Monte Carlo Study of Critical Relaxation near a Surface

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We report the first Monte Carlo simulation on the critical relaxation of the three-dimensional kinetic Ising model with free surfaces. The surface-layer magnetization is shown to relax as $t^{-\beta_1/\nu z}$ at $T=T_c$, while the bulk magnetization relaxes as $t^{-\beta/\nu z}$. The dynamic bulk-to-surface crossover is discussed in view of the dynamic scaling theory.

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The time scale characterizing the dynamics of a system becomes longer near a second-order phase transition point. This phenomenon is called critical slowing down. The dynamic property of critical phenomena is one of the most attractive subjects in statistical mechanics.[1]

The existence of a surface brings about several interesting effects on critical phenomena.[2] Various theoretical techniques have been successfully applied to the study of the surface effects on static critical phenomena.[3–9] However, little attention has been given to dynamic properties. One exception is the recent work by Dietrich and Diehl.[10] Using the renormalized field theory, they have investigated the effects of surfaces on dynamic critical behavior. They assert that the surface dynamic critical phenomena are described in terms of static bulk and surface critical exponents, and the dynamic bulk exponent; there exists no dynamic exponent peculiar to the surface.

The Monte Carlo method is a powerful technique for the simulation of a wide variety of physical problems of interest. The static properties of surface critical phenomena have been recently investigated by means of Monte Carlo simulation.[11–13] This Letter is the *first* report on the Monte Carlo study of the dynamic critical behavior of a system with surfaces. We investigate the critical slowing down at the critical temperature $T=T_c$ for the three-dimensional kinetic Ising model with free surfaces. We restrict ourselves to the ordinary transition[2] in this Letter. We show that the critical slowing down of the magnetization of the surface layer differs from that of the bulk magnetization. We also point out that the dynamic behavior of the inner-layer magnetization shows a crossover from bulklike relaxation to surfacelike relaxation with time.

Let us study first the surface dynamic critical phenomena from the viewpoint of scaling theory. Our treatment has something in common with Suzuki's theory[14] of dynamic finite-size scaling. The parameters of the present system are the reduced temperature $\epsilon=(T-T_c)/T_c$, magnetic field h, surface magnetic field h_1, and time t. Following Suzuki's idea,[14] we consider the generating function of the nonequilibrium system, which is a generalization of the free energy. In the present case, the scaling assumption implies that the surface part of the generating function, Φ_s, can be written in the following scaling form:

$$\Phi_s(\epsilon,h,h_1t) \sim \epsilon^{2-\alpha_s}\tilde{\Phi}_s(h\epsilon^{-\Delta},h_1\epsilon^{-\Delta_1},t\epsilon^{\nu z}), \tag{1}$$

where z is the dynamic critical exponent, and other exponents are static bulk and surface ones. From Eq. (1), it follows that the surface magnetization m_s $(=-\partial\Phi_s/\partial h)$ and the layer magnetization m_1 $(=-\partial\Phi_s/\partial h_1)$ scale as

$$m_s(\epsilon,h,h_1t) \sim \epsilon^{\beta_s}\tilde{m}_s(h\epsilon^{-\Delta},h_1\epsilon^{-\Delta_1},t\epsilon^{\nu z}), \tag{2}$$

$$m_1(\epsilon,h,h_1t) \sim \epsilon^{\beta_1}\tilde{m}_1(h\epsilon^{-\Delta},h_1\epsilon^{-\Delta_1},t\epsilon^{\nu z}), \tag{3}$$

respectively. The scaling relations among static critical exponents have been used in deriving Eqs. (2) and (3). In the same way the surface susceptibility $\chi_s(=\partial m_s/\partial h)$, the layer susceptibility χ_1 $(=\partial m_1/\partial h)$, and the local susceptibility $\chi_{1,1}$ $(=\partial m_1/\partial h_1)$ scale as

$$\chi_s(\epsilon,h,h_1t) \sim \epsilon^{-\gamma_s}\tilde{\chi}_s(h\epsilon^{-\Delta},h_1\epsilon^{-\Delta_1},t\epsilon^{\nu z}), \tag{4}$$

