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Short-time dynamics of first-order phase transition in a disordered system

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Abstract

Nonequilibrium short-time dynamics of first-order phase transition in a driven-disordered system at zero temperature is investigated. In a random-bond Ising model under external field, the largest discontinuous jump of order parameter shows a power-law evolution in short times: $\Delta M(t) \sim t^{\theta}$. The scaling exponent θ is equal to $(d - \beta/\nu)/z$, where d is the dimensionality; β, ν and z are the critical exponents of the system. θ is found to be a universal exponent for any metastable relaxation in the short-time regime. This investigation suggests that the short-time dynamics is valid for the first-order phase transition in the driven disordered system and the critical phenomenon of the disordered system can be understood in the framework of nonequilibrium dynamics.

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1. Introduction

Critical short-time dynamics has attracted a lot of attention in the past decade. In their pioneering work, Jassen, Schaub and Schmittmann [1] proved that at the critical temperature of a second-order phase transition, the system quenched from a high-temperature disordered state shows an 'initial slip' kinetic scenario in the short-time regime. In contrast to the decay of evolution process in the long-time regime [2], the order parameter $M(t)$ grows as a power law in time:

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

where the initial-order parameter m_0 is small. $\theta = (x_0 - \beta/\nu)/z$ is a new dynamic exponent. x_0 is the scaling dimension of m_0. β, ν and z are the critical exponents. Because of critical slowing down, it is difficult to characterize the kinetics of phase transition in long times at the critical temperature. Therefore, the critical short-time dynamics is very useful for the characterization of second-order transitions. The short-time scaling relations have been checked in many well-defined models [3] and are used to characterize the critical phenomena, for example, the critical exponents of the phase transition. So far, most of the studies have been focused on the critical short-time dynamics of systems without impurities [3]. The critical short-time dynamics could be of great importance to the study of phase transitions in disordered systems, since the relaxation time is extremely long and it is difficult to characterize phase transitions in disordered systems by conventional equilibrium and nonequilibrium methods. Unfortunately, recent investigations on the second-order phase transition in disordered models indicate that the power-law scaling relations do not hold and the corrections to the power-law scaling depend on the system and the nature of disorder [4–7]. This issue deserves to be further analysed.

The first-order phase transition (FOPT), in nature, is a kinetic process because of nucleation and growth of the domain structures. Experimental and theoretical investigations have shown that the domain growth at the late stages can be well described by the scaling form or by the Kolmogorov–Johnson–Mehl–Avrami (KJMA) equation [8],

$$f = 1 - \exp(bt^n) \tag{2}$$

where f is the fraction of new phase. $b < 0$ is a constant that depends on the nucleation rate. n depends on the dimensionality and the heterogeneity of nucleation and growth. However, equation (2) is only valid at the late stages of FOPT. At short times and for a FOPT, there is little understanding of the kinetics in short times because the formation of nuclei is very rapid in a pure system. If impurities are present in a FOPT, the short-time regime may be long and the kinetics can be observed. It is, therefore, interesting to investigate the kinetics of FOPT in a disordered system at short times.

The effect of disorder on a phase transition is an important issue in statistical physics. For example, in a disordered Ising model at zero temperature, there is a second-order transition induced by the disorder in the system without applied field [9]. When the magnetic field is applied, there is a field-driven FOPT [10, 11] if the strength of the disorder is smaller than the critical strength of the disorder. Nonequilibrium short-time dynamics may play an important role in the simulation studies of disorder-related phase transitions (second order and first order), since there are a lot of local energy minima introduced by the disorder, and the relaxation times of the metastable states in both the second-order and first-order transitions are extremely long. However, at zero temperature, Monte Carlo simulation of the critical behaviour is almost impossible since the system is usually trapped in metastable states. All these issues imply that the characterization of phase transitions in disordered systems at zero temperature is a subject of great interest.

In this paper, I use Monte Carlo simulation to investigate the short-time dynamics of second-order and first-order phase transitions in a random-bond Ising model. The understanding of critical phenomenon in the framework of nonequilibrium dynamics will be analysed.

2. Model system

Disordered Ising models are important model systems for phase transitions in disordered systems. The effect of quenched-in defects on equilibrium phase transitions has been extensively studied [9]. Here I consider a two-dimensional random-bond Ising system. The Hamiltonian of this system can be written as

$$\hat{H} = -\sum_{\langle ij \rangle} J_{ij} S_i S_j - H \sum_i S_i \tag{3}$$

where $S_i = \pm 1$ are spin variables and $\langle ij \rangle$ denotes the summation extending over all nearest-neighbour spins. H is a homogeneous external field; J_{ij} is the exchange interaction strength with uniform distribution between $J_0 - D$ and $J_0 + D$. D measures the strength of random bonds. H and D are in units of J_0. The random-bond Ising model described by equation (3) at zero temperature can be mapped exactly to a maximum-flow problem [9].

