Monte Carlo Simulation of the Short-time Behaviour of the Dynamic XY Model

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Abstract

Dynamic relaxation of the XY model quenched from a high temperature state to the critical temperature or below is investigated with Monte Carlo methods. When a non-zero initial magnetization is given, in the short-time regime of the dynamic evolution the critical initial increase of the magnetization is observed. The dynamic exponent $\theta$ is directly determined. The results show that the exponent $\theta$ varies with respect to the temperature. Furthermore, it is demonstrated that this initial increase of the magnetization is universal, i.e. independent of the microscopic details of the initial configurations and the algorithms.

PACS: 64.60.Ht, 75.10.Hk, 02.70.Lq, 82.20.Mj
1 Introduction

Recently much attention has been drawn to the short-time universal scaling behaviour of critical dynamic systems. A typical example is the dynamic relaxation of magnetic systems quenched from a high temperature state to the critical temperature. After a time period enough long in the microscopic sense, during which the non-universal short wave behaviour is swept away, the universal scaling behaviour appears. Such a time period is called the microscopic time scale $t_{\text{mic}}$. $t_{\text{mic}}$ is in general very small compared with the macroscopic time scale, which is typically $t_{\text{mac}} \sim \tau^{-\nu z}$ or $t_{\text{mac}} \sim L^z$. Here $\tau$ is the reduced temperature and $L$ is the lattice size of the systems, while $\nu$ and $z$ are the critical exponents. At this macroscopic early stage of the time evolution, important is that even though the spatial correlation length of the systems is still very small in the macroscopic sense, due to the infinite time correlation length the dynamic systems already evolve universally. This is out of the traditional belief that the universal dynamic scaling emerges only when the spatial correlation length becomes very big.

One interesting phenomenon is that, if a non-zero magnetization is given to the initial state at very high temperature, at the macroscopic early time the magnetization surprisingly undergoes a critical initial increase \[ M(t) \sim m_0 t^\theta, \] where $\theta$ is a new critical exponent which is independent of the static exponents $\beta$, $\nu$ and the dynamic exponent $z$. The exponent $\theta$ is related to the dimension $x_0$ of the initial magnetization $m_0$ by $\theta = (x_0 - \beta/\nu)/z$. The magnetization continues the increase in a time scale $t \sim m_0^{-z/x_0}$, then reaches its maximum and crosses over to the well known long-time universal behaviour.

Numerically the critical increase of the magnetization has directly been observed \[ \text{[3, 4, 5, 6, 7, 8].} \] The critical exponent $\theta$ was determined to a satisfactory accuracy for the two dimensional Ising model and Potts model \[ \text{[9] as well as the 6-state clock model [7].} \] Numerical results show rather clean short-time scaling behaviour. However, all these models are relatively simple and the spins locate in discretized configuration spaces. It would be very interesting to investigate whether there exists short-time scaling behaviour in more complex models.

More important, up to now almost all the numerical simulations for the short-time dynamics have been done with the heat-bath algorithm. For the heat-bath algorithm the microscopic time scale $t_{\text{mic}}$ for the two dimensional Ising and Potts model is not bigger than one or two Monte Carlo time steps. This is a miracle. If one Monte Carlo time step is typically the microscopic time unit, one would expect that $t_{\text{mic}}$ should be around $10 \sim 50$ Monte Carlo time steps. Even though the scaling form in the short-time dynamics and its applications have extensively been investigated, it is already overdue to understand universality in
the short-time dynamics, i.e. whether the short-time scaling behaviour is really independent of the algorithms, lattice types and other microscopic details.

In a recent paper [9], the authors have carefully analysed the short-time behaviour of the critical dynamics for the two dimensional Ising model and Potts model. Simulations have been performed with both the heat-bath and the Metropolis algorithm. Indeed, it is only by chance that for the heat-bath algorithm $t_{mic}$ is negligibly small. Actually for the Metropolis algorithm, $t_{mic} \sim 30$. Within the time period up to $t_{mic}$, the dynamic behaviour for the Metropolis algorithm is very different from that of the heat-bath algorithm. When $t > t_{mic}$, however, the dynamic systems with both algorithms present the same universal behaviour. The measured values of the critical exponent $\theta$ are compatible within the statistical errors. This is a first step to the verification of universality in the short-time dynamics. More understanding is urgent and important.

