PHYSICAL REVIEW E **75**, 040104(R) (2007)

Short-time critical dynamics and aging phenomena in the two-dimensional *XY* model

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(Received 6 August 2006; published 12 April 2007)

With Monte Carlo methods, we simulate dynamic relaxation processes of the two-dimensional *XY* model at the Berezinskii-Kosterlitz-Thouless phase transition temperature and below, starting from both ordered and disordered initial states. The two-time correlation function $A(t',t)$ is measured, and aging phenomena are investigated. The power-law correction in the spatial correlation length $\xi(t)$ for relaxation with an ordered initial state and the logarithmic correction for relaxation with a disordered initial state are carefully analyzed. The scaling functions of $A(t',t)$ are then extracted.

DOI: 10.1103/PhysRevE.75.040104 PACS number(s): 64.60.Ht, 02.70.Uu, 75.10.Hk

I. INTRODUCTION

In recent years, many activities have been devoted to dynamic processes far from equilibrium. Examples are spin glass dynamics, structural glass dynamics, phase ordering dynamics, and nonequilibrium critical dynamics, etc. For nonequilibrium critical dynamics, the universal dynamic scaling form has been extended to dynamic processes far from equilibrium, which is valid up to the macroscopic short-time regime [1–7]. It is important that new critical exponents must be introduced to describe the scaling behavior of the macroscopic initial conditions. Based on the short-time dynamic scaling form, new techniques for the measurements of both dynamic and static critical exponents as well as the critical temperature have been developed [7–9]. Recent progress includes, for example, numerical study of *XY* models and Josephson junction arrays [10–13], critical dynamics at surfaces [14,15], and various critical systems [16–22]. Dynamic reweighting methods have been suggested [23,24].

In glassy systems, the aging behavior is one of the central phenomena. For a spin glass, for example, the energy landscape has complex metastable states, and therefore there is slow dynamics below the spin-glass phase transition temperature T_c. In a broad range of temperatures between $T=0$ and T_c, the aging phenomenon is characterized by dynamic scale invariance [25]. Very recently, the aging phenomenon at and around a continuous phase transition has also been intensively studied [26–31]. In this case the aging phenomenon exhibits a dynamic scaling behavior far from equilibrium, induced by the long-range time correlation. This is different from the aging phenomena induced by metastable states in glassy systems below T_c. In a second-order phase transition, the power-law behavior of the nonequilibrium spatial correlation length and two-time correlation function, etc., is relatively clear already in the short-time regime. The aging phenomena may be identified with no difficulty and the critical exponents can be extracted rather accurately.

In a Berezinskii-Kosterlitz-Thouless (BKT) phase transition [32,33], however, the critical dynamics is slower due to the existence of dynamic vortices. For example, the power-law growth of the nonequilibrium spatial correlation length usually undergoes strong corrections to scaling, and the scaling function of the two-time correlation function also approaches the power-law form relatively slowly. These effects together make it difficult to identify the aging phenomena, and to extract the corresponding critical exponents and scaling function. A typical physical system with a BKT phase transition is the two-dimensional (2D) *XY* model [10,34]. With spin-wave approximations or similar assumptions [28,35,36], attempts have been made to identify the aging phenomena and extract the scaling function, taking into account the corrections to scaling. These *Ansätze* could fit the numerical data at lower temperatures.

Based on general scaling arguments, in this paper we suggest a theoretical approach to the aging phenomena of slow dynamics, especially when the spatial correlation length and the scaling function of the two-time correlation function have not yet reached the power-law limits. We present the results for the 2D *XY* model, and the method applies to different dynamical systems.