At zero temperature and $H = 0$, the system changes from the ferromagnetic state to the paramagnetic state when the random-bond strength D increases. This so-called disorder-induced phase transition at zero temperature is a second-order phase transition [10, 11]. If an external field is applied, the driven-disordered system described by equation (3) has a field-driven first-order phase transition when the disorder strength D is below the critical value D_c [10, 11]. Because the metastable relaxation times have a wide range of distribution due to the disorder nature of random bonds, it is possible to investigate the critical short-time dynamics in the driven-disordered system and its relation with the equilibrium critical scaling for the disorder-induced phase transition in the system without an applied field.

The system described by equation (3) is investigated by Monte Carlo simulation. Glauber kinetics at zero temperature is used. Physical quantities are averaged over 5000–50 000 random-bond configurations, dependent on the system size. The system size varies from $L = 256$ to $L = 1024$. To speed up the simulation, a fast algorithm similar to the sort-list algorithm is used. This is based on the fact that when $D \leqslant 1$ a spin will never flip back under a decreasing field once it is flipped. All spins are updated simultaneously. One time step, or one Monte Carlo step (MCS), in the simulation is defined as one attempt to update all spins. A spin will flip if its local field $f_i = \sum J_{ij} S_j + H$ changes sign. For the field-driven first-order transition, the external field is decreased from $+\infty$ to $-\infty$ by dH and then is fixed until all spins have been updated. An infinite slow driving field or static driving field is achieved by adjusting dH to the minimum local field f_i after a metastable state is reached. Thus dH is not a constant.

3. Critical dynamics of disorder-induced phase transition

Let us first look at the critical dynamics of disorder-induced phase transition in the system without applied field. In order to compare with other studies, here we choose the Gaussian distribution of random bonds: $P(J_{ij}) = \exp[-(J_{ij} - J_0)^2/2\sigma^2]/(2\pi\sigma^2)^{1/2}$. The strength of the random bonds is characterized by the standard deviation σ and the critical strength σ_c was found to be 0.44 in the literature [11]. We now let the system start from either a completely ordered state or disordered state and evolve according to the Glauber dynamics [12]. Figure 1 shows that the evolution of the system started from a disordered state ($M_0 = 0$). The evolution of magnetization $M(t)$ can be fitted to a stretched exponential relation:

$$M(t) = M_\infty - a\mathrm{e}^{-bt^\gamma} \tag{4}$$

where a and b are constants and γ depends on random-bond strength σ. At $\sigma = \sigma_c$, there is no power-law scaling relation such as that in the short-time dynamics, e.g. equation (1). Figure 1 indicates that short-time dynamics is obviously not applicable to the disorder-induced transition in the random-bond Ising model at zero temperature. The reason is that at zero temperature the local energy minimum generated by the random-bond defects can trap the system in metastable states. Although equation (4) is approximated as a power law when t is small, γ is not related to the critical exponents of phase transition. γ seems to characterize the disorder nature of system and is related to the random walk kinetics.

In order to use the Monte Carlo simulation to investigate the disorder-induced phase transition at zero temperature in the disordered system, we should explore an alternative method. Because the disordered system trapped in local energy minimum can be activated by an external field, we may study the kinetics of random-bond Ising model driven by an applied field, i.e. a driven disordered Ising model. The critical phenomena of the disorder-induced

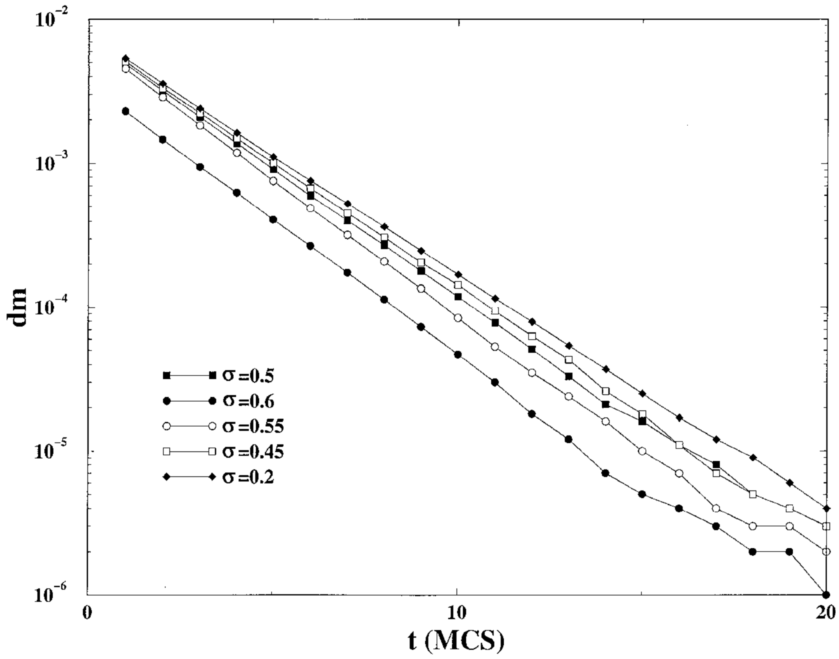

Figure 1. Dynamics of RBIM started from a completely disordered state. $\mathrm{d}m(t) = M_\infty - M(t)$. The y-axis is a logarithmic scale.

transition, therefore, can be understood in the framework of nonequilibrium dynamics of the driven disordered system.

