Dynamic critical exponents and sample independence times for the classical Heisenberg model

Robert G. Brown and Mikael Ciftan
Department of Physics, Duke University, Durham, North Carolina 27708-0305
(Received 16 July 1996)

The critical dynamics of the scalar order parameter autocorrelation function, the total vector spin autocorrelation function, and the energy autocorrelation function for the classical $\mathcal{O}(3)$ three-dimensional Heisenberg ferromagnet are studied both algebraically and with heat bath Monte Carlo simulations. It is shown from a group decomposition of the canonical Markov transitions used in a Monte Carlo study of this model ferromagnet that the *vector* spin autocorrelation relaxation time currently used to estimate both the dynamical critical exponent and the statistical sampling efficiency of the *scalar* order parameter (and other quantities of interest) contains an uncontrolled dependence upon irrelevant symmetric diffusion processes and is therefore unsuitable for this purpose. The central limit theorem is quantified as the fundamental basis of estimates of error and, separately, estimates of statistical sampling efficiency in importance sampling Monte Carlo simulations. A simple but interesting estimate of $z_R = d - 2\beta/\nu$ for the dynamical critical exponent of the ergodicity-restoring thermal-rotational motion of the total vector spin is presented. Various relaxation times are numerically measured and their dynamic critical exponents extracted via finite-size scaling theory to illustrate these points and compare with theoretical predictions. [S0163-1829(96)06345-X]

I. INTRODUCTION

The microscopic Hamiltonian used to study the critical dynamics of the isotropic classical $\mathcal{O}(n)$ d-dimensional Heisenberg ferromagnet (CHF) in the absence of a symmetry-breaking external field is

$$\mathcal{H} = -J \sum_{i<j}^{\text{neighbors}} \vec{S}_i \cdot \vec{S}_j + \mathcal{H}_{\text{bath}}(\{\vec{S}_i\}, T), \tag{1}$$

where the spins $\vec{S}_i$ are n-dimensional unit vectors distributed on i-labeled sites in a d-dimensional lattice. The first term describes a nearest-neighbor exchange interaction between spins and the second describes the coupling between the spin system and a generic, non-spin-conservative ''heat bath'' at temperature T. In this work only the $\mathcal{O}(n=3)$ CHF on a $d=3$ simple cubic lattice with periodic boundary conditions will be considered, although the primary algebraic results can readily be extended to other fields and models.

At the critical temperature for this model the relaxation time τ for the critical mode of the system diverges. This divergence is characterized in terms of the temperature deviation $|T-T_c|$ by the dynamical critical exponent z such that $\tau \sim |T-T_c|^{-z\nu}$ or in terms of the (also diverging) correlation length $\xi \sim |T-T_c|^{-\nu}$ of the system such that $\tau \sim \xi^z$. According to the ideas underlying finite-size scaling theory (FSST),[1] one can therefore obtain the critical exponent in terms of the numerically evaluated relaxation times $\tau(L)$ of a series of large but finite systems with characteristic size L by fitting the relation $\tau(L) \sim L^z$ (plus confluent correction terms that, one hopes, vanish as L becomes ''large'').

Alternatively, the dynamical critical exponent can be obtained algebraically by studying the order parameter autocorrelation function and determining the scaling of the longest time scale appearing in a modal decomposition of the problem. From this, the conventional (van Hove) theory of critical dynamics predicts that $z = 2 - \eta$ (Ref. 2) for ordinary ferromagnet models, but this simple theory does not include mode-mode coupling. Halperin, Hohenberg, and Ma[3] (HHM) and De Dominicis, Bre'zin, and Zinn-Justin[4] (DBZ) use the renormalization group (RG) approach to obtain z for various ferromagnetic spin models; this and other work on critical dynamics is summarized in a paper by Hohenberg and Halperin[5] (HH). From a RG calculation for the $d = 3 = 4 - \epsilon$ Heisenberg model with a nonconservative bath (HH model A), DBZ obtained (to order ϵ^2) $z = 2 + c\eta$, where $c \approx 0.7261(1 - 1.687\epsilon) \approx -0.5$ [see Eq. (69) in DBZ I or (4.39) in HH]. This result is contrasted with the conventional theory, for which $c = -1$.

It has proved remarkably difficult to test these theoretical predictions with Monte Carlo (MC) methods, at least for $\mathcal{O}(n>1)$ (continuous) models. Autocorrelation functions are time-displaced susceptibilities, that is, dynamic measures of fluctuating quantities. It is necessary to numerically obtain them to very high accuracy at T_c and for ''long'' time displacements, where the autocorrelation functions themselves are extremely small but the fluctuations summed to form them are not; convergence is extremely slow. The autocorrelation functions themselves are typically multiexponential decay functions numerically evaluated at a finite set of discrete time points; their broad, continuous decay spectrum is therefore nontrivial to analyze. Both the conventional and the RG predictions apply to the critical scaling of the *longest* (asymptotic) time scale appearing in the decay spectrum, which is exquisitely sensitive to small fluctuations in MC data being fit on a finite interval with nonlinear least squares to a multiexponential form. Very high accuracy data is therefore required just where it is expensive (in computer time) to obtain.

In addition, at the critical temperature the $\mathcal{O}(n=3)$ symmetry of the model is broken. The *vector* total spin splits into distinct components with lower symmetry; specifically the one dimensional (scalar) ''massive'' order parameter mode

 © 1996 The American Physical Society

and $n-1=2$ dimensional ''massless'' (Goldstone) modes appear.[6] Only the *magnitude* of the vector order parameter is related to the degree of order in the system. We will call this magnitude the *scalar* order parameter as it is this scalar quantity, formally conjugate to a symmetry-breaking external field, whose spontaneous appearance at T_c defines the phase transition and its critical exponents. For this reason, it is only the scalar order parameter that is evaluated or studied in Monte Carlo studies of ferromagnetism and its critical properties.

As we shall show below, the *scalar* order parameter relaxes on a very different time scale, driven by a completely different physical mechanism, than the *vector* order parameter. At a given lattice size, the asymptotic time scale of *vector* order parameter relaxation (which describes the restoration of broken symmetry) appears to be strictly larger, under the action of a local, δ-correlated relaxation mechanism, than any of the relaxation time scales of the scalar order parameter. In addition to therefore being the ''slowest'' identifiable decaying mode of a ferromagnetic system, it is also the time scale associated with the breaking and restoring of ergodicity[7] and hence by some reasonable definitions is the ''critical'' mode. It is not, however, equivalent or obviously related to the relaxation time scales of the scalar order parameter and the appearance of long-range order in the system. Further, the ordering of limits in any application of the canonical prescription supresses the vector motion and renders it irrelevant.[7] The time-displaced susceptibility studied in both the conventional approach and the RG approach respects the canonical prescription and therefore *neglects* the vector motion of the order parameter.

Although it is perfectly reasonable to expect that the time scales of vector and scalar relaxation in some way are related, there are currently no comparative theoretical studies of the two distinct motions. Yet the two motions are distinct and experimentally observable—the thermal motion of the total vector spin is the basis for ''superparamagnetism'':[8,9] the anomalous, nonlinear paramagnetic relaxation response observed experimentally in small (single-domain) isotropic ferromagnetic clusters. Only the dynamic critical exponent of the asymptotic autocorrelation time of the scalar order parameter has been theoretically predicted or extensively measured thus far, and the dynamic critical exponent of the autocorrelation of the total vector spin could in principle be different.

Not only are these dynamic critical relaxation rates and their L scaling of both intrinsic and experimental interest; they are also important for one very practical reason. The integrated autocorrelation time [see Eq. (14) and surrounding text for definition and discussion of both integrated and asymptotic autocorrelation times] has long been used as a ''sample independence time'' to correct variance-based error estimates obtained from a single-quench (internally correlated) MC data stream in a prescription first given by Müller-Krumbhaar and Binder[10] (MKB).

The only FSS MC studies of the critical dynamics of the CHF completed to date evaluated the *vector* autocorrelation function decaying under the action of a Metropolis[11] Markov process, extracted its relaxation times, and used FSST to obtain its vector dynamic critical exponent.[12,13] These vector autocorrelation relaxation times, obtained only for the Metropolis MC method, have been used as estimates of order parameter sample independence times for local MC methods in general.[14] They are very long even for modest lattice sizes; this has been a primary motivation for the application of cluster MC methods[15] to this model.[16,17]

A simple, symmetry-based argument is given below that shows that the vector autocorrelation relaxation time is not an accurate predictor of the scalar autocorrelation relaxation time and hence of the scalar order parameter sample independence time. Only the much smaller integrated scalar order parameter autocorrelation time can be used to rescale the partially sequentially correlated sample variance of (only) the scalar order parameter obtained from a single-quench importance sampling MC (ISMC) run according to the MKB prescription. However, the vector autocorrelation time is still of experimental interest in the context of superparamagnetism and related phenomena as noted above. It is also the basis for the breaking and restoration of symmetry and ergodicity in dynamic interpretations of statistical mechanics that *avoid* the ordering of limits implicit to the classical prescription[7] and hence is fundamental to the phase transition itself. Its dynamic critical exponent has not previously been theoretically estimated.

The rotational-diffusion motion of the order parameter under the action of a *local* Markov process (such as the heat bath MC process[18,19]) is analyzed theoretically below, and from this analysis a simple, random walk based estimate of $z_R=d-2\beta/\nu=\gamma/\nu=2-\eta$ is obtained for the dynamical scaling of its longest relaxation time scale. Although this exponent is identical to the conventional one for the order parameter's critical exponent, its theoretical basis is quite different and it is not clear that it would be similarly modified by the mode-mode coupling included in the superior RG prediction.

Recently, a method of evaluating sample independence times that utilizes only *static* averages obtained from many independent ISMC runs has been introduced by Kikuchi and Ito[20] (KI), who also reestablished the MKB connection of these sample independence times to integrated autocorrelation times. The KI result, like the closely related result of MKB, is directly based upon the central limit theorem (CLT) which underlies the assessment of error and assignment of confidence intervals in many statistical and experimental methodologies, including the ISMC method. The relations between the CLT, error analysis, sample independence, and method efficiency will be carefully derived below. From this derivation several obscure points in the literature will be elucidated and an obvious ISMC methodology proposed that assures *a priori* that one's error estimates are reliable. Thereby, the use of this methodology eliminates altogether the need to consider ''sample independence times'' or the ''number of independent samples'' in a given calculation for the purpose of *a posteriori* evaluation or correction of the error estimates.