The 2D *XY* model is defined by the Hamiltonian

$$-\frac{1}{kT}H = K\sum_{\langle ij\rangle} \vec{S}_i \cdot \vec{S}_j, \tag{1}$$

where $\vec{S}_i=(S_{i,x},S_{i,y})$ is a planar unit vector at site i of a square lattice, the sum is over the nearest neighbors, and T is the temperature. For convenience, here we simply take the notation $T=1/K$. In the literature, the transition temperature T_{BKT} is reported to be between 0.89 and 0.90 [37–39]. Below T_{BKT}, the system remains critical. In this paper, we consider the Monte Carlo dynamics, which is believed to be in the same universality class as Langevin dynamics. Following Refs. [10,34], we adopt the heat-bath algorithm in which a trial move is accepted with probability $1/[1+\exp(\Delta E/T)]$, where ΔE is the energy change associated with the move. The dynamic process we simulate is that a system initially in a completely ordered or disordered state is suddenly quenched to the transition temperature T_{BKT} or below, and then released to the dynamic evolution of model A.

We define the two-time correlation function with $t' < t$ as

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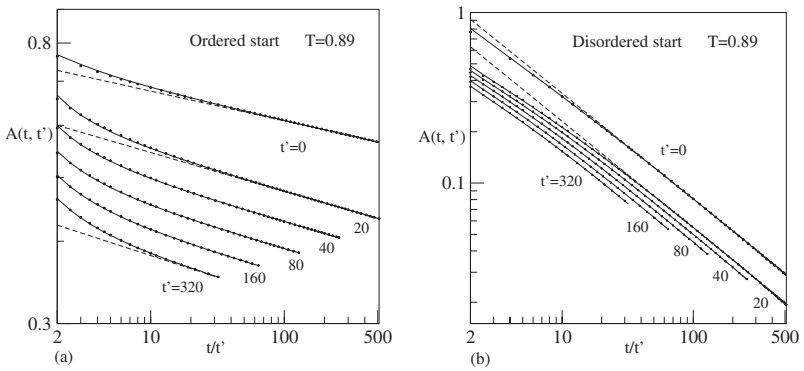

FIG. 1. $A(t',t)$ is displayed with solid lines on a log-log scale, in (a) and (b) for the ordered and disordered initial states, respectively. The time scale for $t'=0$ is $t/10$. Dashed lines show the power-law fits. Dotted lines in (a) are the curves fitted with $A(t',t)=a_1(t/t')^{-\eta/2z}[1+a_2/(t/t')]$. Dotted lines in (b) are the curves fitted with $A(t',t)=a_1\{(t/t')/[a_2+\ln(t/t')]\}^{-\lambda/z}$.

$$A(t',t) \equiv \langle \sum_i \vec{S}_i(t') \cdot \vec{S}_i(t) \rangle / L^d. \tag{2}$$

Here L is the lattice size, and $d=2$ is the spatial dimension. From general scaling arguments, $A(t',t)$ should obey a scaling form at the critical temperature or the critical regime of

$$A(t',t) = [\xi(t')]^{-\eta+2-d} F(\xi(t)/\xi(t')), \tag{3}$$

after a time scale t_{mic} that is sufficiently long in the microscopic sense, but still short in the macroscopic sense. Here $-\eta+2-d$ is the scaling dimension of the magnetic field $\langle \vec{S}_i \rangle$, $\xi(t)$ is the nonequilibrium spatial correlation length, and the scaling function $F(\xi(t)/\xi(t'))$ represents the scale invariance in the critical regime. Such a scaling form of $A(t',t)$ holds for both disordered and ordered initial states. But the forms of $\xi(t)$ and $F(x)$ depend on the initial states. Except for the dependence on the initial states, $F(x)$ is universal even in the finite-x regime. Due to corrections to scaling, $\xi(t)$ is not universal in the finite-t regime. In the large-x limit, $F(x)$ takes a power-law form. Here we emphasize that the scaling form in Eq. (3) is essentially the same as is written down in the literatures [28,31,35,36], and we only assume $\xi(t)$ to have a specific form including the correction to scaling.

