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Large-scale Monte Carlo simulations for the depinning transition in Ising-type lattice models

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ABSTRACT

With the developed "extended Monte Carlo" (EMC) algorithm, we have studied the depinning transition in Ising-type lattice models by extensive numerical simulations, taking the random-field Ising model with a driving field and the driven bond-diluted Ising model as examples. In comparison with the usual Monte Carlo method, the EMC algorithm exhibits greater efficiency of the simulations. Based on the short-time dynamic scaling form, both the transition field and critical exponents of the depinning transition are determined accurately via the large-scale simulations with the lattice size up to L = 8912, significantly refining the results in earlier literature. In the strong-disorder regime, a new universality class of the Ising-type lattice model is unveiled with the exponents $\beta = 0.304(5)$, $\nu = 1.32(3)$, z = 1.12(1), and $\zeta = 0.90(1)$, quite different from that of the quenched Edwards–Wilkinson equation.

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1. Introduction

Driven by a constant force in the presence of the quenched disorder, the interface moves with a steady-state velocity, while it is pinning when the force is weak compared to the random noise. Between them, there exists a second-order dynamical phase transition, called as the "depinning transition" [1-8]. For several decades, the depinning transition has been the focus of the experimental and theoretical research, which are common to a wide variety of phenomena, including the liquid invasion in porous media [9], the contact line in wetting [10], the vortices in type-II superconductors [11,12], the charge-density waves [13], the fracture propagation [14,15], the dislocation dynamics in crystal plasticity [16], and the domain-wall motions in ferromagnetic and ferroelectric materials [17-20]. Practically, understanding the fundamental mechanism of the depinning transition plays an important role in predicting and controlling the motions of the magnetic domain walls in nanomaterials [21–23], thin films [8,24], and semiconductors [20,25], which is key to the realization of the new classes of potential nonvolatile storage-class devices [26,27].

Theoretical approaches to the domain-wall dynamics are typically based on the phenomenological models, such as the Edwards–Wilkinson equation with quenched disorder (QEW) and its

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http://dx.doi.org/10.1016/j.cpc.2016.08.009 0010-4655/© 2016 Elsevier B.V. All rights reserved. variants [28-31]. With these equations, the domain wall in a twodimensional system can be effectively described by a single-valued elastic string, and the static and dynamic critical exponents of the depinning transition, i.e., β , ν , z, and ζ , are measured numerically, though the discrepancies are still large in the literature [32-35]. For example, it reaches nearly 30 percent in the velocity exponent β . Recently, extensive simulations of the OEW at the depinning transition have been performed with a lattice size up to L = 8192[28]. Based on the short-time dynamics method, the universality class of the depinning transition is identified with the exponents $\beta = 0.245(6), z = 1.433(7), \zeta = 1.250(5), \text{ and } \nu = 1.333(7),$ which are robust under the changes of the disorder realization including the random-bond and random-field characters. Moreover, the scaling relation $\beta = \nu(z - \zeta)$ is revealed, consistent with the prediction of the functional renormalization group theory [36,37]. However, most experiments reported that the roughness exponent is $\zeta \approx 0.6-0.9$ [1,15,31,38,39], smaller than that of the QEW equation, suggesting that detailed microscopic structures and interactions of real materials should be concerned.

Besides, the dynamical behaviors of the domain walls in ferromagnetic nanowires are also investigated via the micromagnetic simulations with the Landau–Lifshitz–Gilbert (LLG) equation depicting the time evolution of the orientation of the magnetization distribution, $m(\vec{r}, t)$ [40–42]. However, the LLG equation is too complicated to be simulated for the depinning transitions in ultrathin ferromagnetic or ferroelectric films. The Ising-type lattice models are then introduced with much simpler microscopic structures and interactions [43–46]. In this paper, we use the random-

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field Ising model with a driving field (DRFIM) and the driven bonddiluted Ising model (DBDIM) as examples. For a long time, it has been invariably stated that the QEW equation and DRFIM model belong to the same universality class [43,46,47]. However, significant deviations of the critical exponents have been reported in recent works [48,49], which could not be ruled out by statistical errors. It was argued that the difference may be induced by the intrinsic anomalous scaling and spatial multiscaling of the DRFIM at the depinning transition. Unfortunately, a weak dependence of the critical exponents on the strengths of the random fields is found in the disorder regime $\Delta \in [0.8, 2.3]$ [50]. Hence, it remains ambiguous that the depinning transition of the DRFIM belongs to a new dynamic universality class or it only has a correction to the universality class of the QEW equation due to the influence of the first-order phase transition occurring at $\Delta < 1$. To solve this issue. we will identify the critical exponents of DRFIM in the regime of the strong disorder $\Delta \gg 1$ in this article, and carefully examine the hyperscalings $\beta = \nu(z - \zeta)$ and $\nu = 1/(2 - \zeta)$ proposed in the QEW universality class.

