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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 θ is directly determined. The results show that the exponent θ 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.

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 long enough 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 timescale t_{mic}. t_{mic} is in general very small compared with the macroscopic timescale, which is typically $t_{\mathrm{mac}} \sim \tau^{-\nu z}$ or $t_{\mathrm{mac}} \sim L^z$. Here τ is the reduced temperature and L is the lattice size of the systems, while ν and z are the critical exponents. At *this macroscopic early stage of the time evolution*, it is important 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 a very high temperature, at the macroscopic early time the magnetization surprisingly undergoes *a critical initial increase* [1, 2]

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

where θ is a new critical exponent which is independent of the static exponents β, ν and the dynamic exponent z. The exponent θ 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 timescale $t \sim m_0^{-z/x_0}$, 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 [3–8]. The critical exponent θ was determined to a satisfactory accuracy for the two-dimensional

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Ising model and Potts model [9] as well as the six-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 short-time scaling behaviour exists in more complex models.

More important, up to now almost all the numerical simulations for the short-time dynamics have been done with the heatbath algorithm. For the heatbath algorithm the microscopic timescale $t_{\rm mic}$ 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 $t_{\rm mic}$ 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, the understanding of universality in the short-time dynamics is already overdue, 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 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 heatbath and the Metropolis algorithm. Indeed, it is only by chance that for the heatbath algorithm $t_{\rm mic}$ is negligibly small. Actually, for the Metropolis algorithm, $t_{\rm mic} \sim 30$. Within the time period up to $t_{\rm mic}$, the dynamic behaviour for the Metropolis algorithm is very different from that of the heatbath algorithm. When $t > t_{\rm mic}$, however, the dynamic systems with both algorithms present the same universal behaviour. The measured values of the critical exponent θ 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 given to universality. In the next section a short description of the XY-model is given. In section 3, the numerical data are presented. Conclusions are given in section 4.

2. The XY-model

The XY-model in two dimensions is defined by the Hamiltonian

$$H = K \sum_{\langle ij \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \tag{2}$$

where $\boldsymbol{S}_i = (S_{i,x}, S_{i,y})$ 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 [11, 12] phase transition. 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 remains 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) σ-model in field theory. Its generalization

† 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 θ there was not confidently extracted due to relatively small lattices or some other reasons [8, 10].

such as fully frustrated XY-model attracts more and more attention [13–15]. 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 θ. Special attention will be given to universality. Different from the case of the Ising model, where the spins take only the values ± 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 *et al*'s idea [1], we investigate a dynamic relaxation process starting from an initial state with a 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 of generating a non-zero initial magnetization in a certain direction is not unique. A natural way is to introduce an initial external field, for example 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

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

If we define the magnetization as

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

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

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

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 $\boldsymbol{M}(0)$ is automatically achieved. However, the practical lattice size is finite and the initial magnetization $\boldsymbol{M}(0)$ 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, 9, 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 efficiently improves 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 as follows.

(i) If the configuration generated by the initial Hamiltonian H_{01} does give the value $\langle S_x \rangle = m$ but not m_0, we update a randomly chosen spin. If the resulting magnetization $\langle S_x \rangle$ 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 δ as a certain given small value. In our simulations we take δ to be 2.5% of m_0.

(ii) After adjusting $\langle S_x \rangle$, we turn to the magnetization $\langle S_y \rangle$. If $|\langle S_y \rangle| > \delta$, we randomly select a spin $\boldsymbol{S}_i = (S_{i,x}, S_{i,y})$ and change the sign of $S_{i,y}$. If $|\langle S_{i,y} \rangle|$ becomes smaller, we accept the new configuration otherwise keep the old one. We continue until $|\langle S_y \rangle| < \delta$. In this procedure (ii), the value $\langle S_x \rangle = m$, 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 heatbath algorithm. We have performed the simulations for lattice sizes $L = 8$, 16, 32, 64, 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 $L \leqslant 64$ 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 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 figure 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 figure 1, $M(t)$ is the x-component of the magnetization $\boldsymbol{M}(t)$. The y-component of the magnetization $\boldsymbol{M}(t)$ 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 timescale t_{mic}. Theoretically one would expect, and it is also observed in the cases of the two-dimensional Ising model and Potts model,

