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Short-time dynamic behaviour of critical XY systems

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Abstract

Using Monte Carlo methods, the short-time dynamic scaling behaviour of two-dimensional critical XY systems is investigated. Our results for the XY model show that there exists universal scaling behaviour already in the short-time regime, but the values of the dynamic exponent z differ for different initial conditions. For the fully frustrated XY model, power law scaling behaviour is also observed in the short-time regime. However, a violation of the standard scaling relation between the exponents is detected. © 1998 Elsevier Science B.V.

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Recently, much progress has been made in critical dynamics. It was discovered that universal scaling behaviour may emerge already in the *macroscopic* short-time regime [1–6]. Extensive Monte Carlo simulations show that the short-time dynamic scaling is not only conceptually interesting but also practically important, e.g. it leads to new ways for the determination of the critical exponents and the critical temperature [6–11,3].

For critical systems with second order phase transitions, comprehensive understanding has been achieved. We consider first a relaxational dynamic process of model A starting from an ordered state. Taking the dynamic Ising model as an example, the scaling form is given for the k th moment of the magnetization at the critical temperature, by [6,3]

$$M^{(k)}(t, L) = b^{-k(d-2+\eta)/2} M^{(k)}(b^{-z}t, b^{-1}L), \quad (1)$$

where t is the time variable, L is the lattice size, η and z represent the standard static and dynamic critical exponents. This scaling form looks similar to that in the long-time regime but it is now assumed to hold also in the macroscopic short-time regime after a microscopic time scale t_{mic} .

For a relaxation process starting from a disordered state with small or zero initial magnetization, the scaling form for the k th moment at the critical temperature is found to be

$$M^{(k)}(t, L, m_0) = b^{-k(d-2+\eta)/2} \times M^{(k)}(b^{-z}t, b^{-1}L, b^{x_0}m_0). \quad (2)$$

Here it is important that a new independent critical exponent x_0 has been introduced to describe the dependence of the scaling behaviour on the initial magnetization. The exponent x_0 is the scaling dimension of the global magnetization $M(t)$ and also of the magnetization density. Therefore, even if $m_0 = 0$, x_0 still

enters observables related to the initial conditions. For example, for sufficiently large lattice size the auto-correlation has a power law behaviour,

$$A(t) \equiv \frac{1}{L^d} \left\langle \sum_i s_i(0) s_i(t) \right\rangle \sim t^{-\lambda}, \quad (3)$$

with s_i being a spin variable. The exponent λ is related to x_0 by [12]

$$\lambda = \frac{d}{z} - \theta, \quad \theta = \left(x_0 - \frac{d-2+\eta}{2} \right) \frac{1}{z}. \quad (4)$$

In general, for arbitrary initial magnetization m_0 between 0 and 1 a generalized scaling form can be written down.

Renormalization group calculations for the $O(N)$ vector model show that the static exponents η and the dynamic exponent z in the scaling forms (2) and (3) take the same values as in equilibrium or in the long-time regime of the dynamic evolution where they are defined. This is also confirmed by Monte Carlo simulations for various critical magnetic systems with second order phase transitions. Furthermore, numerical results indicate in good accuracy that the values of the exponents η and z are independent of the initial conditions, i.e. the values of the exponents in scaling form (1) are the same as in scaling forms (2) and (3). This prominent property has been used to extract all the dynamic and static exponents from the short-time dynamic scaling forms. Since the measurements are carried out in the short-time regime, the short-time dynamic approach is free of critical slowing down. One may believe that the scaling forms (1), (2) and (3) hold also in the crossover regime where the time t is not small but also not asymptotically large.

In this Letter we investigate numerically whether critical systems with a Kosterlitz–Thouless phase transition show also a clean scenario as stated above. For this purpose, we should answer the following questions: at first, whether there exists universal scaling behaviour in the short-time regime; secondly, whether the dynamic exponent z and the static exponent η in the short-time scaling forms (1), (2) and (3) are independent of the initial conditions and take the same values as in equilibrium or in the long-time regime where they are defined¹; finally whether the scaling

relations between the exponents for the second order phase transitions, e.g. that between x_0 and λ in Eq. (4), hold also for Kosterlitz–Thouless phase transitions.

As examples, let us consider the two-dimensional classical XY model and the fully frustrated XY ($FFXY$) model. The dynamic process starting from an ordered state has been investigated with Monte Carlo methods at the Kosterlitz–Thouless phase transition T_{KT} and below [13]. Nice power law scaling behaviour was observed, and the static exponent η extracted from scaling form (1) is consistent with that measured in equilibrium. The dynamic exponent z is a constant for all temperatures at and below T_{KT} and slightly smaller than 2.0, but within errors it coincides with the theoretical prediction $z = 2$ [14].

