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LETTER TO THE EDITOR

Critical slowing down in local dynamics simulations

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Abstract. We report some universal and non-universal aspects of the critical dynamics of the three-dimensional Ising model, obtained in recent extensive Monte Carlo finite-size simulations. We show that the time-dependence of the magnetization of finite lattices is composed of two kinds of fluctuations at the critical point: (i) phase fluctuations from one metastable minimum of the free energy to the other, dominating the long-time behaviour of the magnetization; (ii) critical fluctuations inside each minimum, decaying on a comparatively short timescale. Both kinds of fluctuations show up the same critical exponent $z = 2.10 \pm 0.02$, which is also in excellent agreement with the exponent z of energy fluctuations.

The dynamical behaviour of spin systems is a long-studied topic in statistical physics. An important feature is the divergence of the characteristic timescale of the system at its critical point [1]. This critical slowing down leads to a divergence $\tau = AL^z$ of the relaxation time with increasing lattice size L at the critical point T_c. As a consequence, the number of uncorrelated data in measurements of the static and dynamic properties of a system are heavily reduced [2]. This effect is very large in local dynamics ($z \simeq 2$) [3–8]. New dynamical algorithms have been proposed which successfully reduce critical slowing down by cluster updating techniques ($z \simeq 0.5$) and are superior for large system sizes [9, 10].

We have studied the local dynamics of a three-dimensional Ising system at its critical temperature T_c [11–13]. The dynamical behaviour is characterized by the correlation function of some quantity $A(t)$ like magnetization energy, defined by

$$\Phi_A(t) = \frac{\overline{A(t'+t)A(t')} - \overline{A(t')}^2}{\overline{A(t')^2} - \overline{A(t')}^2}. \tag{1}$$

where the bar denotes the time average over the whole Markov sequence of states generated according to the local dynamics. The long-time behaviour of $\Phi_A(t)$ is dominated by a single exponential decay [14], characterized by the asymptotic relaxation time τ of A. We have used the finite-scaling law [15] $\tau = AL^z$, valid at T_c, for the calculation of the critical exponent z.

We have invested about 9×10^{12} single spin-flips for this project, more than ever before on a general purpose computer. This was achieved by a considerable amount of computing time at HLRZ and by a program based on multispin coding which runs at a speed of 335 million spins per second per CRAY-processor [16].

We first discuss some qualitative aspects of the dynamical behaviour of finite systems at the critical point. Then, we present our results concerning the dynamical critical exponent z.

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It is well known that finite systems do not show the perfect symmetry breaking and ergodicity breaking as the infinite system does. As a consequence, finite systems display phase changes in the ordered phase which do not occur in the infinite system. It has been shown in an instanton calculation within the GLW-model [17] that finite systems in the low-temperature region $T \ll T_c$ tunnel from one metastable state to the other with a relaxation time $t_R \sim e^{2\sigma(T)L^{d-1}}$. The mechanism of this phase change is the activated movement of the interface between up- and down-oriented domains. This tunnelling phenomenon has been investigated numerically and the interface tension $\sigma(T)$ has been determined via the relaxation time t_R [18].

We first show that this tunnelling phenomenon even exists at the critical point T_c where it is mixed with critical fluctuations. As opposed to the low-temperature regime, the timescale of phase fluctuations increases with a power law and with the same exponent z as critical fluctuations. We have sampled the magnetization

$$S = 1/N \sum_{i=1}^{N} \sigma_i \tag{2}$$

and the energy

$$E = J/N \sum_{i,j=1}^{N} \sigma_i \sigma_j \tag{3}$$

normalized to the number of spins $N = L^3$ in the lattice. As usual in Monte Carlo studies of dynamics [7, 8], the definition of the magnetization includes the sign or phase of the system. To give a qualitative impression of the dynamics, figure 1(a) shows the magnetization S of a 60^3-system at the critical temperature $T_c/J = 4.511\,536$ [11-13] of the infinite system. Data points are shown every 160 updates of the whole lattice. The system fluctuates critically within one of the metastable states $S(T)$. At large time intervals, a phase change occurs from one minimum of the free energy to the other, leading to a sign change of S. This is indicated by additional data points on top and bottom of the figure. The characteristic time for staying in a minimum depends on the system size and on the temperature. Figure 1(b) displays a short time interval of figure 1(a) with a better time resolution (data points every 16 updates). It becomes evident that critical fluctuations inside the metastable minima occur on a much shorter timescale compared to phase fluctuations.