4. Short-time dynamics of first-order transition in a driven disordered system

4.1. Stationary scaling

A random-bond Ising model under an applied field is simulated using the same algorithm as that stated in section 3. Figure 2 shows a typical magnetization curve at zero temperature. There are a lot of discontinuous jumps in the magnetization curve, which are caused by the evolution of the system among metastable states. When $D < D_c$, there is a field-driven first-order phase transition, as shown in figure 2. This first-order phase transition driven by the magnetic field can be characterized by the largest discontinuous jump in the magnetization curve at the critical field H_c.

The stationary scaling for this system can be obtained by defining one half of the largest jump ΔM (M is the magnetization) in the magnetization reversal curve as an order parameter. In an infinitely large system and near critical disorder strength $D_c(\infty)$, the critical scaling can be written as [10, 11]:

$$\Delta M \sim (D_c - D)^{\beta\nu} \qquad t_0 \sim (D_c - D)^{-\nu z} \tag{5a}$$

where t_0 is the duration time of the largest jump ΔM.

In the Monte Carlo simulation, the magnetization M is measured after the system achieves a metastable state, i.e. no spin is updated unless the external field is further decreased. Equations (5a) are shown in figures 3(a) and (b), respectively. The system sizes are $L =$ 1024, 512 and 256.

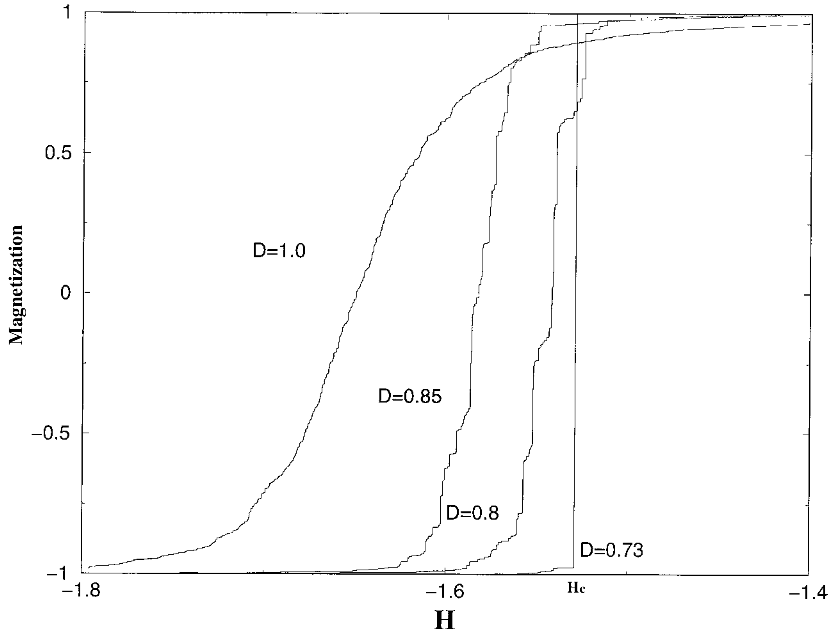

Figure 2. Typical magnetization curve in a driven-disordered RBIM with $L = 512$. The critical disordered strength is $D_c(L) = 0.76$. When $D = 0.73$, the largest magnetization jump in FOPT is defined as ΔM at magnetic field H_c.

Table 1. The critical exponents and $D_c(\infty)$ determined by (a) stationary scaling and (b) nonequilibrium dynamics. The critical exponent is the average of those calculated from the finite-size scaling in small systems and the critical scaling in large systems. $D_c(\infty)$ is determined by the relations $D_c(L) - D_c(\infty) \propto L^{-1/\nu}$.

	β	$1/\nu$	z	$D_c(\infty)$
(a)	0.01 ± 0.04	0.6 ± 0.1	1.2 ± 0.1	0.70 ± 0.03
(b)	0.05 ± 0.02	0.7 ± 0.1	1.28 ± 0.05	0.70 ± 0.02

Since ΔM and t_0 are used as the order parameter and relaxation time, respectively, the finite-size scaling for ΔM and t_0 can be written as [11]

$$\Delta M[L, (D_c - D)/D_c] = b^{\beta/\nu}\, \Delta M[bL, b^{1/\nu}(D_c - D)/D_c] \tag{5b}$$

$$t_0[L, (D_c - D)/D_c] = b^{z}\, t_0[bL, b^{1/\nu}(D_c - D)/D_c] \tag{5c}$$

where b is the size scaling factor. Here D_c is defined as $D_c(L)$ in a system with size L and $D_c(L) - D_c(\infty) \propto L^{-1/\nu}$. Equation (5*b*) is shown in the inset of figure 3(*a*) and equation (5*c*) is shown in the inset of figure 3(*b*). The critical exponents β, ν and z and the critical disorder strength $D_c(\infty)$ can be calculated from finite-size scaling (equations (5*b*) and (5*c*)), or from the critical scaling in the large system ($L = 1024$) using equation (5*a*). They are found to be consistent with each other.