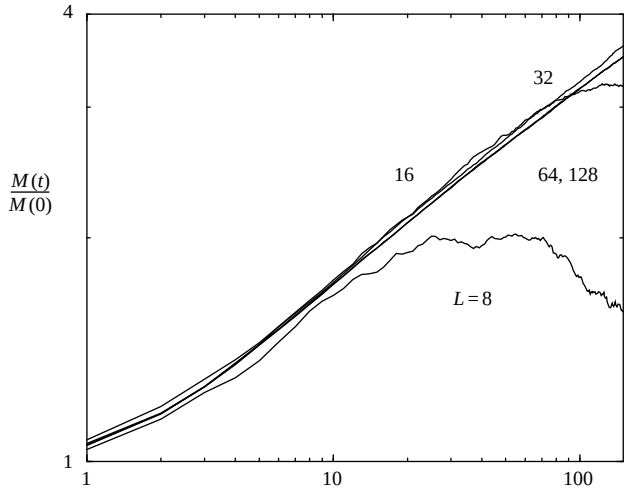

Figure 1. The time evolution of the magnetization for the XY-model with $m_0 = 0.02$ for different lattice sizes with the Metropolis algorithm is plotted on double-log scale. $M(t)$ is the x-component of the magnetization $\boldsymbol{M}(t)$. The sharp preparation technique for the initial magnetization is adopted.

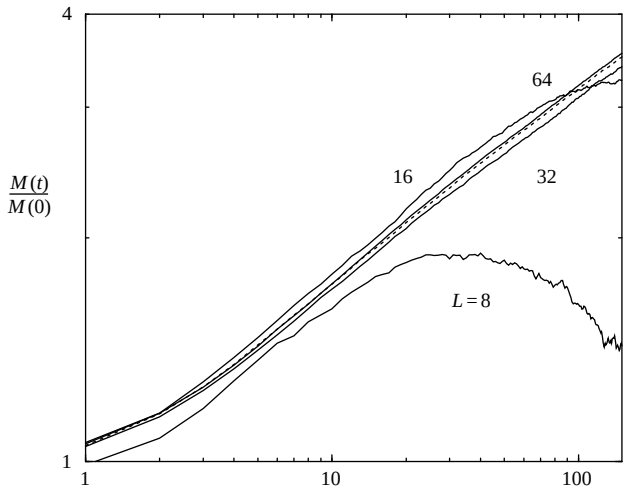

Figure 2. The time evolution of the magnetization for the XY-model with $m_0 = 0.02$ for different lattice sizes with the Metropolis algorithm is plotted on double-log scale. The sharp preparation technique for the initial magnetization is *not* adopted. The dotted curve shows the magnetization with the sharp preparation for $L = 64$ for comparison.

that $t_{\rm mic}$ is in general around $10 \sim 50$. In figure 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 θ.

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

With the sharp preparation of the initial magnetization, the exponent θ measured from lattice size $L = 64$ and 128 are $\theta = 0.250(1)$ and $0.249(4)$ respectively. Within the statistical errors we cannot yet 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 of 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 etc? 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

$$H_{02} = \sum_i \ln(c_2\delta(\phi_i) + 1). \tag{6}$$

Here the angle ϕ_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 y-direction, we give a slightly bigger probability to generate spins in the positive x-direction than in others. The corresponding initial Hamiltonian is

$$H_{03} = \sum_i \ln(c_3\delta(\phi_i) + \delta(\phi_i - \pi) + \delta(\phi_i - \pi/2) + \delta(\phi_i + \pi/2)). \tag{7}$$

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

In figure 3 the time-dependent magnetization for different types of initial configurations is plotted for the lattice size $L = 128$. The full curves 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 curve is the magnetization with $m_0 = 0.02$ from H_{02}, and the broken curve corresponds to that of $m_0 = 0.01$ with H_{03}. In table 1 the corresponding θ 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

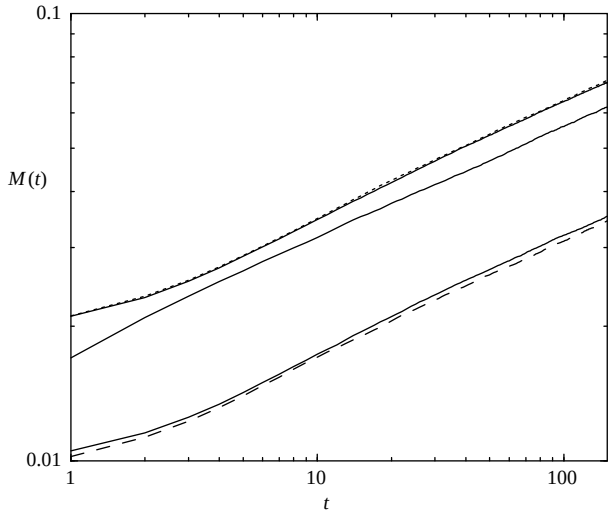

Figure 3. The time evolution of the magnetization for the XY-model for lattice size $L = 128$ with different types of initial configurations and algorithms is plotted on double-log scale. The sharp preparation technique for the initial magnetization is adopted. The full curves are those obtained with the initial Hamiltonian H_{01}. The full curve above and below correspond to $m_0 = 0.02$ and 0.01 with the Metropolis algorithm. The full curve in between is that for the heatbath algorithm with $m_0 = 0.01$. The dotted curve is for the Metropolis algorithm with $m_0 = 0.02$ prepared with H_{02} and the broken curve is for the Metropolis algorithm with $m_0 = 0.01$ prepared with H_{03}.

