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LETTER TO THE EDITOR

Monte Carlo simulation of universal short-time behaviour in critical relaxation

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Abstract. The time evolution of the three-dimensional critical Ising model relaxing from a non-equilibrium initial state is studied by means of Monte Carlo simulation. We observe the characteristic *initial increase* of the (spatially) averaged magnetization predicted by Janssen *et al*. The exponent θ' that governs the initial behaviour is determined, and the dependence of the long-time linear decay on the initial magnetization, m_0, is analysed. Our simulation corroborates earlier results derived from continuum models.

Five years ago Janssen *et al* [1] discovered that under certain circumstances relaxation processes in Ising-like systems near criticality show strong anomalies. When, for example, a system belonging to the dynamic universality class of model A [2] is quenched from a state with temperature $T \gg T_c$ to the critical point, an initially existing small magnetization will grow for a *macroscopic* time span before the actually expected decay towards equilibrium takes over. The *initial increase* of order, which was later also found in other dynamic models [3], is described by a universal power law with a new dynamic exponent, θ', that *cannot* be expressed in terms of a scaling relation between the static exponents and the dynamic exponent z. The reason for the short-time anomaly has to be sought in the initial conditions, more precisely, in the behaviour of the initial magnetization m_0 under renormalization-group transformations. As found by Janssen *et al*, the operator m_0 has a scaling dimension x_0 that is, in general, different from the dimension of the equilibrium magnetization, $x_\phi = \beta/\nu$. As a detailed scaling analysis reveals [4], this gives rise to a *macroscopic* time-scale

$$t_0 \sim m_0^{-z/x_0} \tag{1}$$

and the exponent θ' is related to x_0 by

$$\theta' = \frac{x_0 - x_\phi}{z}\,. \tag{2}$$

Numerical values for the new exponents have been obtained by means of the ϵ-expansion [1].

More recently, Diehl and Ritschel [4] extended the above-mentioned considerations to systems of finite size. In the following these results, which have been obtained by finite-size scaling analysis and with the help of continuum field theory, will be summarized because they are essential for the interpretation of the Monte Carlo data. The basic quantities that

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enter the scaling analysis are the time t, the lattice size L in units of the lattice constant a, and the spatially averaged magnetizations m_0 and $m(t)$. At bulk criticality and for L and t much larger than any microscopic scales, one expects the following scaling form of the magnetization:

$$m(t, L, m_0) \sim l^{-\beta/\nu} m(l^{-z}t, l^{-1}L, l^{x_0}m_0). \tag{3}$$

By choosing the arbitrary rescaling parameter $l \sim t^{1/z}$, one can rewrite (3) as

$$m(t, L, m_0) \sim t^{-\beta/\nu z}\mathcal{F}(t/t_L, t/t_0) \tag{4}$$

where the initial time-scale t_0 is given in (1), and t_L is the well known finite-size relaxation time $t_L \sim L^z$ [6].

Thus, as stated in (4), the relaxational behaviour of the critical Ising system starting from a non-equilibrium initial state with small correlation length $\xi \ll L$ and initial magnetization m_0 is governed by *two* macroscopic time-scales. This gives rise to clearly distinguishable stages of the relaxational process. First, the characteristic initial increase of order

$$m(t) \sim t^{\theta'} \tag{5}$$

discovered in [1] for the infinite system, is also found in the finite system [4] when $t < t_0, t_L$. The only condition for the increase is that t_0 remains macroscopic which, in turn, means that m_0 has to be small (cf (1)). Second, at time $t_{\max}$ the magnetization reaches its maximum and then starts to decrease towards the equilibrium value $m(t \to \infty) = 0$. For $t_L \gg t_0$, the time $t_{\max}$ is roughly given by t_0, but $t_{\max}$ decreases with decreasing t_L and can be much smaller than t_0 for $t_L \ll t_0$. Further, when $t_L \gg t_0$ the system goes through a regime of nonlinear decay with $m \sim t^{-\beta/\nu z}$ for $t_0 \ll t \ll t_L$, whereas this stage is missing completely for $t_L \ll t_0$. Third, the long-time behaviour for $t \gg t_L$ is described by an exponential

