Roughening Dynamics of Systems with Latent Heat

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We study the dynamics of the roughening of a surface between two coexisting phases using a novel Monte Carlo algorithm. Our model Hamiltonian explicitly contains a latent heat whose value directly influences the growth law. We observe a crossover between short-wavelength, short-time behavior controlled by the surface tension and long-wavelength, long-time behavior controlled by the diffusion of heat. The results are in excellent agreement with recent theoretical predictions.

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The characteristics of interfaces such as vapor-liquid or liquid-solid boundaries are of interest to those seeking to understand phenomenon like dendritic instabilities, crystal growth, and nucleation. Of primary importance is the equilibrium state on a stable interface which is “rough” at temperatures above the roughening transition temperature $T_r$ and smooth or “faceted” below. For systems in the Ising universality class, the width of the interface in 3D and in the rough phase depends on the logarithm of the interface length, whereas in 2D, where $T_r$ is exactly zero, the roughening depends on the square root of the length.

The relaxation of perturbed interfaces to their equilibrium roughened state is a simple example of a dynamical process. In particular, the growth of thermal fluctuations on an initially flat interface can be used to characterize the relaxation of various types of dynamical systems which share common static properties but differ in their dynamics.

Three such systems are models $A$, $B$, and $C$ of critical dynamics. The behavior of models $A$ and $B$ are defined by their respective nonconservation and conservation of the order parameter. Their dynamics have been examined theoretically and by simulation and are well understood. Of these, the most important is the recent work of Zia, Bausch, Janssen, and Dohm, which relates the crossover to an asymmetry between two bulk phases, showing that it arises from a transition between uncoupled rapid growth at short length scales and slower growth of fluctuations at long length scales. The importance of model $C$ is also apparent in recent studies of the dynamics of unstable interfaces in Ising-type systems where it provides an ideal forum for examining dynamics which are heat-diffusion dependent and involve first-order phase transitions.

In this Letter we present the first Monte Carlo simulations of the roughening of an interface constrained by model-$C$ dynamics. We observe the crossover from rapid early growth to slower late-time behavior, and show that it depends upon the latent heat of our model, in agreement with theoretical predictions. The growth laws that we observe are precisely those required by theory.

Our novel Monte Carlo algorithm, which combines elements of the microcanonical and canonical schemes, has been described in a number of recent publications which examine equilibrium and nonequilibrium steady-state configurations of various Ising-type systems. Consequently, it will be mentioned only briefly here. The evolution of an Ising-type spin system is governed by one or more Maxwell “demons.” Each demon is responsible for administering the rules of spin flip for a subset of the spin population, thus acting as a heat transport mechanism, and either measuring or controlling the local temperature. In the present application, for a system of $N\times M$ spins, coupled to $N\times M$ demons, the $2N$ demons on the free boundaries of the system are used to set the temperature, and the spins in the bulk each have access to their own demons and to the demons of their nearest neighbors. Since the total energy of the combined demon and spin system is conserved while the average spin magnetization (the order parameter) is nonconserved, this is model $C$.

The algorithm is employed here to simulate the relaxation to equilibrium of interfaces in a 2D ferromagnetic Ising-type model. The basic Ising Hamiltonian is

$$ H = -J \sum_{ij} \sigma_i \sigma_j - \Delta \sum_i \sigma_i , $$

where $J$ is the spin coupling, the interactions are nearest neighbor, the spins are $\sigma_i = \pm 1$, and $\Delta$ represents a uniform external field. In the absence of $\Delta$ the second-order phase transition is at $T_c = 2.269J$, but in order to induce a first-order transition and a stable region of phase coexistence, the upper spin state is given a degeneracy $\delta > 1$. This introduces a latent heat $\Delta$ which is of order $\Delta$, and defines the melting temperature as $T_m = 2\Delta/\ln\delta$. 

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Consequently, $\Lambda$ can be increased at constant $T_m$ by increasing $\delta$ and $\Lambda$ in the appropriate manner.

The initial spin state is prepared as two bulk phases with an exactly flat interface between them. The demons are prepared by randomly distributing the energy estimated to place them in thermal equilibrium with the spins (i.e., at $T_m$). This is done such a way as to minimize the time taken for this equilibrium to be established. The boundary conditions at the sides of the spin system are periodic (the spin array is one dimensional and arranged in a spiral of circumference $N$ and height $M$). The top and bottom are maintained at constant $T_m = 0.9 T_c$, with a Boltzmann-probability technique identical to the standard Metropolis method. This choice of $T_m$ permits a sufficiently fast relaxation for observation while avoiding the influence of critical fluctuations: The thermal correlation length is approximately 5 lattice units. The spin degeneracy is varied over a range of $1.0 \leq \delta \leq 5.0$, with $\Lambda$ therefore varying between 0 (Ref. 16) and 0.53$J$. The interfaces are subsequently allowed to relax towards equilibrium, with time measured in units of MCS, Monte Carlo steps per spin, such that every spin site is visited once in each MCS.

The interface was defined as a single-valued function, ignoring overhangs and bubbles in the bulk; in general, this was a more-than-reasonable approximation since the interface was always distinct and well behaved. The interface width was defined as $\xi_{rms}^2 = \langle (\xi - \langle \xi \rangle)^2 \rangle$. After 5000 MCS, the mean width of the interface was $\sim 10$ lattice units, while the average interface position remained roughly constant (± 1 lattice unit) throughout the run. Saturation of the roughening was observed in systems smaller than $N = 512$, and, consequently, the system size was set at $N = 1024$ and $M = 64$, the initial interface running parallel to the $N$ axis. Because of the lack of self-averaging in the roughening behavior, it was necessary to take an ensemble average of the growth of interface fluctuations, and therefore of order 50 trials for each value of $\delta$ were made.

