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Crossover scaling in the dynamics of driven systems

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We study growing interfaces in two- and three-dimensional systems by the numerical integration of the Kardar-Parisi-Zhang equation and the Monte Carlo simulation of a solid-on-solid model with asymmetric rates of evaporation and condensation. A crossover scaling ansatz is proposed, which we find accounts for the dependence of growth on the driving force, as we crossover from the dynamic roughening regime, where that force is identically zero, to driven growth, where a nonzero driving force is present. We thus estimate the crossover scaling exponents, as well as the scaling functions.

Dynamics of driven interfaces separating two phases is an important subject of fundamental as well as practical interest, which is currently receiving much attention. Examples include layered growth using molecular-beam epitaxy or chemical vapor deposition,[1] crystal growth into a supercooled melt,[2] and propagation of flame fronts.[2] Since driven interfaces are far from equilibrium, they often involve strong nonlinearities, which thus pose a serious challenge to theoretical understanding. An important model for driven interface growth was recently proposed by Kardar, Parisi, and Zhang[3] (KPZ). It is a nonlinear differential equation for the time t dependence of the interface height variable $h(\mathbf{x},t)$ in a d-dimensional system, above a $(d-1)$-dimensional plane,

$$\frac{\partial h}{\partial t}=\nu\nabla^2 h+\frac{\lambda}{2}(\nabla h)^2+\eta\,, \tag{1}$$

$$\langle\eta(\mathbf{x},t)\eta(\mathbf{x}',t')\rangle=2D\delta^{d-1}(\mathbf{x}-\mathbf{x}')\delta(t-t')\,, \tag{2}$$

where ν, λ, and D are constants, η is a random noise satisfying Gaussian statistics, $\langle\,\rangle$ represents ensemble averages, and $h(\mathbf{x},t)$ is single valued. The nonlinear term breaks the symmetry of positive and negative h and provides the driving force for the growth. This term cannot be derived from a Hamiltonian and has a kinetic origin.[3] The long-time, long-wavelength behavior of the model can be probed by measuring the width, $W\equiv[\langle(h-\langle h\rangle)^2\rangle]^{1/2}$, of the interface as a function of time and system size. W is often found to obey a scaling relation: $W(L,t)\sim L^{\chi}\times F(tL^{-z})$ or $W(L,t)\sim t^{\beta}G(tL^{-z})$, where t is the time, L is the linear size of the system, and F and G are scaling functions. The exponent z characterizes the approach to a steady state, χ is the roughening exponent describing the roughness of the interface at late stages of the growth, and $\beta\equiv\chi/z$ is the growth exponent.

Without the nonlinear term ($\lambda=0$), Eq. (1) describes the dynamics of roughening and one can easily find $\chi_0=(3-d)/2$ and $z_0=2$. We have used the subscript 0 to denote zero driving force. For $\lambda>0$, the asymptotic behavior of Eq. (1) is not known and Kardar, Parisi, and Zhang (KPZ) carried out a dynamical renormalization-group analysis.[3] They found that the critical dimension of the nonlinear term is $d_c=3$, with a hyperscaling relation $\chi+z=2$. While no stable strong-coupling fixed point was found at $d=d_c$, a fluctuation-dissipation theorem exists at $d=2$ which allowed them to obtain the exact results $\chi=\frac{1}{2}$ and $z=\frac{3}{2}$. These are consistent with many numerical simulations of lattice models,[4,5] and are different from the roughening results quoted above. At the critical dimension, the perturbative solution of the KPZ equation fails. Numerical solutions of the equation[6,7] give the growth exponent $\beta\approx0.13$ which is also consistent with that of an asymmetric solid-on-solid (SOS) model.[6]

Since the presence or absence of the nonlinear driving force determines the dynamic universality class (driven or roughening), a natural analogy arises with the critical phenomena. In the latter case, competing interactions lead to crossover behavior between different universality classes. For example, adding a cubic anisotropic interaction to the N-vector model can give crossover from Ising to Heisenberg fixed points.[8] For the driven growth problem described above, a crossover regime is thus expected when the driving force is small, and t or L is not asymptotically large.