Early studies of the depinning transition were always focused on the steady-state velocity v(L) of the domain wall [4,35,43,51]. Suffering from severe critical slowing down, however, it is quite arduous to obtain the exact transition field H_c and critical exponents. Adopting the short-time scaling form [52,53], both the static and dynamic exponents β , ν , ζ , and z can be easily and accurately determined from the nonsteady relaxation of the domain interface since the spatial correlation length is short [28,33,48]. Due to the limitation of the computing resources, however, the system size and simulation time are insufficient in previous work for the depinning transition in the DRFIM, which are up to L = 1024 and $t_{max} = 2000$ [48,50], much smaller than those in the QEW equation, L = 8192 and $t_{max} = 8000$ [28]. It may result in a systematic error in the determination of the critical driving field H_c . Accordingly, larger spatial and temporal scales are needed in the simulations to obtain more precise results for the depinning transition in the DRFIM.

In this paper, an optimized Monte Carlo method is developed, termed as the "extended Monte Carlo" (EMC) algorithm. Adopting the EMC, much smaller time of the Central Processing Unit (CPU) is taken for the depinning transition, in comparison with that of the usual Monte Carlo method. By extensive simulations, the transition point and critical exponents of the DRFIM are then accurately determined for various strengths of the quenched disorder, and a new universality class is unveiled. In addition, the depinning transition in another Ising-type lattice model, DBDIM, is also investigated for comparison. In Section 2, the models, EMC algorithm, and scaling analysis are described, and in Section 3, the numerical results are presented. Finally, Section 4 includes the conclusion.

2. Methodology

2.1. Model

The DRFIM is one of the simplest demonstration to study the depinning transition in the disorder media with microscopic structures and interactions. The Hamiltonian of the DRFIM can be written as

$$\mathcal{H} = -J \sum_{\langle ij \rangle} S_i S_j - H \sum_i S_i - \sum_i h_i S_i, \tag{1}$$

where $S_i = \pm 1$ is the classical Ising spin of the two-dimensional rectangle lattice with $2L \times L$, the random field h_i is uniformly distributed within an interval $[-\Delta, \Delta]$, and H is a homogeneous driving field. An unbounded Gaussian distribution of the random field h_i leads to similar results, but the fluctuations induced by the



Fig. 1. Time evolution of the spin configurations under the uniform distribution of the random fields. The black and white correspond to the spin up ($S_i = 1$) and down ($S_i = -1$), respectively, and the stars denote the activated spins within the domain interface. As the time *t* grows, overhangs and islands are created.

disorder are stronger, and numerical simulations are technically more complicated. Hence, we concentrate on the bounded uniform distribution of h_i in this paper. The initial state that spins are positive in the sublattice on the left side and negative on the right side, is used to build a perfect domain wall, also referred to as a "domain interface", in the *y* direction. The direction perpendicular to the domain interface is then set to the *x* axis. Antiperiodic and periodic boundary conditions are used in *x* and *y* directions, respectively. To eliminate the pinning effect irrelevant for disorder, we rotate the square lattice such that the initial domain wall orients in the (11) direction of the square lattice, as shown in Refs. [43,48,51,54].

After preparing the initial state, a usual Monte Carlo method is adopted with standard one-spin flips in the simulations. Simply speaking, we update each spin with the following procedure. First, we randomly choose a single spin S_i in the two-dimensional lattice. The change of the total energy is then calculated after we flip the spin $S_i \rightarrow S'_i$,

$$\delta E = \mathcal{H}(S_i) - \mathcal{H}(S'_i)$$

= $(S'_i - S_i) \left[-J \sum_j S_j - H - h_i \right].$ (2)

Only when $\delta E < 0$, the flip is accepted, otherwise the spin state S_i remains. A Monte Carlo time step (MCS) is defined by $2L^2$ single-spin updates. As time evolves, the domain wall moves and roughens, while the bulk, i.e., spins far away from the domain interface, keeps invariant. As shown in Fig. 1, the time evolution of the spin configuration is displayed with the black and white squares, corresponding to $S_i = \pm 1$, respectively. Complicated spin structures are found nearby the domain interface, such as overhangs and islands at the time t = 1000 MCS. Where overhanging profile means that the front of the domain wall cannot be directly described as a single-value function of the coordinate *y*, which has been observed in experiments for magnetic materials [38,55].

According to literatures [1,38,49], there are many different ways to define the domain interface. In this paper, we adopt a simple and popular definition based on the magnetization [43,46, 47,51]. Denoting a spin at site (x, y) by $S_{xy}(t)$, a microscopic height function of the domain interface is introduced,

$$h(y,t) = \frac{L_x}{2} [m(y,t) + 1],$$
(3)

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