Roughening Dynamics of Systems with Latent Heat

Loki Jörgenson, R. Harris, and Martin Grant
Department of Physics, McGill University, Rutherford Building, 3600 University Street, Montréal, Québec, Canada H3A 2T8
(Received 28 July 1989)

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.

PACS numbers: 68.10.−m, 82.65.Dp

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 of a stable interface which is "rough" at temperatures above the roughening transition temperature T_r and smooth or "faceted" below.[1] 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.[2]

Three such systems are models A, B, and C of critical dynamics.[3] 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:[4,5] In addition, there is considerable literature on the dynamics of their interfaces.[6–10] For model C, interest has focused on crossover behavior of the growth exponents, which is induced by the coupling of an unconserved order parameter to a conserved field. However, there are relatively few results.[2,8,11] Of these, the most important is the recent work of Zia, Bausch, Janssen, and Dohm,[2] 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[12] 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.[12,13] 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

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

where J is the spin coupling, the interactions are nearest neighbor, the spins are $\sigma_i = \pm 1$, and Δ represents a uniform external field. In the absence of Δ the second-order phase transition is at $T_c \approx 2.269J$, but in order to induce a first-order transition and a stable region of phase coexistence, the upper spin state is given a degeneracy $\delta > 1$.[14] This introduces a latent heat Λ which is of order Δ, and defines the melting temperature as $T_m = 2\Delta/\ln\delta$.

Consequently, Λ can be increased at constant T_m by increasing δ and Δ 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 is such a way as to minimize the time taken for this equilibrium to be established.[15] 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 $T_m = 0.9T_c$ 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 Λ therefore varying between 0 (Ref. 16) and $0.53J$. 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 $\xi^2_{\rm rms} = \langle [\xi - \langle \xi \rangle]^2 \rangle$. After 5000 MCS, the mean width of the interface was ~ 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 δ 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 $\Lambda = 0$, $0.20J$, $0.33J$, and $0.53J$. 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 $\xi_{\rm rms} \sim N^{\chi} f(t/N^z)$, where f is a scaling function.[18] Thus, when finite-size effects are unimportant, $\xi^2_{\rm rms} \propto t^{2\chi/z}$, where, from equilibrium,[7,8] one has $2\chi = 3 - d = 1$. 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 Λ. As Λ tends to zero, approaching the standard field-free Ising model, the growth rate is well described by $z = 2$.[17]

Linear analysis provides the framework within which to interpret these results. Within models A, the growth rate is well known to be $z = 2$,[7] and within model B the rate is $z = 3$.[8] By contrast, the linearized solution of Zia *et al.*[2] for model-C dynamics predicts a rate which contains elements of both model A and B behavior. Zia *et al.* describe a dispersion relation for overdamped surface modes of the form $\omega(q) \sim Aq^3/(\Lambda^2 + Bq)$, where A includes factors describing the heat diffusion and the surface tension, q is the wave number, and Λ, as before, is the latent heat. The term Bq is the leading order of an

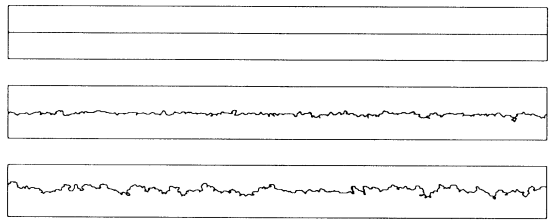

FIG. 1. The evolution of the roughening on a typical interface between coexisting phases. The system size is 1024×64, but the vertical scale has been enhanced by a factor of 1.66 for clarity. The interfaces are represented by a continuous trace; those shown are for $t = 0$, 100, and 5000 MCS with $\Lambda = 0.33J$ and $T_m = 0.9T_c$.

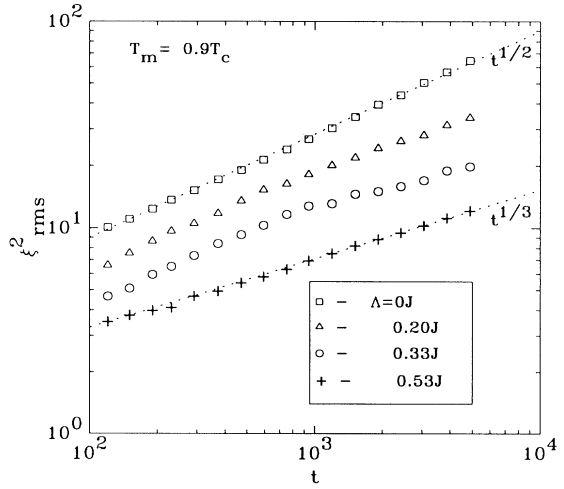

FIG. 2. The ensemble-averaged growth of the mean interface width for various values of the latent heat, $\Lambda = 0$ (Ising), $0.20J$, $0.33J$, and $0.53J$. The mean deviation from the average is smaller than the symbol size in all cases. For clarity, not all data points are shown. The dotted lines, given for comparison, are exactly $t^{1/2}$ and $t^{1/3}$. In the case of the Ising results, the data are shown with an offset of 2.53 (Ref. 17).

