Determination of the correlation length from short-time dynamics

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Abstract

We investigate the short-time dynamic relaxation of the two-dimensional XY model in the high temperature phase. Starting from the ordered state, we measure the autocorrelation function and determine the autocorrelation time. It is shown that apart from a constant the equilibrium spatial correlation length can be calculated in this way.

Key words: Short-time dynamics; Non-equilibrium kinetics; Monte Carlo simulation; spin model

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Simulations in the short-time regime [1] gain more and more importance since Janssen, Schaub and Schmittmann [2] showed that universality exists already in this early time of the evolution. Traditionally, it was believed that universal scaling behaviour can be found only in the long-time regime. However, Janssen et. al discovered that a magnetic system with non-conserved order parameter (model A[3]) quenched from a high temperature state to the critical temperature shows universal scaling behaviour already at short times. After a microscopic time $t_{\text{mic}}$, the magnetization undergoes an initial increase of the form $M(t) \sim m_0 t^\theta$, where $\theta$ is a new dynamic exponent. This prediction was supported by a number of Monte Carlo (MC) investigations [1]. These simulations offer also a possibility to determine the conventional (static and dynamic) critical exponents [4–6] as well as the critical temperature [6]. This may eliminate critical slowing down, since the measurements are performed in the early part of the evolution.

First numerical simulations of the short-time dynamical relaxation at criticality started from a high temperature initial state. However, dynamical scaling exists also for an ordered initial state. No analytical calculations exist for this situation, but MC investigations were done [1]. All static and dynamic expo-
ments — expect for the new exponent $\theta$ — as well as the critical temperature can be also obtained with an ordered initial state.

Up to now, simulations of the short-time dynamics are performed at the critical point to determine most of the critical exponents or in vicinity of the critical point to determine the exponent $1/\nu z$ and the critical temperature. However, a further important aspect of simulations is the determination of the (spatial) correlation length in the long-time regime for temperatures above $T_c$. In this letter we investigate the XY model in the high temperature phase, i.e. at finite correlation lengths. Starting from the ordered state, we measure the autocorrelation function and from this we determine the (exponential) autocorrelation time $\xi_t$. After that we test the predicted scaling behaviour with the (spatial) correlation length $\xi_s$, where the values for $\xi_s$ are taken from conventional simulations in equilibrium [7]. It is shown, that this relation can be used to calculate the correlation length (up to a constant), i.e. $\xi_s$ is determined completely from simulations in the short-time regime.

The XY model in two dimensions provides a simple model of a system with continuous symmetry. It is defined by the Hamiltonian

$$H = -\beta \sum_{\langle ij \rangle} S_i \cdot S_j,$$  \hspace{1cm} (1)

where $S_i$ denotes a planar spin of unit length at site $i$, $\beta$ is the inverse temperature ($k=J=1$) and the sum is over all nearest neighbours. This system has an exponential singularity, i.e. the correlation length diverges as $\xi_s \sim \exp(b \tau^{-\nu})$ for $\tau = (T - T_c)/T_c \to 0^+$. This behaviour is different from that of a second-order transition, where the correlation length diverges with a power law. Also, the XY system remains critical below $T_c$, i.e. the spatial correlation function decays algebraically to zero (quasi-long-range order). This absence of conventional long-range order for two-dimensional systems with continuous symmetry was proven by Mermin and Wagner [8]. A theoretical description of the transition derived from renormalization group treatment was given by Kosterlitz and Thouless (KT) [9,10]. The KT mechanism is based on a topological defect (called vortex) unbinding scenario.

Most of the simulations of the XY model are performed in the thermodynamical equilibrium. The properties at the critical line (e.g. critical exponents, critical temperature) as well as in the high temperature phase (e.g. correlation length) were examined. In general, simulations at or near the transition point are affected by the critical slowing down, i.e. an increase of autocorrelation time with $\xi_s \sim \xi_s^{\nu z}$. For some special cases, such as the Ising model or the XY model, this problem was overcome by the cluster algorithm [11,12]. Unfortunately, no generalization of this algorithm exists for most of the models (e.g. lattice QCD).
An alternative for the determination of critical exponents is short-time dynamics. The power law behaviour in the short-time regime of different observables, such as the magnetization or the cumulant as a function of time, can be used to extract all static and dynamic critical exponents. The advantage — compared to conventional simulations in equilibrium — is that critical slowing down is eliminated independently from the updating scheme, since the simulations are performed in the early part of the evolution. Therefore, in principle this method should work for any model. For the XY model the behaviour of the magnetization as a function of time starting from an unordered state was investigated and the critical exponent \( \theta \) was determined \([13]\). Also, the time evolution of the magnetization and the cumulant starting from the ordered state as well as the corresponding critical exponents were studied \([14]\). However, no simulations in the short-time regime far away from the critical line were made.

