling effect. We took the derivatives at the same time for all lattices whereas the inherent time scale of the system varies with the lattice size.

C. Critical dynamics for $T \neq T_c$

When moving away from T_c, the relaxation times drop sharply, following approximately [see Eq. (15)]

$$\tau_L \propto \epsilon^{-z\nu} = \epsilon^{-1.28} . \tag{17}$$

The relaxation functions can therefore be described by a single exponential decay at very short times as opposed to the case at T_c. For our data for Φ_M away from T_c it was not possible to make a significant fit to more than one exponential term. Also, the dependence of the relaxation times on the length of the Monte Carlo simulation could not be significantly analyzed within the accuracy of our data.

In Fig. 6 we show the relaxation time τ_L plotted versus ϵ. The temperature- and lattice-size-dependent relaxation times $\tau_L(\epsilon)$ for $T > T_c$ were plotted in a finite-size-scaling plot as shown in Fig. 7. There the data are plotted according to

$$\tau_L(\epsilon) L^{-z} = f(\epsilon L^{1/\nu}) . \tag{18}$$

Our calculations for $T \neq T_c$ were much less accurate than those at T_c. Thus, we did not determine an independent estimate of z. For the straight line in Fig. 6 which represents the asymptotic behavior of $f(\epsilon/L^{1/\nu})$ according to Eq. (15b), we therefore used the value for z calculated at T_c. This value is obviously compatible with the data calculated for $T \neq T_c$. In Fig. 6 we also plot τ_L for $T < T_c$. These data are less complete than those for $T > T_c$ but allow us to estimate the dynamic critical amplitude ratio $A_+/A_- = 3.35$.

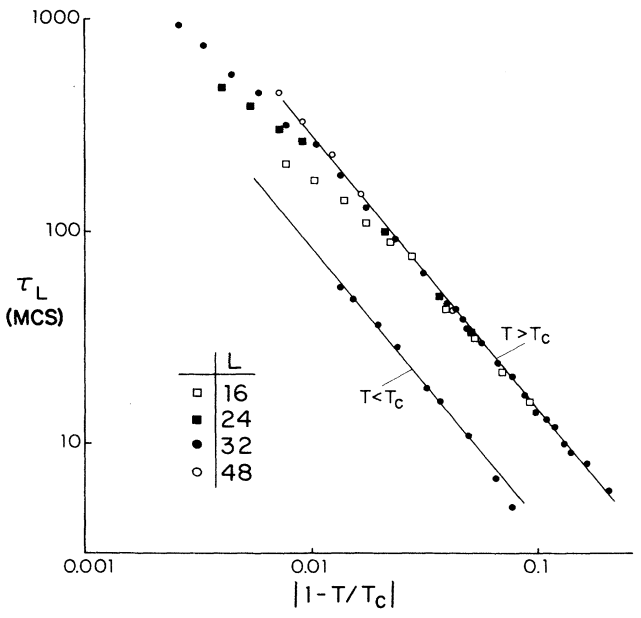

FIG. 6. Relaxation times τ_L for different lattice sizes as a function of $\epsilon = |1 - T/T_c|$.

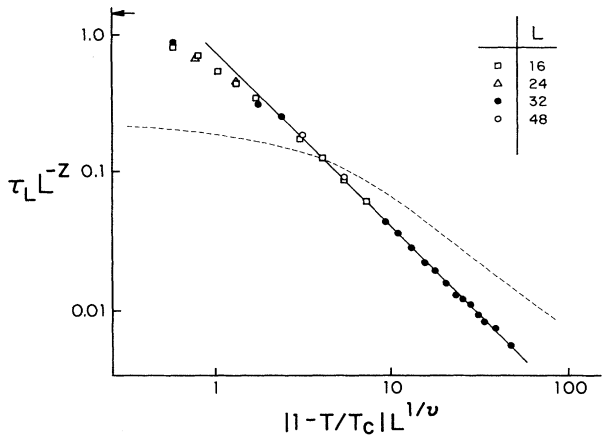

FIG. 7. Finite-size-scaling plot for the relaxation time τ_L for $T > T_c$ as a function of $\epsilon = (T - T_c)/T_c$. The dashed curve is predicted by Ref. 18.

