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Monte Carlo simulations and numerical solutions of short-time critical dynamics [☆]

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Abstract

Recent progress in numerical study of the short-time critical dynamics is briefly reviewed.
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1. Short-time dynamic scaling

For a critical dynamic system in the *long-time* regime, it is well known that there exists a universal dynamic scaling form. This is more or less due to that the correlation time is divergent and the spatial correlation length is also very large in the long-time regime.

Is there any universal behavior in the macroscopic short-time regime of the critical dynamic evolution? The traditional answer is no. However, this has been changed in recent years. In the macroscopic short-time regime, the spatial correlation length is also small in the macroscopic sense. However, the large correlation time induces a memory effect. The memory effect is represented by a scaling form.

Let us consider that a magnetic system initially at high temperature and with a small magnetization is suddenly quenched to the critical temperature, then released to dynamic evolution of model A. A universal dynamic scaling form, which sets in right after a time scale t_{mic} which is large enough in *microscopic* sense but still very small in *macroscopic* sense, has been derived with an ε -expansion [1]. Important is that extra critical exponents should be introduced to describe the dependence of the

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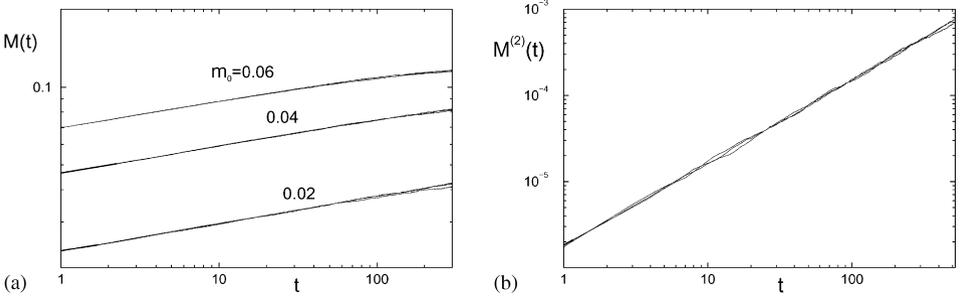


Fig. 1. (a) The magnetization of the 3D Ising model with $L = 128$. (b) The second moment.

scaling behavior on the initial conditions. For example, for the k th moment of the magnetization, the finite size scaling form is written as [1]

$$M^{(k)}(t, \tau, L, m_0) = b^{-k\beta/\nu} M^{(k)}(b^{-z}t, b^{1/\nu}\tau, b^{-1}L, b^{x_0}m_0). \quad (1)$$

Here β , ν are the well-known static critical exponents and z is the dynamic exponent, while the *new independent* exponent x_0 is the scaling dimension of the initial magnetization m_0 .

In this and the next sections we discuss the dynamics generated by Monte Carlo algorithms, which belongs to model A [2].

For a large lattice ($L = \infty$) and $\tau = 0$, from the scaling form (1) one derives for small enough t and m_0 [1,3],

$$M(t) \sim m_0 t^\theta, \quad \theta = (x_0 - \beta/\nu)/z. \quad (2)$$

For almost all statistical systems studied up to now, the exponent θ is *positive*, i.e., the magnetization undergoes surprisingly *a critical initial increase* [1,3]. The time scale of this increase is $t_0 \sim m_0^{-z/x_0}$. In Fig. 1(a), the magnetization for the 3D Ising model with the heat-bath algorithm has been displayed in log–log scale. Power-law behavior is observed at beginning of the time evolution. The microscopic time scale t_{mic} is extremely small in this case. Extrapolating the results to $m_0 = 0$ one obtains $\theta = 0.108(2)$ [4].

Other two interesting observables in short-time dynamics are the auto-correlation and the second moment of the magnetization. For $\tau = 0$ and $m_0 = 0$, it is well known [5,3] that

$$M^{(2)}(t) \sim t^{c_2}, \quad c_2 = (d - 2\beta/\nu)/z. \quad (3)$$

In Fig. 1(b), the second moment for the 3D Ising model with the heat-bath algorithm is plotted in log–log scale [4]. Almost perfect power law is seen. Careful analysis reveals [6] the auto-correlation ($\tau = 0$)

$$A(t) \sim t^{-c_a}, \quad c_a = \frac{d}{z} - \theta. \quad (4)$$

Here it is interesting that even though $m_0 = 0$, the exponent θ still enters the auto-correlation. The behavior in Eq. (4) has been confirmed in many systems [3,5].

Table 1
The exponents of the 3D Ising model

θ	c_a	z	c_2	$2\beta/\nu$
0.108(2)	1.36(1)	2.04(2)	0.970(11)	1.02(3)

In Table 1, we have summarized the measured critical exponents of the 3D Ising model. Taking the exponent θ as an input, from c_a we estimate the dynamic exponent z . With z in hand, from c_2 we obtain the static exponent $2\beta/\nu$. The values of z and β/ν agree nicely with those measured in equilibrium, $z = 2.04(3)$ [7] and $2\beta/\nu = 1.036(14)$ [8]. This fact, on the one hand, strongly supports the short-time dynamic scaling, and on the other hand, provides new ways for the numerical measurements of the critical exponents.