Table 1 lists the results determined by the stationary scaling for metastable states. The critical strength of disorder for the random-bond Ising model described by equation (3) is $D_c(\infty) = 0.70 \pm 0.03$.

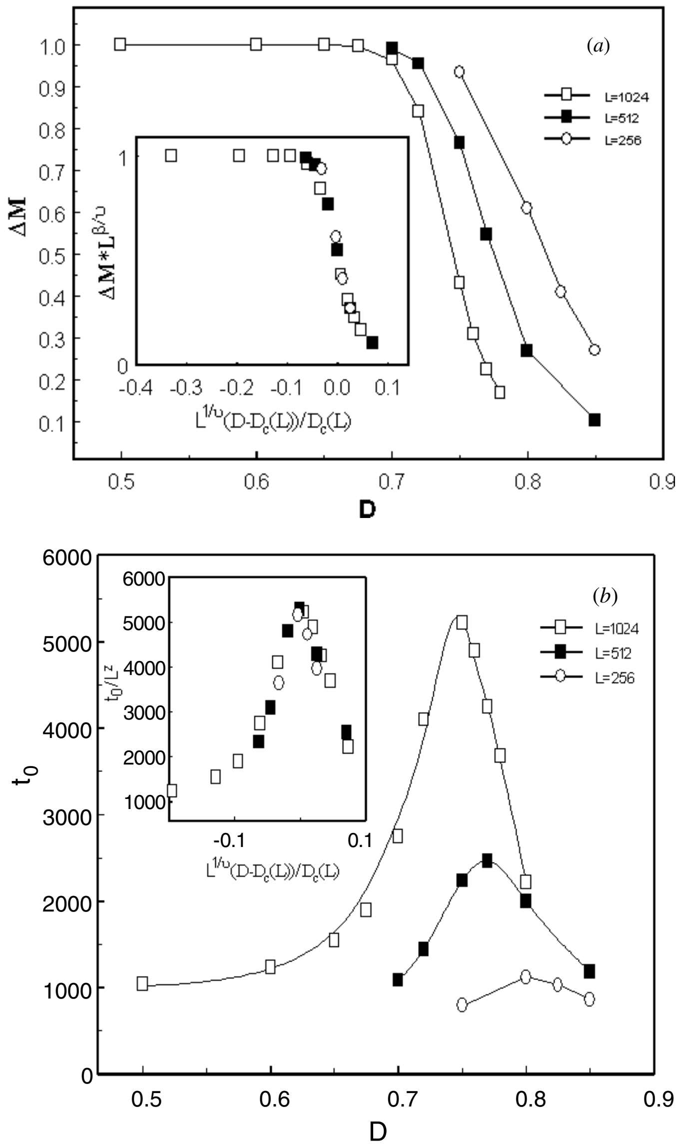

Figure 3. Stationary critical scaling for metastable states. (*a*) The largest jump ΔM in the magnetization curve. The inset is the finite-size scaling. (*b*) The duration time t_0 of the largest jump. The inset is the finite-size scaling. The exponents are listed in table 1.

4.2. Short-time dynamics of field-driven first-order transition

In section 4.1 we characterize the first-order transition using the stationary scaling for the metastable states. In this section, we are interested in the possibility of determining the critical exponents by nonequilibrium dynamics of FOPT. The nonequilibrium kinetics of the first-order transition, i.e. how the metastable state evolves at different random-bond strengths, may also be used to determine the critical exponents. Because ΔM measures the maximum discontinuity in the first-order transition, we can characterize the kinetics of the first-order transition by defining the time-dependent largest jump that occurs at the critical field H_c as $\Delta M(t) \equiv [M(t) - M_c(D)]/2$, where $M_c(D)$ is the magnetization just before the largest jump occurs.

The procedures of simulation are described as follows. (1) The initial configuration of the system is set to have all spins up ($M = 1$). The system is then allowed to evolve under a decreasing external field; (2) set the time to zero ($t = 0$), then the external field is decreased by dH and is kept as a constant; (3) at time t, a Glauber update is applied and the size of discontinuous jump $m(t)$ is calculated using the relation $m(t) = [M(0) - M(t)]/2$; (4) step (3) is repeated until time T when the metastable state is achieved, i.e. no spin flips at time step T (T is defined as the duration time).

The procedures (2), (3) and (4) are carried out until the magnetization saturates at $M = -1$. In a finite-size system the critical field H_c (L, D) is defined as the field value at which $m(T)$ is the largest jump ΔM or the duration $T = t_0$ is the longest.

