

## Non-equilibrium critical dynamics of the two-dimensional XY model with Hamiltonian equations of motion

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2007 J. Phys. A: Math. Theor. 40 9957

(<http://iopscience.iop.org/1751-8121/40/33/001>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.144

The article was downloaded on 03/06/2010 at 06:09

Please note that [terms and conditions apply](#).

# Non-equilibrium critical dynamics of the two-dimensional XY model with Hamiltonian equations of motion

A Asad<sup>1,2</sup> and B Zheng<sup>1</sup>

<sup>1</sup> Zhejiang University, Zhejiang Institute of Modern Physics, Hangzhou 310027, People's Republic of China

<sup>2</sup> Pakistan Atomic Energy Commission, PO Box 1114, Islamabad, Pakistan

E-mail: [zheng@zimp.zju.edu.cn](mailto:zheng@zimp.zju.edu.cn)

Received 31 May 2007, in final form 28 June 2007

Published 1 August 2007

Online at [stacks.iop.org/JPhysA/40/9957](http://stacks.iop.org/JPhysA/40/9957)

## Abstract

Non-equilibrium critical dynamics of the two-dimensional XY model is investigated with Hamiltonian equations of motion. Critical relaxation starting from both ordered and random states is carefully analyzed, and the short-time dynamic scaling behavior is revealed. Logarithmic corrections to scaling are detected for relaxation with a random initial state, while power-law corrections to scaling are observed for relaxation with an ordered initial state. The static exponent  $\eta$  and dynamic exponent  $z$  are determined around and below the Kosterlitz–Thouless phase transition temperature. Our results show that the deterministic dynamics described by Hamiltonian equations is in the same universality class as the stochastic dynamics described by Monte Carlo algorithms and Langevin equations.

PACS numbers: 64.60.Ht, 05.20.-y

## 1. Introduction

It is believed that statistical mechanics was developed for describing statistical properties of many-body systems, when microscopic dynamics was inaccessible to any kind of investigations. For an equilibrium state, for example, the ensemble theory provides an effective description. It allows the prediction of static properties of many-body systems directly from the underlying interactions between molecules or spins etc, without solving microscopic equations of motion. During recent decades, however, the advent of powerful computers has made possible, to some extent, direct access to microscopic dynamics through molecular dynamic simulations of macroscopic systems [1–8]. For example, Hamiltonian equations of the  $O(N)$  vector model and XY model have been numerically solved [9–14]. Since the energy is conserved during the time evolution, solutions of the Hamiltonian equations in the long-time

regime actually generate a *microcanonical* ensemble for the equilibrium state. Performing the time average of physical observables, phase transition temperatures and corresponding critical exponents have been estimated by introducing standard techniques developed in statistical mechanics. The results are in agreement with those obtained from a canonical ensemble.

In principle, microscopic equations of motion should describe not only equilibrium properties but also dynamic properties of many-body systems. In statistical mechanics, under certain conditions the dynamic evolution may be approximately described by stochastic equations of motion, typically at the mesoscopic level, e.g., Langevin equations or Monte Carlo algorithms. For stochastic dynamics, *critical slowing down* and *dynamic scaling behavior* around a continuous phase transition are characteristic dynamic properties. Microscopic equations of motion such as Newton equations and Hamiltonian equations are much different from stochastic equations of motion, and essentially *deterministic* in nature. Stochastic features come only from initial states. It is naturally important to study dynamic properties of microscopic equations of motion, and to investigate whether microscopic dynamics and stochastic dynamics belong to a same dynamic universality class. Due to critical slowing down and errors induced by a finite  $\Delta t$  in numerical solutions, however, it is rather difficult to investigate the critical dynamic behavior in the long-time regime.

In the past years critical dynamics far from equilibrium has been systematically investigated with Langevin equations and Monte Carlo methods [15–21]. The results confirm the existence of a rather general dynamic scaling form *at macroscopic early times*, when the dynamic systems are still far from equilibrium. The physical origin of the dynamic scaling behavior is the divergent correlating time around the phase transition temperature. Recent progress includes, for example, theoretical calculations and numerical simulations of XY models and Josephson junction arrays [22–24], various critical systems [25–31] and ageing phenomena [32–35]. Application of the dynamic approach to the weak first-order phase transitions is also inspiring [36–38].

Now it is challenging whether microscopic equations of motion also lead to a dynamic scaling form at the short-time regime, and especially whether the dynamic universality class of microscopic dynamics is the same as that of stochastic dynamics. Since here only the dynamic behavior at early times is concerned, one does not suffer from critical slowing down, and errors induced by a finite  $\Delta t$  are also under control in numerical solutions. It is possible to draw a relatively convincing conclusion. Such an effort has been made in Ref. [5], taking the  $\phi^4$  theory as an example. The dynamic relaxation starting from a *random* state is carefully examined, and the short-time dynamic scaling form is revealed. Somewhat surprisingly, the dynamic exponent  $z$  is determined to be  $z = 2.15(2)$ . This value of  $z$  is in agreement with  $z = 2.16(2)$  estimated for the Monte Carlo dynamics of the two-dimensional (2D) Ising model, and far from  $z = 1$  naively expected from the power counting and/or Lorentz invariance of the  $\phi^4$  theory. Possibly, the initial condition plays an important role. For example, it violates the Lorentz invariance, and may essentially contribute to the renormalization of time.