In this paper, we will report results for the numerical simulations of the short-time dynamics of the two dimensional XY model. Special attention will be put on universality. In the next section a short description of the XY model is given. In the section 3, the numerical data are presented and conclusions are given in section 4.

## 2 The XY model

The XY model in two dimensions is defined by the Hamiltonian

$$H = K \sum_{<ij>} \vec{S}_i \cdot \vec{S}_j,$$  \hspace{1cm} (2)

where $\vec{S}_i = (S_{i,x}, S_{i,y})$ is a planar unit vector at site $i$ and the sum is over the nearest neighbours. In our notation the inverse temperature has been absorbed in the coupling $K$.

The XY model is the simplest statistical system which exhibits a continuous symmetry. It is known that at a certain critical temperature the XY model undergoes a Kosterlitz-Thouless phase transition [11, 12]. Near the critical temperature the spatial correlation length diverges exponentially rather than by a power law as in the normal second order phase transition. Below the critical temperature the system remains critical in the sense that the spatial correlation length is divergent. No real long range order emerges in the XY model. The $O(2)$ symmetry of the XY model stays unbroken in the whole temperature regime.

The XY model is a very important model since it describes the critical properties of the superfluid helium. It is closely related to the $O(2)$ $\sigma$-model in field

\[1\] Very recently some discussions on universality in short-time dynamics for the two dimensional Ising model have also been made with respect to the lattice types and update schemes even though the critical exponent $\theta$ there was not confidently extracted due to relative small lattices or some other reasons [8, 10].
theory. Its generalization such as fully frustrated XY model attracts more and more attention [13, 14, 15]. The XY model is also a good laboratory to study the more general Heisenberg model.

However, due to the exponentially divergent spatial correlation length, the numerical simulation of the XY model is very difficult. Even though some papers can be found concerning the dynamic properties of the XY model [16, 17], our knowledge about the dynamic XY model is still very poor. In this paper we will investigate the short-time universal behaviour of the dynamic XY model. We will concentrate on the critical initial increase of the magnetization and measure the critical exponent $\theta$. Special attention will be put on universality. Different from the case of the Ising model, where the spins take only the values $\pm 1$, the spin configuration space for the XY model is a unit circle. This non-trivial configuration space allows us to investigate whether the short-time universal behaviour depends on the microscopic details of the initial configurations.

3 Numerical simulations

Following Janssen, Schaub and Schmittmann’s idea [1], we investigate a dynamic relaxation process starting from an initial state with very high temperature and small magnetization. As a first approach to the dynamic XY model, we do not consider the effects of the vortices. The very high initial temperature requests that the spin at each lattice site is generated independently. However, the way how to generate a non-zero initial magnetization in a certain direction is not unique. A natural way is to introduce an initial external field, e.g. in the $x$ direction, as it was used in the numerical simulation of the clock model [7]. Then the initial Hamiltonian, i.e. that for generating the initial magnetization, can be written as

$$H_{01} = 2\sum_i S_{i,x}. \tag{3}$$

If we define the magnetization as

$$\vec{M}(t) = \frac{1}{L^2} \sum_i \vec{S}_i \tag{4}$$

with $L$ being the lattice size, the initial Hamiltonian $H_{01}$ gives an initial magnetization

$$\vec{M}(0) = (m_0, 0) \approx (h, 0), \quad h \to 0. \tag{5}$$

In this paper we are only interested in the case of small $m_0$.

To prepare the initial state, we update the system described by the initial Hamiltonian $H_{01}$ until it reaches equilibrium. Then the generated configurations of this initial system are used as the initial configurations of the dynamic system. If the lattice size is infinity, in each initial configuration an exact value $(m_0, 0)$ of
the initial magnetization $\vec{M}(0)$ is automatically achieved. However, the practical lattice size is finite and the initial magnetization $\vec{M}(0)$ fluctuates around $(m_0, 0)$. This is a kind of extra finite size effect. It causes a problem in a high precision measurement. In order to reduce this effect, a sharp preparation technique has been introduced to adjust the initial magnetization in the numerical simulations of the Ising model and the Potts model [3, 4, 18]: we randomly take one spin on the lattice and flip the spin if the updated magnetization comes nearer to the expected value; we repeat this procedure until the expected initial magnetization is achieved. Numerical data show that the sharp preparation technique improves efficiently the results and especially helps to obtain better results in relatively small lattices.