IV. DISCUSSION

Although our Monte Carlo estimate for z agrees well with the prediction of the ϵ expansion, it is still somewhat disconcerting that previous Monte Carlo studies produced such a wide range of results. There can be several reasons why different investigations disagree. First of all, there are several asymptotic limits which must be reached before one can expect to extract a correct estimate for z: (1) scaling limit, i.e., $T \to T_c$, (2) finite-size-scaling limit, i.e., $L \to \infty$, (3) dynamic-scaling limit, i.e., $t \to \infty$. Failure to be in the asymptotic regime may bias the analysis and yield an incorrect result; however, the determination of whether or not these criteria have been met is not straightforward. Note, in particular, that Suzuki's dynamic-scaling ansatz implicitly assumes that the time scale of dynamic processes is given by only one characteristic time. Our results show that this is true only in the very long-time regime and that MCRG methods based on comparison between relaxation functions obtained from different size lattices may give spurious results if the dynamic-scaling limit is not reached. The analysis of "short-time" data generally leads to an underestimate of z. This is most obvious when we look at the size dependence of effective relaxation times at fixed displaced time t as shown in Fig. 9 for $\Phi_E(t)$. For very small t, the effective relaxation times diverge not with the exponent z but with the critical exponent γ/ν which describes early time relaxation in the infinite system. In the

most recent dynamic MCRG calculation,[6] for instance, a simple dynamic-scaling ansatz was used for lattices up to $32\times32\times32$. The author reports on a considerable shift of the estimate for the critical exponent z to smaller values with increasing lattice size, leading to an extrapolated value 1.95 which is smaller than the exactly known lower bound $\gamma/\nu=1.96$. According to our analysis, we believe that this shift can be traced back to not matching one or both of the last two conditions listed above.

Pearson *et al.*[7] estimated the relaxation time by assuming an exponential decay and analyzing the time derivative of the relaxation function to extract τ. We have carried out a similar procedure for $\Phi_E(t)$ for the $16\times16\times16$ lattice at T_c. Figure 8 shows the decay rate

$$\tau_L^{-1}=\Gamma(t)=\frac{\ln\Phi_E(t)-\ln\Phi_E(t+\delta t)}{\delta t} \tag{19}$$

determined from data separated by $\delta t=20$ Monte Carlo steps (MCS) in time ($\delta t=20$ was chosen since it corresponds roughly to the value used in Ref. 6). Choosing the value at $\sim\tau_L/2$, as was done in Ref. 6, we obtain a relaxation time which is $\sim7\%$ too small. Although we were not able to provide an error estimate because of the way data were stored, the fluctuations which occur at long times provide an estimate of the errors. An apparent "asymptotic plateau" is reached beyond ~120 MCS but this yields an estimate for τ^{-1} which is also too large. If we fix τ_1 at this value and then carry out a three-exponential-decay analysis as shown in Fig. 9, we obtain values for $\Phi(t)$ which are systematically low for large t. We believe that our procedure is superior in that it uses values of $\Phi(t)$ over a wide range of time to extract τ.

Our data show that corrections to finite-size scaling are present for $L=8$ so that an analysis such as that shown in Fig. 4 yields too large a slope if the lattices used are small and $L=8$ is included. Corrections are negligible for $L\geq12$, but only if fully periodic boundary conditions

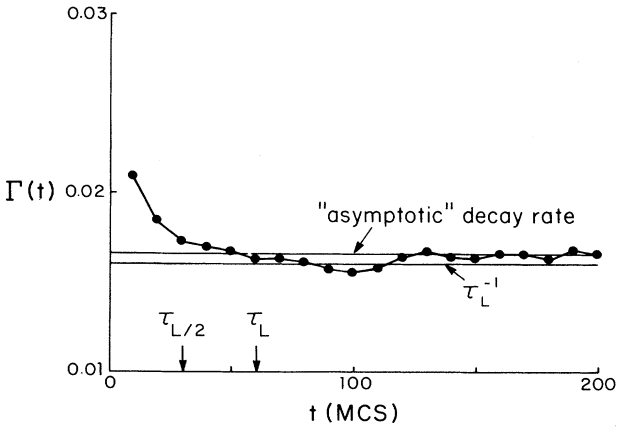

FIG. 8. The decay rate $\Gamma(\tau)$ defined in Eq. (19) extracted from $L=16$ data.

