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Non-equilibrium critical dynamics with domain interface

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Abstract – With Monte Carlo simulations, we investigate the non-equilibrium critical dynamics with a domain interface, taking the two-dimensional Ising model as an example. Starting from a semi-ordered state, the domain interface grows as time evolves. Dynamic scaling behavior is carefully analyzed. The magnetization and Binder cumulant inside the domain interface are governed by critical exponents different from those outside the domain interface. The ageing phenomenon is identified. For comparison, additional simulations starting from an ordered state have been performed with a free surface and a disordered surface.

In the past decades, much progress has been achieved in understanding non-equilibrium dynamic processes. Important examples are spin glass dynamics, structural glass dynamics, phase ordering dynamics, non-equilibrium critical dynamics and interface growth, etc. For the non-equilibrium critical dynamics at a continuous phase transition, the universal dynamic scaling form has been extended to the *macroscopic short-time* regime [1–4], when the system is still far from equilibrium. 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 [4–6]. Recent activities include, for example, theoretical calculations and numerical simulations of XY models and Josephson junction arrays [7–10], magnets with quenched disorder [11–14], various critical systems [15–18], and ageing phenomena [19–24]. Dynamic reweighting methods have been suggested [12,25]. Application of the dynamic approach to the weak first-order phase transitions is also inspiring [12,26].

For the dynamic relaxation starting from a *random* state at a continuous phase transition, renormalization group calculations and numerical simulations show that an independent critical exponent x_0 must be introduced to describe the scaling behavior of the initial magnetization [1–4]. This also explains the relevant experiments in spin glasses. For the dynamic relaxation starting from an *ordered* state, numerical study indicates that the dynamic behavior is controlled only by the static exponents and the dynamic exponent z [4,5,27,28]. Very recently, this result is derived with renormalization group methods [29]. Obviously, the initial condition plays an important role in the dynamic relaxation far from equilibrium.

The first purpose of this letter is to study the dynamic effect of a *semi-ordered* initial state. For the two-dimensional (2D) Ising model, the semi-ordered initial state consists of two fully-ordered domains with opposite spin directions. As the dynamic evolution starts, the domain wall grows and looks like an interface. Such a dynamic process is theoretically and practically important. In refs. [15], a relevant dynamic process of driven diffusive lattice gases has been considered. Since it is actually a model B dynamics and includes the dynamic transportation, the dynamic behavior is rather complicated [30]. In this letter, we intend to clarify first the dynamic scaling behavior with a simpler system, and to pave the way for settling the controversy in refs. [15,30]. Therefore, we consider a model A dynamics, which is purely relaxational and with no conservation laws [31].

On the other hand, the non-equilibrium critical dynamics and the surface critical phenomenon in equilibrium share some common features. At the ordinary phase transition of a free surface, for example, the magnetization at surface is governed by an exponent β_1, different from β at bulk. Naturally, the non-equilibrium critical dynamics at a surface is also an important topic [32–35]. For the dynamic relaxation starting from the random state, the dynamic evolution of the magnetization at surface is controlled by both x_0 and β_1 [34,35]. For the dynamic relaxation starting from the ordered state, however, it

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is theoretically expected that β_1 is sufficient to describe the dynamic evolution of the magnetization at surface. In the present letter, we study the dynamic relaxation *without a surface* but starting from the semi-ordered state. It looks somewhat as if there existed a fictitious surface, *i.e.*, the so-called *domain interface*. The width of the domain interface grows as time evolves. The dynamic evolution of the magnetization within the interface is governed by an exponent β_1. But this β_1 does not correspond to a static exponent in equilibrium, and it is induced by the semi-ordered initial state. The second purpose of this letter is to compare the dynamic relaxation starting from the semi-ordered state with the dynamic relaxation near a surface, but starting from the ordered state.

With Monte Carlo simulations we first study the critical relaxation starting from the *semi-ordered* state, taking the two-dimensional (2D) Ising model as an example. The Ising model is defined on a rectangular lattice $2L \times L$, with a linear size $2L$ in the x direction and L in the y direction. Periodic boundary conditions are used in both x and y directions. The semi-ordered state is taken to be that spins are positive on the square sublattice $L \times L$ on the right side, and negative on the left side. For convenience, we put the x-axis such that the domain wall between the positive and negative spins is located at $x = 0$. After preparing the semi-ordered initial state, we update the spins with the heat-bath algorithm at the critical temperature, up to a maximum time $t_M = 25600$. The main results are presented with $L = 512$, and additional simulations with $L = 1024$ and 256 confirm that the finite-size effect is negligibly small. The total samples for average are 24000, and statistical errors are estimated by dividing the total samples into subgroups. If the fluctuation in the time direction is comparable with or larger than the statistical error, it will be taken into account. Due to the semi-ordered initial state, the dynamic behavior is inhomogeneous in the x direction. Therefore, we measure the magnetization and its second moment as a function of x and t,

$$M^{(k)}(t,x) = \frac{1}{L^k}\left\langle \left[\sum_{y=1}^{L} S_{xy}(t) \right]^k \right\rangle, \quad k = 1, 2. \qquad (1)$$