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

	Metropolis				Heatbath
m_0	0.02		0.01		0.01
	H_{01}	H_{02}	H_{01}	H_{03}	H_{01}
θ	0.249(4)	0.252(4)	0.248(4)	0.252(7)	0.253(5)

time step. Furthermore, the difference of θ measured from different initial magnetizations m_0 is quite small and already within the statistical errors. Therefore the extrapolation of θ 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 to discuss the numerical data, we would like to make some comments. For years it has been believed that two exponents β and ν 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 θ) 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. There have recently been some discussions concerning what is a better choice of the scaling variable [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 θ 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 on the numerical results. In figure 3 the time evolution of the magnetization with $m_0 = 0.01$ with the heatbath algorithm is also displayed by the full curve in between. In the first $20 \sim 30$ time steps, its behaviour is different from that of 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 figure 4 we have plotted the exponent θ as a function of the time t for both the heatbath and the Metropolis algorithm. The exponent θ 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 timescale $t_{\rm mic} \sim 20$–30, the exponents θ for both the heatbath and the Metropolis algorithm overlap each other. The relatively small error bars for the exponent θ at certain time periods may come from the fact that the errors are estimated from only three groups of data. The final values for θ are given in table 1. The results for both the heatbath 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 figure 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

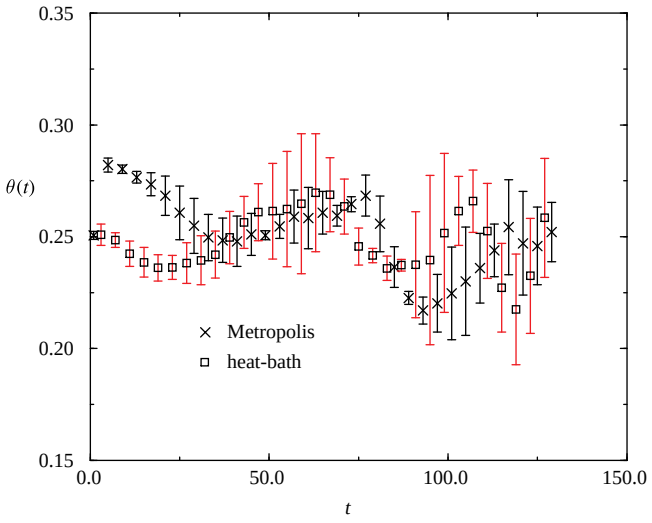

Figure 4. The exponent θ measured as a function of time t for both the heatbath and the Metropolis algorithm with $m_0 = 0.01$ and $L = 128$. $\theta(t)$ is obtained in a time interval $[t, t+20]$. The sharp preparation technique for the initial magnetization is adopted.

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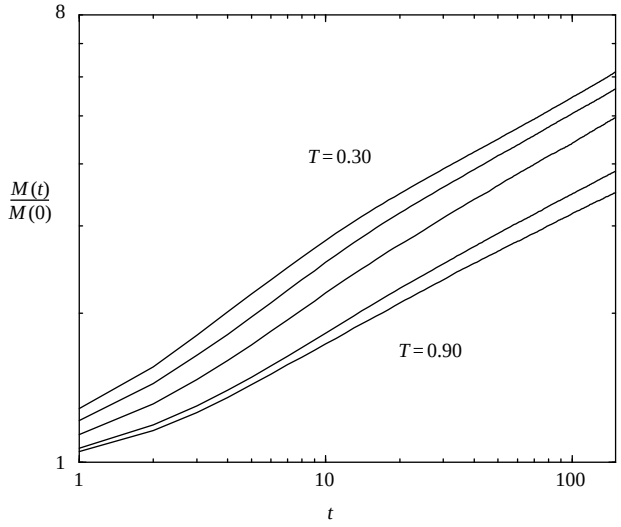

Figure 5. The time evolution of the magnetization for lattice size $L = 64$ and different temperatures with the Metropolis algorithm is plotted on double-log scale. The sharp preparation technique for the initial magnetization is adopted. The temperature parameters are $T = 0.90$, 0.86, 0.70, 0.50 and 0.30 (from below).

the initial magnetization is $m_0 = 0.01$. As before, the weak dependence of the exponent θ on m_0 has not been considered since it is within our statistical errors. The exponent θ 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 that the exponent θ also varies with respect to the temperature. This situation

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

T	0.90	0.86	0.70	0.50	0.30
θ	0.250(1)	0.264(5)	0.287(3)	0.283(4)	0.282(1)

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 θ is determined. The results show that as the temperature decreases, the exponent θ 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 timescale $t_{\rm mic} \sim 30$. Universality in the short-time dynamics is confirmed. A 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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