It is well known that in equilibrium states, the  $\phi^4$  theory and Ising model belong to a same static universality class. For the dynamic process starting from a random state, as stated above, the Hamiltonian dynamics of the  $\phi^4$  theory falls into the dynamic universality class of the Monte Carlo dynamics of the Ising model [5]. This phenomenon is unusual, and it needs further investigation. In this paper, we present numerical solutions of the Hamiltonian equations of the 2D XY model, and examine the dynamic scaling behavior in dynamic processes starting from both *ordered* and *random* states. Results will be compared with those of the Monte Carlo dynamics. The motivation for choosing the 2D XY model is the following.

The 2D XY model may describe the critical behavior of thin films of superfluid helium, and has been extensively studied in the past years. It is the simplest model exhibiting a

Kosterlitz–Thouless (KT) phase transition. At the transition temperature  $T_{\text{KT}}$ , the spatial correlation length diverges exponentially. Below  $T_{\text{KT}}$ , the system remains critical and no real order emerges. These features together make the KT phase transition in the 2D XY model much different from the second-order one in the  $\phi^4$  theory. The Hamiltonian dynamics of the 2D XY model has been investigated in various aspects, such as the KT phase transition and its relation to geometry and topology etc [6, 11–14]. All these works concentrate mostly on the equilibrium state or the dynamic indication in the equilibrium state. Therefore, it is important to explore the critical dynamic behavior of the Hamiltonian dynamics, when the system is still far from equilibrium. Especially, one should examine whether the short-time dynamic scaling form holds in the whole critical regime, and how the static and dynamic critical exponents depend on temperatures.

In addition, the 2D XY model allows a more systematic study of the Hamiltonian dynamics in non-equilibrium states. For the  $\phi^4$  theory, for example, it is hard to address the relaxation process starting from an ordered state, in comparison with the Ising model. The reason might be that in connecting the  $\phi^4$  theory to the Ising model, one already assumes that around the critical temperature, the order parameter  $\phi$  is not too far from zero. For the 2D XY model, however, dynamic processes with any initial state can be considered.

On the other hand, due to the continuous rotational symmetry, there exist vortices and vortex pairs in the 2D XY model. These topological excitations lead to nontrivial dynamic effects. In the stochastic dynamics described by Langevin equations or Monte Carlo algorithms, for example, there emerge logarithmic corrections to scaling in critical relaxation starting from a random state [22, 39, 40]. It is instructive to examine the dynamic effects of topological excitations in the deterministic dynamics described by Hamiltonian equations. Detecting logarithmic corrections to scaling needs much more computer times than the calculation without corrections to scaling [5]. But it is now possible, for computers at our hand are much more powerful than a few years ago.

The model, Hamiltonian equations and scaling analysis of the non-equilibrium dynamic behavior are described in section 2. Numerical solutions are presented in section 3. The final section contains the conclusion.

## 2. Scaling behavior and corrections to scaling

### 2.1. Model

In statistical mechanics, the 2D XY model is defined by the Hamiltonian

$$H_{XY} = J \sum_{\langle ij \rangle} [1 - \vec{S}_i \cdot \vec{S}_j] = J \sum_{\langle ij \rangle} [1 - \cos(\theta_i - \theta_j)], \quad (1)$$

where  $i$  and  $j$  label the lattice sites on a square lattice,  $\vec{S}_i$  and  $\vec{S}_j$  are planar unit vectors,  $\theta_i$  and  $\theta_j$  are the rotation angles of  $\vec{S}_i$  and  $\vec{S}_j$  respectively, and  $J > 0$  is the coupling constant. The summation is extended over all the nearest neighbors. In the following, without loss of generality, we set  $J = 1$ , and the lattice spacing equal to unity. It is well known that the 2D XY model undergoes a Kosterlitz–Thouless phase transition at the temperature  $T_{\text{KT}}$ . Below  $T_{\text{KT}}$ , the system remains critical and no real order emerges.

Similar as the Ising model, the XY model does not possess an intrinsic dynamics from the Hamiltonian  $H_{XY}$  itself. Langevin equations, Monte Carlo algorithms and Hamiltonian equations may be introduced to describe the dynamic evolution of the system. For example, one usually adds a kinetic energy term to introduce the Hamiltonian dynamics,

$$H = \sum_i^L \left[ \frac{p_i^2}{2} + H_{XY} \right], \quad (2)$$

where  $p_i = \dot{\theta}_i$  is the spin momentum. The choice  $J = 1$  is equivalent to setting the time unit and to rescaling the momentum accordingly. With the kinetic energy term, spins in fact become rotators, and the XY model becomes a system of coupled rotators. The Hamiltonian equations of motion are

$$\ddot{\theta}_i(t) = - \sum_{j(i)}^4 [\sin[\theta_i(t) - \theta_j(t)]], \quad (3)$$

where the summation is over the four neighbors of site  $i$ . We choose periodic boundary conditions in both  $x$  and  $y$  directions. Both ordered and random initial states are considered in our numerical solutions. Spins are randomly chosen with  $\theta_i(0) \in [0, 2\pi]$  for the random initial state, and fixed at the  $x$  direction for the ordered initial state. A Gaussian distribution is assumed for the initial momenta  $p_i(0)$ , and its width is fixed by the energy density  $\varepsilon = E/L^2$ , with  $E$  being the total energy and  $L$  being the lattice size. Numerical integration of equation (3) is performed using the velocity Verlet algorithm. Thermodynamical quantities are computed by averaging over time. This computation is repeated for several values of the energy density at the critical regime.