For the dynamic process starting from a disordered state, however, the situation is complicated. For a quench to zero temperature, it was suggested some years ago that the dynamic scaling is violated [15]. However, recent numerical simulations show that at least for a quench to not so low temperatures the magnetization undergoes a universal power law initial increase if the initial magnetization is small but nonzero [16,17]. Therefore, a comprehensive understanding of the short-time behaviour of this dynamic process is important and necessary.

Our strategy is to simulate a dynamic relaxational process starting from a disordered state with zero magnetization and to measure the auto-correlation and the second moment of the magnetization. Then from the scaling forms (2) and (3), we obtain the static exponent η and the dynamic exponent z and compare them with those measured from the scaling form (1). Indeed, to simulate a dynamic process starting from a disordered state with zero magnetization is more difficult than that from an ordered state. This is very probably due to the effect of the vortices. We need very large lattices and update the system to fairly long time t .

The XY model and the $FFXY$ model in two dimensions can be defined by the Hamiltonian

¹ In Eqs. (1)–(3), the dynamic exponent z and even the static exponents could be initial condition dependent and different from those in equilibrium since they are defined in different fixed points of the time t and different initial conditions.

¹ In principle, even if there exist the short-time scaling form as

$$H = K \sum_{\langle ij \rangle} f_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (5)$$

where $\mathbf{S}_i = (S_{i,x}, S_{i,y})$ is a planar unit vector at site i , and the sum extends over the nearest neighbours. In our notation, K is just the inverse temperature. Here f_{ij} take the values $+1$ or -1 , depending on the model. For the XY model, $f_{ij} = 1$ on all links. A simple realization of the $FFXY$ model is by taking $f_{ij} = -1$ on half of the vertical links (negative links) and $+1$ on the others (positive links) [18].

In this paper, only the dynamics of model A is concerned. The dynamics of model A is a relaxational dynamics without energy and magnetization conservation. Starting from a completely random configuration, we update the system at the temperature T_{KT} or below with the standard Metropolis algorithm. The trial state of each spin is randomly taken in the unit circle since the acceptance rate is high in the short-time regime of the dynamic evolution. Updating is stopped at Monte Carlo time step $t = 1500$. The procedure is repeated with another initial configuration and different random numbers. We have tested that for updating time $t = 1500$, a big lattice size like $L = 512$ is needed. An updating time $t = 1500$ is necessary for reliable measurements of the observables since the microscopic time scale is here around $t_{mic} \sim 100$ or more. For the average a total of 800 samples has been taken. Errors are estimated by dividing the samples into four groups.

We measure the auto-correlation

$$A(t) \equiv \frac{1}{L^d} \left\langle \sum_i \mathbf{S}_i(0) \cdot \mathbf{S}_i(t) \right\rangle \quad (6)$$

and the second moment of the magnetization

$$M^{(2)}(t) \equiv \frac{1}{L^{2d}} \left\langle \left(\sum_i \mathbf{S}_i(t) \right)^2 \right\rangle. \quad (7)$$

For the $FFXY$ model, the second moment must be calculated in four sublattices separately, and the results are summed up after average. Keeping in mind that spatial correlation is very small in the short-time regime of the dynamic evolution, from the finite size scaling in Eq. (2) one may easily deduce the short-time power law behaviour for the second moment,

$$M^{(2)}(t) \sim t^\nu, \quad (8)$$

with

$$y = (2 - \eta)/z. \quad (9)$$

In Fig. 1, the auto-correlation for both the XY and the $FFXY$ model is displayed in log-log scale for different temperatures at and below T_{KT} . After a certain microscopic time scale t_{mic} , power law behaviour is clearly observed. Careful analysis shows that for temperature T not so far from T_{KT} , $t_{mic} \sim 100$ – 200 but as T decreases, t_{mic} gradually increases. Actually, this tendency can also be seen roughly by eyes from the figure. For example, for the XY model at $T = 0.70$, $t_{mic} \sim 300$ – 400 . This increase of t_{mic} for lower temperatures was also noticed in the measurements of the critical initial increase of the magnetization [16,17]. This phenomenon is somehow understandable since at low temperatures the configuration tends to be frozen. As the temperature T approaches zero, we may believe that t_{mic} becomes considerable big. Numerical simulations of the short-time behaviour for very low temperatures are much more difficult. It requests long updating time t and correspondingly large lattices. This might explain the violation of dynamic scaling observed for a quench to zero temperature [15].