In the numerical simulation of the XY model, we also implement the sharp preparation technique. However, due to the fact that spins in the XY model are planar unit vectors, this procedure becomes slightly more complicated. We proceed in the following way:

(i) If the configuration generated by the initial Hamiltonian $H_0$ does give the value $<S_x> = m$ but not $m_0$, we update a randomly chosen spin. If the resulting magnetization $<S_x>$ is nearer to $m_0$, we accept it otherwise keep the old configuration. We continue in this way until the difference $|m - m_0| < \delta$ with $\delta$ being a certain given small value. In our simulations we take $\delta$ to be 2.5 percent of $m_0$;

(ii) After having adjusted $<S_x>$, we turn to the magnetization $<S_y>$. If $|<S_y>| > \delta$, we randomly select a spin $\vec{S}_i = (S_{i,x}, S_{i,y})$ and change the sign of $S_{i,y}$. If $|<S_{i,y}|$ becomes smaller, we accept the new configuration otherwise keep the old one. We continue until $|<S_y>| < \delta$. In this procedure (ii), the value $<S_x> = m$ already prepared in (i) remains unchanged.

After the preparation of the initial configuration, the system is released to a dynamic evolution at the critical temperature or below with the Metropolis or the heat-bath algorithm. We have performed the simulations for lattice sizes $L = 8, 16, 32, 64$ and 128. The magnetization is measured up to Monte Carlo time step $t = 150$. The average is taken over 40 000 samples with independent initial configurations for the lattice size $L \leq 64$ and 12 000 – 30 000 samples for the lattice size $L = 128$ depending on the initial magnetization. For smaller $m_0$ we take relatively large statistics. Errors are estimated by dividing the data into three or four groups. In this paper we take the critical temperature of the XY model from the literature [19], $T_c = 1/K_c = 0.90$. Unless we explicitly specify, all the discussions below are assumed to be at the critical temperature.

In Fig. 1, the time evolution of the magnetization at the critical temperature with the initial magnetization $m_0 = 0.02$ for the Metropolis algorithm is displayed for different lattice sizes. In the figure $M(t)$ is the $x$ component of the magnetization $\vec{M}(t)$. The $y$ component of the magnetization $\vec{M}(t)$ remains zero since the initial value is zero. From the figure we can see that for $L = 64$ the finite size
effect is already very small and the curve almost completely overlaps with that of $L = 128$. We have discussed above that the universal behaviour appears only after a microscopic time scale $t_{\text{mic}}$. Theoretically one would expect and it is also observed in the cases of the two dimensional Ising model and Potts model that $t_{\text{mic}}$ is in general around $10 \sim 50$. In Fig. 1 one can see this clearly. In the first 30 time steps there is no universal power law behaviour but after that it indeed appears. From the slope of the curve one may measure the critical exponent $\theta$.

How important is the sharp preparation of the initial magnetization? This practically depends on how big the lattice size and how small the initial magnetization $m_0$ is. On the other hand, since the exponent $\theta$ is defined in the limit $m_0 = 0$, the practically measured exponent $\theta$ from the power law behaviour (1) shows in general some weak dependence on $m_0$ when $m_0$ is finite. The stronger the dependence of $\theta$ on $m_0$ is, the more important becomes the sharp preparation. In Fig. 2, the magnetization without a sharply prepared initial magnetization is displayed for different lattice sizes. For comparison, the dotted line shows that with a sharply prepared initial magnetization for the lattice size $L = 64$. Comparing Fig. 1 and Fig 2 we see that the difference between the curves with and without the sharp preparation of the initial magnetization becomes already quite small when the lattice size reaches $L = 64$. Such a small difference is also partly due to the quite weak dependence of $\theta$ on $m_0$, which can be seen later.

With the sharp preparation of the initial magnetization, the exponent $\theta$ measured from lattice size $L = 64$ and 128 are $\theta = 0.250(1)$ and $0.249(4)$ respectively. Within the statistical errors we already can not distinguish the results for the lattice size $L = 64$ and $L = 128$. Without the sharp preparation of the initial magnetization, we get the exponent $\theta = 0.252(2)$ for lattice size $L = 64$, which shows a slightly bigger value and fluctuation compared with that with the sharp preparation of the initial magnetization even though the difference is small. In the following simulations, the sharp preparation technique is always adopted.

Is the power law scaling behaviour (1) really universal? Would it depend on the microscopic details of the initial configurations, algorithms and lattice types and so on? In this paper we will show that the power law behaviour is indeed independent of the microscopic details of the initial configurations and the algorithms.