Finally, to illustrate all of these points, a complete FSS heat bath ISMC study of the CHF will be presented. This study was conducted in parallel on over 100 workstations (accumulating many GFLOP months of total CPU). All error estimates are obtained from collectively statistically analyzing the averages obtained from these manifold *independent* runs using the CLT-based methods derived herein and hence

are fundamentally reliable. This degree of numerical effort was necessary to statistically resolve the autocorrelation functions to the extremely high accuracy necessary for a careful nonlinear least squares analysis of the multiexponential relaxation functions to yield sensible results for the integrated and asymptotic relaxation times.

From these times (evaluated for various $L \geqslant 5$) the integrated and asymptotic dynamical critical exponents z are extracted via FSST and compared both to theoretical predictions and to the related dynamical critical exponents obtained by FSST applied to the sample independence times themselves, independently obtained following the general ideas presented in KI and below. In all cases the agreement is entirely satisfactory and consistent with theoretical expectations, although our results are still of insufficiently high precision to be able to resolve the tiny difference between the conventional and RG predictions.

II. ISMC METHOD

ISMC methods are in widespread use in physics [see MKB or Binder and Heerman[21] (BH), especially Secs. 2.1 and 2.2, for examples and a more complete explanation of the ISMC method with references and specific examples of its application]. A canonical Markov process $P(W)$ consisting of a stochastically selected transition W_{ij} from the ith to the jth state of a model system is sequentially applied. If the forward and backward transition probabilities are in the canonical ratio

$$\frac{P(W_{ij})}{P(W_{ji})} = \exp\left(- \frac{E_j - E_i}{kT} \right), \tag{2}$$

then the repeated application of the Markov process generates a phase space trajectory that (after a transient period that ''quenches'' the system) ''ergodically'' visits the neighborhood of each point with a frequency proportional to its canonical weight. Equilibrium averages can be evaluated by sampling quantities of interest along this trajectory for a series of finite system sizes whose critical properties are then extrapolated via FSST.

The constraint (2) leaves one considerable freedom in selecting Markov processes $P(W)$. In particular, suppose $\mathcal{R}$ is a proper subgroup of the symmetry group of the Hamiltonian with very few parameters. Then the transitions in $\mathcal{R}$ (by hypothesis) generate a trivial configurational degeneracy in the system, with nonextensive associated entropy. For any transition $W \in \mathcal{W}$ (the full transition group), there exists a *coset* of transitions $\{RW\}$, $\forall R \in \mathcal{R}$, which form an *orbit* in $\mathcal{W}$. The transitions in this orbit generate spin configurations that are *statistically equivalent*. The set of all the orbits is the factor group $\mathcal{W}/\mathcal{R}$.

Since the R transitions conserve energy, the coset $\{RW\}$ satisfies condition (2) and is itself a valid Markov process for use in the ISMC method. Markov chains $RWRWRW\ldots$ [with W from any valid Markov process $P(W)$] sample the relevant features of phase space for any or all R. R becomes important only when the dynamics of thermalization are being studied, for example, when the MC method is being used to study the restoration of the ergodicity and symmetry broken at a critical point (typically $\mathcal{R}$ itself) with some *physically motivated* choice for $P(W)$ (see, for example, the review of broken ergodicity by Palmer[7]). In this latter case, $P(W)$ is typically a local, δ-correlated transition corresponding to the canonical noise term for model A discussed in, e.g., HH.

There are several distinct processes that equivalently generate a new state for any given spin from the canonical distribution of possible final states in the field of its nearest neighbors [the essential element of condition (2)] that have been used in ISMC methods, including the Metropolis transition,[11] the Glauber transition,[22] and the heat bath transition.[18,19] Since both the Glauber MC and Metropolis MC methods select new spin states by accept-reject methods, they are both fundamentally less efficient than the heat bath method of directly (always) generating a new state for problems where it can be applied.

This group factorization has significant implications in the analysis of errors in some quantity (such as the magnetization M or energy E) sampled from a given Markov chain of W. For illustrative purposes, in the following discussion and calculations the three-dimensional $\mathcal{O}(3)$-symmetric CHF on a simple cubic lattice whose Hamiltonian is given above [Eq. (1)] is used, although the results can readily be generalized.

The set of all $R \in \mathcal{O}(3)$ operations applied uniformly to all the spins in the lattice (i.e., rotating all the spins together) forms a proper subgroup $\mathcal{R}$ of energy-conserving transitions. These R exactly preserve the relative orientations of the spins and the detailed structure of the energy at each spin site. The different configurations generated by the application of distinct R are distinguished at most by three angles independent of the size of the system and hence have essentially the same free energy and entropy. To the degree that a given Markov chain can be R factored, the states that it generates cannot be counted as ''independent'' samples from the statistical point of view. This complicates error analysis in the model.

A discrete pseudodynamic time in the ISMC method (''Monte Carlo time''; see BH) is generally defined to be the suitably normalized count of the applications of the Markov process and is usually less than or equal to the sampling interval. A ''MC sweep'' is defined to be the application of a local (single spin) Markov process (which may or may not result in a transition) an average of once per spin. Alternatively the time can be counted as one or more single-cluster transitions in a nonlocal cluster method,[15] although the numerical effort associated with such a time step varies considerably from step to step. We will refer to the time units of a given ISMC methodology generically as ''Monte Carlo steps'' (MCS) below.

To obtain error estimates from a single, partially sequentially correlated thread of data, the usual practice in ISMC studies of magnetism has been to determine a ''sample independence time'' $\tau_{s,X}$ (for a given quantity X), shown in MKB and elsewhere to be equal to twice the integrated autocorrelation relaxation time of X, measured in pseudodynamic units of MCS. (In the following, $\tau_{[s,i,a],[R,M,E]}$ will be used to represent the exponential time scales of sample dependence decay, the integrated autocorrelation decay, and the asymptotic autocorrelation decay of the rotational mode, the order parameter, and the energy, respectively. The integrated and asymptotic autocorrelation times and the rota-

tional autocorrelation will be defined and discussed below.) This sample independence time is defined to be the correct interval to scale the number $\mathcal{N}$ of partially sequentially correlated samples obtained according to some sampling schedule given in MCS. It is used to obtain the number of effectively ''independent'' samples contained in the data set, which can be used, together with the measured sample variance, to construct a sample standard deviation that is a valid error estimator (see MKB, Sec. 4, or BH, Secs. 2.2.3–2.2.4 for the general argument, or Refs. 12–14, 16, and 17 for applications to the CHF). The sample independence time is generally evaluated for the order parameter, which sometimes (but not always[23]) has the slowest relaxation times. It will be derived from the CLT and discussed in detail in a later section.

In at least the case of the CHF the MKB prescription has been misapplied to determine erroneous sample independence times that, unfortunately, have been widely accepted in the literature. In addition, the use of nonoptimal sampling schedules that skip many steps between samples (to increase the effective independence of the samples accumulated) has reduced the statistical efficiency of the ISMC method in application. Finally, the common reliance on irrelevant and misleading descriptors such as ''the number of independent samples'' in a calculation makes it extremely easy to generate incorrect error estimates for quantities other than the single quantity to which that number applies, e.g., the order parameter. These statements will be proved and discussed in the following sections.

III. SYMMETRY AND SAMPLE INDEPENDENCE

Previous studies of the dynamic critical properties of the CHF have numerically evaluated the *vector* spin autocorrelation function

$$A_R(t)=\langle \mathbf{M}(0)\cdot\mathbf{M}(t)\rangle \tag{3}$$

[where $\mathbf{M}(t)=(1/L^3)\,\Sigma_i \mathbf{S}_i(t)$ is the ''vector'' order parameter and $\langle\ \rangle$ denotes a thermal average], determined its integrated autocorrelation time $\tau_{i,R}$, and used $\tau_{s,M}=2\tau_{i,R}$ as an estimate of the configurational sample independence time required to correct error estimates in ISMC CHF calculations.[12–14] In addition, the dynamic critical exponent of the relaxation time(s) associated with this autocorrelation function has been evaluated from finite-size scaling theory and compared to theoretical predictions.[12,13]

The resulting dynamical scaling law, obtained for the Metropolis ISMC method[11] applied to the CHF, has extremely long vector order parameter relaxational time scales $\tau_{i,R}$. These, in turn, have been used as the basis of estimates of sample independence times $\tau_{s,M}$ that are remarkably large (and hence poor, from the point of view of MC efficiency) for quite modest lattice sizes: e.g., according to these estimates $\tau_{s,M}\approx 1000$ MCS by $L=12$. Much larger L are necessary to successfully apply FSST to extract critical exponents, but according to this estimate local methods would become prohibitively expensive. This has been a major factor motivating the development of nonlocal (cluster) methods[15,16] in static finite-size scaling studies of the static exponents of this model conducted at much higher L.[16,17,24]

However, it is incorrect to use the relaxation times of the total vector spin to predict the sample independence time of the scalar order parameter. This is clear from the analysis presented in MKB or BH (which shows that the sample independence time that corrects error estimates for a given quantity is the integrated autocorrelation time *of that quantity*, be it the *scalar* order parameter, the energy, or any of their moments).

It might be thought that, following the canonical prescription, the vector relaxation time and scalar relaxation times are equivalent. This is not the case for relaxation driven by a Markov process that does not conserve the vector spin direction, which includes all ISMC Markov processes used to study the CHF, other isotropic vector spin $[\mathcal{O}(n)]$ models with spin dimensionality $n>1$, and still more general models with group properties that should be obvious from the following discussion. A given autocorrelation relaxation process may be *separable* with a part that depends upon $\mathcal{R}$ and a distinct part that depends only on the factor group $\mathcal{W}/\mathcal{R}$ described in the previous section. The *correct* $\tau_{s,M}$ depends on the rate of motion between orbits derived from the factor group, but $A_R(t)$ can easily be shown to decay under the action of the elements of $\mathcal{R}$ as well.

An example illustrates the general problem of using the asymptotic decay time τ_R of $A_R(t)$ (or other vector autocorrelation times) as estimates of sample independence times. Consider the ''random rotation'' heat bath transition for the CHF, $W_{\rm rand}=R_{\rm rand}W$, where $R_{\rm rand}$ is a *random* element from $\mathcal{R}$ that rotates the entire configuration and W is a heat bath transition with the usual canonical weight and sample independence time $\tau_{s,M,\rm hb}$. $W_{\rm rand}$ is a valid Markov process that satisfies condition (2). Clearly $\tau_{s,M,\rm rand}=\tau_{s,M,\rm hb}$. However, since $R_{\rm rand}$ randomly rotates the configuration (and hence **M**) between samples, $A_R(t>0)$ clearly vanishes. This specific counterexample shows that $2\tau_{i,R,\rm rand}\approx 0\neq\tau_{s,M,\rm rand}$ is an *incorrect* application of the criterion established in MKB.