For a second-order phase transition, for example in the 2D Ising model, corrections to scaling are rather weak and negligible. After a microscopic time scale t_{mic}, typically tens of Monte Carlo time steps, the spatial correlation length grows by a power law $\xi(t) \sim t^{1/z}$, independently of the initial conditions [1,7]. z is the so-called dynamic exponent. In addition, for a medium ratio $x=\xi(t)/\xi(t')$ (e.g., $x \geqslant 2$), the scaling function $F(x)$ already shows a power-law decay, $F(x) \sim x^{-\alpha}$. The exponent $\alpha=(\eta-2+d)/2$ for an ordered initial state, while $\alpha=\lambda$ for a disordered initial state [1,7,26,31].

For a BKT phase transition, for example in the 2D XY model, corrections to scaling are strong [10,34]. In Fig. 1, $A(t',t)$ of the 2D XY model is displayed with solid lines on a log-log scale. The data are obtained with the lattice size $L=256$, and 10 000 samples are collected on average. Additional simulations with $L=128$ and 512 confirm that the finite-size effect is negligible. Obviously, the curves in Fig. 1 do not obey a power law. The deviation of $A(t',t)$ from a power law comes from both the scaling function $F(x)$ itself and the corrections to scaling in $\xi(t)$.

In Refs. [28,35,36], efforts have been made to understand the aging behavior of the 2D XY model. Based on the spin-wave approximation, one can derive

$$A(t',t) = (t-t')^{-\eta/z}[4(t/t')/(1+t/t')^2]^{-\eta/2z} \tag{4}$$

for a dynamic process with an ordered initial state. Further, it is assumed that [36]

$$A(t',t) = (t-t')^{-\eta/z} f(\xi(t)/\xi(t')), \quad \xi(t) \sim (t/\ln t)^{1/z} \tag{5}$$

for a dynamic process with a disordered initial state. For the 2D XY model, it is well known that the dynamic exponent $z=2$ for Monte Carlo or Langevin dynamics. These *Ansätze* hold only at lower temperatures. In Fig. 2, we have analyzed the numerical data of $A(t',t)$ with Eqs. (4) and (5) at the temperature $T=0.89$. According to Eqs. (5), for example, $A(t',t)(t-t')^{\eta/2}$ as a function of $x=(t/t')/(\ln t/\ln t')$ should be independent of t'. This kind of data collapse is not observed in Fig. 2.

Now let us start our analysis based on Eq. (3). For a dynamic process starting from an ordered state, the form

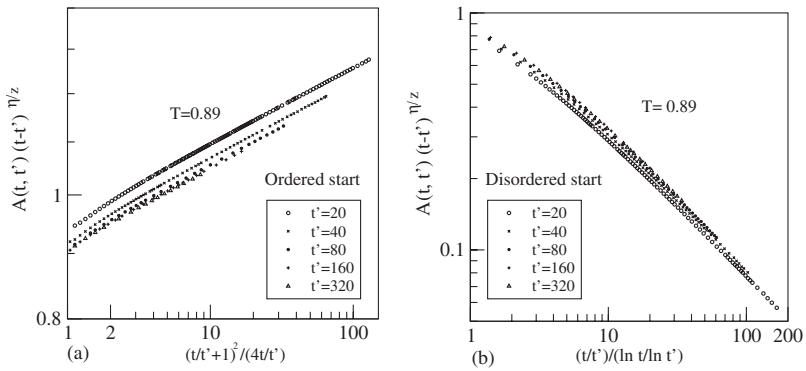

FIG. 2. Scaling plot of $A(t',t)$: (a) for the ordered initial state, based on Eq. (4); (b) for the disordered initial state, based on Eq. (5). η/z is taken to be 0.118 for $T=0.89$ and 0.0715 for $T=0.70$. Data collapse is not observed.

TABLE I. Critical exponents η/z and λ/z, as well as c, c', c_1, and c_1' in Eqs. (6), (7), (9), and (10) extracted from Figs. 1 and 3.