$$\chi_1(\epsilon,h,h_1t) \sim \epsilon^{-\gamma_1}\tilde{\chi}_1(h\epsilon^{-\Delta},h_1\epsilon^{-\Delta_1},t\epsilon^{\nu z}), \tag{5}$$

$$\chi_{1,1}(\epsilon,h,h_1t) \sim \epsilon^{-\gamma_{1,1}}\chi_{1,1}(h\epsilon^{-\Delta},h_1\epsilon^{-\Delta_1},t\epsilon^{\nu z}). \tag{6}$$

In particular, at criticality, $\epsilon=h=h_1=0$, we find that the layer magnetization relaxes as $m_1 \sim t^{-\beta_1/\nu z}$, in contrast to the relaxation of the bulk magnetization, $m_b \sim t^{-\beta/\nu z}$. Since $\beta_1>\beta$ for the ordinary transition, the relaxation rate of m_1 is expected to be faster than that of the bulk magnetization.

We study the critical slowing down of the three-dimensional kinetic Ising model by the Monte Carlo method. We deal with a simple cubic lattice of sizes $64\times64\times32$, $128\times128\times32$, and $256\times256\times32$, with the free boundary condition on the short direction and periodic boundary conditions otherwise for taking account of the surface effects. The simulation is performed at $T=T_c$ $(1/T_c=0.221\,654)$,[15] with no magnetic field, $h=h_1=0$. The critical behavior varies as the value of the surface-to-bulk ratio of the exchange interaction, $w=J_s/J$.[2] We restrict ourselves to the ordinary transition and take w as 0.25, 0.5, and 0.75, which are typical values of w for an ordinary transition. For the initial condition, we start with all spins up. We flip spins according to the transition probability $p=[1+\exp(\Delta E/T)]^{-1}$, where ΔE denotes the energy change at the spin flip. We employ the Tausworthe-Lewis-Payne method[16] for generating random numbers, and apply multispin coding[17] to the surface problem.

The variations of the Lth-layer magnetization m_L with time for $L=1$, 2, 4, 8, and 16 are shown in Fig. 1. We use a log-log plot, and the time is measured by the number of Monte Carlo steps per spin. We show the result of the $128\times128\times32$ lattice for $w=0.75$, and the average is taken over forty samples. The straight lines with the slope $-\beta_1/\nu z$ $(=-0.613)$ and $-\beta/\nu z$ $(=-0.255)$ are also shown. For the bulk exponents, we have used $\beta=0.325$,[18] $\nu=0.630$,[18] and $z=2.02$.[19,20] The surface exponent β_1 was estimated by the static Monte Carlo study[11,12] as $\beta_1=0.78$, which is consistent with the high-temperature expansion[6,7] and the ϵ expansion[3,4] through the scaling relations. Figure 1 shows that the surface-layer magnetization relaxes as $t^{-\beta_1/\nu z}$ with time, while the bulk magnetization relaxes as $t^{-\beta/\nu z}$. In the case of different w, we have obtained the same result except for the shift of the effective surface, which will be discussed later. The effect of surface size has not been detected in this simulation.

Next we consider the crossover behavior. From Fig. 1, we find that the magnetization of the inner layer, for example, $L=4$, shows bulklike relaxation for small t, and that for large t, the slope of the magnetization becomes the same as that of m_1. This variation is due to the crossover of the critical slowing down from bulklike to surfacelike with time. Moreover, the characteristic time for the crossover becomes longer as L becomes larger. We can interpret this from the scaling argument that the distance from the surface is scaled by time with the dynamic critical exponent as $t^{1/z}$. In our previous paper[12] we showed that the *static* magnetization profile for various w can be expressed in a single scaling function using $L'=L-1+\lambda$ for the distance from the surface. Here λ represents the extrapolation length,[21] and the lattice spacing is taken as unity. Then we may write the dynamic scaling function for the Lth-layer magnetization $m_L(t)$ as