$$m(t \gg t_L) \approx M_\infty \mathrm{e}^{-t/t_L}. \tag{6}$$

While the time-scale in this 'linear' regime is not influenced by the initial state [5], the amplitude M_∞ is a *universal* function of both m_0 *and* L. It may be written in the form [5]

$$M_\infty(L, m_0) \approx \text{constant} \times L^{-\beta/\nu}\mathcal{G}(t_0/t_L). \tag{7}$$

In the limit $t_L \gg t_0$, the scaling function $\mathcal{G}$ approaches a constant. Hence, in this case the dependence on t_0 (and therefore on m_0) drops out of the long-time behaviour of $m(t)$. On the other hand, for $t_L \ll t_0$ the scaling function behaves as $\mathcal{G}(w) \approx w^{-x_0/z}$. Thus, the amplitude becomes [4]

$$M_\infty(L, m_0) \approx \text{constant} \times m_0 L^{z\theta'} \tag{8}$$

i.e. it is proportional to the initial magnetization m_0, and the exponent θ' that in the infinitely *extended system only appears in the short-time regime now governs the* L*-dependence of* M_∞. In other words: In the finite system there is a long-time memory of the initial condition in the sense that the asymptotically leading term depends on it.

For the Ising model the scaling function $\mathcal{G}$ has not been calculated so far. However, for the general n-vector model an exact solution for $n \to \infty$ has been obtained by Diehl and Ritschel [4]. For the special case of fixed L, their result for the amplitude takes the simple form

$$M_\infty^{(n\to\infty)} \approx \frac{A\, m_0}{\sqrt{1 + B\, m_0^2}} \tag{9}$$

with non-universal constants A and B. For the Ising system ($n = 1$) we expect a qualitatively similar behaviour of the asymptotic amplitude, i.e. the linear dependence for small m_0 and asymptotically independence of the initial magnetization for large m_0.

Now, the question asked in this letter is: do the results on universal short-time behaviour reported above stand up to the Monte Carlo 'experiment'?

Much numerical work has been devoted to the simulation of time-displaced correlation functions in equilibrium [8, 9] and to relaxational processes starting from an completely ordered state [10], but to our knowledge the process described above has not been studied in the literature so far. However, projects similar to ours are at present under investigation [11]. For the time being, our major aims may be summarized as follows.

- Simulation of the short-time behaviour of the relaxational process starting from the non-equilibrium initial state as explained above and measurement of the exponent θ'.
- Measurement of the universal amplitude of the exponential decay for late times and comparison with (9).
- Test of the scaling form (3) and thereby determine the scaling dimension x_0.

An initial state with non-vanishing magnetization and small correlation length can, in principle, be generated by letting the system evolve to thermal equilibrium with temperature $T \gg T_c$ within an external magnetic field. However, this procedure turns out to be unpractical because it is too time consuming, and, more importantly, due to the finite number of degrees of freedom, even for $T \gg T_c$ and strong magnetic field, fluctuations of the initial magnetization of the canonical ensemble cannot be neglected. As a consequence, the width of the distribution of the initial magnetization gives rise to an additional scale which may alter the simple relation (3). (In the continuous system the same phenomenon occurs if the initial temperature is close to T_c [1, 4].) In order to avoid this, we start from an initial state with *fixed* m_0 and small correlation length. It consists of a fixed number of 'up' spins distributed randomly over the lattice and the remaining spins pointing in the opposite direction.

Then the standard heat-bath formalism is used to trace the time evolution of the system [7]. Time is measured as usual in Monte Carlo steps per spin (MCS) and measurements are carried out after each sweep. We work at the (bulk) critical temperature $J/T_c = 0.2216$ [12]. For each magnetization profile we have averaged over 150 000 to 400 000 statistically independent histories of the system or runs, up to $t = 100$–200 MCS. Further, for each run a new initial configuration is generated and a new sequence of random numbers is used for the ensuing relaxational process.