The procedures (1)–(4) are repeated 5000–50 000 times with different random-bond configurations. The time-dependent largest jump $\Delta M(t)$ is averaged and is shown in figure 4. Near the critical disorder strength $D_c(L)$ in systems with different sizes L, $\Delta M(t)$ evolves as a power law in the short-time regime. In an infinite system, the characteristic time of this power-law regime could diverge when the disorder strength approaches $D_c \equiv D_c(\infty)$. In a finite-size system with $D < D_c(L)$, $\Delta M(t)$ can be used to characterize the kinetics of a field-driven first-order phase transition, therefore, the short-time dynamics (equation (1)) is applicable to the first-order transition in the disordered system.

We may analyse the short-time scaling based on a dynamical finite-size scaling relation [6]. In the short-time regime, since the size of the largest jump is small and the correlation among flipped spins is weak, the dynamic finite-size scaling for $m(t)$ at $D = D_c(\infty)$ and $H = H_c$ is written as

$$m(L, t) = b^{\beta/\nu}\, m(bL, tb^{-z}) \tag{6}$$

where b is a size scaling factor. z is the dynamical exponent. In an infinitely large system equation (6) leads to the critical dynamic scaling for $m(t)$ in short times:

$$m(t) \sim t^{[d-\beta/\nu]/z} \sim t^{\theta} \tag{7}$$

where $d = 2$ is the dimensionality. Although equation (7) is exact only at the critical point, i.e. $D = D_c(\infty)$ and $H = H_c$, it is also valid for the first-order transition at short times, as shown in figure 4. For the first-order transition in the system with $L = 1024$, the characteristic time scale (the duration of the largest jump) is about several thousand time steps dependent on $D_c(L) - D$. Therefore equation (7) holds in the first-order transition at short times and the scaling exponent θ can be determined accurately. In figure 4 the exponent θ is measured at $D = D_c(L)$ in systems with different sizes and is extrapolated to $L \to \infty$. $\theta = 1.52 \pm 0.02$ is found to be equal to $(d - \beta/\nu)/z$, compared with the critical exponents listed in table 1. The dynamical finite-size scaling for $m(t)$ at $D = D_c(\infty)$ and $H = H_c$ is shown in figure 5. It can be seen from figure 5 that equation (6) is valid for the first-order transition at short times. The critical exponents β/ν and z are calculated from equations (6) and (7) and are listed in table 1.

Equation (7) can also be used to determine the critical disorder strength $D_c(\infty)$ and the crtical exponent ν. In a finite-size system, $m(t)$ is fitted to equation (7) at the critical disorder strength $D_c(L)$ with the least error. Therefore, $D_c(\infty)$ is estimated by the relation $D_c(L) - D_c(\infty) \propto L^{-1/\nu}$. Table 1 lists β, ν, z and $D_c(\infty)$ measured by this method.

Figure 6 shows the configuration of flipped spins at various times during the largest discontinuous jump. The Fourier transform of the correlation function of these flipped spins is written as