In this paper we show that there indeed exists a crossover behavior between the dynamic roughening and the driven growth, which is a consequence of the competing relaxation and driving forces for large, but not infinite, time regimes. We propose a scaling ansatz, which is found to account for the dependence of growth on driving force, as we crossover from the dynamic roughening regime, where that force is identically zero, to driven growth, where a nonzero driving force is present.[9] We compute the crossover scaling functions and associated exponents in two and three dimensions for the KPZ equation, and confirm the results by simulating a SOS model at $d=2$, which we expect has the same universality class as the KPZ equation.[6] While the usual crossover phenomena are between two or more *stable* fixed points, we are now dealing with a situation where the crossover is to a strong-coupling fixed point where dimensional analysis is of little utility (since the $\epsilon=d_c-d$ expansion involves an unstable fixed point). As a consequence, the usual dimensional and scaling analysis cannot predict the crossover exponents. Thus a numerical study, as we present below, is required.

To motivate our crossover scaling ansatz, note that for any driving force $\lambda>0$, the dynamics in the hydrodynamic limit is controlled by the driven growth exponents.[3] Thus it is natural to make the following ansatz to account for the crossover from the dynamic roughening regime involving exponents χ_0 and z_0, to the driven growth regime

$$W(L,t,\lambda)\sim t^{\beta_0}f_d(Lt^{-1/z_0},t\lambda^{\phi}), \tag{3}$$

where f_d is the crossover scaling function. Setting $\lambda=0$, we simply recover the roughening results. When $t\ll L^{z_0}$ (or for $L=\infty$), the growth is not limited by the system size L and one can drop the first argument of f_d,

$$W\sim t^{\beta_0}f_d(t\lambda^{\phi}). \tag{4}$$

If $\lambda>0$, the growth will eventually be controlled by the unknown strong-coupling fixed point with exponent χ and z, and we must have $W\sim t^{\beta}$. Thus $f_d(u)\sim u^{\beta-\beta_0}$ for large u. This gives, for $d=2$,

$$W\sim t^{\beta}\lambda^{\phi(\beta-\beta_0)}\approx t^{1/3}\lambda^{\phi/12}. \tag{5}$$

We expect (4) and (5) to hold in the large-L limit.

While the above is sufficient for $d=2$, for $d=3$ the crossover behavior is more complicated because the roughening dynamics is marginal, i.e., $W^2\sim A_0\ln t$ where A_0 is a constant. Therefore, we propose the following crossover scaling ansatz

$$W^2(L,t,\lambda)\approx A_0[f_3(t\lambda^{\phi})-\phi\ln\lambda], \tag{6}$$

where the scaling function satisfies $f_3(u)\sim\ln u$, for $u\to 0$, and $f_3(u)\sim u^{2\beta}$, for $u\to\infty$. Again we require times $t\ll L^{z_0}$ so that any size dependence can be neglected. Our goals in this paper are to compute the crossover exponents ϕ, the scaling functions, and to test the scaling ansatz equations (4) and (6).

Although no perturbable strong-coupling fixed point has been found for the KPZ equation in $d\le 3$, it is still worthwhile to show how ϕ would be determined by simple scaling arguments, if such a fixed point existed. First, one makes a scale transformation in space and time of the KPZ equation, using the exponents for $\lambda=0$: $\mathbf{x}'=e^{-l}\mathbf{x}$, $t'=e^{-z_0l}t$, $h'=e^{-\chi_0l}h$. Second, the transformed equation is restored to the original form by redefining the constants: $\nu\to\nu'=\nu e^{(z_0-2)l}$, $\lambda\to\lambda'=\lambda e^{(\chi_0+z_0-2)l}$, and $D\to D'=De^{(z_0-d+1-2\chi_0)l}$. Finally, the transformation $h'(\mathbf{x}',t',\lambda')=e^{-\chi_0l}h(\mathbf{x},t,\lambda)$ implies