Profiles for various L and m_0 are displayed in figures 1 and 2. In figure 1 both axes are logarithmic to show clearly the power-law behaviour (5) for early times, whereas in figure 2 only the m-axis is plotted logarithmically to bring out the linear decay for long times. All curves show the initial increase, and θ' is determined by fitting a straight line to the short-time regime.

Because we expect the universal initial increase only for small m_0, we calculate θ' from eight profiles with $0.02 \leqslant m_0 \leqslant 0.10$ and $4 \leqslant L \leqslant 16$. The results and their statistical errors are displayed in table 1. (The figure for $m_0 = 0.04$ and $L = 10$ is included in the table but the corresponding curve is not shown in figure 2.) They have to be compared with 0.08 from first-order and 0.13 from second-order ϵ-expansion [1]. In the range of L and m_0 we consider, the scattering of the data is small. Closest to the truth is probably the $\theta' = 0.102(2)$ from $L = 16$ and $m_0 = 0.06$.

The dependence of the amplitude of the linear decay has been obtained from the data of figure 2. The results which are displayed in figure 3 clearly show the linear increase for small m_0 and the tendency to become independent of m_0 for larger values. Fitted to the numerical data is the analytic large-n solution (9) with constants $A = 1.98$ and $B = 14.2$. We actually do not expect that the large-n result also holds in exactly the same form for

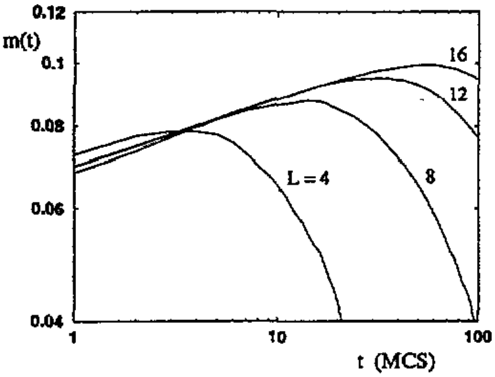

Figure 1. Magnetization profiles for $m_0 = 0.06$ and $L = 4, 8, 12, 16$ in double-logarithmic representation.

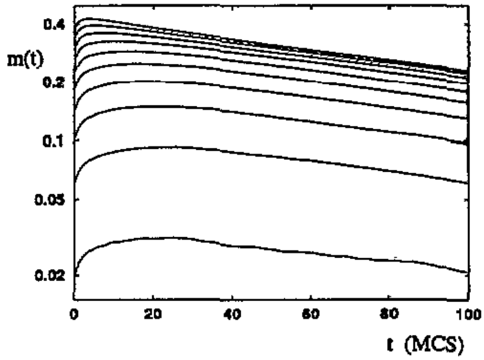

Figure 2. Magnetization profiles for $L = 10$ and $m_0 = 0.02, 0.06, \ldots, 0.38$ in semi-logarithmic representation.

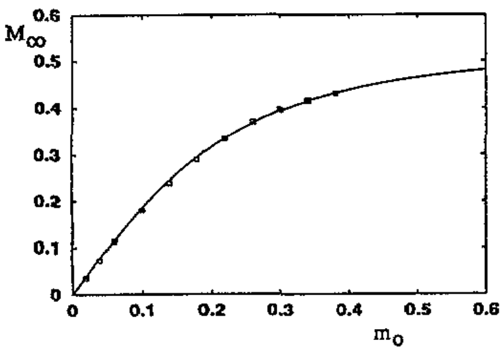

Figure 3. Amplitude of the linear decay as a function of m_0 for $L = 10$. The squares respresent the Monte Carlo results. The function fitted to them is the exact large-n solution (9).

Table 1. Monte Carlo results for θ' and x_0.