$$m_L(t)\sim L'^{-\beta/\nu}f(tL'^{-z}). \tag{7}$$

The scaling function f has the asymptotic behavior

$$f(t)\propto t^{-\beta/\nu z}\quad (t\to 0), \tag{8}$$

$$f(t)\propto t^{-\beta_1/\nu z}\quad (t\to\infty). \tag{9}$$

We give the scaling plot of our data for $w=0.75$, 0.5, and 0.25 in Fig. 2. We have used the values of λ which were determined by the measurement of the static magnetization profile.[12,22] The data for various L are collapsed on a single curve. It should be emphasized that the shift of distance by λ is essential for expressing all the data for different w in a single function, as in the static case.[12] Figure 2 explicitly provides the scaling description of the bulk-to-surface crossover with time. We have taken the dynamic exponent z as given in this study. It should be noted that we can use the scaling analysis of Monte Carlo data based on Eq. (7), conversely, for determining the exponent z.

We make a short comment on the transition probability. We have taken p as $[1+\exp(\Delta E/T)]^{-1}$. We have also made a simulation by using the usual Metropolis probability, $\min\{1,\exp(-\Delta E/T)\}$. A parallel shift of the curve in Fig. 1 is observed, but the

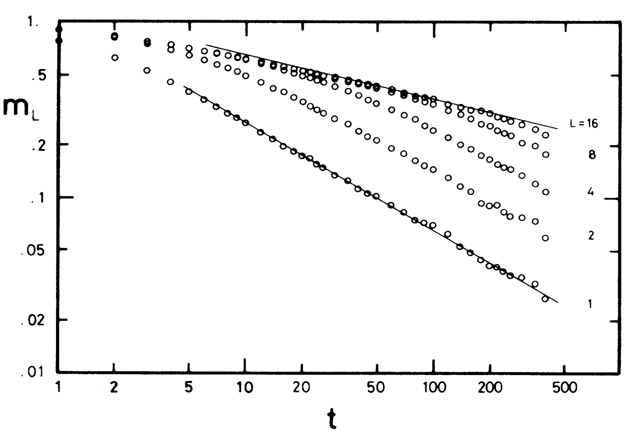

FIG. 1. Variations of the Lth-layer magnetization with time, i.e., the number of Monte Carlo steps per spin, for $L=1$, 2, 4, 8, and 16. The system size is $128\times128\times32$, and $w(=J_s/J)=0.75$. The straight lines with the slope $-\beta_1/\nu z$ $(=-0.613)$ and $-\beta/\nu z$ $(=-0.255)$ are also shown.

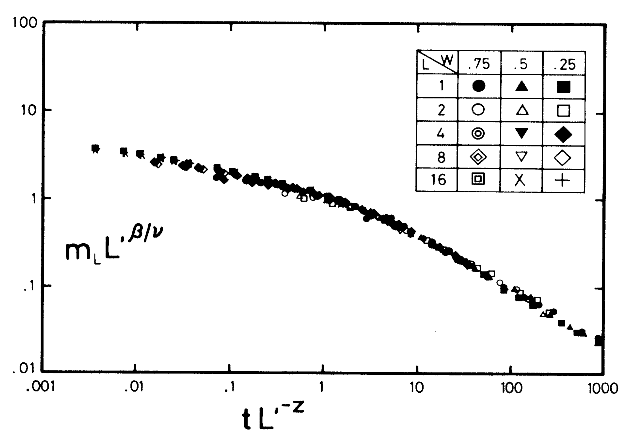

FIG. 2. Scaling plot of time-dependent Lth-layer magnetization for $w=0.75$, 0.5, and 0.25 based on Eq. (7). The table in the figure gives the explanation of symbols.

relaxation rate remains the same. This is, the choice of the probability affects only the time scale, which is the same as the bulk case.

In summary, we have performed the first Monte Carlo simulation of the dynamic critical behavior of the Ising model with surfaces. We have obtained the fast relaxation for the surface layer, which is consistent with the scaling prediction, and observed the dynamic bulk-to-surface crossover phenomenon.

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