In order to generate an initial state with a non-zero magnetization, using the initial Hamiltonian $H_{01}$ given in (3) is a natural way but by no means unique. An example of alternative methods may be the following: in each lattice site, the spin orients towards the pure positive $x$ direction ($S_{i,x} = 1$, $S_{i,y} = 0$) with a certain probability, otherwise randomly. This initial state can be described by an initial Hamiltonian

$$H_{02} = \sum_i \ln (c_2 \delta(\phi_i) + 1).$$

Here the angle $\phi_i$ is defined by $S_{i,x} = \cos \phi_i$ and $S_{i,y} = \sin \phi_i$. Properly choosing the constant $c_2$ one obtains the expected initial magnetization $m_0$. Another
possibility is: assuming that the orientation of initial spins is restricted to either pure $x$ or pure $y$ direction, we give a slightly bigger probability to generate spins in the positive $x$ direction than in others. The corresponding initial Hamiltonian is

$$H_{03} = \sum_i \ln \left( c_3 \delta(\phi_i) + \delta(\phi_i - \pi) + \delta(\phi_i - \pi/2) + \delta(\phi_i + \pi/2) \right).$$

(7)

It is clear that the preparation of the initial configurations given by $H_{02}$ and $H_{03}$ is rather simple [3, 4, 9].

| $m_0$ | $0.02$ | $0.01$ |
|-------|--------|--------|
| $H_{01}$ | $0.249(4)$ | $0.252(4)$ |
| $H_{02}$ | $0.248(4)$ | $0.252(7)$ |
| $\theta$ | $0.248(4)$ | $0.252(7)$ |

Table 1: The exponent $\theta$ measured for lattice size $L = 128$ with different types of initial configurations and algorithms.

| $T$ | $0.90$ | $0.86$ | $0.70$ | $0.50$ | $0.30$ |
|-----|--------|--------|--------|--------|--------|
| $\theta$ | $0.250(1)$ | $0.264(5)$ | $0.287(3)$ | $0.283(4)$ | $0.282(1)$ |

Table 2: The exponent $\theta$ measured for different temperatures with the Metropolis algorithm. The lattice size is $L = 64$.

In Fig. the time dependent magnetization for different types of initial configurations is plotted for the lattice size $L = 128$. The solid lines above and below are the results for an initial magnetization $m_0 = 0.02$ and $m_0 = 0.01$ generated from $H_{01}$. The dotted line is the magnetization with $m_0 = 0.02$ from $H_{02}$, and the dashed line corresponds to that of $m_0 = 0.01$ with $H_{03}$. In Table 1 the corresponding $\theta$ measured in a time interval $[40, 150]$ are listed. We see that all three initial Hamiltonians give almost the same results. The difference of the initial configurations is swept away in more or less one Monte Carlo time step. Furthermore, the difference of $\theta$ measured from different initial magnetizations $m_0$ is quite small and already within the statistical errors. Therefore the extrapolation of $\theta$ to the limit $m_0 = 0$ is not necessary here. This is also one of the reasons why the results with and without the sharp preparation of the initial magnetization are not so different.

Before we continue the discussions of the numerical data, we would like to make some comments here. For years it is believed that two exponents $\beta$ and $\nu$ sufficiently describe the critical scaling properties of most magnetic systems in
equilibrium and the dynamic scaling properties can be described by the dynamic exponent $z$. An essential point in the short-time dynamic scaling exists in the claim that an independent critical exponent $x_0$ (or $\theta$) should be introduced to specify the dependence of the scaling behaviour on the initial magnetization. In principle, however, there are other choices for the scaling variable. For example, the initial magnetic field $h$ in $H_{01}$ may also be used. Some discussions concerning what is a better choice of the scaling variable has recently been made \[20, 18, 21\]. In our numerical simulations, we have demonstrated that a non-zero initial magnetization $m_0$ can be realized in different ways, by introducing either an initial magnetic field with $H_{01}$ or some other initial systems described by $H_{02}$ or $H_{03}$. However, the exponent $\theta$ is the same for different types of initial configurations. Therefore these different ways may be considered as the microscopic details for the initial state. Introducing an initial magnetic field is only one possibility to generate a non-zero initial magnetization. In this sense, the scaling variable $m_0$ seems to be more general.