$L = 10$		$m_0 = 0.06$		Scaling analysis		
m_0	θ'	L	θ'	(L, L')	x_0	θ'
0.02	0.115(11)	16	0.102(2)	(16, 6)	0.725(13)	0.100(6)
0.04	0.105(5)	12	0.102(3)	(10, 6)	0.738(26)	0.107(13)
0.06	0.106(5)	8	0.114(10)	(16, 10)	0.710(22)	0.093(11)
0.10	0.102(6)	4	0.096(43)			

the Ising system, but apparently the scaling function for the latter is quite similar.

Finally, we test the scaling form (3) and determine directly the scaling dimension x_0 by comparing profiles from systems of different size. If (3) is satisfied, it should be possible to map curves onto each other by appropriate rescalings of m_0, m and t. To this end, we have calculated one profile for lattice size L and initial magnetization m_0 and several curves for a smaller lattice L' and a certain range of m_0'. Now the curves from the primed system can be mapped to the unprimed system by (i) multiplying by an overall factor $b^{\beta/\nu}$ and (ii) by stretching the time axis by b^z with $b = L/L'$. Here we have used the literature values $z = 2.04$ [8] and $\beta/\nu = 0.52$ [12], which are, by the way, consistent with our own data. For one example the result is shown in figure 4. The full curve is from $L = 16$ and $m_0 = 0.06$, and the three broken curves are those from $L' = 10$ and $m_0' = 0.082, 0.084$ and 0.086, respectively. (Note that due to the finite number of the degrees of freedom the increment

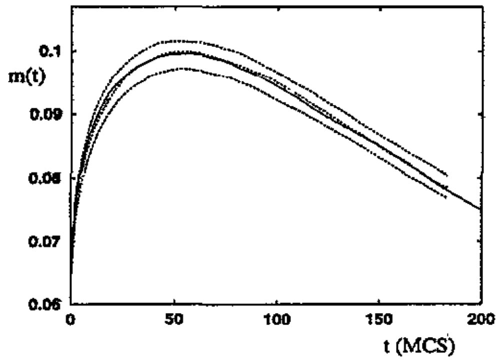

Figure 4. Test of finite-size scaling relation (3). Compared are profiles for $L = 16$ and $m_0 = 0.06$ (full curve) and $L = 10$ and $m_0 = 0.082$, 0.084, 0.086 (broken curves, from bottom to top). For details see text.

for changes of m_0' here is 0.002.) After matching the magnetizations by linear interpolation of m_0', x_0 is determined with the help of $m_0' = (L/L')^{x_0} m_0$. The results for x_0 and θ'—the latter has been computed with the help of (2)—obtained from $(L, L') = (16, 10)$, $(16, 6)$ and $(10, 6)$ are displayed in table 1. Again this may be compared to 0.67 and 0.77 from first- and second-order ϵ-expansion.

In summary, we have investigated the influence of the initial conditions on the relaxational behaviour of the three-dimensional Ising model by means of Monte Carlo simulation. The measured values of the exponents θ' and x_0 are consistent with those found by renormalization-group improved perturbation theory [1]. As demonstrated in figure 3, also the dependence of the amplitude of the linear decay on the initial magnetization agrees very well with the expectation from continuum calculations [4, 5]

Compared with what is standard today in Monte Carlo simulations in critical dynamics [8, 9], the lattices we have studied are relatively small. However, we think the results derived from our small systems are very well suited as a first step to verify the anomalous initial behaviour and other universal properties related to it, e.g. the universal dependence of the amplitude of the linear decay on m_0 and the scaling behaviour (3) as shown in figures 3 and 4. Especially, we point out that the dependence of θ' on the lattice size in the range of L studied is very weak (cf table 1). Thus, we do not expect qualitative or dramatic quantitative changes for the simulation on larger lattices, which, of course, should be carried out in the future. Besides there remains a number of other extensions of our present work, such as the investigation of correlation functions, the influence of initial correlations on the process, and the temperature dependence when one moves away from T_c.

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