T	$\eta/2z$	c	c'	λ/z	c_1	c_1'
0.89	0.0587(5)	0.92	0.22	0.738(5)	0.22	0.26
0.70	0.0358(3)	0.50	0.15	0.694(4)	0.56	0.50

$A(t',t)=a_1(t/t')^{-\eta/2z}[1+a_2/(t/t')]$ fits the numerical data well, with a_1 and a_2 being t' dependent. For $T=0.89$, the fitted curves are shown by the dotted lines in Fig. 1(a), and the exponent $\eta/2z=0.0587(5)$ is extracted from the curves of different t'. Similar fitting yields $\eta/2z=0.0358(3)$ for $T=0.70$. These values of $\eta/2z$ are in good agreement with those reported in Refs. [10,40]. Based on this analysis and the numerical study in Ref. [10], we assume that there exists a power-law correction to scaling for the nonequilibrium spatial correlation length,

$$\xi(t) \sim t^{1/z}(1+c/t)^{-2/\eta}, \tag{6}$$

and the scaling function in Eq. (3) takes the form

$$F(x) \sim x^{-\eta/2}(1+c'/x^2). \tag{7}$$

It is important that c and c' are constants. Assuming Eq. (6) rather than $\xi(t)\sim t^{1/z}(1+c/t)$ is just for convenience.

We will numerically verify Eqs. (3), (6), and (7). In fact, the scaling form in Eq. (3) can be easily demonstrated, if $\xi(t)$ in Eq. (6) is known. Direct measurements of $\xi(t)$ from the spatial correlation function are, however, not so accurate. Our strategy is to determine $\xi(t)$ from $A(t'=0,t)\sim[\xi(t)]^{-\eta/2}$, following the scaling analysis above. Such a fitting for $T=0.89$ has been done in Fig. 1(a), and the extracted $\eta/2z$ and c are given in Table I. With $\xi(t)$ in hand, and keeping $z=2$ in mind, we plot $A(t',t)[\xi(t')]^{\eta}$ as a function of $x=\xi(t)/\xi(t')$ in Fig. 3(a). Obviously, the data of different t' collapse nicely onto a single curve. This proves the scaling form in Eq. (3). Here we note that, to identify the aging phenomenon described by Eq. (3), it is not necessary to specify the concrete form of the scaling function $F(x)$.

With the data in Fig. 3(a), we now fit the scaling function $F(x)$ to Eq. (7), and the fitted curve is displayed by the solid lines. The fitting is already good for $x\geqslant 1.5$, and the values of c' are listed in Table I. Finally, inserting Eqs. (6) and (7) into Eq. (3), simple calculations lead to

$$A(t',t) \sim t'^{-\eta/z}(1+c/t')(t/t')^{-\eta/2z}[1+(c/t'+c')/(t/t')]. \tag{8}$$

This equation explains the numerical data in Fig. 1(a).

For a dynamic process starting from a disordered state, $A(t',t)$ is dominated by logarithmic corrections, $A(t',t)=a_1[(t/t')/(a_2+\ln(t/t'))]^{-\lambda/z}$, as shown with dotted lines in Fig. 1(b). a_1 is t' dependent, and both a_2 and λ/z are weakly t' dependent. Such a logarithmic correction to scaling has been reported in the literature, e.g., in Refs. [10,34,36]. Following the theoretical argument in Ref. [34],

$$\xi(t) \sim [t/(\ln t - c_1)]^{1/z}, \tag{9}$$

with c_1 being a constant. From our analysis, the scaling function $F(x)$ does not include a logarithmic term;

$$F(x) \sim x^{-\lambda}(1-c_1'/x) \tag{10}$$

fits the numerical data well. Here the convergence of $F(x)$ to a power law is somewhat slower than in the case with an ordered initial state.