As noted above, if one applies the methodology of MKB exactly as prescribed, $\tau_{s,M}=2\tau_{i,M}$ (twice the integrated autocorrelation time of the order parameter M). The scalar autocorrelation function can be evaluated numerically (with considerable effort) and its decay times extracted and used to predict sample independence times; the results of this evaluation are presented in a later section. However, it is simpler and more accurate to evaluate $\tau_{s,M}$ directly from an analysis of independent static averages by applying the CLT.

IV. CLT AND ERROR ESTIMATION IN THE ISMC METHOD

To begin with, it is worth noting that the CLT is the fundamental basis for all error estimates in the ISMC method (not to mention most statistical error estimates everywhere else). In particular, the MKB result is derived directly from it, although it is not invoked by name. It is easy to deduce directly from the CLT itself an ISMC methodology that does not require any *a posteriori* correction of sample standard deviations from tediously evaluated autocorrelation functions and their integrated autocorrelation times.

There are several advantages of this approach. It avoids the use of autocorrelation times altogether and directly yields demonstrably valid (Gaussian) error estimates from static av-

erages. It protects one from errors of the sort analyzed in the previous section, where an autocorrelation function that is certainly not *obviously* incorrect is used to determine sample independence times. It requires considerably less numerical effort than the accurate evaluation of autocorrelation times for each quantity studied in a calculation. It can, in principle, be applied to more general problems than just ISMC methods in physics. Finally, it automatically corrects for and reveals more subtle correlations than the decaying multiexponential sequential correlations produced by a δ-correlated Markov process.

This general methodology was recently described by Kikuchi and Ito[20] (KI) in application to the three-dimensional (3D) Ising model although, again, in their discussion the CLT was not explicitly invoked. The derivation and discussion below, therefore, is somewhat different and emphasizes the fundamental and direct connection of the variance of an internally correlated set of samples, whatever the nature of their internal correlation, to the variance of the corresponding number of *independent* samples deduced by directly measuring the variance of a distribution of independent sample means and applying the CLT. The emphasis is on arriving at reliable error estimates and confidence intervals without necessarily addressing sample independence times at all.

In the following few paragraphs, we will first give some definitions that will make the following discussion easier to follow. Then we will present the CLT as it is usually applied, i.e., for *a priori* independent random data. We will then discuss various ways that ISMC data might *not* be independent. Finally, we will introduce a simple ''meta'' extension of the CLT that allows *a priori* reliable error estimates to be made from a set of independent *static* ISMC runs. This final methodology turns out to be very powerful and yields useful information about the internal data dependencies of each independent ISMC run.

Let X be an arbitrary, normalized distribution with finite mean $\mu(X)$ and variance $\sigma^2(X)$. Suppose a random process can generate $\mathcal{N}$ ''independent, identically distributed'' (IID) samples $\{x_i\}=x_1,x_2,\ldots,x_\mathcal{N}$ from this distribution. This $\mathcal{N}$ sample has a sample mean of $\overline{x}=(1/\mathcal{N})\Sigma_i x_i$ and an unbiased sample variance $\sigma_x^2=[1/\mathcal{N}(\mathcal{N}-1)]\Sigma_i(x_i-\overline{x})^2$.

The CLT states that for sufficiently large $\mathcal{N}$ the *distribution of sample means* generated in this way from independent sets of IID data will be normal—$N(\mu(X),\sigma^2(X)/\mathcal{N})$—regardless of the shape of the underlying distribution.[25] The usual application of this theorem involves a single set of IID data, and in this case it is shown in virtually any book on statistics that σ_x^2 as defined above is an unbiased self-consistent estimate of $\sigma^2(X)/\mathcal{N}$.

From this result and the CLT, confidence intervals can be assigned to any given sample mean $\overline{x}$ in terms of the sample standard deviation $\sigma_x=\sqrt{\sigma_x^2}$ from integrals of the normal distribution, i.e., the error function. For example, it is roughly 96% probable that the sample mean $\overline{x}$ is within two sample standard deviations σ_x of the true mean $\mu(X)$.

The number $\mathcal{N}$ of independent samples required to cause the distribution of sample means $\overline{x}$ to become normal (within some resolution) is not determined by the CLT itself. It can be related to the size of the higher-order cumulants of the underlying distribution (see, for example, the discussion in Ma[26]). A commonly used rule of thumb is that for ''well-behaved'' distributions, $\mathcal{N}>30$ is sufficiently large for the CLT to validate error estimates based on the standard deviation.[27] This is no burden in general as one usually wishes to make $\mathcal{N}$ far larger anyway to obtain an accurate result. For this reason the CLT is more or less taken for granted and the unbiased standard deviation is commonly used for error estimates and confidence intervals of directly measured or sampled IID quantities throughout experimental and theoretical science.

For completeness it should be noted that for quantities $f(x)$ that are *not* directly sampled but are rather functionals of directly sampled quantities x (e.g., susceptibilities, cumulants), a jackknife estimate of the mean $\langle f\rangle$ and standard deviation σ_f,

$$f_i=\frac{1}{\mathcal{N}-1}\sum_{j=1}^{\mathcal{N}}(1-\delta_{ij})f(x_j), \tag{4}$$

$$\langle f\rangle=\frac{1}{\mathcal{N}}\sum_{i=1}^{\mathcal{N}} f_i, \tag{5}$$

$$\sigma_f=\sqrt{\frac{\mathcal{N}-1}{\mathcal{N}}\sum_{i=1}^{\mathcal{N}}(\langle f\rangle-f_i)^2}, \tag{6}$$

yields an equivalently useful unbiased error estimator (see, e.g., Efron[28]). In fact, the jackknife standard deviation can be used as an error estimate for *all* quantities because (a) it is algebraically equivalent to the usual standard deviation for directly sampled quantities; (b) it generally derives its validity as an unbiased error indicator from the CLT and will fail when the CLT for the underlying directly sampled quantities fails. The jackknife standard deviation does not address or ameliorate the problem of underlying data dependences; its axioms still require that the underlying directly sampled quantities be IID.

From all this it should be apparent that error estimates and confidence intervals in the ISMC method are derived from the CLT. The moment distributions for the CHF, $X=P(M),P(M^2),\ldots,P(E),P(E^2),\ldots$, are all smooth, single peaked, and have compact support for all finite lattice sizes L and temperatures T and hence have the finite mean and variance required for the CLT to hold for sample sets drawn from them. However, the numerical Markov processes that underlie ISMC methods do *not*, in general, generate independent sequential samples.

If the elements of a set of identically distributed samples, $\{x_i\}=x_1,x_2,\ldots,x_N$, are *not* independent, then their standard deviation is *not* an axiomatically valid estimator of the error in their mean. Suppose that a data set $\{x_i\}$, $i=1,\ldots,\mathcal{N}$ really contained only $\mathcal{N}_{\rm ind}<\mathcal{N}$ ''independent'' samples, where the internal sample dependences might be well hidden. A real-world ISMC calculation is fully capable of introducing a number of distinct kinds of correlation (some of which are summarized below), and so it is worthwhile to develop a methodology capable of revealing and correcting for as many of them as possible.

In ISMC methods generally, only partial configuration randomization occurs between steps and samples. Samples

(multiexponentially) approach zero covariance as the number of steps between samples is increased, and, as already shown by MKB, the integrated autocorrelation time is then an accurate scale factor that can be used to correct the associated sample variance. This diminishing sequential correlation is the only kind of internal data correlation corrected for by the MKB approach as it is generally applied.

However, there may also be occult long-time-scale nonsequential correlations, for example, full or partial periodicity. This can occur in the random number generator for certain seeds or in the more interesting relatively slow internal reversible dynamics that might appear in a Langevin model like that underlying the phenomenon of spin echos or photon echos,[29] or in HH model J. In any of these cases samples might *appear* to have reached zero covariance by virtually any autocorrelation-based measure evaluated on shorter time scales than the periods of the hidden motion, which can clearly be much longer than the intervals in which autocorrelation functions are typically evaluated, and a MKB-based correction of the sample variance might result in error estimates that are artificially small. As an explicit example of this, the reversible spin-wave-based transverse autocorrelation relaxation time obtained in HH model J is completely irrelevant to the sample independence times, since the latter derives only from *irreversible* bath interactions.

There may also be hidden dependencies or symmetries generated by group transformations like R that alter the relationship between an autocorrelation time and the sample independence time. It has already been shown above with some mathematical effort that, canonical prescription aside, vector order parameter autocorrelation times do not in general predict scalar order parameter sample independence times; it is not ''obvious'' from the MKB prescription alone that this would be the case.

Finally, one's numerical code itself can contain errors or bugs that introduce subtle correlations that defy simple categorization. For example, the random number generator may be internally correlated at the bit level even though it is not periodic. Roundoff errors may be accumulating and robbing a result of precision at a greater level than indicated by the MKB correction of the observed sample variance. A programming error may cause, e.g., an internal array boundary to be infrequently overwritten. These kinds of errors are extremely subtle as one's code may ''work'' just fine and produce numbers that are close to the correct results and quite reasonable at a glance. The results can even produce reasonable theoretical fits if the confidence intervals around each point are large enough. Usually, though, the results obtained from flawed methodology are ultimately quite incompatible with predicted theoretical forms when accurate confidence intervals are obtained that are small enough to reveal the problem. In this case the problem is not just being able to correct for occult correlation; one also needs high-resolution results capable of demonstrating the method errors when a fit is attempted to an assumed theoretical form.

It can be difficult to recover a meaningful estimate of the error in the mean of a single set of data $\{x_i\}$ under any of these sets of circumstances. The methodology of MKB is designed to yield a correct error estimate only if the correlations are the decaying sequential correlations produced by the Markov process itself. However, it requires the tedious evaluation of the integrated autocorrelation time of each quantity studied and can easily be misapplied. The CLT itself, however, suggests a simpler method that will nearly always lead to axiomatically reliable error estimates in an ISMC calculation. These reliable, Gaussian error estimates, in a high-resolution calculation, give one at least a chance of discovering many subtle errors in methodology that would otherwise be hidden.