Here $S_{xy}(t)$ is the spin at the time t on the lattice site (x, y), and $\langle ... \rangle$ represents the statistical average. For convenience, we also use $M(t,x) \equiv M^{(1)}(t,x)$ to denote the magnetization. Similarly, we define the two-time correlation function,

$$A(t,t',x) = \frac{1}{L}\left\langle \sum_{y=1}^{L} S_{xy}(t) S_{xy}(t') \right\rangle, \quad t > t'. \qquad (2)$$

At the critical temperature T_c and in the thermodynamic limit $L \to \infty$, there are two length scales in the dynamic system, *i.e.*, x and the non-equilibrium spatial correlation length $\xi(t) \sim t^{1/z}$. General scaling arguments

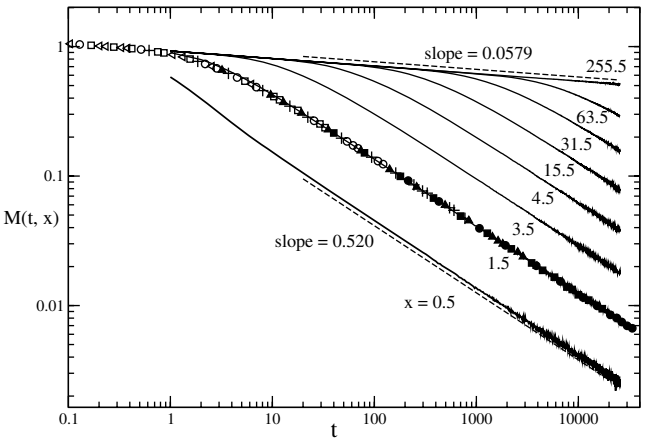

Fig. 1: Time evolution of the magnetization starting from the semi-ordered state is plotted with solid lines on a double-log scale. Dashed lines show the power law fits. According to eq. (3), data collapse is observed for different x. Solid circles, solid squares, solid triangles, pluses, open circles, open squares and open triangles correspond to $x = 0.5, 1.5, 3.5, 7.5, 15.5, 31.5$ and 63.5 respectively.

lead to the scaling form of the magnetization and its second moment

$$M^{(k)}(t,x) = t^{-k\beta/\nu z}\tilde{M}^{(k)}(t^{1/z}/x), \quad k = 1, 2. \qquad (3)$$

Here β and ν are the static exponents and z is the dynamic exponent. Similarly, we may write down the scaling form for the two-time correlation function,

$$A(t,t',x) = t'^{-2\beta/\nu z}\tilde{A}(t/t', t'^{1/z}/x). \qquad (4)$$

In eqs. (3) and (4), the overall factors $t^{-\beta/\nu z}$ and $t'^{-2\beta/\nu z}$ indicate the scaling dimensions of $M(t,x)$ and $A(t,t',x)$, and the scaling functions $\tilde{M}(t^{1/z}/x)$ and $\tilde{A}(t/t', t'^{1/z}/x)$ represent the scaling invariance. The scaling forms in eqs. (3) and (4) may also apply to the dynamic relaxation *with a surface* but starting from the *ordered* state, and one should only keep in mind that β, ν and z are the exponents *at bulk*. Based on our numerical simulations, we investigate whether the scaling forms in eqs. (3) and (4) hold for the dynamic relaxation without a surface but starting from the semi-ordered state, and compare the results with those near a surface but starting from the ordered state. In addition, we expose the features of the scaling function in eqs. (3) and (4), and extract the exponent β_1 for the domain interface and at a surface.

In fig. 1, $M(t,x)$ is displayed for the dynamic relaxation starting from the semi-ordered state on a log-log scale. For a sufficiently large x, *e.g.*, $x = 255.5$, $M(t,x)$ approaches the non-linear decay *at bulk*, $M(t,x) \sim t^{-\beta/\nu z}$. The exponent $\beta/\nu z = 0.0579(3)$ measured from the slope of the curve is well consistent with $\beta = 1/8$, $\nu = 1$ and $z = 2.16(1)$ reported in the literature [4]. For a sufficiently small x, *e.g.*, $x = 0.5$, $M(t,x)$ exhibits also a power law behavior,