expansion in q. At a critical q, $q_c \sim \Lambda^2/B$, $\omega(q)$ 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,[19] the value of q_c appears as the inverse of the capillary length $d_0 = \gamma T_m C_p/\Lambda^2$, where γ 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 grow with $z=3$. If $Bq/\Lambda^2 \ll 1$, the neat 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 $z=3$ when all of the fluctuations shorter than q_c have grown into their equilibrium values and the long-length-scale relaxation dominates. This will continue until the system saturates at its equilibrium width ($\xi_{eq}^2 \propto N$).

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 $\Lambda \sim 0.5J$, 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. The data between $t=200$ MCS and the time of transition show $z \sim 2$, but the amount of data involved is not sufficient for much precision. After the transition, the growth rate approaches but does not reach $z \sim 3$. Both results are subject to improvement with larger systems and longer runs.

To conclude, we have presented the results of simulations of the roughening of flat interfaces, based on a novel Monte Carlo technique. Our approach, which is especially useful for modeling situations involving heat diffusion, provided the means to confirm the predictions of recent theoretical work regarding model-C dynamics. By controlling the strength of the latent heat of transition, the effect of coupling the interface and bulk modes was demonstrated, showing the transition from model-A-like to model-B-like behavior. In the future, with data from further simulations, the dispersion relation $\omega(q)$ 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.

This work was supported by the Natural Sciences and Engineering Research Council of Canada, and by the Fonds pour la Formation des Chercheurs et l'Aide à la Recherche de la Province du Québec.

[1]Recent reviews are J. D. Weeks, in *Ordering in Strongly Fluctuating Condensed Matter Systems,* edited by T. Riste (Plenum, New York, 1980); J. D. Weeks and G. H. Gilmer, Adv. Chem. Phys. **40**, 157 (1979); H. van Beijeren and I. Nolden, in *Topics in Current Physics,* edited by W. Schommers and P. von Blackenhagen (Springer-Verlag, Berlin, 1987), Vol. 43, p. 259.

[2]R. K. P. Zia, R. Bausch, H. Janssen, and V. Dohm, Mod. Phys. Lett. B **8**, 961 (1988).

[3]P. C. Hohenberg and B. I. Halperin, Rev. Mod. Phys. **49**, 435 (1977).

[4]Model *A*: S. M. Allen and J. W. Cahn, Acta Metall. **27**, 1085 (1979).

[5]Model *B*: I. M. Lifshitz and V. V. Slyosov, J. Chem. Phys. Solids **19**, 35 (1961).

[6]R. Lipowsky, J. Phys. A **18**, L585 (1985); F. Family, J. Phys. A **19**, L441 (1986).

[7]M. Grant, Phys. Rev. B **37**, 5705 (1988).

[8]D. Jasnow and R. K. P. Zia, Phys. Rev. A **30**, 2243 (1987).

[9]S. T. Chui and J. D. Weeks, Phys. Rev. Lett. **40**, 733 (1983).

[10]M. Grant, K. Kaski, and K. Kankaala, J. Phys. A **20**, L571 (1987); D. Stauffer and D. Landau, Phys. Rev. B **39**, 9650 (1989); R. C. Desai and D. Stauffer, J. Phys. A **21**, L59 (1988); T. Ala-Nissila, K. Kankaala, and K. Kaski, J. Phys. A (to be published).

[11]A. Sadiq and K. Binder, J. Stat. Phys. **35**, 617 (1984); A. Chakrabarti, J. B. Collins, and J. D. Gunton, Phys. Rev. B **39**, 1506 (1989); W. W. Mullins, and J. Viñals, Acta Metall. **37**, 991 (1989).

[12]R. Harris and M. Grant (to be published).

[13]R. Harris and M. Grant, Phys. Rev. B **38**, 9323 (1988).

[14]R. Harris, Phys. Lett. **111A**, 299 (1985).

[15]L. Jörgenson, M.Sc. thesis, McGill University, 1989 (unpublished).

[16]It 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 region 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.

[17]Because 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 ξ_0. Linear theory (Ref. 7) gives $C \sim \xi_0 T_m/\gamma\pi^2$, which is in the range 0.5–5. With values of C 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 $\Lambda \simeq 0.5$, d_0 is very small (Rev. 12) so that corrections to the $t^{1/3}$ form are not important.

[18]The notation is that of M. Kardar, G. Parisi, and Y.-C. Zhang, Phys. Rev. Lett. **56**, 889 (1986).

[19]J. S. Langer, Rev. Mod. Phys. **52**, 1 (1980).