When the MKB result was derived, most computing was done on large mainframe computers in a time-sharing environment. Computer time was ''expensive'' and access limited, as is still the case in many supercomputing centers. The computers themselves were sufficiently slow that it was always difficult to study large enough L to be able to eliminate or correct for finite-size effects in order to extract critical exponents. In this environment, it was natural to perform single, monolithic ISMC calculations from a single quench, and rely on sampling and accumulating data from this single ''run.'' All error estimates had to be performed on this one data set, which was *a priori* contaminated with sequential correlation. Under these circumstances, the MKB approach was necessarily near optimal, since measuring autocorrelation times and applying dynamical scaling laws produced the best possible error estimates in most cases.

Now, however, most computing is done on small, inexpensive workstations, each of which is considerably more powerful than those original mainframes. Many of these workstations can be simultaneously accessed over a network, and it is a simple matter to perform calculations in parallel upon them. In this sort of environment, the CPU ''cost'' of a quench on any given machine becomes much less important. One can routinely perform multiple ISMC calculations with the same parameters, each with its own *independent* quench from isotropic initial conditions using a unique, randomly chosen, random number seed to begin the calculation. This allows reliable error estimates to be trivially obtained directly from the CLT.

The methodology (described in the context of a CHF ISMC calculation) is as follows: First, let us modify the notation previously introduced so that i *internally* indexes the samples produced by a Markov process in the jth independent calculation. Each j-indexed ''thread'' of the calculation produces a set of data $\{x_{ij}\}$ and is assumed to have been begun from unbiased initial conditions with a unique random number seed. Consequently, the i-averaged moments of each thread [e.g., $\overline{x_j}=(1/\mathcal{N})\Sigma_i x_{ij}$] are themselves j-IID samples generated from a random process that satisfies the axioms of the CLT. The CLT and the standard tools of statistical error analysis can thus be applied to the distribution of j-indexed, i-averaged moments *regardless* of the degree or nature of internal correlation in each thread, provided only that all distinguishing parameters (e.g., the random number seed and the random number generator itself) are sufficiently ''random.''

Practically speaking, then, one generates $\mathcal{M}=j_{\max}$ threads, each containing $\mathcal{N}=i_{\max}$ (not necessarily independent) samples x_{ij} for $x=E,E^2,\ldots$ or $M,M^2,\ldots$. From these data form the i mean $\overline{x_j}=(1/\mathcal{N})\Sigma_i x_{ij}$. It is recommended that $\mathcal{N}\gg 30\tau_{s,x}$ (where $\tau_{s,x}$ is self-consistently determined) so that the $\overline{x_j}$ themselves will be approximately normally distributed. The mean of all the data,

$\overline{x}=(1/\mathcal{M})\Sigma_j \overline{x_j}=(1/\mathcal{M}\mathcal{N})\Sigma_{i,j}x_{ij}$, is the best estimate for the true mean of X. The standard deviation of the distribution of j-indexed sample means $\overline{x_j}$,

$$\sigma_x=\left(\frac{1}{\mathcal{M}(\mathcal{M}-1)}\sum_j (\overline{x_j}-\overline{x})^2\right)^{1/2},$$

is the optimal unbiased estimate of the error in $\overline{x}$ that in no way relies on a knowledge of the autocorrelation times and can equally well be applied to static averages and averages of dynamic quantities (like the autocorrelation functions themselves). Clearly this methodology can be applied to more general mathematical and statistical problems than just the ISMC method in physics; any time one can isolate and randomize a single random variable that makes distinct internally correlated sample sets themselves IID, applying statistics at that level will result in reliable error estimates.

These error estimates (the standard deviations) contain useful information concerning the *internal* sample independence of the partially correlated $\{x_i\}$ threads of data. The CLT states that $\sigma^2_{x,\mathcal{N}}$ (the numerically evaluated variance of the distribution of the $\mathcal{N}$ sample means $\overline{x_j}$) is equal to $\sigma^2(x)/\mathcal{N}_{\rm ind}$, where $\sigma^2(x)=\overline{x^2}-\overline{x}^2$ is the variance of the random process X (numerically estimated from all the x_{ij} and the x_{ij}^2 data). This effectively defines $\mathcal{N}_{\rm ind}$ in a correlated sequence of data. From this one can quantify the degree of internal sample dependence in each thread. The ratio

$$F=\frac{1}{\mathcal{N}}\left(\frac{\sigma^2(x)}{\sigma^2_{x,\mathcal{N}}}\right)=\frac{\mathcal{N}_{\rm ind}}{\mathcal{N}} \tag{7}$$

is the average ''fractional independence'' of each sample x_i in a thread or the inverse of the number of sequential x_i that must be collected and averaged to create precisely one IID sample as far as collective CLT scaling of the sample standard deviation is concerned (a quantity clearly closely connected to the sample independence time $\tau_{s,X}$). Note as well that F is well defined and the error estimates are accurate whether or not the hidden correlation involved is periodic, multiexponential, or even quasiperiodic (associated with Poincaré cycles, for example, that repeatedly visit the same neighborhood of configuration and phase space without returning to the same point) provided only that $\mathcal{M}$ and $\mathcal{N}$ are large enough.

KI effectively worked the algebraic result of MKB backwards from this result (which they also obtained, but without explicit reference to the CLT) to reconnect the sample independence time of a quantity (the inverse of the fractional independence measured for that quantity, given a sampling interval of unity in MCS and a multiexponential decay process) to the integrated autocorrelation time for that quantity. However, as one can already see, F is an interesting quantity in its own right and deserves further examination.

One can freely choose a sampling interval in a given ISMC calculation. If one samples after an interval of $\Delta t \gtrsim \tau_{s,X} \gg 1$ MCS, one will clearly increase the independence of the samples of X. However, doing so will usually significantly *decrease* the accuracy of the results obtained for a given investment in computer time as we will now show. F is itself a *function* of the sampling interval Δt. As might be expected, it exponentially approaches 1 as $\Delta t \to \infty$ and samples become uncorrelated (see Fig. 3 below). This exponential defines the sample independence time $\tau_{s,X}$ for the quantity X. Since $\tau_{s,X} \gg 1$ for most cases of interest, $\tau_{s,X}=F(1)^{-1}$ to an acceptable degree of precision.

Knowledge of the form of $F(\Delta t)$ permits the definition and analysis of the *sampling efficiency* and the closely related definition of *numerical efficiency*. The latter is the quantity that must be optimized by one's sampling schedule. The sampling efficiency $\epsilon_{\rm samp}$ is just the fractional independence obtained per sample, divided by the number of MCS required to generate the sample. It is clearly optimized (maximized) by selecting the shortest possible sampling interval. If sampling were ''free'' (required neglible CPU time compared to the time to make an MCS in the first place) it would thus be most efficient numerically to sample every MCS or even more often (if it were truly free one would sample after every local single-spin transition). In practice, sampling costs are smaller than the cost of an MCS but not quite negligible; they generally require some fixed fraction <1 of the numerical effort required to make a MCS. This fraction must thus be added to the numerical effort required to generate a sample to define the numerical efficiency $\epsilon_{\rm num}$. Thus

$$\epsilon_{\rm samp}(\Delta t)=\frac{F(\Delta t)}{\Delta t}\approx\frac{1}{\Delta t}(1-e^{-\Delta t/\tau_{s,x}}), \tag{8a}$$

$$\epsilon_{\rm num}(\Delta t)=\frac{F(\Delta t)}{(\Delta t+\delta t)}\approx\frac{1}{(\Delta t+\delta t)}(1-e^{-\Delta t/\tau_{s,x}}), \tag{8b}$$

where δt is the MCS-scaled numerical effort required to actually tally a sample. For $\delta t \approx 0.2$ MCS (a reasonable figure according to our profiling measurements) a numerically optimal sampling schedule can be anything from $\Delta t=1$ to 20 MCS for $\tau_s=10$–500. A typical efficiency curve for $\delta t=0.2$, $\tau_s=19.2$ is shown in Fig. 1. This can readily be compared to Fig. 3 in the numerical results section below.

From this figure it should be clear that the common practice of discarding the partially correlated data in $\Delta t \approx \tau_{s,x}$ steps between samples of a quantity x (see Sec. 2.2.4 or pp. 100–101 in BH) to make sequential samples ''independent'' does not take into account the actual cost of sampling and fails to optimize either the sampling or the numerical efficiency. For the ranges of values most often encountered in ISMC calculations, sampling every $\tau_{s,x}$ steps yields only 60%–80% of the optimum number of independent samples for a given investment in computer time and hence wastes roughly 10%–30% of the achievable relative accuracy.

On the basis of these results it is possible to examine in some detail the relationship between the oft-quoted ''number of independent samples'' in a given ISMC calculation and its relative accuracy. It can be seen that the number of independent samples in a given data set is strictly determined by the CLT scaling of the variance of the distribution of (possibly internally correlated but externally IID) sample means of similarly prepared data sets. It is also seen that if one evaluates many independent threads of data to obtain the standard deviation of the distribution of thread sample means, it is not necessary to know the number of independent samples at all in order to calculate accurate confidence intervals; rather one

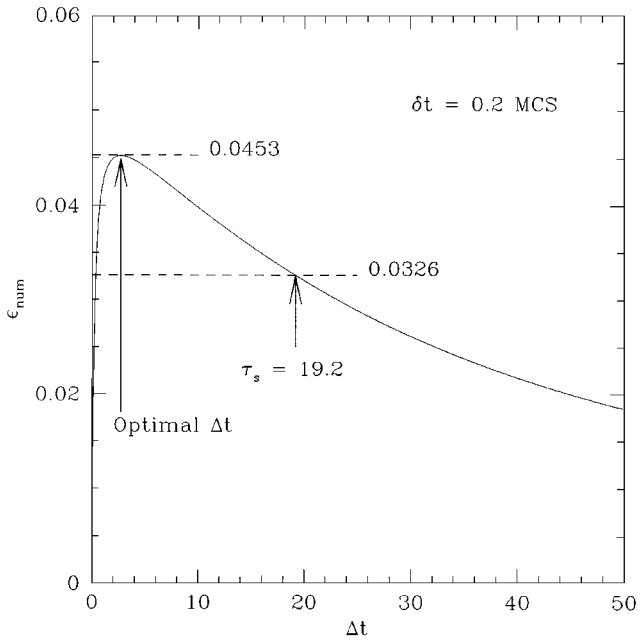

FIG. 1. The numerical efficiency plotted as a function of sampling interval for $\delta t = 0.2$, $\tau_s = 19.2$ (in units of MCS), typical of energy sampling at $L = 12$ (see Fig. 3). Sampling once every $\Delta t = \tau_s = 19.2$ MCS costs approximately 28% of the numerical accuracy achievable by sampling every $\Delta t = 2$ or 3 MCS.

can work backwards and obtain the number of independent samples from the *a priori* reliable variance of the distribution of sample means.