$$W(L,t,\lambda)\sim t^{\beta_0}F(Lt^{-1/z_0},t\lambda^{z_0/(\chi_0+z_0-2)}), \tag{7}$$

where a choice of l has been taken such that $e^l=t^{1/z_0}$. This implies that the crossover exponent $\phi=z_0/(\chi_0+z_0-2)$. For example, for $d=2$, this implies $\phi=4$. However, as we shall show below, a numerical solution of the KPZ equation gives $\phi\approx 3.0$, and thus does not agree with the scaling argument. As mentioned above, this is because no stable fixed point exists in the strong-coupling regime for the KPZ equation. Indeed, the dimensional analysis above is intimately related to the existence of a stable $\epsilon=d_c-d$ expansion, since power counting by the Ginzburg criterion, $\chi_0+z_0-2=0$, determines the critical dimension. For cases where a stable fixed point exists,[10] we expect this analysis to give the right crossover exponent.

To test the crossover scaling ansatz, we first solved the KPZ equation numerically, using a finite difference scheme.[6] In $d=2$, the constants ν and D were taken to be 1.0 and 0.01, respectively. A space mesh 1.0 and time mesh 0.01 were used; reducing the time mesh gives essentially the same results. A system size of $L=4096$ was used throughout, which was sufficiently large for our purposes. For large values of $\lambda(\lambda\ge 40)$, we recovered the KPZ result $\beta=\frac{1}{3}$. However, for $0<\lambda<40$, a crossover regime exists where β has effective values between $\frac{1}{4}$ and $\frac{1}{3}$, over the time regime studied. The inset to Fig. 1 shows $f_2=W/t^{1/4}$ as a function of t for several values of λ. The curves, each of which corresponds to an average of 100 independent runs, are well separated and considerable curvature exists indicating that the growth is faster than $t^{1/4}$. Indeed, those curves include large-λ data which can be well fit by $\beta\approx\frac{1}{3}$. Figure 1 gives the test of the crossover scaling ansatz equation (4), where f_2 is plotted as a func-

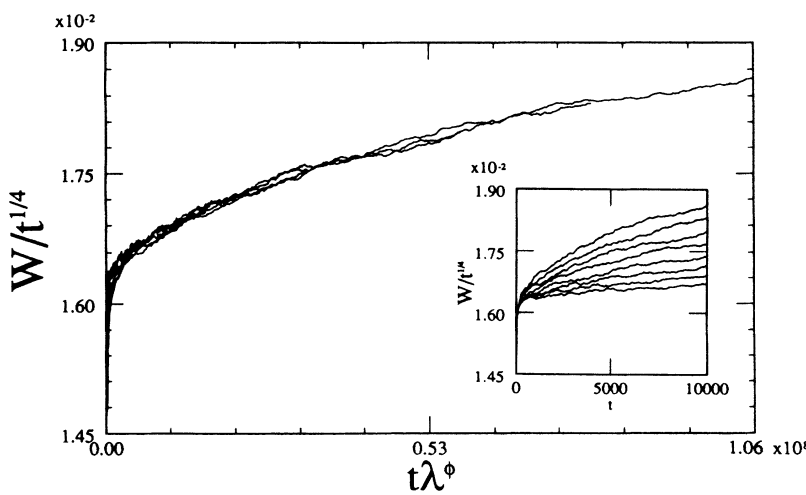

FIG. 1. Plot of the crossover scaling function $f_2=W/t^{1/4}$ vs $t\lambda^{\phi}$ of the KPZ model in $d=2$. Good data collapsing is achieved for $\phi=3.0$. System size $L=4096$. Data for $\lambda=8$–22 in steps of two were used to get the scaling curve. Inset shows curves before data collapsing.

tion $t\lambda^{\phi}$. Using $\phi=3.0$, reasonable data collapsing is indeed observed, so that Fig. 1 gives our estimate of the crossover scaling function f_2.