The dynamical behaviour of a finite system at the critical point is suspected to be a mixed process in language of stochastic processes: critical fluctuations are mixed with phase fluctuations in a temperature interval $T_l(L) < T < T_u(L)$ around the critical point. In order to analyse this mixed process quantitatively, we have studied separately the time-dependence of the phase $p = \mathrm{sign}(S)$ and of the absolute value of the magnetization $M = |S|$. As an example, figure 2(a) shows the correlation function Φ_S, Φ_p and Φ_M in a logarithmic plot, calculated from a simulation of 50^3-lattices at T_c. It is obvious that the correlations of the magnetization are completely determined by the correlations of the sign S alone. The quantitative analysis shows that both correlation functions Φ_S and Φ_p decay with the same asymptotic relaxation time which is considerably larger than that of Φ_M. However, the initial relaxation of Φ_S and Φ_p is different. This is shown in figure 2(b), which displays the relaxation during the first 100 Monte Carlo steps. The sign-correlation decreases sharply within the first 10 Monte Carlo steps compared to the magnetization correlation Φ_S. The reason is that zero-passage of S give a large contribution to Φ_p but almost no contribution to Φ_S since the absolute value of S is small when passing $S = 0$.

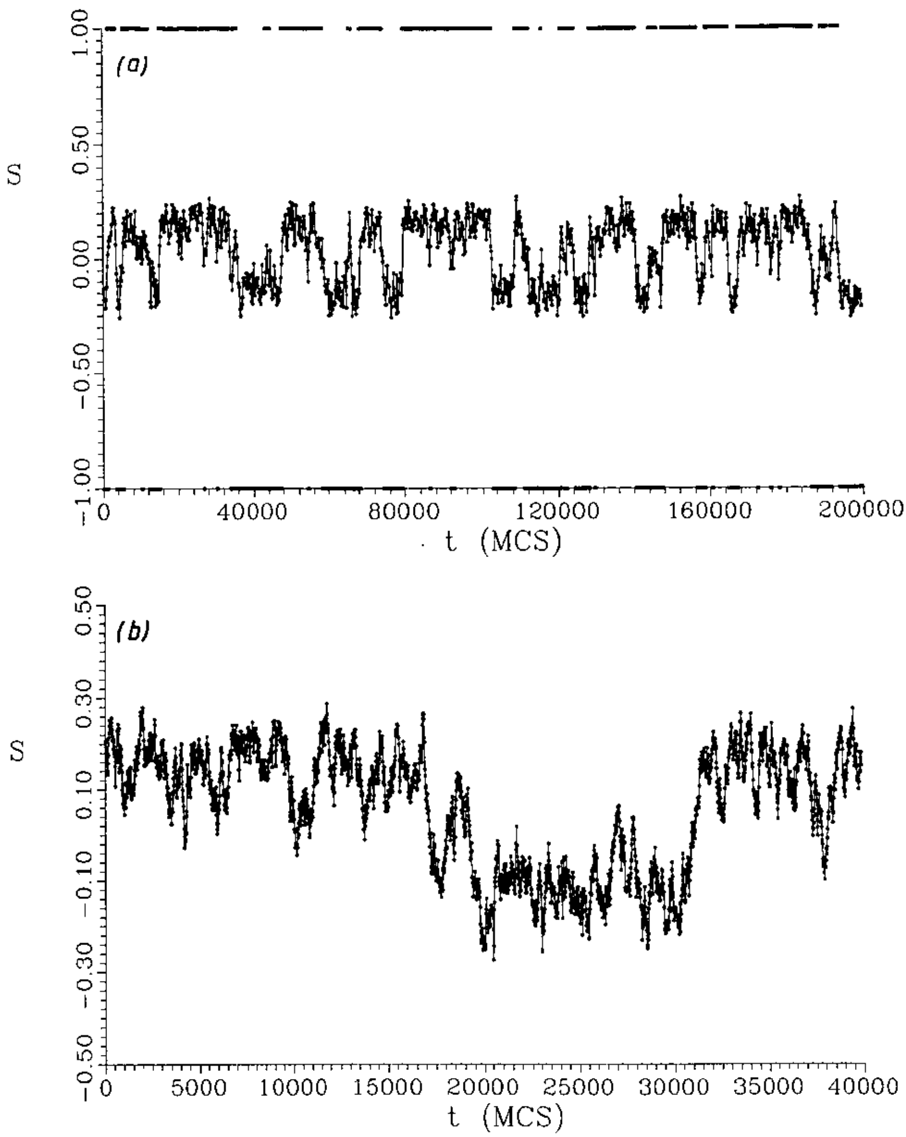

Figure 1. (a) Time-dependence of the magnetization S of a 60^3-system at the critical temperature of the infinite system $T_c = 4.511\,536$ (data points every 160 lattice updates). Phase fluctuations and critical fluctuations form a mixed process near T_c. (b) A short time interval of (a) (data points every 16 lattice updates). Critical fluctuations within a minimum of the free energy are well distinguished from fluctuations from one phase to the other.