However, it is clear that there is no advantage to be gained from backtracking in this way to obtain the number of independent samples. The ''number of independent samples'' in a given ISMC calculation is, by itself, a useless and misleading indicator of the overall precision obtained in a given calculation. This can be seen from the following observations.

First, when the number of independent samples (and, implicitly, the confidence intervals around measured points) is evaluated from autocorrelation times it is easy to get the wrong result. This can occur because one is using the wrong autocorrelation function, as shown in the previous section. It can also occur because it is relatively difficult to evaluate accurate autocorrelation functions at all, especially at large L; one typically needs to numerically evaluate an extremely large number of independent sets of sequentially correlated samples and average their sequential autocorrelation decay functions. At large L it can easily require GFLOP-months of numerical effort to get 10% relative accuracy in integrated autocorrelation times. Even if one parallelizes this evaluation process with a calculation of static averages, the evaluation of autocorrelation can increase the numerical work required for the static calculation alone many fold at the considerable expense of accuracy.

Second, the average energy (per spin) and the order parameter, and all the moments of these quantities, as distinct x with their own distributions and internal properties, typically have *different, method-dependent sample independence times* for any given lattice size L. Therefore, a given number of sequential MCS produced by an ISMC method typically contains different numbers of ''independent'' energy E samples, ''independent'' order parameter M samples, and ''independent'' moment (M^2, E^2, etc.) samples. Either one (the number of M samples or the number of E samples) can be the larger quantity and there can even be L-dependent crossovers. It is not possible to relate the number of independent energy samples to the number of independent order parameter samples by any simple rule that will work for all ISMC methodologies, and there is little point in developing such a rule for individual ones. Using the number of independent order parameter samples to generate an MKB-corrected error estimate (the sample standard deviation) for the energy from its measured single-thread sample variance will, in general, result in a significant overestimate or underestimate of its true, unbiased expected error.

Descriptions of confidence interval estimation methodology in the ISMC literature are rarely complete enough to be able to tell whether or not this error has been made (or not made) in any particular paper, but, given the frequency with which the ''number of independent samples'' is quoted as a number with some universal validity, it seems likely that it has occurred more than once.

Even when the number of independent samples *is* quoted appropriately and used in the correct context (the number of independent M samples is quoted when discussing errors in M only, for example) it is still misleading. The error estimate or confidence interval for any *single* quantity depends, according to the CLT, *both* on the number of independent samples *and* on the intrinsic variance of the quantity. *Both* of these scale with L, and so citing one without the other (and L) is not useful. To be concrete, millions of independent samples from an $L = 4$ lattice can easily produce larger absolute or relative errors for some quantity than tens of thousands of independent samples of the same quantity from an $L = 32$ lattice. At best, this number can be used only to compare the relative accuracy of two calculations of the same quantity, at the same value of L. This comparison is surely better made between the achieved confidence intervals themselves.

The autocorrelation times themselves, of course, are quantities with independent interest in cases with a ''physical'' model for the thermalizing Markov process and in this case it is useful to evaluate them even if they are not to be used as estimators of sample independence. Theories of dynamical scaling and critical slowing down make concrete predictions for the dynamical critical exponents of at least some autocorrelation times. It is here that the work of MKB and KI relating sample independence times to integrated autocorrelation times, $\tau_{s,x} = 2\tau_{i,x}$, becomes most valuable.

V. AUTOCORRELATION TIMES AND THE DYNAMIC CRITICAL EXPONENTS

The $\tau_{s,x}$ extracted from the direct (CLT) measurements of ISMC statistical efficiency can be numerically compared to various (integrated) vector and scalar autocorrelation times to verify the conclusions of the group theoretical analysis above. The total vector spin autocorrelation function is

$$A_T(t) = \left\langle \frac{1}{L^3} \sum_i \left[\mathbf{S}_i(0) \cdot \mathbf{S}_i(t) \right] \right\rangle . \tag{9}$$

$A_R(t)$ (its asymptotic form) is already defined above, where we note that $\mathbf{M}(0)\cdot\mathbf{M}(t)$ is just the instantaneous projection of the vector order parameter, rotated by the canonical Markov process through some angle, on its original direction. For that reason we call $A_R(t)$ the *rotational* autocorrelation[23] although length fluctuations in $\mathbf{M}$ also modify the decay at short times.

It is expected that all vector-based MC autocorrelation functions like $A_T(t)$ and $A_R(t)$ will depend strongly on the uncontrolled R factor in their Markov process $P(W)$ and are therefore unreliable indicators of order parameter sample independence. However, the energy autocorrelation

$$A_E(t)=\langle E(0)E(t)\rangle-\langle E\rangle^2 \tag{10}$$

is invariant under the action of $R\in\mathcal{R}$ by definition. The *scalar* order parameter autocorrelation (or the time-dependent order parameter covariance)

$$A_M(t)=\langle M(0)M(t)\rangle-\langle M(0)\rangle\langle M(t)\rangle \tag{11}$$

[where $M(t)=|\mathbf{M}(t)|$] is also invariant with respect to the action of members of $\mathcal{R}$. $M(0)$ and $M(t)$, as samples of the order parameter length, are independent when their (average) covariance vanishes. These are therefore valid quantities to study from the point of view described in MKB and BH, and their integrated autocorrelation times (defined next) are related by KI to the sample independence time $F(1)^{-1}$ obtained above from the CLT.

In general all of the autocorrelation functions considered above are multiexponential, with a continuous spectrum of characteristic relaxation timescales, e.g.,

$$A_X(t)=\int_0^\infty \hat{A}(\tau^{-1})e^{-t/\tau}d(\tau^{-1}) \tag{12}$$

(for $X=M,E,R$). They can often be acceptably fit in MC studies (via nonlinear least squares methods) with a discrete sum of exponentials:

$$A_X(t)\approx\sum_i A_{i,X}e^{-t/\tau_i}, \tag{13}$$

where care must be exercised to ensure that the fit is not poor as a result of using too few basis functions or ill conditioned by too many basis functions for the precision or amount of the data obtained (as unambiguously signaled by a divergent covariance matrix). This fit is also limited and complicated by the fact that data are usually only available at certain discrete times (i.e., at MCS) that can be commensurate with the smallest τ_i.

This multiexponential behavior complicates the numerical extraction of a uniquely defined time constant, e.g., τ_M, to study scaling with. Two time constants that are uniquely specifiable for all such decay functions are the *asymptotic* time scale $\tau_{a,M}$ (the exponential time constant of the slowest decay mode) and the *integrated* time scale

$$\tau_{i,M}=\int_0^\infty A_M(t)dt\approx\sum_j A_M(t_j)(t_j-t_{j-1})\approx\sum_i A_{i,M}\tau_i. \tag{14}$$

The first sum approximates the integral via the rectangle rule on (e.g.) discrete MC steps and the second is the formal integral of the multiexponential fit (13). The rectangle rule may not be a good approximation to the continuous integral unless the time constants $\tau_i\gg 1$, a condition that is not always met.

At the critical temperature the relaxation time scale of the order parameter diverges. This divergence is characterized in terms of the correlation length ξ of an infinite system or in terms of the size L of a finite system by the dynamic critical exponent z_M such that $\tau_M\sim\xi^{z_M}\sim L^{z_M}$.[1] This finite-size-scaling form is convenient for defining (possibly different) dynamic critical exponents for the other diverging time scales studied, with the notation $\tau_E\sim L^{z_E}$ and $\tau_R\sim L^{z_R}$.

We take care to distinguish between energy exponents and order parameter exponents, and further between integrated and asymptotic exponents because ''the'' critical exponent z_M for the model is only derived for the asymptotic time constant (the slowest mode) of the order parameter. There is (to our knowledge) no comparable theoretical result for z_E describing the critical slowing down of energy fluctuations or energy autocorrelation decay. Nor is there a proof that the integrated and asymptotic times (which are certainly different quantities) necessarily diverge with the same exponent. We therefore distinguish them notationally as $z_{i,M}$ and $z_{a,M}$; similar notation indicates which time constants are being studied. Unfortunately, only the *integrated* time constants are accessible from the CLT-based static approach, although the difference in the z's thus obtained does not exceed the error in this calculation (see Fig. 3 below). This point seems to have been missed in KI, and complicates the direct comparison of CLT-derived exponents to the predictions of theory.

Although the integrated and asymptotic time constants themselves can be quite close, they are generally different, with the asymptotic constant strictly greater than the integrated constant, for multiexponential decay functions like Eq. (13). Although the order parameter autocorrelation decay for the CHF often appears to the eye (or even to a fitting routine if the data is not sufficiently precise) to be single exponential (see, e.g., Fig. 2 below), this can be misleading. At the very high precision obtained in this study, the best single-exponential fit of the $A_M(t)$ data for $L=12$ has a χ^2 of 430, compared to $\chi^2=5$ for a well-conditioned, well-separated, two-exponential fit. This two-exponential fit yields $\tau_{a,M}=19.1\pm 1.9>\tau_{i,M}=18.3\pm 1.8$. Note that although these time constants are within each other's mutual error bars, they cannot be equal.

It could well be that the relative difference between $\tau_{i,M}(L)$ and $\tau_{a,M}(L)$ vanishes for sufficiently large L [that is, $\lim_{L\to\infty}\tau_{i,M}(L)=\tau_{a,M}(L)$]. In this case, the difference would amount to an additional finite-size correction and both forms would eventually have the same dynamic critical exponent. However, in the absence of a proof that this is the case, the difference (built of the faster, short-range decay terms) might equally well scale in such a way that both decay times could have different dynamic critical exponents. This ambiguity is something that will have to be carefully investigated before adopting the KI, CLT-based prescription for obtaining high-precision dynamic critical exponents for comparison to theoretical predictions.

There seem to be no theoretical predictions for the dynamic critical scaling of τ_R or τ_E (in any form). Nevertheless, both diverge at T_c with an exponent, and together describe the dynamic breaking of $\mathcal{O}(3)$ symmetry and energy ergodicity at the critical point, which is at least as interesting as the relaxation (or sample independence) of the scalar order parameter itself. A particular question of physical interest is, which process experiences the greatest critical slowing down? That is, does $\mathcal{O}(3)$ symmetry break ''faster'' than energy ergodicity disappears or than the order parameter length relaxes? Which dynamic critical exponents are the largest, or are they all equal?