An independent check on the value of ϕ was carried out by studying the amplitude of the growth of the interface width, Eq. (5), for large λ's, where the $t^{1/3}$ growth was unambiguously observed. In Fig. 2, we plot $\ln W$ as a function of $\ln\lambda$. The data fall on a straight line of slope 0.23 ± 0.02 implying a power-law dependence. From Eq. (5), that slope is consistent with our estimate of above $\phi=3.0$, which would imply a slope $\phi/12=0.25$. These results show that the crossover scaling ansatz Eq. (4) does hold for the two-dimensional driven growth described by the KPZ equation. Combining the two independent calculations of ϕ, our best estimate is $\phi=3.0\pm0.2$.

Another $d=2$ model we have studied is the asymmetric SOS model.[6,11] We use the SOS Hamiltonian $H=\sum_{\langle ij\rangle}|h_i-h_j|$ for Monte Carlo attempts, but bias those attempts by an amount λ_a, which is the fractional amount of extra attempts made on one side. This implies that $\lambda_a=0$ gives equilibrium, while $\lambda_a>0$ cause the interface to drift. We expect that the asymmetry allow terms even in ∇h to appear in the equation of motion in the hydrodynamic limit, so that this model is in the same universality class as the KPZ equation. In a previous paper,[6] we have found that this model has the same growth exponents χ and z as the KPZ equation in $d=2$ and 3.

We used systems with size $L=2000$ and times up to 4000 Monte Carlo steps per site. Here a Monte Carlo step corresponds to an attempt of growing the height by one unit. 250 independent runs were averaged for each λ_a to get reasonable statistics. The system temperature was kept[12] at 0.5. For any nonzero λ_a we expect $\beta=\frac{1}{3}$, but crossover phenomena are important for smaller values of λ_a. Figure 3 shows the crossover scaling function after data collapsing for several λ_a's. The exponent ϕ is again found to be approximately 3.0 ± 0.4. Thus not only do the growth exponents χ and z agree between the KPZ equation and the asymmetric SOS model, the crossover scaling

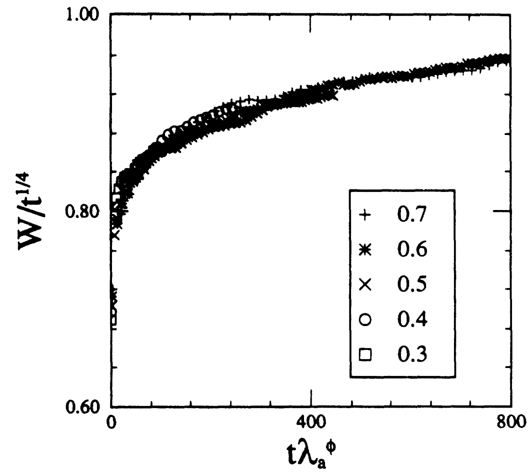

FIG. 3. Crossover scaling function for the $d=2$ asymmetric SOS model. System size $L=2000$. Data from five different λ_a's (values as indicated) were collapsed onto a single curve using $\phi\approx3.0$.

exponent ϕ also agrees.

In $d=3$, we performed numerical solutions of the KPZ equation with $\nu=1.0$, $D=5\times10^{-4}$, and the time mesh was[6] 10^{-3}. We studied λ ranging from 120 to 240 in increments of 20 (smaller $\lambda<120$ required much longer simulations to observe crossover behavior). This range includes large-λ data which can be well fit by[6] $\beta\approx0.13$. Systems of size 128^2 were studied and integrated over 40000 time steps, with 50 independent runs averaged. We also studied systems of size 256^2 to ensure no finite-size effects were present. Equation (6) was tested by plotting $f_3=W^2/A_0+\phi\ln\lambda$ vs $t\lambda^{\phi}$, where A_0 is obtained from $W^2=A_0\ln t$ for runs with $\lambda=0$. Our best data collapse is shown in Fig. 4 for $\phi=4.5\pm0.5$. Nevertheless, we caution that systematic errors could be present in our estimation of exponents in $d=3$, because it is a marginal dimension.