Since equation (3) conserves the energy, its solutions in the long-time regime are assumed to generate a micro-canonical ensemble for the equilibrium state. In this case, the temperature could not be introduced externally as in a canonical ensemble, but can be defined internally by the averaged kinetic energy. In our short-time dynamic approach, the total energy density  $\varepsilon$  is actually a more convenient controlling parameter, since it is conserved and could be input from the initial state. Previous study of the static properties of equation (3) shows that at low temperatures, i.e.,  $T \leq T_{KT}$ , the equipartition of kinetic energy and potential energy gives  $\varepsilon(T) \sim T$  [11, 12]. This is the so-called linear regime, where angles between neighboring spins are small. In the literature, the transition temperature  $T_{KT}$  is reported to be between 0.89 and 0.90 [11, 41]. In this paper, we concentrate also on the regime  $T \leq T_{KT}$ .

Equation (3) is deterministic in nature, and the randomness of the dynamic system comes from initial conditions. In both *ordered* and *random* initial states, the initial momenta  $p_i(0)$  are *randomly* distributed according to a Gaussian distribution. In the random initial state, the initial spin angles  $\theta_i(0)$  are also distributed randomly and uniformly between  $[0, 2\pi]$ . The randomness in the initial state leads to the stochastic evolution of the kinetic energy. The stochastic kinetic energy serves as a kind of noises or a heat bath to the potential energy. This is similar to the case of stochastic dynamics, where the Hamiltonian of the system is simply the potential energy  $H_{XY}$ , but coupled to a heat bath with the temperature  $T$ , such as in Langevin equations or Monte Carlo algorithms.

Denoting a spin at the time  $t$  as  $\vec{S}_i(t)$ , as usual, we define the magnetization, its second moment and the autocorrelation function at the time  $t$  as

$$\vec{M}(t) \equiv \left\langle \sum_i \vec{S}_i(t) \right\rangle / L^2, \quad (4)$$

$$M^{(2)}(t) \equiv \left\langle \left[ \sum_i \vec{S}_i(t) \right]^2 \right\rangle / L^4, \quad (5)$$

and

$$A(t) \equiv \left\langle \sum_i \vec{S}_i(0) \cdot \vec{S}_i(t) \right\rangle / L^2, \quad (6)$$

respectively. Here  $L$  is the lattice size.

## 2.2. Ordered start

For the dynamic process starting from an ordered state, e.g.,  $\vec{M}(0) = (M_x(0), M_y(0)) = (1, 0)$ , we assume a universal dynamic scaling form for the  $k$ th moment of the magnetization, which is valid up to the macroscopic short-time regime,

$$M^{(k)}(t, L) = \lambda^{-k\eta/2} M^{(k)}(\lambda^{-z}t, \lambda^{-1}L), \quad k = 1, 2. \quad (7)$$

Here  $M(t) \equiv M^{(1)}(t)$  is the  $x$  component of the magnetization vector,  $\eta$  is the usual static exponent,  $z$  is the dynamic exponent and  $\lambda$  is an arbitrary scale factor. The scaling form in equation (7) has been suggested for the Monte Carlo dynamics in the past years [16, 17, 19, 20], and recently confirmed by renormalization group calculations with Langevin equations [21]. We will show that it holds also for the Hamiltonian dynamics.

Taking  $\lambda = t^{1/z}$  and neglecting the finite size effect in equation (7), one immediately obtains the power-law behavior of the magnetization

$$M(t) \sim t^{-\eta/2z}. \quad (8)$$

To determine  $z$  independently, we introduce a time-dependent Binder cumulant

$$U(t, L) = (M^{(2)} - M^2)/M^2. \quad (9)$$

When the nonequilibrium spatial correlation length at the time  $t$  is much smaller than the lattice size  $L$ , the Binder cumulant  $U \sim 1/L^d$ . Simple finite size scaling analysis [20] leads to

$$U(t, L) \sim t^{d/z}. \quad (10)$$

Here  $d = 2$  is the spatial dimension.

In general, the scaling behavior in equations (8) and (10) is reached only in the large- $t$  limit. Before reaching the limit, in principle, there exist corrections to scaling. In the cases of the simple Ising and Potts models, correction to scaling are rather weak [20]. For the statistical systems with disorder, frustration or at a KT phase transition, however, corrections to scaling could be strong due to existence of many meta stable states. For accurate estimate of critical exponents, one needs to take into account corrections to scaling. For the 2D XY model, for example, Monte Carlo simulations suggest that there may exist power-law corrections to scaling for the ordered start [22],

$$M(t) \sim t^{-\eta/2z}(1 + c/t), \quad (11)$$

$$U(t) \sim t^{d/z}(1 + c/t). \quad (12)$$

## 2.3. Random start

For the dynamic process starting from a random state with a zero or small initial magnetization  $\vec{M}(0) = (m_0, 0)$ , a generalized dynamic scaling form can be written down, e.g., for the  $k$ th moment of the magnetization

$$M^{(k)}(t, m_0, L) = \lambda^{-k\eta/2} M^{(k)}(\lambda^{-z}t, \lambda^{x_0}m_0, \lambda^{-1}L), \quad k = 1, 2. \quad (13)$$

Here  $x_0$  is an independent exponent describing the scaling behavior of  $m_0$ . This dynamic scaling form was first derived with renormalization group methods for the Langevin dynamics [15], then confirmed with Monte Carlo simulations [5, 18, 20]. It also explains the experiments in spin glasses.