$$C(q, t) = [\langle S_q(t) S_{-q}(t)\rangle] \tag{8}$$

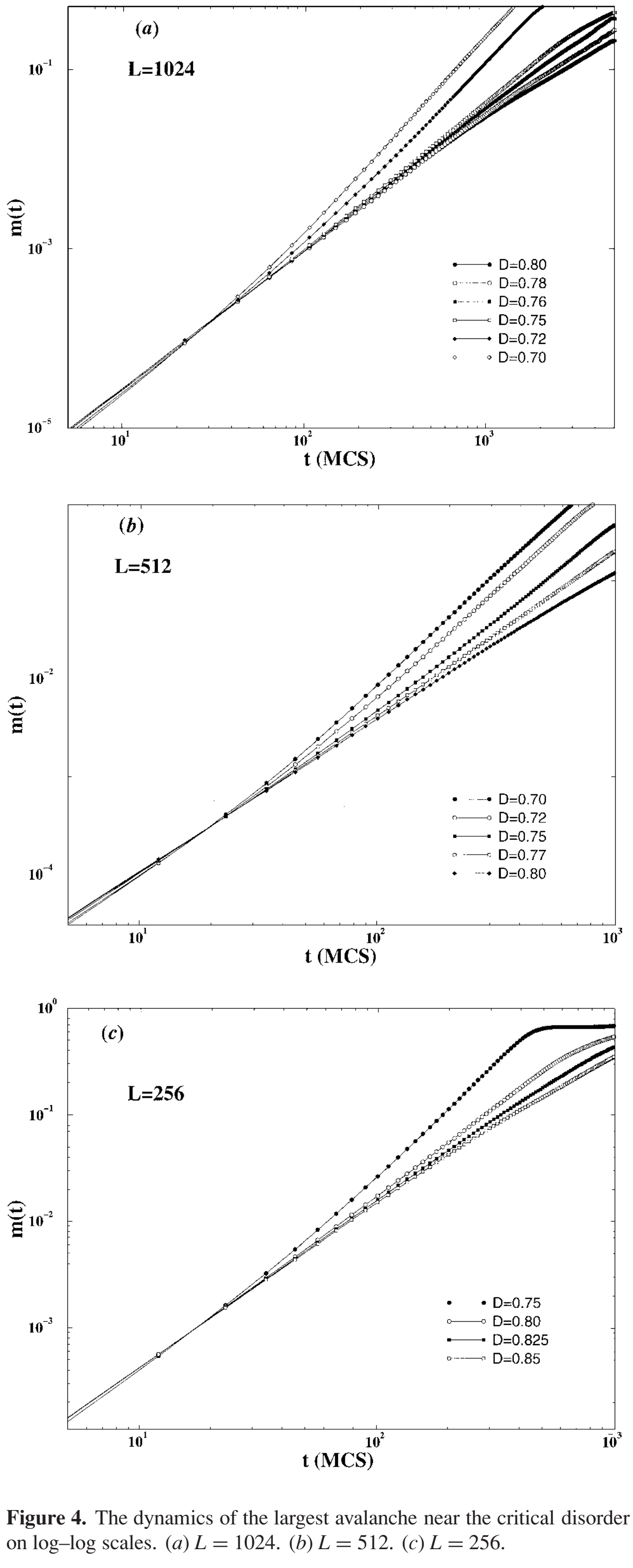

Figure 4. The dynamics of the largest avalanche near the critical disorder strength. The plots are on log–log scales. (*a*) $L = 1024$. (*b*) $L = 512$. (*c*) $L = 256$.

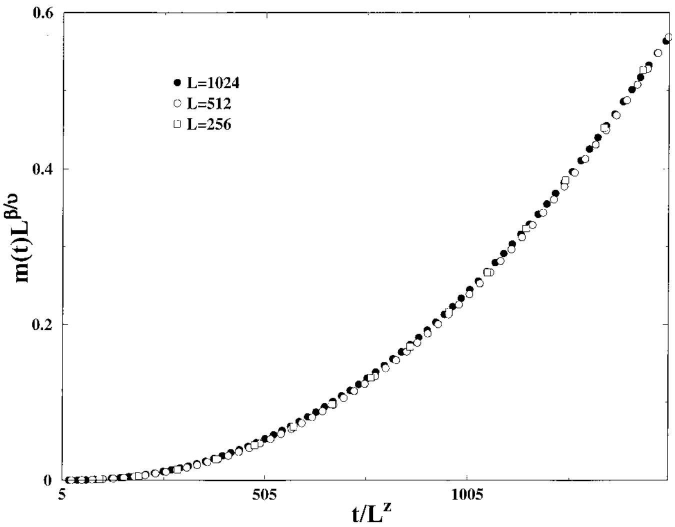

Figure 5. The dynamic finite-size scaling for the largest avalanche size $m(t)$.

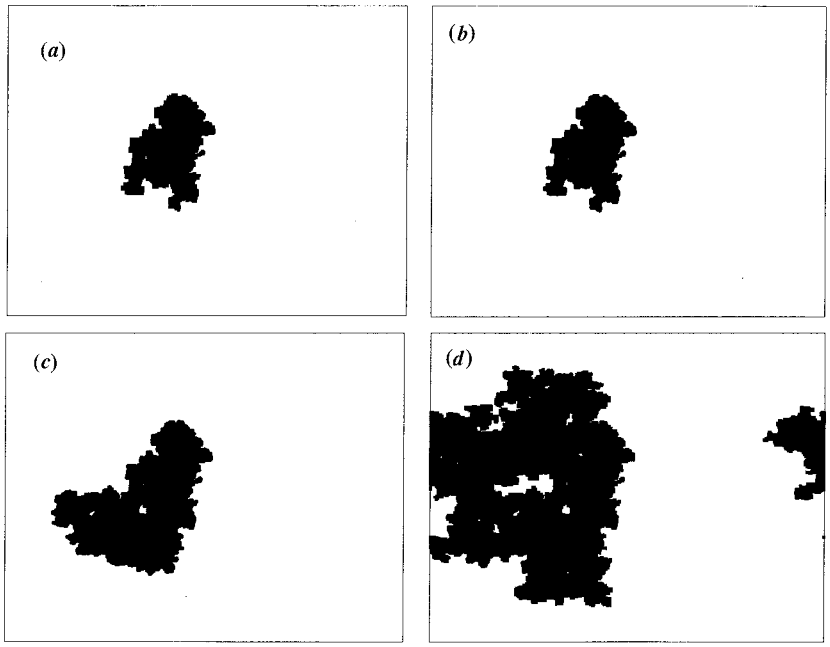

Figure 6. The evolution of the largest avalanche at different times. (a) $t = 100$ μs. (b) $t = 1000$ μs. (c) $t = 2000$ μs. (d) $t = 5000$ μs.

where $S_q(t)$ is the Fourier transform of the flipped spin during the first-order transition. $\langle \cdots \rangle$ denotes ensemble average and $[\cdots]$ denotes average over random-bond configurations. Figure 7 shows the data collapse of $C(q, t)$ at different times. q_0 is defined as the wave vector at which $C(q_0, t)/C(0, t) = 1/2$. This data collapse suggests that the avalanches of spins during FOPT at short times have self-similarity [10].