2. Dynamic measurements of critical exponents

For critical dynamics, correlation times are very large. Therefore, for standard Monte Carlo simulations in equilibrium it is very difficult to generate independent spin configurations. This is the so-called *critical slowing down*. One of the most successful methods to overcome critical slowing down is the non-local cluster method. However, it does not apply to systems with quenched randomness or/and frustration.

In short-time dynamics, we do not have the problem of generating independent spin configurations. Therefore, one does not suffer from critical slowing down. The 2D fully frustrated XY (FFXY) model is a typical example where critical slowing down is severe.

In general, for determination of the dynamic exponent z and static exponents a dynamic process starting from a completely *ordered* state is more favorable, since fluctuation is much less. The completely ordered state in the 2D FFX model is the ground state where spins on four sublattices orient in different directions. Here we only concern the chiral degrees of freedom and the phase transition is of the second order. Assuming the lattice is sufficiently large, around the critical point the dynamic scaling form of the magnetization is written as

$$M(t, \tau) = t^{-\beta/\nu z} F(t^{1/\nu z} \tau). \quad (5)$$

If $\tau = 0$, the magnetization decays by a power law $M(t) \sim t^{-\beta/\nu z}$. If $\tau \neq 0$, the power-law behavior is modified by the scaling function $F(t^{1/\nu z} \tau)$. From this fact, one determines the critical point and the critical exponent $\beta/\nu z$.

In Fig. 2(a), the magnetization at $T = 0.452, 0.454$ and 0.456 is plotted in double-log scale. The Metropolis algorithm has been used in simulations. Extrapolating $M(t)$ to other temperatures, from the time interval [200,2000] we measure the critical temperature to be $T_c = 0.4545(2)$ and $\beta/\nu z = 0.0602(2)$ [9]. To determine the exponent $1/(\nu z)$, we differentiate $\ln M(t, \tau)$ and obtain

$$\partial_\tau \ln M(t, \tau) |_{\tau=0} \sim t^{1/\nu z}. \quad (6)$$

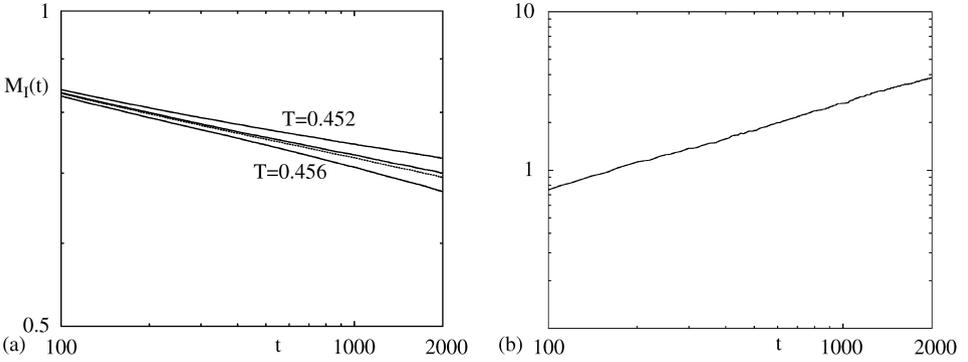


Fig. 2. (a) The chiral magnetizations of the 2D FFX model starting from an ordered state. From above, the solid lines represent $M_I(t)$ at $T = 0.452, 0.454$ and 0.456 . The dotted line is at $T_c = 0.4545$. (b) The derivative $\partial_\tau \ln M_I(t, \tau)|_{\tau=0}$.

Table 2

Dynamic measurements of the exponents of the 2D FFX model compared with those in recent references. For the Ising model, the exponent θ is taken from Ref. [14]. The exponent z in literature ranges from 2.155 to 2.172 [3]. Here an ‘average’ value is given

	Ref. [9] (1998)	Ref. [10] (1996)	Ref. [11] (1995)	Ref. [12] (1994)	Ref. [13] (1993)	Ising
T_c	0.4545(2)	0.451(1)	0.452(1)	0.454(2)	0.454(3)	
ν	0.81(2)	0.898(3)	1	0.813(5)	0.80(5)	1
$2\beta/\nu$	0.261(5)			0.22(2)	0.38(2)	0.25
z	2.17(4)					2.165(10)
θ	0.202(3)					0.191(3)

This power-law behavior is shown in Fig. 2(b) [9].

In order to estimate the dynamic exponent z *independently*, we introduce a Binder cumulant $U = M^{(2)}/M^2 - 1$, and finite size scaling analysis shows

$$U(t, L) \sim t^{d/z} . \tag{7}$$

Now we complete the measurements of the critical exponents. The results are given in Table 2, in comparison to those obtained in equilibrium simulations. Our results obviously support that the exponent ν of the 2D FFX model is different from that of the 2D Ising model. But other exponents of both models look similar.