Now let us come back to our discussions of the numerical results. In Fig. 3 the time evolution of the magnetization with $m_0 = 0$ is also displayed by the solid line in between. In the first $20 \sim 30$ time steps, its behaviour is different from that with the Metropolis algorithm. After that, however, as in the case of the Metropolis algorithm it stabilizes to the universal power law behaviour. To see this more clearly, in Fig. 4 we have plotted the exponent $\theta$ as a function of the time $t$ for both the heat-bath and the Metropolis algorithm. The exponent $\theta$ at time $t$ is measured as the slope of the curve in a time interval $[t, t + 20]$. Error bars are estimated by dividing the total sample into three groups. After a microscopic time scale $t_{mic} \sim 20 - 30$, the exponents $\theta$ for both the heat-bath and the Metropolis algorithm overlap each other. The relatively small error bars for the exponent $\theta$ at certain time periods may come from the fact that the errors are estimated from only three groups of the data. The final values for $\theta$ are given in Table 1. The results for both the heat-bath and the Metropolis algorithm are also consistent within the statistical errors. All these results strongly support universality in the short-time dynamics.

Finally we have also performed the simulations with the Metropolis algorithm for the temperature below the critical temperature. Since the XY model remains critical, a similar scaling form is expected. In Fig. 5, the magnetization for $L = 64$ and different temperatures is plotted versus time $t$ in double-log scale. For the temperatures $T = 0.90$ and $0.86$ the initial magnetization is $m_0 = 0.02$. For the temperatures $T = 0.70, 0.50$ and $0.30$ the initial magnetization is $m_0 = 0.01$. As before, the weak dependence of the exponent $\theta$ on $m_0$ has not been considered since it is within our statistical errors. The exponent $\theta$ measured in a time interval $[40, 150]$ for different temperatures is listed in Table 2. It is known that in the equilibrium the critical exponents in general depend on the temperature. Here we see the exponent $\theta$ also varies with respect to the temperature. This situation is similar to that of the clock model \[7\].
4 Conclusions

We have numerically investigated the short-time behaviour of the dynamic relaxation of the two dimensional XY model at the critical temperature and below, starting from an initial state with a very high temperature and non-zero magnetization. The critical initial increase of the magnetization is observed and the exponent $\theta$ is determined. The results show that as the temperature decreases, the exponent $\theta$ first increases rather rapidly and then decreases slowly. The independence of the scaling behaviour on the microscopic details of the initial configurations and the algorithms is demonstrated and the microscopic time scale $t_{\text{mic}} \sim 30$. Universality in the short-time dynamics is confirmed. Further extension of this work remains important, such as the determination of the critical temperature and the static exponents from the short-time dynamics and an investigation of the effects of the vortices.
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Figure 1: The time evolution of the magnetization for the XY model with $m_0 = 0.02$ for different lattice sizes with the Metropolis algorithm is plotted in double-log scale. $M(t)$ is the $x$ component of the magnetization $M(t)$. The sharp preparation technique for the initial magnetization is adopted.
Figure 2: The time evolution of the magnetization for the XY model with \( m_0 = 0.02 \) for different lattice sizes with the Metropolis algorithm is plotted in double-log scale. The sharp preparation technique for the initial magnetization is not adopted. The dotted line shows the magnetization with the sharp preparation for \( L = 64 \) for comparison.
Figure 3: The time evolution of the magnetization for the XY model for lattice size $L = 128$ with different types of initial configurations and algorithms is plotted in double-log scale. The sharp preparation technique for the initial magnetization is adopted. The solid lines are those obtained with the initial Hamiltonian $H_{01}$. The solid lines above and below correspond to $m_0 = 0.02$ and 0.01 with the Metropolis algorithm. The solid line in between is that for the heat-bath algorithm with $m_0 = 0.01$. The dotted line is for the Metropolis algorithm with $m_0 = 0.02$ prepared with $H_{02}$ and the dashed line is for the Metropolis algorithm with $m_0 = 0.01$ prepared with $H_{03}$. 
Figure 4: The exponent $\theta$ measured as a function of time $t$ for both the heat-bath and the Metropolis algorithm with $m_0 = 0.01$ and $L = 128$. $\theta(t)$ is obtained in a time interval $[t, t + 20]$. The sharp preparation technique for the initial magnetization is adopted.
Figure 5: The time evolution of the magnetization for lattice size $L = 64$ and different temperatures with the Metropolis algorithm is plotted in double-log scale. The sharp preparation technique for the initial magnetization is adopted. The temperature parameters are $T = 0.90, 0.86, 0.70, 0.50$ and $0.30$ (from below).