For the random start, however, corrections to scaling are very strong for the 2D XY model. In [39], with Langevin equations one shows that the corrections to scaling are logarithmic. It

is believed that the logarithmic corrections are induced by the vortex-pair annihilation, and do not disappear within early times [39].

We first consider the case of  $m_0 = 0$  and with a sufficiently large lattice. Assuming the logarithmic correction for the nonequilibrium spatial correlation length, scaling analysis leads to the dynamic scaling forms for the second moment and autocorrelation function [39]

$$M^{(2)}(t) \sim [t/(\ln(t) + c)]^{(2-\eta)/z}, \quad (14)$$

$$A(t) \sim [t/(\ln(t) + c)]^{\theta-d/z}. \quad (15)$$

These logarithmic corrections to scaling have been confirmed with Monte Carlo simulations [22, 35]. Since the logarithmic correction to scaling is an important feature of the 2D XY model and essentially affects the measurements of the critical exponents, it is important to investigate whether such a logarithmic correction to scaling emerges also in the Hamiltonian dynamics.

For a nonzero but sufficiently small  $m_0$  and with a sufficiently large lattice, one can deduce from equation (13)

$$M(m_0, t) \sim t^\theta. \quad (16)$$

Here  $\theta$  is related to  $x_0$  by  $\theta = (x_0 - \eta/2)/z$  [15, 20]. Careful scaling analysis shows that the above power-law behavior holds within a time scale  $t_0 \sim m_0^{-z/x_0}$ . Typically, the exponent  $\theta$  is positive [5, 15, 20, 22]. Therefore, this anomalous behavior is also called a critical initial increase of the magnetization. Usually, the correction to scaling for  $M(m_0, t)$  is weak, since the nonzero  $m_0$  could suppress the dynamic effect of the vortex pairs. Even if there is a correction, it does not affect so much our estimate of the dynamic exponent  $z$  with equation (15), for  $\theta$  usually is rather small, in comparison with  $d/z$ .

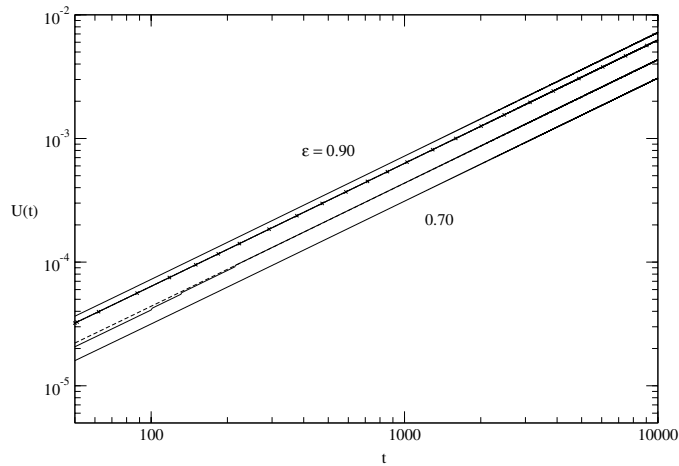
### 3. Numerical solutions

Our aim is to investigate whether the dynamics scaling behavior including the corrections to scaling in equations (11), (12) and (14)–(16) holds for the Hamiltonian dynamics, up to macroscopic early times. In order to detect the corrections to scaling, and obtain accurate values of the critical exponents, we solve equation (3) up to  $t = 10\,000$  with a lattice size  $L = 256$ . An exceptional case is for the random start with a small initial magnetization  $m_0$ , where it is only up to  $t = 1000$ . Due to the small  $m_0$ , one suffers from large fluctuations at longer times. To study possible finite size effects, numerical solutions are also performed with  $L=128$  maximally to  $t = 10\,000$ . Samples of the initial configurations for average are 15 000. To estimate the statistical errors, total samples are divided into a few subgroups. If the fluctuation along the time direction is comparable with the statistical error, it will also be taken into account.

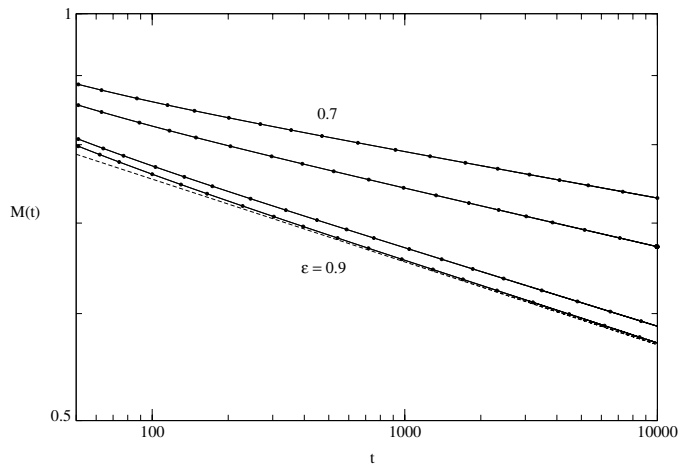
Our main results are obtained with  $\Delta t = 0.05$  for the energy densities  $\varepsilon = 0.90, 0.89, 0.80$  and 0.70. We have also performed the numerical solutions with  $\Delta t = 0.01$ , and confirmed that the errors induced by the finite  $\Delta t$  have been negligibly small.