In the following, we investigate the two-dimensional XY model in the high temperature phase with short-time dynamics. We use inverse temperatures of \( \beta = 0.82 \) - 1.02, i.e. below the critical point of \( \beta_c \approx 1.1199(1) \) \([15]\). We start the relaxation process from the ordered initial state. This means that the absolute value of the magnetization \( M(t) = \frac{1}{L^2} \sum_i S_i \) at \( t = 0 \) is one, where \( L \) denotes the lattice size. The system is then released to a dynamic evolution with the Metropolis or the heatbath algorithm and the autocorrelation

\[
A(t) = \frac{1}{L^2} \left\langle \sum_i S_i(t) \cdot S_i(0) \right\rangle
\]

is measured. The autocorrelation (of the spins) \( A(t) \) is identical to the autocorrelation of the magnetization \( \langle M(t) \cdot M(0) \rangle \), since all spins in the initial state are in the same direction. Depending on the updating scheme and \( \beta \), the autocorrelation is measured up to \( t = 40000 \) MC sweeps. The lattice size range from \( L = 128 \) for \( \beta = 0.82 \) to 1024 for \( \beta = 1.02 \). In the first case we performed 4000 independent measurements (i.e. we used different random numbers), while in the latter case the average was taken over 22 independent samples.

\(^1\) Of course, the expectation value of the magnetization in the XY model in equilibrium at non-zero temperatures is zero. However, the time dependence for non-zero initial magnetization is studied.
At the critical line the autocorrelation obeys a power law \([1]\)

\[ A(t) \sim t^{-\eta/2z}, \quad (4) \]

while in the high temperature phase the behaviour can be described by the ansatz

\[ A(t) \sim t^{-\eta/2z} \exp(-t/\xi_t). \quad (5) \]

The autocorrelation measured for different values of \(\beta\) is plotted in Fig. 1, where we used the Metropolis algorithm. Figure 1(a) shows the autocorrelation in a log-log scale to clarify the power law behaviour for small \(t\), while the lin-log scale of Fig. 1(b) exhibits the exponential decay at larger times.

Statistical errors of \(A(t)\) are of the order of 1%. For microscopic times \(t_{mic}\) up to approximately 50 sweeps\(^2\) there are deviations from the ansatz (5). This is similar to simulations at the critical point [1]. Therefore, we left out the data for such small \(t\), when we determined the (exponential) autocorrelation time \(\xi_t\) by fitting the data according to Eq. (5). In all fits the value of \(\eta/2z\) is an independent fit parameter, i.e. the value depends on the temperature. The value decreases from about 0.14 at \(\beta = 0.82\) to approximately 0.11 at \(\beta = 1.02\). The autocorrelation is always well described by the ansatz (5), i.e. the \(\chi^2\) per degree of freedom is smaller than one. Statistical errors of \(\xi_t\) are obtained by dividing the data into subsamples and performing the analysis on these independent sets. The usage of different time intervals (i.e. different

\(^2\) The exact value depends on \(\beta\). The criterion for the determination of \(t_{mic}\) was that increasing the value does not lead to an essential change in the fit parameter or \(\chi^2\). At \(\beta = 0.81\) we left out 10 – 80 sweeps, while we skipped the values of the first 20 – 800 sweeps at \(\beta = 1.02\).
Fig. 2. Autocorrelation as a function of time at $\beta = 0.98$ in a lin-log scale for different system sizes.

$t_{\text{mic}}$ yields an estimate for the systematic error. The quoted error is the sum of statistical and systematic error.

Finite-size effects were studied for lattice sizes of $L = 32, 64, 128, 256$ and $512$ at $\beta = 0.98$. Figure 2 shows the result for $L = 32, 64$ and $512$. Only the two smallest lattices show finite-size effects, while the results for $L = 128$ and $256$ coincide within statistical errors with the data of the largest lattice in the time interval $t = [0, 4000]$. For that reason, we omitted these curves in the figure. The MC time when a system starts to show finite-size effects scales with $L^z$. Thus the lattice size of $L = 512$ — which was used to determine $\xi_t$ at $\beta = 0.98$ — is large enough to avoid additional errors coming from a too small system. Correspondingly, also the lattice sizes for the simulations at the other temperatures are chosen large enough.