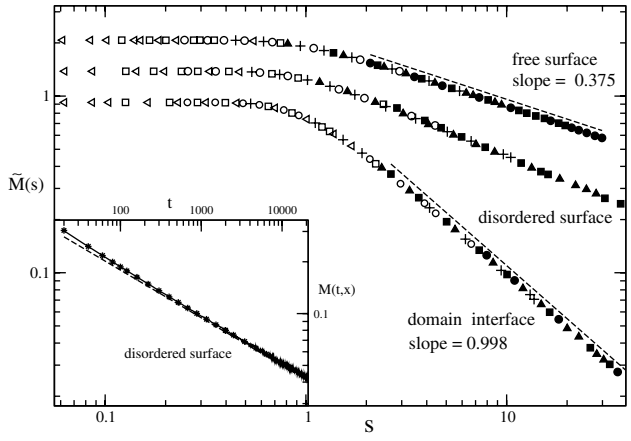

Fig. 2: The scaling function $\tilde{M}(s)$ is plotted on a double-log scale, for the free surface, disordered surface and domain interface (from above). Data collapse is observed for different x. In the inset, the magnetization at $x = 0.5$ for the disordered surface is shown with the solid line. The dashed line shows a power law fit. Dots fitted to the solid line are with the logarithmic correlation to scaling in eq. (6).

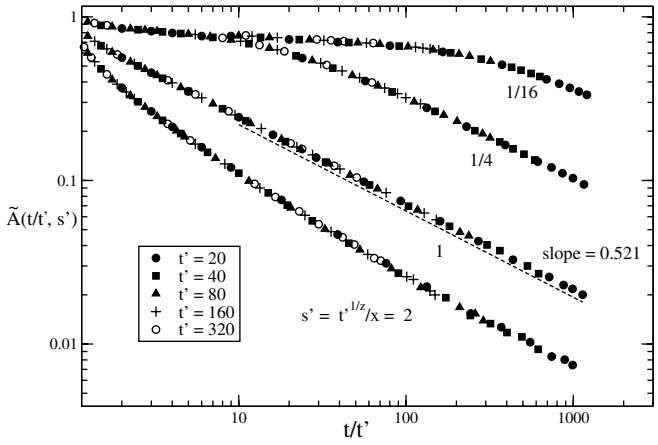

Fig. 3: $\tilde{A}(t/t', s')$ is displayed for fixed values of $s' = t'^{1/z}/x$ on a double-log scale. Data collapse is observed for different t'. The dashed line shows a power law fit.

but decays much faster than at bulk. In other words, the scaling function $\tilde{M}(s) \to \text{const}$ when $s \to 0$, while

$$\tilde{M}(s) \to s^{-\beta_0/\nu}, \quad \text{when} \quad s \to \infty. \tag{5}$$

In the limit $s \to \infty$, one may define an exponent β_1 such that $M(t,x) \sim t^{-\beta_1/\nu z}$ with $\beta_1 = \beta + \beta_0$. This behavior characterizes the domain interface, whose width grows in time in the form $\xi(t) \sim t^{1/z}$. Inside the interface, the power law decay of the magnetization is governed the exponent β_1, while outside the interface, it is controlled by the bulk exponent β. From fig. 1, one measures $\beta_1/\nu z = 0.520(2)$, and calculates $\beta_1 = 1.123(5)$, therefore, $\beta_0 = 0.998(5)$. Similar to the exponent x_0 in the dynamic relaxation starting from the random state [1–4], β_0 here is induced by the semi-ordered initial state. Taking into account the error, one may believe $\beta_0/\nu = 1$, which suggests that $M(t,x)$ is an analytic function of x. This result is also supported by our preliminary simulations of the 3D Ising model.

To fully confirm the scaling form in eq. (3), for example, we fix $x_f = 1.5$, and change the time scale t of another x to $(x_f/x)^z t$, and the scale of $M(t,x)$ to $(x_f/x)^{-\beta/\nu} M(t,x)$. As shown in fig. 1, all data of different x nicely fit to the curve of $x_f = 1.5$. This validates eq. (3). Alternatively, we may plot $t^{\beta/\nu z} M(t,x)$ as a function of $s = t^{1/z}/x$. If eq. (3) holds, all data of different x collapse onto the master curve $\tilde{M}(s)$. This is shown in fig. 2. Clearly, $\tilde{M}(s) \to \text{const}$ when $s \to 0$, while $\tilde{M}(s) \to s^{-\beta_0/\nu}$ when $s \to \infty$.