As a first step toward answering these questions, we offer the following estimate for a scaling relation that might be satisfied by the asymptotic rotational autocorrelation exponent.

VI. ROTATIONAL DYNAMICAL CRITICAL EXPONENT

As noted above, both $A_T(t)$ and its asymptotic form $A_R(t)$ depend strongly upon the R components of the thermalizing transitions W.[24] For the W used in ''heat bath'' ISMC,[18,19] the R components are small but strictly greater than zero and cause the thermal rotational diffusion of the *direction* of the vector order parameter, a process that is completely supressed in the canonical prescription by the ordering of limits.[7] This ergodicity-restoring motion dominates the long-time behavior of $A_R(t)$ and hence $A_T(t)$ and can be physically understood.

Each spin has instantaneous components that lie parallel to ($||$) and transverse to ($\perp$) the total spin of the system $\mathbf{S}_T$. At T_c, $|\mathbf{S}_T| \sim NM(L) \sim L^d L^{-\beta/\nu} \gg 0$ from finite-size scaling theory. The single-spin heat bath transition (or other related Markov processes) produces microscopic fluctuations of $\mathbf{S}_T$, $\delta\mathbf{S} = \delta\mathbf{S}_{||} + \delta\mathbf{S}_{\perp}$.

At equilibrium, the $\delta\mathbf{S}_{||}$ leave $|\mathbf{S}_T|$ unchanged on the average ($\langle \delta\mathbf{S}_{||} \rangle = 0$) and drive the relaxation of $A_M(t)$. These fluctuations produce the ''massive'' part of the susceptibility. The transverse fluctuations $\delta\mathbf{S}_{\perp}$ are azimuthally distributed approximately uniformly with respect to the direction of the instantaneous $\mathbf{S}_T$. These (Goldstone) fluctuations are ''massless'' and are responsible for the slow restoration of the broken $\mathcal{O}(3)$ symmetry. At all $T > 0$, $\delta S_{\perp} = \sqrt{\langle \delta\mathbf{S}_{\perp} \cdot \delta\mathbf{S}_{\perp} \rangle} > 0$. $\delta S_{\perp,c}$ is defined to be its magnitude at T_c.

In the absence of a confining field and presence of a local thermalizing Markov process, the vector order parameter of continuous $\mathcal{O}(n>1)$ models (and real single-domain ferromagnets) will therefore wander about randomly in direction via small rotations while fluctuating longitudinally about its mean length. This quasicontinuous thermal-rotational behavior *disappears* for $n=1$ Ising models which have no continuous transverse subspace to support a random-walk–diffusion process with no free energy cost.

The critical exponent of τ_R can be estimated by analyzing this motion as a random walk with the assumption that the azimuthal direction of each transverse step $\delta S_{\perp,c}$ is uniformly randomly distributed. Thus $\langle \hat{\mathbf{x}}(0) \cdot \hat{\mathbf{x}}(t) \rangle = \exp(-\Delta\theta^2 t/2)$ for a random walk of a unit three-vector $\hat{\mathbf{x}}$ consisting of t azimuthally random rotations through the constant angle $\Delta\theta \ll \pi$ (a relation that was carefully tested). Note that this assumption of azimuthal randomness is only approximately correct as natural clustering in the overall spin distribution can create second-order correlations in the direction distribution of distinct transverse steps. This might give rise to renormalization corrections to the simple estimate below.

We approximate $\Delta\theta \approx \delta S_{\perp,c}/|\mathbf{S}_T|$ so that

$$\tau_{\text{microscopic}} = \frac{2L^{2d-2\beta/\nu}}{(\delta S_{\perp,c})^2}, \tag{15}$$

where τ is measured in the number of microscopic fluctuations (random walk steps). Converting to macroscopic time units measured in ''MC sweeps'' (MCS, defined to be $N = L^d$ fluctuations or heat bath ''moves''):

$$\tau_R = \tau_{\text{microscopic}}/L^d \sim L^{d-2\beta/\nu}. \tag{16}$$

We conclude that $z_R \approx d - 2\beta/\nu = \gamma/\nu = 2 - \eta$. This crude estimate is thus identical to the van Hove estimate and is slightly smaller than the renormalization estimate.

Although simple, this argument illuminates the fundamental mechanism underlying the breaking and restoration of symmetry and ergodicity at the critical point of systems with a trivial continuous symmetry group. The L scaling of a random walk, the order parameter length, and the system volume all contribute in distinct ways. The connection of this process to the appearance and properties of Goldstone modes at and below T_c is an interesting topic of future research.

Along this line it is useful to note that in the ferromagnetic phase the argument above [modified only by the scaling of $|\mathbf{S}_T| \sim NM(L) \sim L^d$] yields $\tau_R \sim L^d \sim N$, that is, the ergodicity-restoring time scales (only) extensively. The ergodicity and symmetry broken by the phase transition is restored remarkably rapidly even below T_c for continuous models like the pure CHF. For comparison, the ergodicity-restoring time for the $\mathcal{O}(1)$ (Ising) model below T_c scales like $\tau_I \sim \exp(aL^{(d-1)/d})$.[7] The difference is due to the existence of a free energy barrier that scales like $L^{(d-1)/d}$ between the discrete symmetry-degenerate components of the Ising model, versus *no* free energy barrier between the continuous symmetry-degenerate components of the CHF. This is physically significant: The (relatively) rapid rotational spin-diffusion process analyzed above has been experimentally observed in small (single-domain) ferromagnetic clusters,[8,9] where ergodicity-restoring ''orientation fluctuations'' are overcome by an applied external field to cause ''superparamagnetic relaxation'' of the magnetic-phase clusters.

VII. NUMERICAL RESULTS

A. Methods

The calculations presented below were run over many months in the background on a 2+ GFLOP virtual parallel supercomputer consisting of more than 100 110-MHz (Sun) Sparcstation 5 workstations (in simultaneous use as student computing cluster workstations) as well as another 20–30 older model Sun Sparc machines. The jobs were managed with EXPECT scripts[30] and required no special privileges and almost no network bandwidth to support. Using this tremendous ''invisible'' computing resource, extremely-high-precision results were obtained, both for the autocorrelation

functions and dynamic scaling reported herein and for static averages reported elsewhere.[24]

The sole negative aspects of this scavenging of the vast quantities of otherwise wasted CPU present in this (or any similar) public cluster environment were that (a) the Solaris 2.3 scheduler in use on these machines was (and still is) extremely poorly configured—consequently the background job negatively affected the foreground usage and response time of the cluster machines even when maximally ''niced''; (b) even though the cluster machines had 64 MB of main memory, the memory demands of the Sun 24-bit X server and its clients and the need to reserve a reasonable amount of system memory for use by the primary users of the clusters (the students) limited somewhat the size of the systems studied. Even working to avoid this limitation, the cluster systems occasionally ran out of real memory and started to page and swap.

The impact of these two problems was that interactive response on the Sparcstation 5 cluster machines running the simulation (or anything else) in the background was sometimes considerably worse than that observed on the older SunOS 4.1.3 Sun Sparc machines, in spite of their being more than 2.5 times as fast and possessing more than twice as much main memory. The problem with the scheduler has presumably been repaired in Solaris 2.4 and Solaris 2.5; however, we will be unable to verify this until an OS upgrade takes place on the cluster machines. In a properly configured public cluster environment (or a public cluster environment running an operating system with a more robust and functional scheduler), though, the negative impact of this sort of background usage should be almost nonexistent. We are currently working to build a distributed parallel supercomputer-workstation environment to augment the existing cluster resource.

Using this computing resource, an extensive heat bath[18,19] ISMC study of the CHF was performed on a simple cubic lattice to directly measure the $A_T(t)$, $A_R(t)$, $A_M(t)$, and $A_E(t)$ as given above, in time units of MCS, for lattices with $L=6,7,8,12,16,24,20,32$ at $T_c \approx 1.4427 \pm 0.0002 \approx 1/\ln(2)$.[24,14,16,17]

This was done for each set of parameters (e.g., L, T, etc.) by initiating a calculation on a CPU from this pool of workstations with its own, random and unique random number seed. The spins were initialized in a high-T (random) state, and the lattice was then quenched to equilibrium by applying the heat bath to all spins in the lattice sequentially (1 MCS) for at least 20 sample independence times in MCS. That the state reached was indeed equilibrium was verified by comparing the states thus obtained to those obtained from similar quenches from low-T initial conditions.

A reference copy of the quenched lattice was then saved. Autocorrelation functions relative to this reference copy were then evaluated and accumulated for each time displacement in MCS in an interval of 25–250 MCS. The reference lattice was then replaced with the current state of the lattice and the process iterated until a finite number of (not necessarily independent) ''samples'' of the autocorrelation function was obtained. This number (which is not important) ranged from at least 100 (at $L=32$) to several million for the smaller lattice sizes. The accumulators were then averaged over this interval, the resulting autocorrelation functions written to disk, and the calculation terminated. Static averages were simultaneously and similarly obtained for the first four moments of E and M accumulated each MCS. The ''internal'' variances of these averages were *not* evaluated at all as the samples that were averaged were not independent.

This entire process was then replicated from hundreds to thousands of times on CPU's selected from the pool, producing hundreds to thousands of *independent* samples of the average autocorrelation functions and static moments. These independent samples were themselves averaged (as described above) and their unbiased sample standard deviation obtained and used as the basis of all further statistical analysis.

The autocorrelations functions themselves were then analyzed with nonlinear least squares fits to various multiple exponential forms. Considerable effort was expended to make these fits robust. A fit was considered acceptable when it (a) had a well-conditioned covariance matrix, (b) produced a ''reasonable'' (and minimum) value for χ^2, given the number of points being fit, and (c) used as many exponential functions as possible, given the first two constraints. In cases where there was any remaining ambiguity in the fit (such as near degeneracy in some of the shorter time scales) we focused on accurately obtaining the asymptotic decay time (the most interesting from a theoretical point of view) at the modest expense of overall χ^2.

It was empirically determined early on that there was very little advantage to be obtained from reinitializing the reference lattice and accumulating long intervals (many times the longest observed decay time constant) at the expense of the number of intervals accumulated. In one case both the lengths of the regions fit and the errors on each point fit were large; in the other the length was much smaller but so were the errors. In test cases where equal amounts of CPU were used each way, the overall accuracy of the time constants obtained was not significantly enhanced either way, even when the time constants were much larger than the interval being fit.

