Microscopic nonuniversality versus macroscopic universality in algorithms for critical dynamics

U. Ritschel and P. Czerner
Fachbereich Physik, Universität GH Essen, 45117 Essen, Federal Republic of Germany
(Received 26 July 1996)

We study relaxation processes in spin systems near criticality after a quench from a high-temperature initial state. Special attention is paid to the stage where universal behavior, with increasing order parameter $m(t) \sim t^{\theta}$, emerges from an early nonuniversal period. We compare various algorithms, lattice types, and updating schemes and find in each case the same universal behavior at *macroscopic* times, despite surprising differences during the early nonuniversal stages. [S1063-651X(97)14103-4]

PACS number(s): 64.60.Ht, 02.70.Lq, 05.50.+q

I. INTRODUCTION

Temperature quenches in spin systems and the ensuing relaxational processes have been a much-studied subject in the recent past [1–19]. Especially for a quench from a high-temperature initial state to the critical region, a new universal regime was predicted by Janssen, Schaub, and Schmittman [2]. In its most pronounced form this phenomenon, termed universal short-time behavior (USTB) in the following, occurs in a model with purely relaxational dynamics (model *A* according to Ref. [20]). Starting from an initial state with $T \gg T_c$ and a *small* initial magnetization m_0, the magnetization increases as [2]

$$m(t) \sim m_0 \, t^{\theta} \tag{1}$$

for a macroscopic time span before it reaches a maximum and eventually decays to the equilibrium value zero. θ is an independent new exponent determined by the nonequilibrium initial state that cannot be expressed in terms of equilibrium exponents. Its value in the two-dimensional Ising system for instance is $\theta \simeq 0.19$ [6,15].

The results of Janssen, Schaub, and Schmittmann [2,3] allowed the interpretation of earlier Monte Carlo (MC) simulations [4], and later the power law (1) was also directly verified in the ''computer experiment'' [5]. Further it was pointed out by Li, Schülke, and Zheng [6] that the USTB can be exploited to determine *equilibrium* exponents from the early nonequilibrium regime. In the sequel, this method was further developed and applied to a number of systems [7,8]. Moreover, USTB in other dynamic universality classes [9], in systems with a tricritical point [10], and in disordered and dilute spin systems, was studied [11]. Finite size effects were analyzed in Refs. [12,13], and the USTB near surfaces was studied in Ref. [14]. Further, the close relationship between USTB and ''damage spreading'' was pointed out [15], USTB in a different context, for quasi-long-range order evolving after a quench to the Kosterlitz-Thouless phase, was investigated [16], and a general scaling invariance in the short-time regime was found [17]. Possibly also related to USTB is the ''overshooting'' of the order parameter beyond the equilibrium domain magnetization for quenches below T_c [18], and the issue whether there exist still more independent exponents for relaxational processes was raised in a recent report [19].

A simple physical argument for the growth of the magnetization in Eq. (1) was given by Janssen [3,21]. Consider a system that is quenched to some final temperature T_f (not necessarily T_c), again with initial magnetization m_0. Then for $T_f \ll T_c$, $m(t)$ should grow after the quench, towards the equilibrium value selected by m_0. If in contrast $T_f \gg T_c$, $m(t)$ is expected to decay to zero rapidly. Hence, there should be a limiting temperature T_l where the qualitative behavior changes.

As the initial correlations are short ranged, the natural candidate for T_l is the critical temperature of the mean-field (MF) theory T_c^{MF}, and with the real T_c of spin systems being always smaller than T_c^{MF}, it would be an immediate consequence that $m(t)$ increases for a quench to the critical point. However, as argued in Ref. [13], it is *not* possible to derive the power law (1) from this scenario. The power-law growth is rather a phenomenon that occurs when the time-dependent (growing) correlation length $\xi(t)$ has become *macroscopic*, i.e., much larger than the lattice spacing a (compare Fig. 1 below). The derivation of Eq. (1) is thus beyond the scope of MF theory.

So far numerical investigations have been mostly carried out with the heat-bath (HB) algorithm [22,23]. A comparison between the HB and the Metropolis (ME) algorithm [22] was performed for the Potts model by Okano *et al.* [8], and it turned out that concerning the universal behavior both algorithms yield compatible results, but differences occur for early times.

The main purpose of this paper is a more systematic examination of the issue of universality. Are equilibrium exponents determined with the USTB really independent of factors like the algorithm (HB or ME), the updating scheme (random or sequential), and the lattice type (nearest or next-nearest neighbor coupling, square or triangular lattice)? How does universal behavior in the regime with $\xi(t) \gg a$ emerge from the nonuniversal early stage with $\xi(t) \simeq a$? And closely related: Is it really a MF ordering process during the *microscopically* early stages, or has this simple picture to be refined?