#### 3.1. Ordered start

Let us start the analysis of our numerical solutions from the dynamic process with an ordered initial state, since corrections to scaling are relatively weaker in this case. In figures 1 and 2, the Binder cumulant and magnetization of the 2 D XY model with an ordered start are displayed with solid lines on a log–log scale. For the Binder cumulant  $U(t)$  in figure 1, careful



**Figure 1.** The time-dependent Binder cumulant of the 2D XY model with the ordered start. Solid lines are for the energy densities  $\epsilon = 0.9, 0.89, 0.8$  and  $0.7$  (from above) with a lattice size  $L = 256$ . The dashed line shows a power-law fit for  $\epsilon = 0.8$ . The crossed line is obtained with  $L = 128$  for  $\epsilon = 0.89$ .



**Figure 2.** The magnetization of the 2D dynamic XY model with the ordered start. Solid lines are for  $\epsilon = 0.9, 0.89, 0.8$  and  $0.7$  (from below) with a lattice size  $L = 256$ . The dashed line shows a power-law fit for  $\epsilon = 0.9$  at later times. Dots fitted to the solid lines are with power-law corrections to scaling.

analysis shows that the correction to scaling is negligibly small. For example, the fluctuation for the measurements of the exponent  $d/z$  in different time intervals is well within 1.0%, smaller than the statistical error. Even if one fits the curves in figure 1 with the Ansatz in equation (12), it gives the same results as those without taking into account the correction to scaling. The relatively worse case is  $\epsilon = 0.8$ . In figure 1, a power-law fit to the curve of  $\epsilon = 0.8$  is shown with the dashed line. The deviation from the power law is still within about 100 time steps. The exponent  $d/z$  measured from the slope of the curves for all the energy densities  $\epsilon = 0.90, 0.89, 0.80$  and  $0.70$  is given in table 1. The dynamic exponent estimated from  $d/z$  is denoted as  $z_1$  in the table, and its values are very close to 2.0 for



**Table 1.** Critical exponents obtained with Hamiltonian equations of the 2D XY model, after taking into accounts logarithmic corrections to scaling for  $M(t)$  and  $U(t)$  with the ordered start, and power-law corrections to scaling for  $M^{(2)}(t)$ ,  $A(t)$  and  $M(m_0, t)$  with the random start.  $z_1$  is the dynamic exponent  $z$  estimated from  $d/z$ , and  $\eta$  is calculated from  $\eta/2z$  by taking  $z_1$  as input.  $z_2$  is estimated from  $(d - \eta)/z$  with  $\eta$  as input, and  $z_3$  is calculated from  $d/z - \theta$  and  $\theta$ . For comparison, the corresponding critical exponents obtained from Monte Carlo simulations are also given. The linear relation  $\varepsilon(T) = T$  between the temperature and energy density is assumed.

		$\varepsilon = 0.9$	0.89	0.8	0.7
$U(t)$	$d/z$	0.998(13)	0.997(10)	0.998(6)	0.994(8)
	$z_1$	2.00(3)	2.00(2)	2.00(1)	2.01(2)
$M(t)$	$\eta/2z$	0.0621(10)	0.0594(12)	0.0461(9)	0.0361(4)
	$\eta$	0.248(7)	0.237(9)	0.184(4)	0.144(5)
[22]	$z_1$	2.00(2)	2.01(1)	2.00(1)	2.01(1)
	$\eta$	0.246(3)	0.234(2)	0.176(2)	0.144(1)
$M^{(2)}(t)$	$(d - \eta)/z$	0.872(15)	0.892(14)	0.907(9)	0.917(8)
	$z_2$	2.01(4)	1.98(3)	2.01(2)	2.02(2)
$A(t)$	$d/z - \theta$	0.763(8)	0.743(6)	0.721(7)	0.701(5)
$M(m_0, t)$	$\theta$	0.235(7)	0.246(5)	0.263(3)	0.279(3)
	$z_3$	2.00(3)	2.02(2)	2.03(2)	2.04(2)
[22]	$(d - \eta)/z$	0.860(12)	0.877(9)	0.897(10)	0.920(8)
	$d/z - \theta$	0.756(5)	0.738(4)	0.711(5)	0.695(6)
	$\theta$	0.241(2)	0.249(2)	0.263(4)	0.280(4)

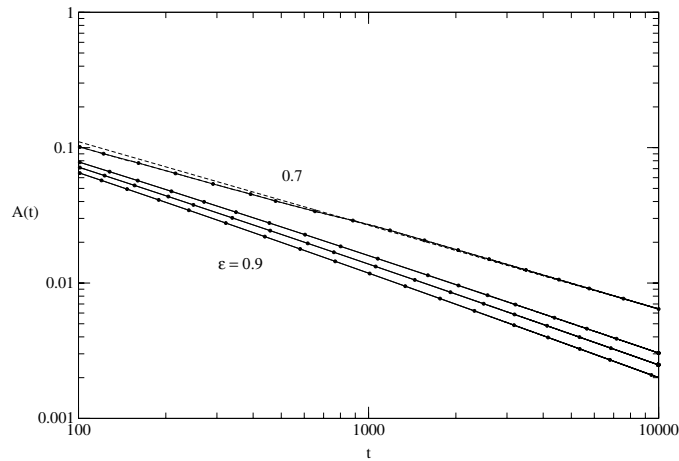
all the energy densities, the same as that for the Langevin dynamics [39] and Monte Carlo dynamics [22].