From the slopes of the curves in Fig. 1, we measure the exponent λ . The results are given in Tables 1 and 2. As the temperature decreases, λ becomes smaller. We should mention that the errors here are only those estimated by dividing the total samples into four groups. Other errors as the fluctuation in time direction and a possible remaining effect of t_{mic} have not been taken into account². In equilibrium, it is well known that critical slowing down is much more severe in the XY and the $FFXY$ model than in the Ising model. Numerical measurements in the XY systems are very difficult. However, the situation is completely different for short-time dynamic measurements. For a lattice size $L = 512$ and updating time $t = 1500$, we already obtain rather accurate results with a total number of 800 samples.

In Fig. 2, the second moment for both the XY and $FFXY$ model is displayed in log-log scale for different temperatures at and below T_{KT} . Again we observe power law behaviour even though the fluctuations here are apparently larger than those of the auto-correlation.

²The effect of t_{mic} may sometimes be a kind of correction to the scaling which may not disappear suddenly, e.g. when the correction obeys power law.

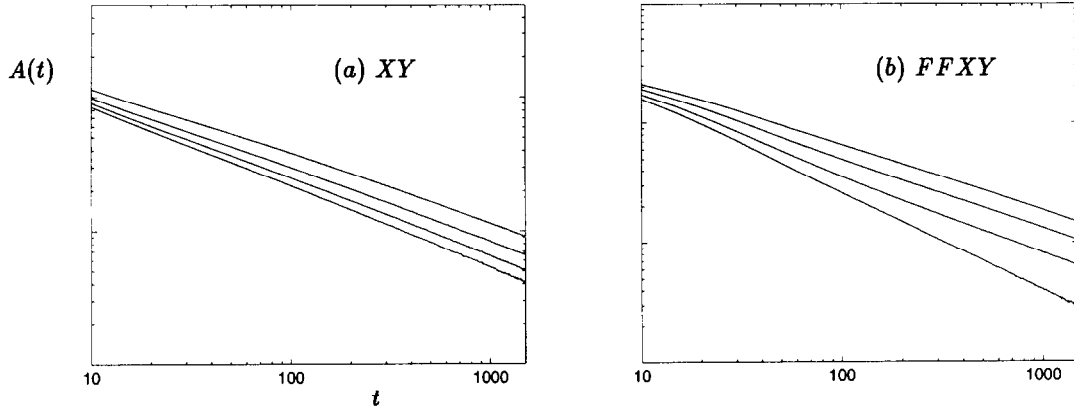


Fig. 1. Auto-correlation in log-log scale (a) for the XY model at the temperatures $T = 0.90, 0.86, 0.80$ and 0.70 (from below); (b) for the FFXY model at the temperatures $T = 0.44, 0.40, 0.35$ and 0.30 (from below).

Table 1

The exponents λ and y measured for the XY model. Values of the exponent θ are taken from Ref. [16], while η and z_1 are from Ref. [13]. z_1 is the dynamic exponent z measured from a quench from an ordered initial state [13].

T	0.90	0.86	0.80	0.70
λ	0.625(4)	0.600(3)	0.569(2)	0.552(4)
y	0.766(16)	0.775(15)	0.780(19)	0.773(24)
θ	0.250(1)	0.264(5)	0.290(1)	0.287(3)
η	0.244(5)	0.212(4)	0.178(2)	0.143(3)
$z = (2 - \eta)/y$	2.292(48)	2.307(45)	2.335(57)	2.402(75)
$z = d/(\theta + \lambda)$	2.286(11)	2.315(16)	2.328(06)	2.384(14)
z_1	1.96(4)	1.98(4)	1.94(2)	1.98(4)

Table 2

The exponents λ and y measured for the FFXY model. Values of the exponents θ are taken from Ref. [17], while η and z_1 are from Ref. [17]. z_1 is the dynamic exponent z measured from a quench from an ordered initial state [13].

T	0.44	0.40	0.35	0.30
λ	0.808(3)	0.622(2)	0.577(2)	0.561(2)
y	0.747(14)	0.835(20)	0.809(15)	0.801(13)
θ	0.079(4)	0.181(5)	0.245(3)	0.263(2)
η	0.243(4)	0.140(2)	0.107(1)	0.086(2)
$z = (2 - \eta)/y$	2.352(44)	2.228(53)	2.340(43)	2.390(39)
$\delta = \lambda - d/z + \theta$	0.037(17)	-0.095(22)	-0.033(16)	-0.013(14)
z_1	1.93(4)	1.95(3)	1.99(7)	1.97(3)

From the slopes of the curves, we measure the exponent y . The results are also listed in Tables 1 and 2. Interestingly, for the FFXY model the exponent y obviously first increases and then decreases as the temperature goes down. This might be related to the rapid drop of the exponent λ near T_{KT} .