Figure 1 shows the growth of thermal fluctuations on a typical interface for typical values of the system parameters, and Fig. 2 shows the observed time dependence of the interface width for $\Lambda = 0$, 0.20$J$, 0.33$J$, and 0.53$J$. Error bars are somewhat smaller than the symbol size. The width was measured every 10 MCS, although for clarity not all data points are shown, and the other system quantities such as the magnetization, demon energy, spin energy, demon temperature, etc., were monitored every 100 MCS. The first 200 MCS were ignored as a (pessimistic) estimate of the time taken for demons and spins to come to equilibrium.

The width is expected to be of the form $\xi_{rms} \sim N^z f(t/N^\nu)$, where $f$ is a scaling function. Thus, when finite-size effects are unimportant, $\xi_{rms}^2 \sim t^{\nu}$, where, from equilibrium, one has $2 \nu = 3 - d = 1$. Power-law fits to our data, see Fig. 2, reveal that systems with latent heats greater than $\Lambda \sim 0.5J$ grow uniformly with $z = 3$, while strong transitional behavior is observed for the smaller values of $\Lambda$. As $\Lambda$ tends to zero, approaching the standard field-free Ising model, the growth rate is well described by $z = 2$.

Linear analysis provides the framework within which to interpret these results. Within models $A$, the growth rate is well known to be $z = 2$, and within model $B$ the rate is $z = 3$. By contrast, the linearized solution of Zia et al. for model-$C$ dynamics predicts a rate which contains elements of both model $A$ and $B$ behavior. Zia et al. give a dispersion relation for overdamped surface modes of the form $\omega(q) = Aq^2/(\Lambda^2 + Bq)$, where $A$ includes factors describing the heat diffusion and the surface tension, $q$ is the wave number, and $\Lambda$, as before, is the latent heat. The term $Bq$ is the leading order of an
expansion in $q$. At a critical $q_c = \lambda^2/B$, $\omega(q)$ will transit from $q^2$ to $q^3$, and thus, through simple dimensional analysis, the growth law will change from $z=2$ to $z=3$. From the linearized continuum equations for the interface, the value of $q_c$ appears as the inverse of the capillary length $d_0 = \gamma T_m C_p/\lambda^2$, where $\gamma$ is the surface tension and $C_p$ is the specific heat.

This critical length scale is a manifestation of the relationship between the rate of generation of latent heat at the interface and the rate of heat diffusion to the bulk phases. If the rate of generation is very much larger than the rate of heat diffusion ($Bq/\Lambda^2 \ll 1$), the relaxation will be retarded by the coupling to the energy field and with $z=3$. If $Bq/\Lambda^2 \ll 1$, the heat produced or absorbed at the interface will be efficiently diffused away and the thermal fluctuations will grow unhindered with $z=2$. Thus, the short-length-scale fluctuations will grow freely at early times, giving a $z=2$ behavior which will eventually be supplanted by $z=3$ for the long-length-scale fluctuations.

This will continue until the system saturates at its equilibrium width ($\xi_{\text{eq}} \gg N$).

The results presented in Fig. 2 are consistent with this picture. The growth of fluctuations in the Ising model ($\Lambda = 0$) is observed to be within error of $z=2$ for the duration of the trial. At $\Lambda = 0.5$, $q_c$ is of the order of the lattice spacing. Consequently, the transition from $z=2$ to $z=3$ occurs very early, well before the 200-MCS limit, and the interface is observed to grow with $z=3$. The intermediate systems show less well-defined but consistent behavior. In both cases, there is apparently a transition region between $z=2$ and $z=3$ behavior, but the growth rates before and after the transition are not distinctly defined.

Consequently, the transition from model-A-like to model-B-like behavior. In the future, with data from further simulations, the dispersion relation $\omega(q_0)$ of the interface will be examined directly to study the transition from $q^2$ to $q^3$ behavior, making the correspondence with theory even more precise.

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16It should be noted that the algorithm used to examine the standard Ising case, $\delta = 1.0$, was a modified version of the code described above. Since there is no spin degeneracy, there is no coexistence regime and, consequently, the interface is not strictly stable: The width of the interface is not limited to $\sqrt{N}$ in the equilibrium limit. Indeed, the equilibrium state of the system at $T = 0.9T_m$ is an ordered state in either phase. However, the interface that we study has a lifetime that is much longer than the time of the simulation, and it roughens in a manner which is similar to the stable interface of the degenerate system.

17Because the run times are relatively short, it is necessary to fit the Ising data with $t^{1/2} - C$, where the constant $C$ arises from the small-length-scale cutoff, namely, the thermal correlation length $\xi_0$. Linear theory (Ref. 7) gives $C \sim \xi_0 T_m / \nu^2$, which is in the range 0.5–5. With values of $\nu$ in this range, the exponent $z$ has the value 2.0±0.2. For the data with nonzero latent heat, the corresponding small length is the capillary length $d_0$, and when $\Lambda = 0.5$, $d_0$ is very small (Rev. 12) so that corrections to the $t^{1/3}$ form are not important.