In figure 2, the dashed line shows a power-law fit to the curve of the magnetization  $M(t)$  with  $\varepsilon = 0.9$  at later times. Obviously, the curve deviates visibly from the power-law behavior in the first some hundred time steps. This leads to an error of a few per cent for the exponent  $\eta/2z$ . For accurate measurements of the critical exponents, therefore, corrections to scaling should be taken into account. In figure 2, dots show the fitting with the correction to scaling in equation (11), and a good fit is observed up to  $t \sim 50$ . We may also vary the form of the correction to scaling to  $M(t) \sim t^{-\eta/2z}(1 + c/t^b)$ , but it turns out that  $b = 1$  yields the best fit. The final values of  $\eta/2z$  are listed in table 1.

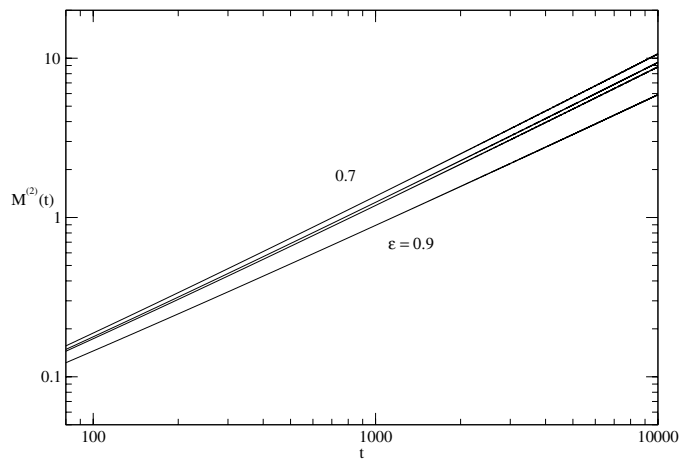
In table 1, the static exponent  $\eta$  is calculated from  $\eta/2z$ , taking the dynamic exponent  $z_1$  as input. For comparison, results obtained from Monte Carlo simulations are also given in table [22]. Assuming  $\varepsilon(T) = T$ , both  $z_1$  and  $\eta$  estimated for the Hamiltonian dynamics agree well with those from Monte Carlo simulations. Since the transition temperature  $T_{KT}$  locates between 0.89 and 0.90,  $\eta$  at  $T_{KT}$  is about 0.24, slightly smaller than the theoretical value  $1/4$ . On the other hand, according to the numerical solutions of equation (3) in equilibrium [11], the linear relation  $\varepsilon(T) = T$  may be modified when the temperature approaches  $T_{KT}$ , e.g., by 3% or 4%. Since the static exponent  $\eta$  is defined in equilibrium and should be independent of dynamics, our results suggest that the modification of the linear relation  $\varepsilon(T) = T$  around  $T_{KT}$  could be smaller. The finite size effects and/or possible errors induced by a finite  $\Delta t$  in the numerical solutions in equilibrium might be responsible for it. Our dynamic approach in the short-time regime is performed with large lattices, and the errors induced by a finite  $\Delta t$  are also under control.

### 3.2. Random start

For the 2D XY model, the dynamic process with a random initial state is somewhat complicated, for there exist logarithmic corrections to scaling. Numerically it is subtle to



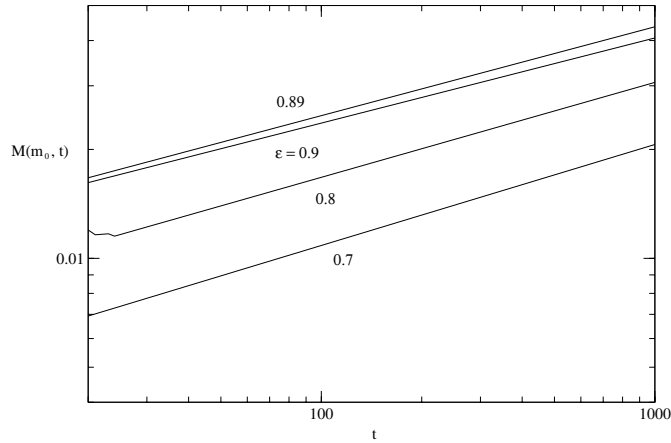
**Figure 3.** The autocorrelation function of the 2D dynamic XY model with the random start. Solid lines are for  $\epsilon = 0.9, 0.89, 0.8$  and  $0.7$  (from below). The dashed line shows a power-law fit for  $\epsilon = 0.7$ . Dots fitted to the solid lines are with logarithmic corrections to scaling. The slope of the dashed line is  $d/z - \theta = 0.617$ , far from  $d/z - \theta = 0.701$  after taking into account the logarithmic correction to scaling.



**Figure 4.** The second moment of the 2D dynamic XY model with the random start. Solid lines are for  $\epsilon = 0.9, 0.89, 0.8$  and  $0.7$  (from below).

detect a logarithmic correction to scaling, although it is strong. In figures 3 and 4, the autocorrelation function and second moment of the 2D XY model with the random start are displayed on a log–log scale. Looking at the curves by eyes, they are not too far from a power-law behavior. If one measures the critical exponents directly from the slopes of the curves, however, the results deviate from real ones by 10% to 20%.