Before we proceed to the determination of the critical exponent z, we point out some practical consequences of the analysis sketched above. It seemed to be a general belief that the largest relaxation time is relevant for statistical errors of magnetic data [19]. Since we have shown that the largest relaxation time is dictated by phase-fluctuations only, this expectation is easily seen to be wrong: we know from the theory of stationary random processes that independent of the physical nature of a process the relevant timescale for statistical errors depends on the process/quantity $A(t)$ under consideration. It is τ_M for the absolute value of the magnetization M and τ_E for the

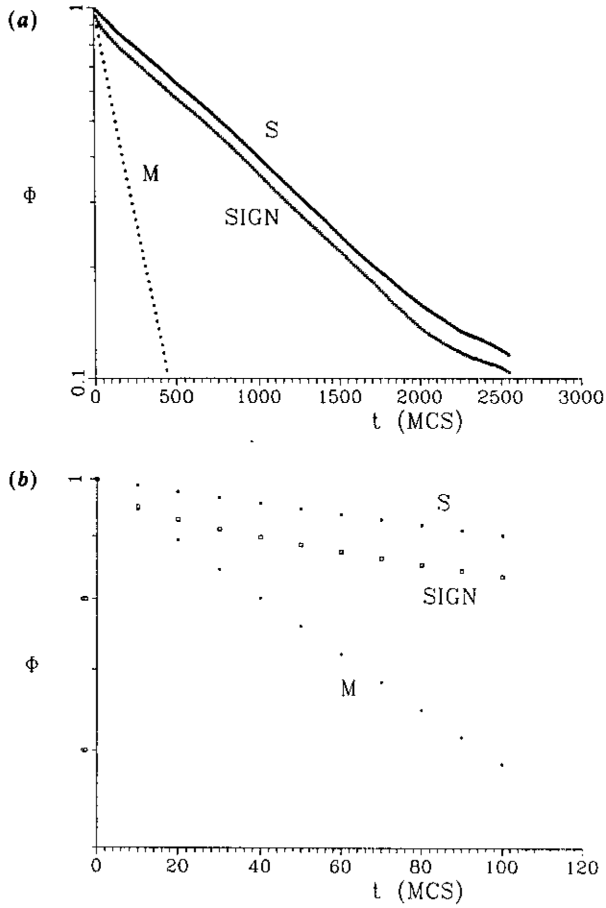

Figure 2. (*a*) Logarithmic plot of the correlation function of *S*, of its sign and its absolute value *M* calculated of a single run with 2.7 million updates of a 50^3-system. The process $S(t)$ is entirely determined by fluctuations of the sign of $S(t)$, i.e. fluctuations from one phase to the other. (*b*) Initial relaxation of correlations within the first 100 Monte Carlo steps.

energy. The relevant relaxation time for the susceptibility, which is proportional to $\langle M^2\rangle(T>T_c)$ and $\langle(M-\langle M\rangle)^2\rangle(T<T_c)$ is τ_{M^2}, which is of the order of τ_M and τ_E. The symmetry of the system under sign-reversal implies that there is no thermodynamic property of the infinite system which depends on the sign or phase of the system; thus, the large relaxation time τ_S is irrelevant for statistical errors Monte Carlo sampling. This has been shown explicitly by a comparison of calculated and measured errors [20].