We now determine the spatial correlation length $\xi(t)$ from $A(t'=0,t)\sim[\xi(t)]^{-\lambda}$. This fitting for $T=0.89$ has been done in Fig. 1(b), and the extracted λ/z and c_1 are given in Table I. The values of λ/z are in good agreement with those reported in Refs. [10]. With $\xi(t)$ in hand, we plot $A(t',t)[\xi(t')]^{\eta}$ as a function of $x=\xi(t)/\xi(t')$ in Fig. 3(b). Data collapse is observed. This proves the scaling form in Eq. (3) for the dynamic relaxation starting from the disordered state. With the data in Fig. 3(b), we fitted the scaling function $F(x)$ to Eq. (10), and the fitted curve is displayed by the solid lines. The fitting is good for $x\geqslant 1.5$, and the values of c_1' are listed in Table I. In Fig. 1(b), $A(t',t)$ is plotted as a function of t/t', and its deviation from a power law comes from both Eqs. (9) and (10). Since the power-law term in Eq. (10) is weaker, it just slightly modifies the exponent λ/z and the constant c_1 if one fits the curves with only the logarithmic correction in Eq. (9).

Finally, we observe that, at lower temperatures, our scaling form in Eqs. (3) and (7) for the ordered initial state is consistent with Eq. (4) from the spin-wave approximation, and the difference is only the power-law correction of $\xi(t)$ in Eq. (6). However, our scaling form in Eq. (3) for the disordered initial state does differ from Eq. (5) due to the factor

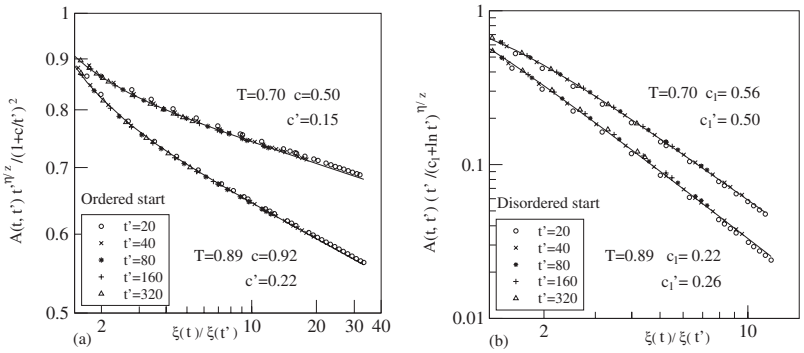

FIG. 3. Scaling plot of $A(t',t)$: (a) for the ordered initial state, based on Eqs. (3) and (6); (b) for the disordered initial state, based on Eq. (3) and (9). Data collapse is observed. Solid lines in (a) and (b) are the curves fitted with Eqs. (7) and (10), respectively.

$(t-t')^{-\eta/z}$, although Eq. (9) is not much different from $\xi(t) \sim (t/\ln t)^{1/z}$ in Eq. (5). The difference will not disappear even for a very large t, for it is logarithmic.

In conclusion, with Monte Carlo methods we have investigated the aging phenomena of the 2D XY model at the BKT transition temperature and below. The dynamic processes starting from both ordered and disordered states are simulated, and the two-time correlation function $A(t',t)$ is measured. The scaling form $A(t',t)=[\xi(t')]^{-\eta+2-d}F(\xi(t)/\xi(t'))$ is numerically verified. We propose to determine the spatial correlation length $\xi(t)$ from $A(t'=0,t)$. It is demonstrated that there exists a power-law correction in $\xi(t)$ for an ordered initial state, and a logarithmic correction for a disordered initial state. Then we extract the scaling function $F(x)$ for both the ordered and disordered initial states. The techniques in this paper can be applied to different dynamic systems, especially when there exist strong corrections to scaling, and/or the ratio $x=\xi(t)/\xi(t')$ is not at the infinite limit.

ACKNOWLEDGMENTS

This work was supported in part by NNSF (China) under Grant No. 10325520 and RPST (China) under Grant No. KJ061208.

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