According to the argument with Langevin equations in [39], the corrections to scaling take the logarithmic forms in equations (14) and (15). In figure 3, for example, dots represent the fitting with the logarithmic correction to scaling, and fit well the numerical data of the autocorrelation functions from rather early times. The situation is similar for the second moments in figure 4. In table 1, the extracted values of the exponents  $(2 - \eta)/z$  and  $d/z - \theta$



**Figure 5.** The initial increase of the magnetization of the 2D dynamic XY model with the random start. The initial magnetization  $m_0$  for  $\varepsilon = 0.9, 0.89, 0.8$  and  $0.7$  are  $0.008, 0.008, 0.005$  and  $0.003$ , respectively.

are given. Here we emphasize that the logarithmic correction is so strong that the effective exponent obtained with a power-law fit would be correct only in the limit of  $t \rightarrow \infty$ . In the measurements of the critical exponents, therefore, it is important to take into account the corrections to scaling.

To complete our investigation, especially to verify the exponent  $d/z - \theta$  in the scaling behavior of  $A(t)$  in equation (15), we finally perform the numerical solutions from a random start but with a nonzero initial magnetization  $m_0$ . Since we need a small initial magnetization  $m_0$  in obtaining the scaling behavior in equation (16) and therefore suffer from large fluctuations in longer times, the solutions are presented only up to  $t = 1000$ . In figure 5,  $M(m_0, t)$  is displayed with solid lines on a log-log scale. From these data, we cannot detect a logarithmic correction. In a time interval  $[10, 1000]$ , direct measurements of the slope yield the same exponents as those with any correction to scaling.

In table 1, we summarize all the exponents extracted from  $A(t)$ ,  $M^{(2)}(t)$  and  $M(m_0, t)$  for different energy densities. For comparison, the critical exponents  $(d - \eta)/z$ ,  $d/z - \theta$  and  $\theta$  measured from Monte Carlo simulations have been also given [22]. Assuming again  $\varepsilon(T) = T$ , the results for the Hamiltonian dynamics agree well with those for the Monte Carlo dynamics. At the temperatures around  $T_{KT}$ , e.g.,  $T = 0.90$  and  $0.89$ , there might be small deviation from  $\varepsilon(T) = T$ , but it looks not so significant.

To understand more the results in table 1, one may calculate the dynamic exponent  $z$  from  $(d - \eta)/z$ , taking  $\eta$  measured from the dynamic process with the ordered start as input. This value of the dynamic exponent is denoted as  $z_2$  in the table. In addition, one may also estimate the dynamic exponent  $z$  from  $d/z - \theta$  and  $\theta$ . This value is denoted as  $z_3$ . Similar as  $z_1$  calculated from the Binder cumulant  $U(t, L)$  in the dynamic process with the ordered start, both  $z_2$  and  $z_3$  are very close to 2.0, which is expected from the Langevin dynamics and Monte Carlo dynamics.

#### 4. Conclusions

We have numerically solved the Hamiltonian equations of the 2D XY model, and investigated the dynamic processes starting from both ordered and random states. The short-time dynamic

scaling behavior is revealed in the whole critical regime, and the static exponent  $\eta$  and dynamic exponent  $z$  are extracted. In different measurements of the physical observables, the dynamic exponent  $z$  takes values well in agreement with 2.0 for all energy densities. In addition, logarithmic corrections to scaling are detected in the dynamic process with a random initial state, while power-law corrections to scaling are observed in the dynamic process with an ordered initial state. All these results indicate that the deterministic dynamics described by Hamiltonian equations is indeed in the same dynamic universality class as the stochastic dynamics described by Langevin equations and Monte Carlo algorithms. The values of the static exponent  $\eta$  are also consistent with those obtained in dynamic Monte Carlo simulations.

In comparison with the numerical solutions of the Hamiltonian equations for the  $\phi^4$  theory in [5], our results for the 2D XY model extend the dynamic scaling form far from equilibrium to the KT phase transition, and provide comprehensive understanding of the Hamiltonian dynamics including critical relaxation starting from an ordered state and corrections to scaling. Naive power counting might expect that the dynamic exponent  $z$  of the Hamiltonian equations is around 1.0, rather than 2.0. It is possible that the initial condition plays an important role here. More theoretical techniques such as renormalization group methods should be developed to understand this phenomenon. Furthermore, the critical dynamic behavior in the long-time regime should be explored.

### Acknowledgments

This work was supported in part by NNSF (China) under grant No. 10325520. The authors would like to thank the Higher Education Commission of Pakistan for financial support.