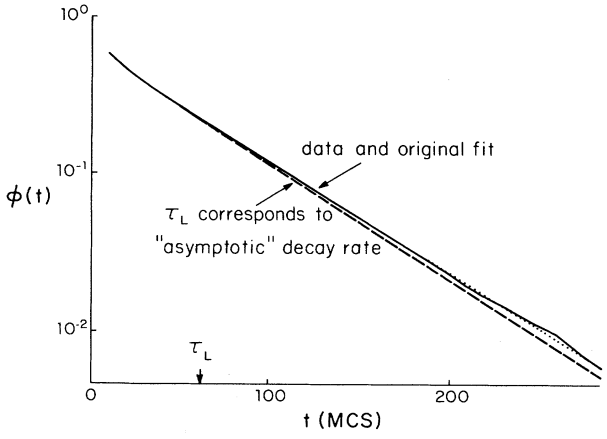

FIG. 9. Relaxation function for the internal energy for $L=16$. The solid curve shows the Monte Carlo data, the dotted line is the original two-exponential fit, and the dashed line is the long-time behavior, obtained from the "asymptotic decay" determined from Fig. 8.

are used. It is not uncommon, however, for skewed (screw periodic) boundary conditions to be used in one or more directions because such a procedure leads to some simplification in the programming. To test the effect of such boundary conditions on the dynamics, we repeated the calculations for the $12\times12\times12$ lattice with skewed boundary conditions and 9×10^6 MCS/site. Following the common practice in high-efficiency programming for the vector and special purpose computer, we implemented the skewed boundary condition in only one lattice direction leaving the remaining lattice boundaries periodically connected. The resultant time-displaced correlation function is shown in Fig. 10 along with that for the

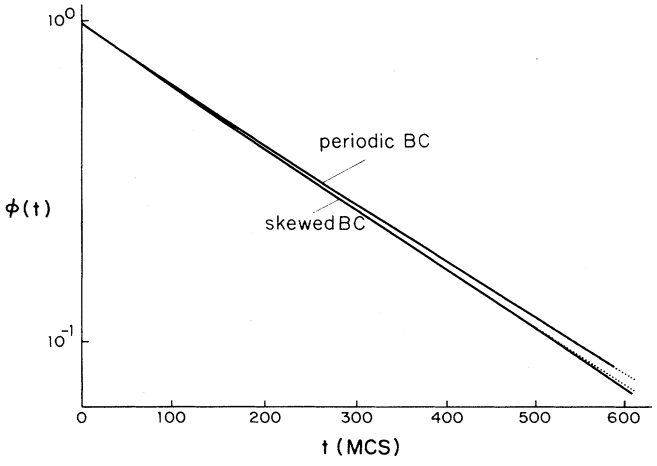

FIG. 10. Relaxation function for the magnetization for $L=12$ lattices with periodic boundary conditions and with skew boundary conditions. The solid curves represent Monte Carlo data for runs of 9×10^6 MCS; dotted curves are two-exponential fits.

fully periodic case. The relaxation time is clearly smaller ($\sim 4\%$) with skewed boundary conditions, but the effect should decrease as the lattice size increases. Nonetheless, for smaller lattices this leads to an "effective" correction to scaling. In summary then, Monte Carlo simulations can easily lead to estimates for z which are either too large or too small if statistical and systematic errors are not carefully taken into consideration.

V. CONCLUSIONS

The main result of our investigation of (equilibrium) critical dynamics at T_c is the value 2.04 ± 0.03 for the dynamical critical exponent z of the 3D Ising model. This is in excellent agreement with the ϵ-expansion result[8] $z = 2.02$. Thus, our investigation gives strong evidence that the ϵ expansion is qualitatively correct and the inequality $z > 2$ for $1 < d < 4$ is obeyed. Our analysis of systematic errors occurring in the Monte Carlo data of relaxation functions gives a satisfying explanation for the variety of previous Monte Carlo results for z, some of which contradict the aforecited inequality. These systematic errors are related to the conditions which have to be satisfied in any Monte Carlo investigation of equilibrium critical dynamics in order to get an unbiased result for the dynamical critical exponent. These conditions are sufficiently large lattice size to reach the scaling region, sufficiently long times to get an unbiased estimate for the dominating relaxation time, sufficiently long Monte Carlo runs for good enough statistics, and a careful analysis of the dependence of the calculated observables on the length of the Monte Carlo simulation itself. If these conditions are not met, the results of the Monte Carlo simulation are not reliable. For too small lattices ($L < 12$), the estimated value of the critical exponent z is too large. This was the case for the first dynamic MCRG calculations[4] where the lattice sizes used were $L = 8$ and 16 and the resulting value for $z = 2.08$. For increasing lattice sizes, corrections to scaling effects are less important but it becomes more difficult to satisfy the last two conditions. In the most recent dynamic MCRG calculation,[6] for instance, a simple dynamic-scaling ansatz was used for lattices up to $32 \times 32 \times 32$. The author reports on a considerable shift of the estimate for the critical exponent z to smaller values with increasing lattice size, leading to an extrapolated value 1.95 which is smaller than the exactly known lower bound $\gamma/\nu = 1.96$. According to our analysis we believe that this shift can be traced back to not matching one or both of the last two conditions listed above. Although we did not explicitly study the nonlinear relaxation of magnetization and energy into the equilibrium in finite systems, it is suggestive that the results of our analysis of systematic errors are, in principle, valid for nonlinear relaxation, too.