We have performed a very detailed analysis of correlation data for lattice sizes L between 20 and 60; details will be presented elsewhere [20]. We have shown that the ansatz of previous Monte Carlo work [8] to fit correlation data in the whole time range to a 2- or 3-exponential ansatz incorrect [20]. The correct way of analysis is to identify the asymptotic time range by deviations of the power spectral densities of M, S and E from their asymptotic Lorentzian form [20]. The 1-exponential fit in the asymptotic time range leads to very precise relaxation times; errors of τ_L have been determined from averaging over several (6–12) runs per lattice size. As a typical example of our

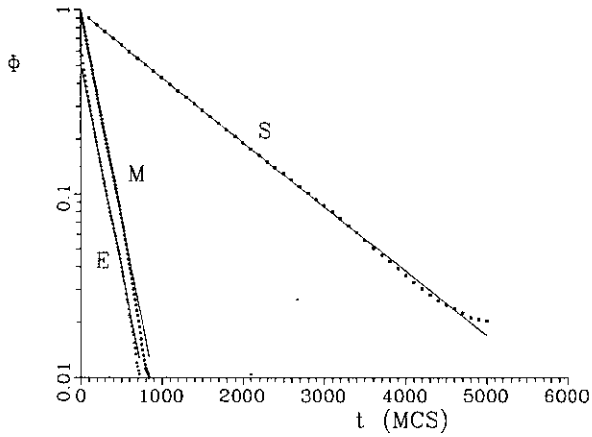

Figure 3. Logarithmic plot of Φ_S, Φ_M and Φ_E and their one-exponential fits in the asymptotic time range. Note that Φ_M and Φ_E are statistically much better than Φ_S. The timescale of these correlations is about six times smaller than the scale of Φ_S.

data and analysis, we show the time-dependence of the correlation data Φ_M, Φ_E and Φ_E and Φ_S of a 50^3 system at the critical temperature T_c (figure 3), calculated from 11 million updates of the lattice. The asymptotic relaxation time obtained from a single exponential fit of Φ_S in the asymptotic time region (solid line) is $\tau_S = 1232$. From the same data set, we show the correlation functions Φ_M and Φ_E with their one-exponential fits in the asymptotic time region, leading to $\tau_M = 195$ and $\tau_E = 195$. Φ_M and Φ_E have the same asymptotic relaxation times, but the initial time-dependence of Φ_M and Φ_E is very different: energy correlations reach their asymptotic exponential behaviour below $\Phi_E = 0.1$, whereas M-correlations are in the asymptotic time range already for $\Phi_M = 0.6$.

As usual we have fitted our results for $\tau(L)$ by a least-squares fit with error weights to the finite-size scaling $\tau(L) = AL^z$. For each of the three quantities M, S and E, we have obtained values of z which are very close to one another:

$$
\begin{aligned}
z_M &= 2.098 \pm 0.006 \\
z_E &= 2.09 \pm 0.02 \\
z_S &= 2.12 \pm 0.02.
\end{aligned}
\tag{4}
$$

We conclude that magnetic and caloric properties are governed by the same exponent $z = 2.10$ within an error bound of 0.02. This verifies universality of dynamic critical phenomena; previous simulations did only arrive at a consistency statement since the errors of z were too large. A fit of the $\tau(L)$-data assuming the same relative error of $\tau(L)$ for all lattice L gives $z = 2.09 \pm 0.01$. The resulting best fits are shown in figures 4 and 5. The non-universal amplitudes obtained from this fit are $A_M = 0.0530$, $A_E = 0.0539$ and $A_S = 0.310$. Thus, the absolute timescale for M- aand E-correlations is the same within our errors. We stress that the exponential increase of τ_S, found below T_c [18], is changed to the power law behaviour at the critical point. Obviously, the dynamics of interface fluctuations becomes triggered by critical fluctuations within the minima, so that the asymptotic relaxation time τ_S scales as L^z with the same exponent z as for M and E.