The autocorrelation time $\xi_t$ is related to the spatial correlation length (in equilibrium) by

$$\xi_t = c \xi_s^z .$$

(6)

This relation is often used to determine the dynamic critical exponent $z$ from simulations in equilibrium [16] by measuring the autocorrelation time\(^3\) as a function of the correlation length. In the following we examine the behaviour of $\xi_t$ as a function of $\xi_s$, where we have taken the values of $\xi_s$ from Ref. [7]. In principle we could simply plot $\xi_t$ versus $\xi_s$ in a double logarithmic scale. However, in case of a dynamic critical exponent of $z \approx 2$ the behaviour can be seen clearer, if we plot $\xi_t^{1/2}/\xi_s$ for $\xi_s \to \infty$. This is done in Fig. 3 for the MC dynamics with the Metropolis algorithm in a double logarithmic scale. For a constant value of $c$ we should see a straight line. The slope gives the value

\(^3\) Usually, in simulations in equilibrium the integrated autocorrelation time is used.
Test of the scaling relation \( \xi_t = c \xi_s^{z/2} \) using the Metropolis algorithm. The slope in the double logarithmic scale gives the value \( z/2 - 1 \). The dashed line shows a linear fit.

\( z/2 - 1 \). It is visualized by a dashed line and was obtained from a linear fit. The data seem to indicate that \( c \) is indeed a constant and the value of \( z \) is 2.19(3).

To clarify the situation we also made simulations using the heatbath algorithm. We expect that corrections to the scaling behaviour (6) far away from the critical point are smaller than in case of the Metropolis algorithm. The reason is that at very high temperatures \( (T \to \infty, \xi_s \to 0) \) the autocorrelation time \( \xi_t \) goes to zero for the heatbath algorithm, while it approaches a non-zero constant in case of the Metropolis algorithm. Our results are visualized in Fig. 4. Again, we see an almost straight line with non-zero slope of about 0.07(1), i.e. \( z = 2.14(2) \). Taking both values together we get \( z = 2.16(2) \). This value is similar to those of two-dimensional systems with a second order transition such as the Ising, 3-state Potts or SU(2) model, and with a KT-like transition as the 6-state clock model [1]. Using Eq. (6) with our value of \( z \) and \( c \), we could now determine the correlation length from short-time dynamics by measuring the autocorrelation time \( \xi_t \).

We have seen that short-time dynamic simulations can be used to determine \( \xi_t \). But also the dynamic critical exponent \( z \) can be easily extracted from short-time critical dynamics simulations. The costs for these measurements are low, because they are not affected by critical slowing down. This can be done, e.g., by measuring the dynamic relaxation of the cumulant

\[
\bar{U}(t) = \frac{M^{(2)}(t)}{(M(t))^2} - 1 .
\]

Here \( M^{(2)}(t) \) is the second moment of the magnetization. At the critical point \( \bar{U}(t) \) obeys a power law \( \bar{U}(t) \sim t^{-d/z} \), where \( d \) is the dimension of the system.
In case of the XY model this was already done for the Metropolis and the heatbath algorithm [14]. However, the result of $z = 1.97(4)$ is different from our value.

Short-time critical dynamics simulations to determine the critical exponents are not effected by the critical slowing down. The situation for the measurement of $\xi_t$ in the high temperature phase is different. The MC time which is necessary to determine $\xi_t$ is $O(\xi_t)$, i.e. it scales with $\xi_s^z$. Therefore, the situation is the same as for the simulations in equilibrium with the same algorithms, i.e. critical slowing down is not eliminated and the the CPU time to determine $\xi_s$ scales in the same way. In our simulations (Metropolis and heatbath algorithm) we have a dynamic critical exponent of $z \approx 2$, but we could also use different algorithms and improve the scaling behaviour. While the scaling behaviour of the CPU time for the determination of $\xi_s$ is the same for simulations in the short-time regime and in equilibrium, the total CPU time can be different. Also, in the short-time simulation there is no problem to warm-up the system. Often a large part of simulations in equilibrium is only used to reach the long-time regime. Of course, in the XY model this problem does not appear, if one uses the cluster algorithm. However, for many other model there exists no generalization of this algorithm.

In summary, we have shown for the XY model that short-time dynamic relaxation can be used to determine the (spatial) correlation length. This can be done by measuring the autocorrelation time and the dynamic critical exponent with short-time dynamic relaxation and using Eq. (6). However, at least one value of the correlation length (preferably near the critical point) is necessary to fix the constant $c$. These measurements did not fight critical slowing down. Nevertheless, the absolute CPU time to measure the correlation length with short-time simulations can be smaller than the corresponding simulations in equilibrium.
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