Lastly, we note that multigrid[24] and cluster-flipping[25] techniques are becoming quite effective for the study of static critical phenomena in very large systems because of reduced critical slowing down. However, any dynamic exponent which is extracted from these is *different* than the exponent z which is determined here. We would nonetheless welcome high-resolution studies of relaxation using these methods so that further progress can be made in understanding dynamic universality.

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[1] P. C. Hohenberg and B. I. Halperin, Rev. Mod. Phys. **49**, 435 (1977).

[2] See, e.g., A. J. Liu and M. E. Fisher, Physica A **156**, 35 (1989); G. S. Pawley, R. H. Swendsen, D. J. Wallace, and K. G. Wilson, Phys. Rev. B **29**, 4030 (1984); H. W. J. Blöte, A. Compagner, J. H. Croockewit, Y. T. J. C. Fonk, J. R. Heringa, A. Hoogland, T. S. Smit, and A. L. van Willigen, Physica A **161**, 1 (1989); A. M. Ferrenberg and D. P. Landau (unpublished).

[3] C. K. Chakrabarti, H. G. Baumgärtel, and D. Stauffer, Z. Phys. B **44**, 333 (1981).

[4] M. C. Yalabik and J. D. Gunton, Phys. Rev. B **25**, 534 (1982).

[5] N. Jan, L. L. Mosley, and D. Stauffer, J. Stat. Phys. **33**, 1 (1983).

[6] C. Kalle, J. Phys. A **17**, L801 (1984).

[7] R. B. Pearson, J. L. Richardson, and D. Touissaint, Phys Rev. B **31**, 4472 (1985).

[8] R. Bausch, V. Dohm, H. K. Janssen, and R. K. P. Zia, Phys. Rev. Lett. **47**, 1837 (1981).

[9] J. K. Williams, J. Phys. A **18**, 49 (1985); S. Tang and D. P. Landau, Phys. Rev. B **36**, 567 (1987).

[10] G. Parisi and F. Rapuanu, Phys. Lett. **157B**, 301 (1985).

[11] G. Bhanot, D. Duke, and R. Salvador, Phys. Rev. B **33**, 7841 (1986).

[12] R. Abe, Prog. Theor. Phys. **39**, 947 (1986).

[13] K. Binder, D. Stauffer, and H. Müller-Krumbhaar, Phys. Rev. B **12**, 5261 (1975).

[14] R. Zwanzig and K. Aliwadi, Phys. Rev. **182**, 182 (1969).

[15] H. Müller-Krumbhaar and D. P. Landau, Phys. Rev. B **14**, 2014 (1976).

[16] See, W. W. Wood, in *Physics of Simple Liquids,* edited by H. N. V. Temperley, J. S. Rowlinson, and G. S. Rushbrooke (North-Holland, Amsterdam, 1958).

[17] M. Suzuki, Prog. Theor. Phys. **58**, 1142 (1977).

[18] Y. Y. Goldschmidt, Nucl. Phys. **B285**, 519 (1987).

[19] S. Wansleben, J. G. Zabolitzky, and C. Kalle, J. Stat. Phys. **37**, 271 (1984).

[20] J. K. Williams, J. Phys. A **18**, 1781 (1985); H. A. Ceccatto and J. A. Riera, Phys. Rev. B **34**, 4874 (1986).

[21] H. Müller-Krumbhaar and K. Binder, J. Stat. Phys. **8**, 1 (1973).

[22] M. Kikuchi and Y. Okabe, J. Phys. Soc. Jpn. **55**, 1359 (1986).

[23] S. Wansleben, Comp. Phys. Commun. **43**, 9 (1987).

[24] J. Goodman and A. D. Sokal, Phys. Rev. Lett. **56**, 1015 (1986); D. Kandel, E. Domany, D. Ron, A. Brandt, and E. Loh, Jr., *ibid.* **60**, 1591 (1988).

[25] R. H. Swendsen and J.-S. Wang, Phys. Rev. Lett. **58**, 86 (1987); U. Wolff, *ibid.* **62**, 361 (1989).