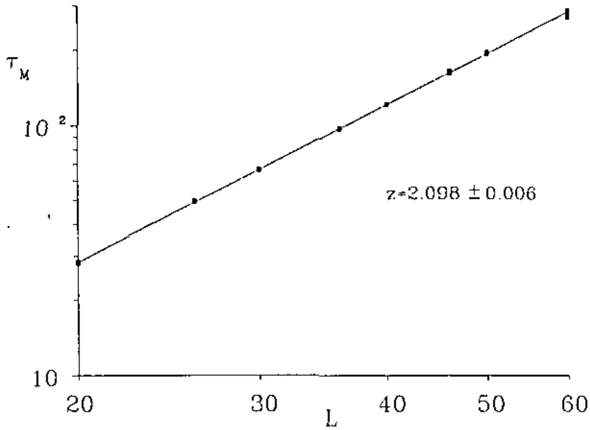

Figure 4. Fit of the asymptotic relaxation times $\tau_M(L)$ to the finite-size scaling form $\tau = AL^z$. The free parameters of the error-weighted fit are the amplitude A and the exponent z. The symbol-size for each τ-value is given by $\tau \pm \Delta\tau$.

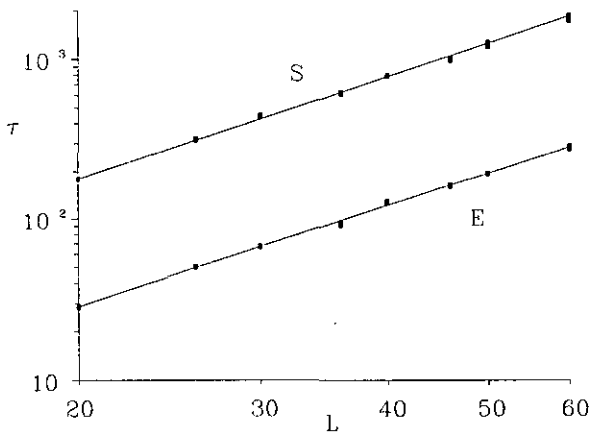

Figure 5. The same error-weighted fit as in figure 4 for the asymptotic relaxation times τ_E and τ_S. The errors of τ_E and τ_S are larger than for leading to a less precise value for z.

The error of our simulation and exponent z is considerably smaller than in previous Monte Carlo works on dynamical behaviour. The reason is that we have sampled more data and we have done a more detailed analysis. Moreover, previous studies, based on Φ_S, have extracted only the fraction $\tau_M/\tau_S \simeq 0.15$ of the statistical contents of their dynamical simulation data compared our analysis of Φ_M. Our value of $z = 2.10 \pm 0.02(4)$ is significantly larger than the RG-estimate $z \simeq 2$ [21–23] and other recent Monte Carlo values [7, 8]. We have therefore analysed our relaxation times by a fit to the power law plus finite-size scaling corrections of the form $\tau = AL^z(1 + BL^{-w})$, assuming a value of $z = 2.02$ and leaving A, B and w to be determined by the data-fit. The data are consistent with such a fit, but at the expense of significant finite-size corrections. The estimator of the corresponding least-squares fit is comparable to the conventional simple power law with $z = 2.10$, but it is not better. If a lower value of z around 2 is asymptotically valid, then finite-size corrections in critical dynamics are much more pronounced than in the static case where finite-size corrections are very small for the lattice sizes considered here. We have checked this with our own susceptibility results. In accord with previous simulations, we have found finite-size corrections of γ/ν from the asymptotic value which are of the order 0.02 and smaller for $L<30$.

Recent results of simple hydrodynamic model equations and their discretized version have shown that the effects of the discrete nature of a dynamical model may be competitive to fluctuation effects [24]. It seems plausible that dynamical critical phenomemna are similarly influenced by the discretization of time and space in Monte Carlo simulations. These effects may account for the deviation between the theoretical value of $z\simeq 2$ [21-23] and the result $z=2.10$ of the present simulation. However, it is not clear whether the discretization of the dynamics leads to strong scaling corrections or even to a new universality class different from the expected GLW-field theory.

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