### References

- [1] Fermi E, Pasta J and Ulam S 1965 *Collected Papers of Enrico Fermi* ed E Segré (Chicago: Chicago University Press)
- [2] Ford J 1992 *Phys. Rep.* **213** 271
- [3] Escande D, Kantz H, Livi R and Ruffo S 1994 *J. Stat. Phys.* **76** 605
- [4] Elskens Y and Antoni M 1997 *Phys. Rev. E* **55** 6575
- [5] Zheng B, Schulz M and Trimper S 1999 *Phys. Rev. Lett.* **82** 1891
- [6] Casetti L, Pettini M and Cohen E G D 2000 *Phys. Rep.* **337** 238
- [7] Delfini L, Lepri S and Livi R 2005 *J. Stat. Mech. Theory Exp.* P05006
- [8] Mossa A, Pettini M and Clementi C 2006 *Phys. Rev. E* **74** 041805
- [9] Caiani L, Casetti L and Pettini M 1998 *J. Phys. A: Math. Gen.* **31** 3357
- [10] Caiani L, Casetti L, Clementi C, Pettini G, Pettini M and Gatto R 1998 *Phys. Rev. E* **57** 3886
- [11] Leoncini X and Verga A D 1998 *Phys. Rev. E* **57** 6377
- [12] Cerruti-Sola M, Clementi C and Pettini M 2000 *Phys. Rev. E* **61** 5171
- [13] Lepri S and Ruffo S 2001 *Europhys. Lett.* **55** 512
- [14] Casetti L, Pettini M and Cohen E G D 2003 *J. Stat. Phys.* **111** 1091
- [15] Janssen H K, Schaub B and Schmittmann B 1989 *Z. Phys. B* **73** 539
- [16] Stauffer D 1992 *Physica A* **186** 197
- [17] Ito N 1993 *Physica A* **196** 591
- [18] Li Z B, Ritschel U and Zheng B 1994 *J. Phys. A: Math. Gen.* **27** L837
- [19] Luo H J, Schülke L and Zheng B 1998 *Phys. Rev. Lett.* **81** 180
- [20] Zheng B 1998 *Int. J. Mod. Phys. B* **12** 1419 review article
- [21] Fedorenko A A and Trimper S 2006 *Europhys. Lett.* **74** 89
- [22] Zheng B, Ren F and Ren H 2003 *Phys. Rev. E* **68** 046120
- [23] Ozeki Y and Ito N 2003 *Phys. Rev. B* **68** 054414
- [24] Granato E and Dominguez D 2005 *Phys. Rev. B* **71** 094521
- [25] Albano E V and Saracco G 2002 *Phys. Rev. Lett.* **88** 145701
- [26] Grandi B C S and Figueiredo W 2004 *Phys. Rev. E* **70** 056109

- [27] Yin J Q, Zheng B and Trimper S 2004 *Phys. Rev. E* **70** 056134
- [28] Ozeki Y and Ogawa K 2005 *Phys. Rev. B* **71** 220407
- [29] Chen Y and Li Z B 2005 *Phys. Rev. B* **71** 174433
- [30] Arashiro E, de Felicio J R D and Hansmanno U H E 2006 *Phys. Rev. E* **73** 040902
- [31] Zhou N J and Zheng B 2007 *Europhys. Lett.* **78** 56001
- [32] Godrèche C and Luck J M 2002 *J. Phys.: Condens. Matter* **14** 1589
- [33] Henkel M, Paessens M and Pleimling M 2004 *Phys. Rev. E* **69** 056109
- [34] Calabrese P and Gambassi A 2005 *J. Phys. A: Math. Gen.* **38** R133
- [35] Lei X W and Zheng B 2007 *Phys. Rev. E* **75** 040104
- [36] Schülke L and Zheng B 2000 *Phys. Rev. E* **62** 7482
- [37] Yin J Q, Zheng B and Trimper S 2005 *Phys. Rev. E* **72** 036122
- [38] Yin J Q, Zheng B, Prudnikov V V and Trimper S 2006 *Euro. Phys. J. B* **49** 195
- [39] Bray A J, Briant A J and Jervis D K 2000 *Phys. Rev. Lett.* **84** 1503
- [40] Bray A J 2000 *Phys. Rev. E* **62** 103
- [41] Zheng B, Schulz M and Trimper S 1999 *Phys. Rev. E* **59** R1351

## Corrigendum

### Corrigendum on 'Non-equilibrium critical dynamics of two-dimensional XY model with Hamiltonian equations of motion'

Asad A and Zheng B 2007 *J. Phys. A: Math. Theor.* **40** 9957–9968

I regret that part of the conclusion in the above paper is incorrect. Under my supervision, the computer simulations of the article were done by my former student A Asad. In the past months, I and my other students were involved in related research topics. We are not able to reproduce part of the results. According to our new computations, the dynamic exponent for the dynamic process starting from an ordered state is  $z = 1$ , different from  $z = 2$  reported in the above paper and in Monte Carlo simulations [1, 2]. For the dynamic process starting from a disordered state, the numerical solutions should be also reformulated. Detailed results will be reported elsewhere.

### References

- [1] Zheng B, Ren F, and Ren H 2003 *Phys. Rev. E* **68** 046120.
- [2] Lei X W and Zheng B 2007 *Phys. Rev. E* **75** 040104.

## Corrigendum

### Non-equilibrium critical dynamics of two-dimensional XY model with Hamiltonian equations of motion

Asad A and Zheng B 2007 *J. Phys. A: Math. Theor.* **40** 9957–9968

I regret that part of the conclusion in the above paper is incorrect. Under my supervision, the computer simulations of the article were done by my former student A Asad. In the past months, I and my other students were involved in related research topics. We are not able to reproduce part of the results. According to our new computations, the dynamic exponent for the dynamic process starting from an ordered state is  $z = 1$ , different from  $z = 2$  reported in the above paper and in Monte Carlo simulations [?, ?]. For the dynamic process starting from a disordered state, the numerical solutions should be also reformulated. Detailed results will be reported elsewhere.

### References

- [1] Zheng B, Ren F, and Ren H 2003 *Phys. Rev. E* **68** 046120.
- [2] Lei X W and Zheng B 2007 *Phys. Rev. E* **75** 040104.