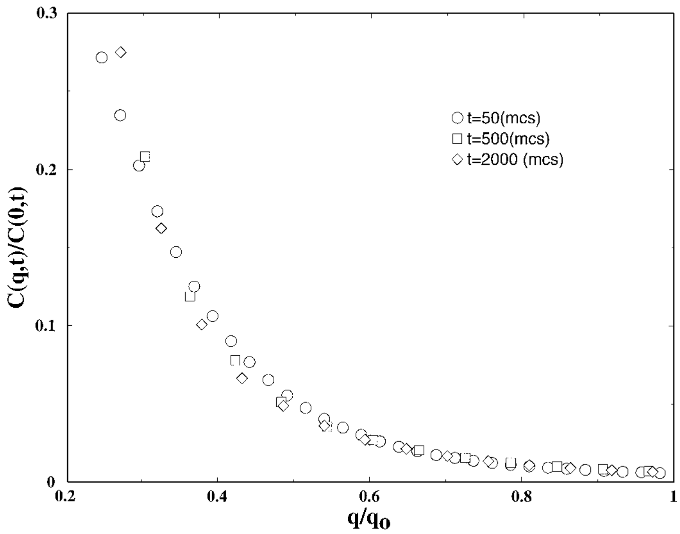

Figure 7. The data collapse of correlation functions at different times.

4.3. Universality of the short-time scaling exponent in FOPT

Besides the largest discontinuous jump ΔM at H_c that is used to characterize the field-driven first-order transition, there are other small jumps in the magnetization reversal process, i.e. small discontinuities in the magnetization curve as shown in figure 2. The evolution of these small jumps characterizes the relaxation of all metastable states that are induced by the impurities. Under an applied field, the metastable states lead to hysteresis, which is a common feature of a first-order transition. We can fit the metastable relaxation to equation (7) in the short-time regime. Assume T is the duration time of a jump and the short-time regime is defined as [5, $T/2$]. The evolution of this jump can be fitted to equation (7). The resulting exponent θ thus becomes the kinetic characteristic of this jump. All discontinuous jumps in the magnetization curve are characterized by equation (7) and the corresponding exponents θ are evaluated. We plot the distribution of all these exponents θ in figure 8. The distribution has two peaks at θ_L and θ_H. θ_L is smaller than θ_H and does not change with the disorder strength D. Since $\theta_L = 1.53$ is independent of D and the same as the exponent of $\Delta M(t)$, i.e. $(d - \beta/\nu)/z$, the exponent of the largest discontinuous jump, *we identify θ_L with the dynamic exponent that characterizes the short-time relaxation of all metastable states, and therefore it is a characteristic dynamic exponent of FOPT*. The evidence that θ_H increases with increasing disorder strength also suggests that θ_H characterizes the kinetics at the late-time regime and should not be fitted to equation (7). These features can be seen in figure 4. At the late stage the evolution of discontinuous jump is much faster than a power-law relation and can be fitted to equation (2), the KJMA equation.

Figure 9 shows the finite-size effect on the distribution of θ at a fixed disorder strength $D = 0.75$. In figure 9, a small number of bins for histogram plots is used so that $P(\theta)$ can be quantitatively compared. In a finite-size system, for example $L = 1024$, 512 or 256, the critical disorder strength $D_c(L)$ is larger than $D = 0.75$, therefore, the system with $D = 0.75$ undergoes a field-driven first-order transition. As L increases, D_c decreases and it becomes difficult to resolve the θ_L peaks related to the late-stage kinetics for the largest system sizes, i.e. 512 and 1024. In contrast, θ_L is clearly seen and well defined. Assume that $P(\theta_L)$ is a Gaussian

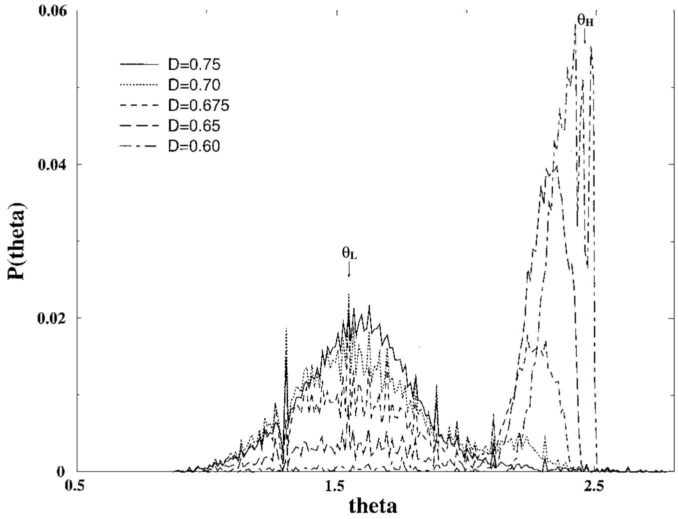

Figure 8. The distributions of dynamic exponent θ near the critical disorder strength. $L = 1024$. The bin size is 0.01.