On the other hand, $L=4$ lattices were evaluated but excluded from the fits due to unacceptable finite-size deviations from scaling and the difficulty of accurately fitting multiple exponential functions with time constants less than or the order of one MCS (the grid size). These small time constant components decay so rapidly that they are not greatly constrained by the particular value of the autocorrelation functions at displacements of a few MCS, while the effect of statistical noise is significantly enhanced.

The autocorrelation times thus extracted are compared to independent, statically measured sample independence times for M and for E. These static sample independence times were determined by comparing the CLT-validated sample standard deviation for E and M to their variances, which were explicitly evaluated from the accurately known values of $\langle E \text{ or } M \rangle$ and $\langle E^2 \text{ or } M^2 \rangle$, respectively.

It was immediately observed that the sample independence times, which are directly related to the integrated autocorrelation times for the given quantity, were much easier to obtain accurately even for the largest lattices. The error was also much easier to numerically control. Unfortunately, as discussed above, it is by no means clear that integrated autocorrelation times should be expected to scale with the same dynamical critical exponent(s) predicted in the litera-

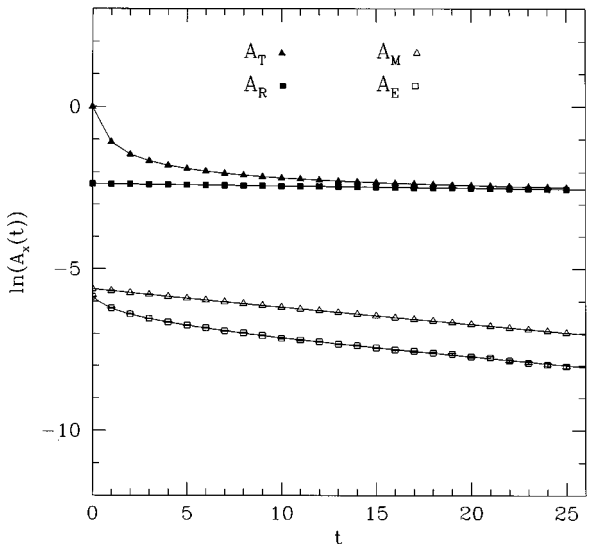

FIG. 2. $A_T(t)$, $A_R(t)$, $A_M(t)$, and $A_E(t)$ for the $L=12$ lattice. The drawn lines are the best nonlinear least squares fits obtained for each curve.

ture, especially for smaller lattice sizes where short-time–short-range interactions make large contributions to the integrated autocorrelation times.

B. Autocorrelation times

The autocorrelation functions $A_T(t)$, $A_R(t)$, $A_M(t)$, and $A_E(t)$ were evaluated in time units of MCS for an $L=12$ lattice and are presented in Fig. 2. The error bars are the standard deviations of sample means from 865 independent MC calculations (threads), each containing 500 000 MCS. The lines through the data are from nonlinear least squares fits used to robustly extract the relaxation times for each autocorrelation function. Two exponentials were fit to A_R, A_M, and A_E and five exponentials were fit to A_T. The resulting fits were in each case very well conditioned because of the extremely high precision of our data (the error bars at most of the points are smaller than the width of the drawn lines). The integrated autocorrelation times thus obtained are $\tau_{i,T}=15\pm1$, $\tau_{i,R}=146\pm2$, $\tau_{i,M}=18\pm1$, and $\tau_{i,E}=9\pm1$.

The variances of the distributions of sample means of M and E were separately evaluated and analyzed to form estimates of F, ϵ, and $\tau_{s,(M,E)}$ for these quantities as described above. Sampling periods of $\Delta t=1,4,10,20,40$ MCS were studied. At least $\mathcal{M}=100$ completely independent (separate quench) threads, each with $\mathcal{N}=100\,000$ samples, were generated for each sampling period. Each thread's sample mean thus contains (self-consistently) from 140 to 80 000 *independent* samples. The CLT is therefore expected to hold for these distributions of sample means and empirically the distributions of sample means were indeed approximately normal.

Figure 3 shows the results. The drawn lines are fits to the form $F(\Delta t)=1-\exp(-\Delta t/\tau_s)$ (in percent) and $\epsilon(\Delta t)=F(\Delta t)/\Delta t$, respectively. For the energy E, $\tau_{s,E}\approx19.2\pm1$ MCS and for the order parameter M, $\tau_{s,M}\approx34.2\pm4$ MCS. These numbers are in good agreement with the CLT-based

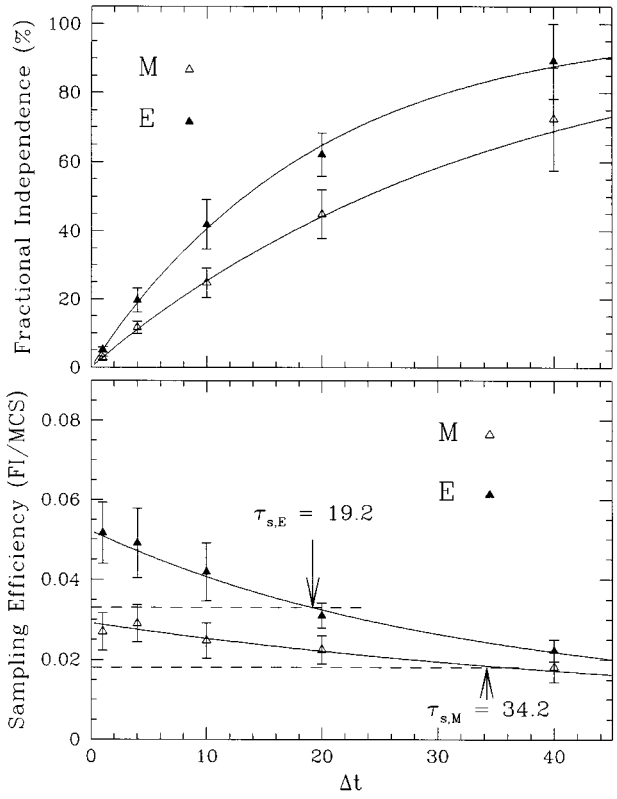

FIG. 3. The fractional independence function $F(\Delta t)$ and statistical efficiency $\epsilon(\Delta t)$, plotted as a function of sampling interval for M and E separately. The curves drawn are the best fits to the forms (8) given above.

estimate obtained from the full 865 runs used in the autocorrelation study with $\Delta t=1$: $\tau_{s,E}\approx F_E(1)^{-1}=19\pm1$ MCS and $\tau_{s,M}\approx F_M(1)^{-1}=38\pm2$ MCS.

It is now possible to proceed to extract the dynamical critical exponents z_M of the order parameter and z_E of the energy for this model in multiple ways. Finite-size scaling of the CLT-measured $\tau_{s,M}(L)$ and $\tau_{s,E}(L)$ is used (exploiting the connection established by KI) and compared to the exponents traditionally evaluated by scaling directly measured integrated and asymptotic autocorrelation times $\tau_{(i,a),E}(L)$ and $\tau_{(i,a),M}(L)$ for a wide range of L. Finally, finite-size scaling theory is used to extract dynamical critical exponents $z_{(i,a),R}$ for the rotational autocorrelation times $\tau_{(i,a),R}(L)$.

In Figs. 4(a)–4(c) the L scaling of (twice the) the asymptotic and integrated τ_M, τ_R, and τ_E are presented and compared to the scaling of the sample independence times. The lines through the data are nonlinear least squares fits to the form $\tau(L)=\tau_0 L^{-z}$. The exponents can be compared to $d-2\beta/\nu=\gamma/\nu\approx1.980\pm0.001$.[24] z_M and z_R are essentially the same regardless of whether asymptotic or integrated τ are fit (the difference tends to vanish for large L). z_E is not very accurately known from the integrated and asymptotic autocorrelation times because the energy autocorrelation is in general small enough in absolute value that it is difficult to get good statistics. However, the static estimation of the sample independence time (which should be identical to twice the integrated autocorrelation time) yields a reasonably precise estimate of $z_E\approx1.62$.