3. Deterministic dynamics

Up to now, we have discussed *stochastic* dynamics induced by Monte Carlo algorithms. However, in general stochastic dynamics is *not* equivalent to real dynamics described by microscopic *deterministic* equations of motion. Only in some cases stochastic dynamics is an effective description of real physical systems. Therefore, it is

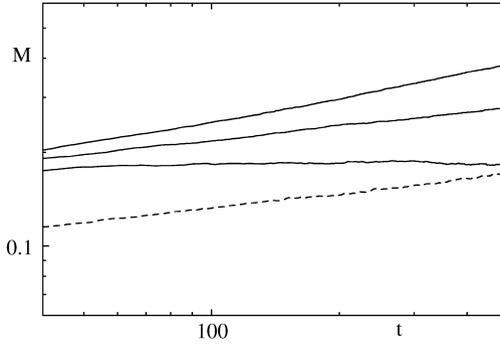


Fig. 3. The magnetization of the ϕ^4 theory in log–log scale. Solid lines are for $m_0 = 0.015$ with energy densities $\varepsilon = 20.7, 21.1$ and 21.5 (from above), while the dashed line is for $m_0 = 0.009$ with $\varepsilon_c = 21.11$.

important and interesting to investigate whether there exists universal scaling behavior in deterministic dynamics.

We consider the 2D ϕ^4 theory. The Hamiltonian on a square lattice is

$$H = \sum_i \left[\frac{\pi_i^2}{2} + \frac{1}{2} \sum_{\mu} (\phi_{i+\mu} - \phi_i)^2 - \frac{m^2}{2} \phi_i^2 + \frac{\lambda}{4!} \phi_i^4 \right] \quad (8)$$

with $\pi_i = \dot{\phi}_i$ and it leads to the equations of motion

$$\ddot{\phi}_i = \sum_{\mu} (\phi_{i+\mu} + \phi_{i-\mu} - 2\phi_i) + m^2 \phi_i - \frac{\lambda}{3!} \phi_i^3. \quad (9)$$

In dynamic evolution governed by Eq. (9), energy is conserved. The solutions are assumed to generate a microcanonical ensemble. The temperature could be defined as the averaged kinetic energy. In the short-time dynamic approach, however, the total energy is a more convenient controlling parameter, since it is conserved and can be input from the initial state. Therefore, from now τ will be understood as a reduced energy density $(\varepsilon - \varepsilon_c)/\varepsilon_c$. Here ε_c is the critical energy density.

The order parameter of the ϕ^4 theory is the magnetization. For the dynamic process starting from a *random* state [15], we assume a same dynamic scaling form as in stochastic dynamics. For sufficiently large L and small enough m_0 and t , from scaling form (1) one deduces

$$M(t) = m_0 t^{\theta} F(t^{1/\nu z} \tau). \quad (10)$$

Similar as the discussion on Eq. (5) in Section 2, we determine the critical energy ε_c and the exponent θ from Eq. (10) and the exponent $1/\nu z$ from its derivative. Finally, the exponent $\beta/\nu z$ and the dynamic exponent z are estimated from the second moment and the auto-correlation.

In Fig. 3, numerical solutions of the magnetization with $m_0 = 0.015$ for parameters $m^2 = 2$ and $\lambda = 0.6$ have been plotted with solid lines for three energy densities $\varepsilon = 20.7, 21.1$ and 21.5 in log–log scale. Careful analysis of the data between $t = 50$ and 500

Table 3

The critical exponents of the ϕ^4 theory in comparison with those of the Ising model Ref. [3]

	θ	$d/z - \theta$	$(d - 2\beta/\nu)/z$	$1/\nu z$	z	$2\beta/\nu$	ν
ϕ^4	0.176(7)	0.755(5)	0.819(12)	0.492(26)	2.148(20)	0.24(3)	0.95(5)
Ising	0.191(1)	0.737(1)	0.817(7)		2.155(3)	1/4	1

leads to the critical energy density $\varepsilon_c = 21.11(3)$ [15]. This agrees well with $\varepsilon_c = 21.1$ given by the Binder cumulant in equilibrium in Ref. [16]. At ε_c , one measures the exponent $\theta = 0.146(3)$. The magnetization with $m_0 = 0.009$ is also displayed in Fig. 3 (dashed line). The corresponding exponent is $\theta = 0.158(2)$. Extrapolating the results to $m_0 = 0$, we obtain the final value $\theta = 0.176(7)$. With the critical energy in hand, we estimate other exponents. In Table 3, we summarize all the critical exponents of the ϕ^4 theory. Remarkably, not only the static exponents, but also the dynamic exponents z of the ϕ^4 theory is the same as those of the Ising model with standard Monte Carlo dynamics.

4. Concluding remarks

We have demonstrated that universal scaling behavior emerges already in the macroscopic short-time regime of the critical dynamic evolution. The short-time dynamic scaling is found not only in stochastic dynamics but also in microscopic deterministic dynamics. Therefore, it is fundamental. Furthermore, it leads to new methods for numerical measurements of both dynamic and static critical exponents. The methods do not suffer from critical slowing down.

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