We answered these questions by solving the master equation for early times (during the first single-spin updates) as well as by MC simulation for later times. Our work reveals a number of interesting and surprising details about algorithms

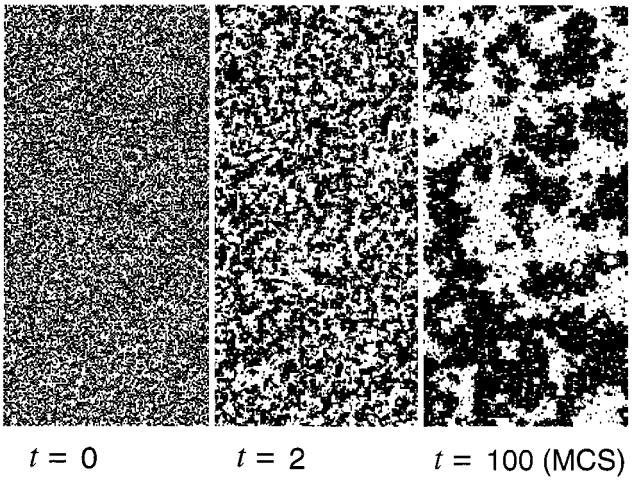

FIG. 1. Three snapshots of the temporal evolution of a spin configuration for $L=300$ and $m_0=0$, generated with the HB algorithm and random updating. Displayed in each picture is half of the system. From the visual appearance there is no difference between HB and ME algorithm.

for critical dynamics, and puts the USTB as a method to access equilibrium properties from a nonequilibrium (though universal) regime on a much firmer basis.

II. SOLUTION OF THE MASTER EQUATION

Information about thermal averages in the early nonuniversal stage of the relaxational process can be obtained by solving the master equation for the Ising system with Glauber dynamics [22]

$$\frac{dP(\mathbf{s},t)}{dt}=\sum_{s'}\ [W(\mathbf{s}'\rightarrow\mathbf{s})\ P(\mathbf{s}',t)-W(\mathbf{s}\rightarrow\mathbf{s}')\ P(\mathbf{s},t)], \tag{2}$$

where $\mathbf{s}$ denotes a spin configuration, $W(\mathbf{s}'\rightarrow\mathbf{s})$ is the transition probability, $P(\mathbf{s},t)$ the probability to find configuration $\mathbf{s}$ at time t, and the sum extends over all possible configurations. The analytic integration of Eq. (2) for large systems of coupled spins is not feasible. However, for the high-temperature initial state consisting of N uncorrelated spins in a magnetic field H, characterized by the Boltzmann factor

$$P(\mathbf{s},0)=Z_0^{-1}\exp\left(H\sum_{i=1}^{N}s_i\right)\quad\text{with}\quad Z_0=(2\ \cosh H)^N, \tag{3}$$

the analytic treatment for very early times, $t\ll 1$, is possible. [The time is expressed in units of MC steps per site (MCS).]

Consider the first single-spin update after the quench. It takes place in an environment that is coupled to a heat bath at the *final* temperature T_f, and H is switched off. Decisive for the very early stage is whether after the *first* update, on average, the magnetization is reduced or increased. The respective tendency survives as long as the system still closely resembles the initial state, i.e., as long as the number of single-spin updates is much smaller than N.

Without loss of generality one may choose spin 1 to be updated. From Eq. (2) one straightforwardly derives $\Delta m:=m(t=1/N)-m_0$ to be

$$\Delta m=2\,N^{-1}\sum_{\mathbf{s}}\ [W(-\rightarrow+)\ P(-,0)-W(+\rightarrow-)\ P(+,0)], \tag{4}$$

where the W's are the probabilities for spin 1 changing sign with all other spins remaining unchanged. Especially for small H (corresponding to small m_0), we find from Eq. (4) the simple result

$$\Delta m=-4\,H\,N^{-1}\sum_{s}\ W(+\rightarrow-)\left(1+\sum_{i\in IN}s_i\right), \tag{5}$$

where the second sum extends over the interacting neighbors of spin 1.