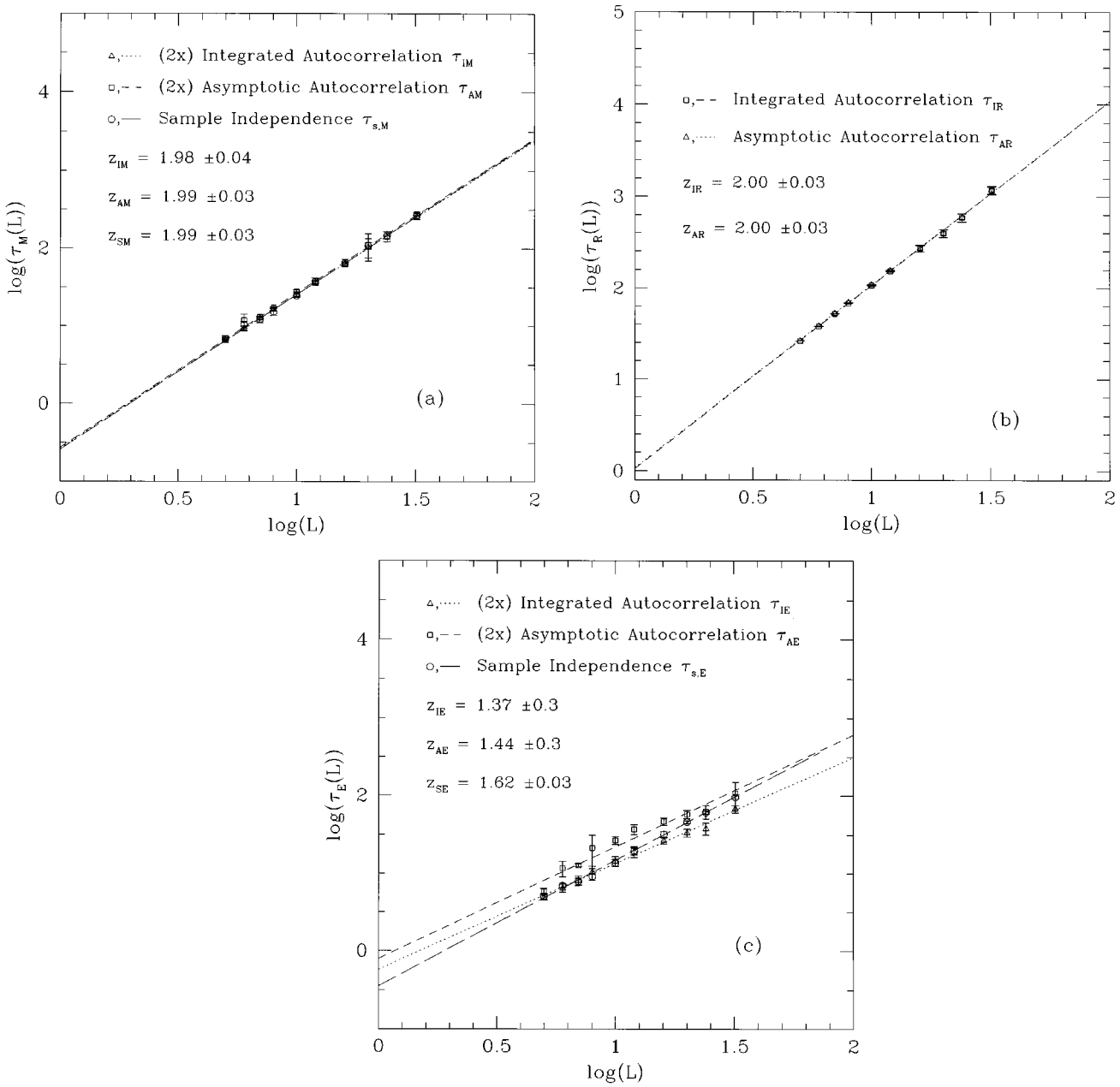

FIG. 4. The integrated and asymptotic relaxation times and sample independence time evaluated from A_M (a), A_R (b), and A_E (c) for various L. The (asymptotic) slope of the log-log fits yields the associated critical exponents. The best nonlinear least squares fit to the data is drawn on for each data set.

These results have several interesting or surprising features. The measured asymptotic autocorrelation exponents compare reasonably well to the theoretical predictions. As measured, $z_M = (1.97\text{–}1.99) \approx (2 - \eta = \gamma/\nu = 1.98) \approx (2 + c\,\eta = 1.99)$ where the former is the conventional prediction and the latter is the RG result. The precision of our results, although quite good, is still not good enough to resolve the ~ 0.01 difference between the conventional and RG predictions. It is possible that extending the calculation to higher L and applying the CLT-based methodology of KI will yield high enough precision to resolve the difference.

$z_R \approx 2.00$, which again agrees reasonably well both with the RG predictions (it is possible that the RG actually evaluates z_R, which is without a doubt the largest relaxational time scale of the system for any finite lattice size) and with our simple estimate. There is a systematic finite-size correction visible in the $\tau_{(i,a),R}$ data; if one fits only the points with $L \geqslant 10$, both $z_R \approx 1.98$. Even allowing for the possibility of other systematic errors, the error estimate of ~ 0.03 seems reasonable.

$z_E \approx (1.4\text{–}1.7)$ (where $z_{s,E} \approx 1.62$, due to the reasonably accurate static sample independence times, is probably the most reliable result) is the first MC measurement of this quantity. This exponent describes the scaling (critical slowing down) of energy relaxation times and the breaking of ergodicity. It is interesting that this exponent is considerably

smaller than the order parameter relaxation dynamic critical exponent, although the integrated energy relaxation time apparently still diverges at T_c. We can therefore conclude that the breaking of symmetry (connected to the appearance of the order parameter direction) occurs ''faster'' than the breaking of energy ergodicity *per se*, at least for a ''typewriter'' heat bath thermalization mechanism that thermalizes all the nearest-neighbor ''bonds'' in the lattice twice per MCS.

This split suggests that large systems near the critical point can exist for considerable times in metastable states that are more or less energy equilibrated but do not have equilibrated order parameters. This metastability can readily be observed to occur in MC simulations [for example, when rapidly quenching from high-temperature initial conditions to a temperature below T_c (Ref. 23)].

VIII. CONCLUSIONS

The primary results of this paper must be considered the categorical numerical evaluation, analysis, and comparison of several distinct autocorrelation functions and their relaxation time scales, the sample independence time scales, and the related dynamical critical exponents that describe critical slowing down, the explicit breaking of symmetry, and the breaking of energy ergodicity. There are, however, quite a number of secondary results of nearly equal significance and utility.

The first estimate for the rotational dynamical critical exponent z_R was derived from a simple random walk argument that illuminates the scaling of the fundamental mechanism of thermodynamic restoration of vector spin ergodicity and symmetry.

The relationship between symmetry and sample independence in the ISMC method was carefully developed, where it was shown that Markov processes in general have two parts: one part that irreversibly moves the system from one distinct configuration to another distinct configuration (distinct in the sense of having vanishing covariance) and another part that transforms a configuration into a symmetry-connected but otherwise identical copy. Although for many Markov processes the latter proceeds slowly, it cannot be neglected and should not be mistaken for the former, which is the only part that contributes to sample independence.

The CLT was shown to be the fundamental basis of error estimates in the ISMC method, and a simple methodology indicated for obtaining *a priori* reliable error estimates without any prior knowledge of the autocorrelation times for a given quantity. Indeed, the reliable, CLT-based sample standard deviations can be worked backwards (much as is done in the approach of KI) to obtain the sample independence times.

This methodology was shown to be robust and accurate for computing integrated autocorrelation times when directly compared to the much more laboriously evaluated autocorrelation times themselves for several quantities. The FSS of the CLT-based sample independence times is generally more accurate than the FSS of directly measured autocorrelation times for estimating dynamic exponents, although (as was noted) it has not been proven that the integrated autocorrelation exponents are identical to the asymptotic exponents derived in most theoretical work. This makes it possible to routinely evaluate dynamic critical exponents (and validate error analysis) in a static exponent calculation.

Finally, a number of minor errors in the literature were addressed. Since the rotational autocorrelation time does not measure or predict the order parameter sample independence time, properly applied local MC methods are considerably more efficient than previously reported.[12,13] The correct functional form of the numerical efficiency was established; this should enable future calculations to realize as much as a 10%–30% increase in numerical efficiency by optimizing the sampling schedule. It was recommended that CLT-based standard deviations replace the ''number of independent samples'' as an objective measure of ISMC result quality.

ACKNOWLEDGMENTS

The authors gratefully acknowledge the support of the Army Research Office. They wish to thank R. G. Palmer, P. Hohenberg, and B. Halperin for useful discussions. They also would like to thank the Duke University Office for Information Technology for technical support and for permission to use the otherwise wasted background time on the academic Unix clusters as part of a parallel supercomputer.

[1] M. N. Barber, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic Press, New York, 1983), Vol. 8, p. 145.

[2] L. Van Hove, Phys. Rev. **93**, 1374 (1954).

[3] B. I. Halperin, P. C. Hohenberg, and S. Ma, Phys. Rev. Lett. **29**, 1548 (1972); Phys. Rev. B **10**, 139 (1974).

[4] C. De Dominicis, E. Bre'zin, and J. Zinn-Justin, Phys. Rev. B **12**, 4945 (1975); **12**, 4954 (1975).

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

[6] J. Goldstone, Proc. Roy. Soc. London A **239**, 267 (1957).

[7] R. G. Palmer, Adv. Phys. **31**, 669 (1982). See especially Secs. 2 (where components and confinement are defined) and 4 (where the role of the confining–symmetry-breaking field in the canonical prescription is explored).

[8] J. P. Bucher, D. C. Douglass, and L. A. Bloomfield, Phys. Rev. Lett. **66**, 3052 (1991).

[9] S. N. Khanna and S. Linderoth, Phys. Rev. Lett. **67**, 742 (1991).

[10] H. Muller-Krumbharr and K. Binder, J. Stat. Phys. **8**, 1 (1973).

[11] N. Metropolis *et al.*, J. Chem. Phys. **21**, 1087 (1953).

[12] P. Peczak and D. P. Landau, J. Appl. Phys. **67**, 5427 (1990).

[13] P. Peczak and D. P. Landau, Phys. Rev. B **47**, 14 260 (1993).

[14] P. Peczak, A. M. Ferrenberg, and D. P. Landau, Phys. Rev. B **43**, 6087 (1991).

[15] U. Wolff, Phys. Rev. Lett. **62**, 361 (1989).

[16] K. Chen, A. M. Ferrenberg, and D. P. Landau, Phys. Rev. B **48**, 3249 (1993).

[17] C. Holm and W. Janke, Phys. Lett. A **173**, 8 (1993); J. Phys. A **27**, 2553 (1994); Phys. Rev. B **48**, 936 (1993); Nucl. Phys. B (Proc. Suppl.) **30**, 846 (1993).

[18] X. Paauw, X. Compagner, and X. Bedaux, Physica **79A**, 1 (1975).
[19] Y. Miyatake *et al.*, J. Phys. C **19**, 2539 (1986).
[20] M. Kikuchi and N. Ito, J. Phys. Soc. Jpn. **62**, 3052 (1993); M. Kikuchi, N. Ito, and Y. Okabe, in *Computer Simulations in Condensed Matter Physics VII*, edited by D. P. Landau, K. K. Mon, and H. B. Schuettler (Springer, New York, 1994).
[21] K. Binder and D. W. Heerman, *Monte Carlo Simulation in Statistical Physics*, Springer Series in Solid State Sciences, Vol. 80 (Springer, New York, 1988).
[22] R. J. Glauber, J. Math. Phys. **4**, 294 (1963).
[23] R. G. Brown and M. Ciftan (unpublished).
[24] R. G. Brown and M. Ciftan, Phys. Rev. Lett. **76**, 1352 (1996).
[25] D. Gillespie, *Markov Processes* (Academic Press, New York, 1992).
[26] S. K. Ma, *Statistical Mechanics* (World Scientific, Philadelphia, 1985). See especially Chap. 12.
[27] G. Smith, *Statistical Reasoning*, 3rd ed. (Allyn and Bacon, Boston, 1991). See remarks on p. 244.
[28] B. Efron, *The Jackknife, the Bootstrap and Other Resampling Plans* (Society for Industrial and Applied Mathematics, Philadelphia, 1982).
[29] R. G. Brown and M. Ciftan, Phys. Rev. A **40**, 3080 (1989).
[30] EXPECT is a (UNIX) scripting language that runs under TCL that parses response lines with regular expressions and then conditionally enters commands. It can be readily used for automating many functions of distributed (networked) computing in general. It is in the public domain and available over the net. A reasonably recent release is available in, e.g., ftp://ftp.cme.nist.gov/pub/expect.