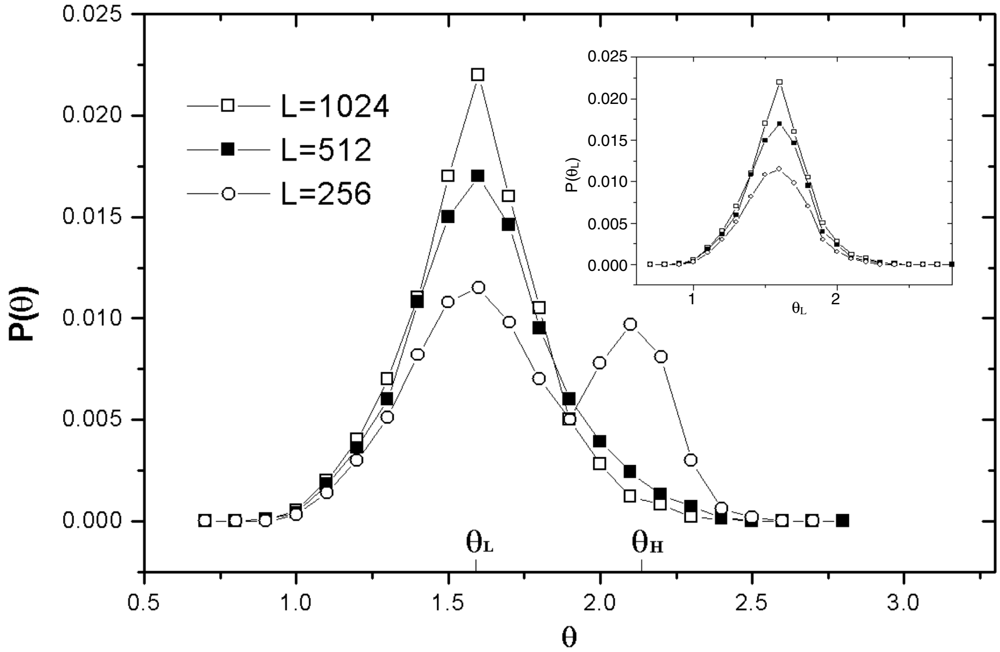

Figure 9. The distributions of the dynamic exponent θ at $D = 0.75$ in finite-size systems. The bin size is 0.1. The inset shows the distributions of short-time dynamic exponent θ_L.

distribution, we can obtain $P(\theta_L)$ from $P(\theta)$. The inset in figure 9 shows the finite-size scaling for $P(\theta_L)$. Figure 9 indicates that θ_L does not change with the system size and the metastable relaxations in the first-order transition are consistent with the power-law short-time dynamics (equation (7)).

5. Discussion and conclusion

Critical short-time dynamics is not applicable to the disorder-induced phase transition at zero temperature. The reason is that there are a lot of energy barriers created by the disorder and the system started from ordered or disordered states will be trapped in the metastable states rapidly. When the external field is applied, the system is activated from the metastable states. Hence metastability and hysteresis are common features in the field-driven first-order phase transition in the disordered system. Based on these features, the critical exponents of disorder-induced transition can be investigated by nonequilibrium dynamics of FOPT.

In FOPT it is difficult to investigate the kinetics at the late stage by Monte Carlo simulation because of the finite-size effect. Instead, the dynamic scaling in short times is independent of the system size and the metastable states. As demonstrated in the random-bond Ising model, the short-time dynamics is well defined in a finite system and the characteristic exponent θ is universal. Therefore, short-time dynamics for the first-order transition has great advantage in determining the critical exponents.

It should be emphasized that short-time dynamic scaling for the first-order transition is also observed in systems other than systems with quenched disorder. Usually the metastable relaxation in a first-order transition is so fast that it is difficult to observe the kinetic process in short times. If a system is composed of multi-species, or is generated by rapid cooling, the energy landscape of the system is very complicated and the relaxation time of the metastable states could be very long. We may observe the short-time kinetics that is obviously different from the late-time kinetics (equation (2)). Glass transition [13] and spinodal decomposition in multi-component system are good examples. In these systems, the kinetics in short times shows dynamic scaling that cannot be described by the KJMA equation.

In the driven-disordered system, two methods can be used to determine the critical exponents. One is the stationary scaling (equations (5)) that describes the critical behaviour of the largest discontinuous jump. Another is the nonequilibrium dynamics scaling for all discontinuous jumps during the FOPT. In a small system ($L < 256$) the stationary scaling relations can be used but the errors in the determined exponents determined are large. In a relative large system ($256 < L < 2048$), the dynamic scaling (equation (7)) holds very well and can serve as an alternative and a more accurate method for determining the critical exponents.

In conclusion, the short-time dynamics is not applicable to the disorder-induced second-order transition in a disordered system at zero temperature. However, the field-driven first-order phase transition is found to follow the short-time dynamics. Any metastable relaxation shows the same power-law kinetics in the short times. The scaling exponent is related to the critical exponents of a disorder-induced transition and can be treated as a new dynamical exponent for the field-driven first-order transition. Compared to the stationary scaling for the metastable states, the nonequilibrium dynamics is more suitable for the investigation of the critical phenomenon in a finite-size system.

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