From Eq. (5) we calculated Δm and the limiting temperature T_l for the Ising model on a square lattice with nearest-neighbor interaction J for HB and ME algorithm. In $d=2$ (the system that will be also studied by MC simulations below) the explicit results are $T_l^{HB}=3.0898\ldots$ and $T_l^{ME}=1.5885\ldots$ for HB and ME algorithm, respectively. (Temperatures are expressed in units of J/k_B.) For comparison, the (exact) critical temperature is $T_c=2.2691\ldots$ and $T_c^{MF}=4$. Hence, for the HB algorithm T_l is indeed above T_c, while, surprisingly, with ME even *at* T_c the magnetization decays $t\ll 1$.

We calculated T_l also for other dimensions. In the limit $d\rightarrow\infty$ (where the number of nearest neighbors becomes infinite) one finds $T_l\rightarrow T_c^{MF}$ for both algorithms considered above. For $d=1$ both yield $T_l=0$.

From this analysis we conclude: First, the limiting temperature in general depends on the algorithm. Only for $d\rightarrow\infty$ it turns out to be T_c^{MF}. Second, we are left with the puzzling result that for the ME algorithm the limiting temperature lies even *below* T_c, and therefore one would not expect to see an increase of the magnetization at T_c. In any event, the simple explanation that the nonuniversal stage preceding the USTB is a MF ordering process is in general not correct.

III. MONTE CARLO SIMULATION OF THE NONUNIVERSAL STAGE

In order to learn about later stages, $t\gtrsim 1$, especially the crossover from microscopic to macroscopic behavior, we had to resort to MC simulations. These were carried out for an Ising system on a square lattice in $d=2$ with a linear dimension L and periodically coupled boundaries. Single spins were randomly selected and updated. In order to obtain thermal expectation values we generated a large number of histories, each starting from a new initial configuration, and calculated mean values [22].

Snapshots of the temporal evolution of a single configuration for a square lattice with $N=90\,000$ spins are displayed in Fig. 1. The left picture shows the initial state. Next to it

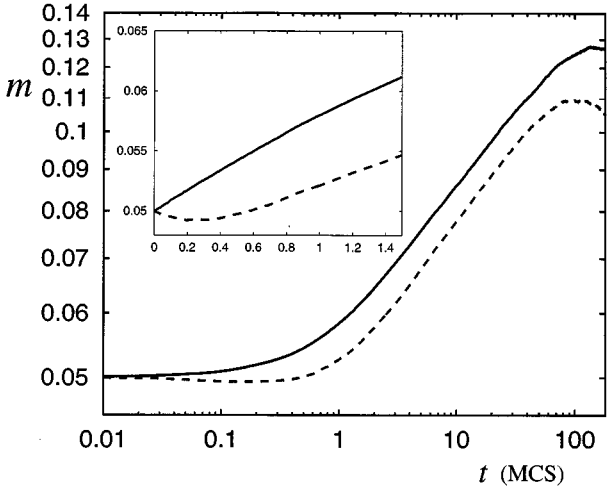

FIG. 2. Order-parameter profiles for $L=20$ and $m_0=0.05$ obtained with HB (solid line) and ME algorithm (dashed line) in double-logarithmic representation. The small diagram inserted shows the data for small times in double-linear representation.

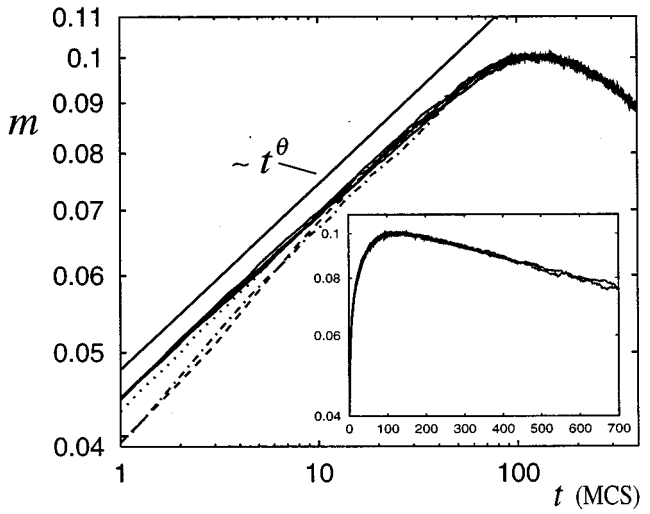

FIG. 3. Data collapse of seven magnetization profiles obtained for $L=40$ and $m_0=0.03$ for different combinations of lattice types, algorithms, and updating schemes (as described in the text) in double-logarithmic representation. The ME results for the square lattice with sequential (dashed line) and random (dotted line), as well as for the triangular lattice with sequential update (dashed-dotted line) are singled out. The small diagram inserted shows the same data in semilogarithmic representation. The power law (1) with $\theta=0.19$ is plotted for comparison.

the configuration after $2N$ updates corresponding to $t=2$ is depicted. At this point the average domain size and (with that) the correlation length are already substantially larger than the lattice spacing. This is the stage where universal (macroscopic) behavior emerges from the nonuniversal (microscopic) regime as discussed in more detail below. At $t=100$ the correlation length is of the order of the lattice size L.