In Tables 1 and 2, the static exponent η is estimated from a dynamic process starting from an ordered state [13]. The results are in good agreement with and improve the measurements in equilibrium. For the XY model, taking the exponents θ and η obtained in Refs. [16,13] as input, one can compute sep-

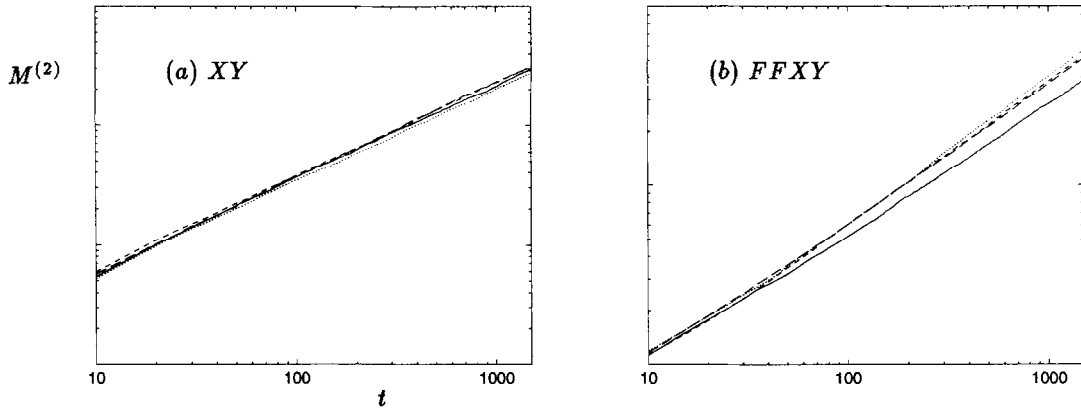


Fig. 2. Second moment in log-log scale (a) for the *XY* model with the solid, dotted, dashed and long dashed lines for the temperatures $T = 0.90, 0.86, 0.80$ and 0.70 , respectively; (b) for the *FFXY* model with the solid, dotted, dashed and long dashed lines for the temperatures $T = 0.44, 0.40, 0.35$ and 0.30 , respectively.

arately the dynamic exponent z from λ and y for different temperatures. The results are given in Table 1. The values of z obtained from the auto-correlation and the second moment agree well within statistical errors. This fact strongly supports the scaling forms in Eqs. (2) and (3) and the scaling relations between the exponents in Eqs. (4) and (9). However, the dynamic exponent z is clearly different from that measured from a dynamic process quenched from an ordered initial state, which is denoted by z_1 in Table 1. As the temperature decreases, z_1 remains a constant near 2, but z is apparently bigger than 2 and increases gradually. The difference is 15 to 20 percent and we regard it as prominent. This indicates that the dynamic scaling behaviour of the *XY* systems with a Kosterlitz–Thouless phase transition is more complicated than the simple scenario of the dynamic scaling for critical systems with second order phase transitions. The dynamic *XY* model has a nontrivial crossover behaviour for the time t macroscopically not small but also not asymptotically large. As mentioned before, the microscopic time scale t_{mic} grows as the temperature decreases. When the temperature approaches zero, it might happen that the system evolves already into the crossover regime at the time $t \sim t_{\text{mic}}$, and thus the simple scaling forms (2) and (3) are not observed.

For the *FFXY* model, the situation is even more complicated. Taking η as input, the resulting dynamic exponent z from the second moment interestingly shows a non-monotonous dependence on the temperature. This was also qualitatively observed by other

authors in calculating the domain growth [19]. However, if we take the exponent θ as input, the dynamic exponent estimated from the auto-correlation with the scaling relation (4) does not coincide with that from the second moment. The difference cannot be explained by the statistical errors. Since the exponent y from the second moment is not directly related to the initial conditions, we believe that the scaling relation (9) holds in any case, i.e. the exponent z computed from y should be correct. However, for the *FFXY* model the scaling relation (4) is violated. The violation can be described by $\delta = \lambda - d/z + \theta$. Values for this quantity are given in Table 2. The origin of this violation may probably be traced back to the chiral degree of freedom. Since the chiral transition temperature T_c is above T_{KT} , ordering dynamics of the chiral magnetization may affect the behaviour of the auto-correlation. However, a complete understanding of this problem remains open.

In conclusion, we have numerically investigated the short-time dynamic behaviour of the two-dimensional *XY* and the fully frustrated *XY* model at the temperature T_{KT} and below. Our results show that there exists indeed dynamic scaling in the short-time regime. However, the dynamic exponent z may depend on the initial conditions. It indicates that a nontrivial crossover behaviour occurs when the dynamic evolution crosses over from macroscopic short-time regime to the long-time regime. This scenario is very different from that of critical systems with second order phase transitions.

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