For comparison, we have performed numerical simulations of the 2D Ising model with a *free* surface and a *disorder* surface, starting from the ordered state. For the disordered surface, the spin S_i on the surface couples to a random field h_i through the interaction $H_i = JS_ih_i$ [36]. Here J is just the coupling constant between two spins in our model, and $h_i = \pm 1$. For the dynamic relaxation with a surface, the scaling analysis in eqs. (3) and (4) also applies, but the scaling functions are different. In fig. 2, we plot the scaling function $\tilde{M}(s)$ for both surfaces. Obviously, data collapse is observed, and in both cases, $\tilde{M}(s) \to \text{const}$ when $s \to 0$. When $s \to \infty$, it is somewhat complicated. For the free surface, $\tilde{M}(s)$ obeys the power law in eq. (5), and the exponent β_0/ν measured from the slope of the curve is 0.375(3). In other words, $M(t,x) \to t^{-\beta_1/\nu z}$ when $x \to 0$, and the surface exponent $\beta_1 = \beta + \beta_0 = 0.500(3)$ is in agreement with the theoretical value 1/2 derived in equilibrium [36]. For the disordered surface, the surface exponent β_1 remains 1/2, but a logarithmic correction to scaling is detected in equilibrium [36]. For the dynamic relaxation, $\tilde{M}(s)$ also undergoes a logarithmic correction to scaling, and it should be written as

$$\tilde{M}(s) \to s^{-\beta_0/\nu}/(1 + b \ln s)^{1/2}, \quad \text{when} \quad s \to \infty. \tag{6}$$

In fig. 2, therefore, $\tilde{M}(s)$ of the disordered surface decays somewhat faster than that of the free surface at the large-s regime. In the inset in fig. 2, the logarithmic correction to scaling is directly shown for $M(t,x)$ at $x = 0.5$.

We emphasize that in the case at the free surface or disordered surface, the exponent β_1 does describe the critical behavior of the magnetization at the surface *in equilibrium*. For the free surface, for example, $M(\tau) \sim (-\tau)^{\beta_1}$ with τ being the reduced temperature. Here it is important that β_1 is induced by the geometric surface. In the case of the domain interface, however, β_1 is induced by the geometric structure of the semi-ordered initial state. When the dynamic system reaches its equilibrium state, the effect of the initial state disappears and the critical behavior of the magnetization is governed by the bulk exponent β *everywhere*. To what extent β_1 is universal needs further investigation.

The scaling form of the two-time correlation function in eq. (4) represents a kind of ageing phenomena. Now $t'^{2\beta/\nu z} A(t,t',x) = \tilde{A}(t/t', t'^{1/z}/x)$ is a function of two

scaling variables, t/t' and $s' = t'^{1/z}/x$. In fig. 3, therefore, we plot $\tilde{A}(t/t', s')$ as a function of t/t' for a couple of *fixed* s' for the domain interface. Obviously, data for different t' but with a fixed s' collapse onto a master curve. This verifies the scaling form in eq. (4). For a small s', $\tilde{A}(t/t', s')$ first decays according to $(t/t')^{-\beta/\nu z}$ in the small t/t' regime, then crosses over to $(t/t')^{-\beta_1/\nu z}$ in the large t/t' regime. This is consistent with the theoretical expectation, since the magnetization $M(t, x)$ shows the power law decay $t^{-\beta/\nu z}$ for a large x, while $t^{-\beta_1/\nu z}$ for a small x. For s' around 1, $\tilde{A}(t/t', s')$ directly enters the power law decay $(t/t')^{-\beta_1/\nu z}$, and $\beta_1/\nu z$ is estimated to be 0.521(4), in agreement with 0.520(2) measured from the magnetization.

To understand the spatial fluctuation, one may construct a time-dependent Binder cumulant $U(t, x) = M^{(2)}(t, x)/[M(t, x)]^2 - 1$. Following the scaling form in eq. (3) and the finite-size scaling analysis [4], one may deduce

$$U(t, x) = \frac{t^{(d-1)/z}}{L^{d-1}} \tilde{U}(t^{1/z}/x), \tag{7}$$

where $d = 2$ is the spatial dimension. Naturally, the scaling function $\tilde{U}(s) \to$ const when $s \to 0$, and we estimate the exponent $(d-1)/z = 0.47(2)$. Interestingly, our numerical data for the domain interface show that $\tilde{U}(s) \to s^{d_0}$ when $s \to \infty$, and $(d - 1 + d_0)/z$ is measured to be 0.93(4). These two measurements are consistent with $z = 2.16(1)$, and indicate $d_0 = 1$. In contrast to this, we obtain $d_0 = 0$ at the free surface. This result indicates that the spatial fluctuation of the domain interface grows faster than that at the free surface.

In summary, with Monte Carlo methods we have investigated the non-equilibrium critical dynamics starting from a semi-ordered state, taking the 2D Ising model as an example. The domain interface grows as time evolves, and the dynamic scaling behavior including the ageing phenomenon is identified. Inside the domain interface, the dynamic evolution of the magnetization is governed by an exponent β_1, different from β at bulk. Compared with the dynamic relaxation at a surface but starting from the ordered state, β_1 for the domain interface does not correspond to a static exponent. The Binder cumulant of the domain interface shows a non-trivial behavior different from that at a surface. It is challenging how to derive the dynamic scaling form for the domain interface with renormalization group methods.

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