Results for $m(t)$ at $T_f=T_c$ with $L=20$ and $m_0=0.05$ are displayed in Fig. 2. The HB curve (solid line) monotonously increases and is consistent with a power law for $t\gtrsim 1.5$. In the case of the ME algorithm (dashed line) the behavior is qualitatively different. As expected from our analytic results, $m(t)$ indeed drops initially, but has a minimum at $t\simeq 0.3$, and then increases to assume the power-law form for $t\gtrsim 2$. Thus, despite the anomalous time dependence of the ME curve in the nonuniversal regime, for macroscopic times, it agrees with Eq. (1). This is in accord with the findings of Okano *et al.*, where sequential updating was used and, thus, the details of the temporal evolution were not uncovered. Later the profiles in Fig. 2 have a maximum and then decay to the equilibrium value zero [24].

Taking into account these results, the natural question to ask is whether there exists an algorithm-independent limiting temperature, a ''dynamic MF temperature,'' where the *macroscopic* behavior changes from increasing (USTB) to decaying. It turns out that for the HB algorithm this limiting value coincides with T_l^{HB}; the profiles have mostly one extremum. In order to determine the corresponding limit for ME, we generated a number of profiles for temperatures above T_c, seeking the one that shows a saddle point. We determined the corresponding temperature as 2.70 (2). Neither did this number depend significantly on the system size nor on m_0. However, it does not agree with the corresponding value of the HB dynamics $T_l^{HB}\simeq 3.1$.

IV. MONTE CARLO SIMULATION OF THE UNIVERSAL STAGES

Eventually we compared magnetization profiles in the *universal* regime for a system with $L=40$ and $m_0=0.03$ at the critical point, $T_f=T_c$, for various combinations of algorithms, lattice types, and updating schemes. For the square lattice with nearest-neighbor interactions, we combined the ME and HB algorithm with random and sequential updating (four curves), for the triangular lattice with nearest-neighbor interactions we used both algorithms and sequential updating (two curves), and for a square lattice with additional next-nearest-neighbor interactions we used the HB algorithm and sequential updating (one curve) [25].

As can be seen already from Fig. 2, even though the initial power law is assumed by both profiles depicted there, the heights and locations of the maxima depend on the details of the method, besides the differences for early times. However, in all cases studied it turned out to be possible to map the data onto a single curve for times $t\gtrsim 20$, by constant rescalings of both axes. The result is shown in Fig. 3. On the semilogarithmic plot (small insertion) the individual profiles cannot be distinguished. When both axes are plotted logarithmically, on the other hand, the short-time regime is more pronounced, and significant differences for $t\lesssim 10$ become visible. The pure power law (solid line above the data) is plotted for comparison.

Singled out are the ME curves, for the square lattice with sequential (dashed) and random (dotted) updating, and for the triangular lattice with sequential updating (dashed-dotted line). In particular, when the ME algorithm is combined with sequential updating, the power law is assumed only for $t\gtrsim 10$. This is consistent with the findings of Okano *et al.* [8] for the Potts model, and can now be interpreted as a consequence of the anomalous behavior of the ME algorithm for $t\lesssim 1$. The HB results assume the power-law form much earlier. Most importantly, however, all seven curves show the USTB as expressed in Eq. (1) for later times, $t\gtrsim 10$.

V. SUMMARY

We investigated the short-time behavior in relaxational processes after a temperature quench. As a concrete example we studied the Ising system with short-range interactions and a nonconserved order parameter (Glauber dynamics). We found surprisingly different temporal evolutions with heat-bath and Metropolis algorithm during early, nonuniversal stages. Nevertheless, the characteristic short-time power law (1) turned out to be a rather robust phenomenon, occurring independently of the algorithm, the lattice type, and the updating scheme, provided the systems belong to the same dynamic universality class and the correlation length has grown substantially larger than microscopic scales.

ACKNOWLEDGMENTS

This work was supported in part by the Deutsche Forschungsgemeinschaft through Sonderforschungsbereich 237 ''Unordnung und groβe Fluktuationen.''

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