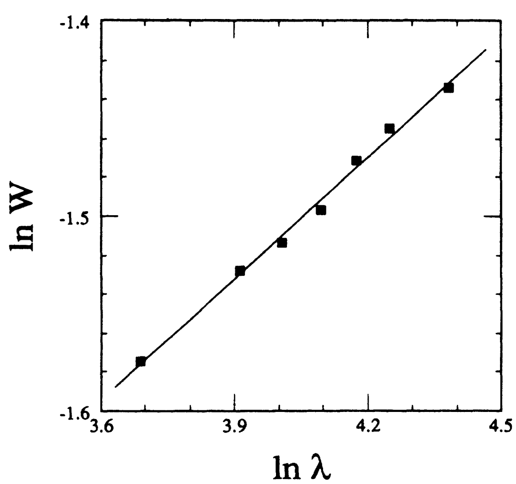

FIG. 2. Typical ln-ln plot of $W(t)$ vs λ at a given time t for the $d=2$ KPZ model. Linear fit to data for all times gives slope of 0.23 ± 0.02, consistent with $\phi\approx3.0$.

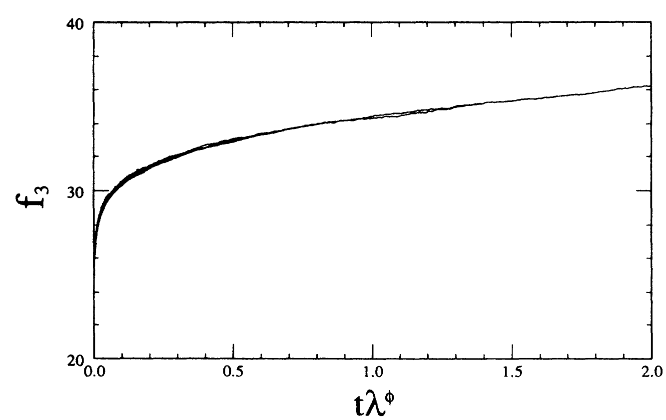

FIG. 4. Plot of the crossover scaling function $f_3=W^2/A_0+\phi\ln\lambda$ vs $t\lambda^{\phi}$ of the KPZ model in $d=3$. Very good data collapsing is achieved with $\phi=4.5$. The system size is 128^2. Data for $\lambda=120$–240 in steps of 20 were used to get the scaling curve.

In summary, we have studied crossover phenomena, described by simple scaling forms, between roughening dynamics and driven growth of interfaces. Extensive numerical simulations of the KPZ equation and an asymmetric SOS model gave the crossover scaling exponents $\phi \approx 3.0$ for $d=2$, and $\phi \approx 4.5$ for $d=3$. Simple dimensional analysis does not give consistent results, indicating the subtlety of driven growth dynamics in the absence of a stable fixed point at the critical dimension.

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[1]*Molecular Beam Epitaxy and Heterostructures,* edited by L. L. Chang and K. Ploog (Martinus Nijhoff, Hingham, MA, 1985); A. W. Vere, *Crystal Growth* (Plenum, New York, 1987).

[2]See, for example, articles in *Dynamics of Curved Fronts,* edited by Pierre Pelce (Academic, New York, 1988).

[3]M. Kardar, G. Parisi, and Y. C. Zhang, Phys. Rev. Lett. **56**, 889 (1986).

[4]M. Plischke and Z. Racz, Phys. Rev. A **31** 985 (1985); F. Family and T. Vicsek, J. Phys. A **18**, L75 (1985); R. Jullien and R. Botet, *ibid.* **18**, 2279 (1985); J. G. Zabolitzky and D. Stauffer, Phys. Rev. Lett. **57**, 1809 (1986); J. Kertesz and D. E. Wolf, J. Phys. A **21**, 747 (1988).

[5]P. Meakin, P. Ramanlal, L. M. Sander, and R. C. Ball, Phys. Rev. A **34**, 5091 (1986); P. Meakin and R. Jullien, J. Phys. (Paris) **48**, 1651 (1987); D. Liu and M. Plischke, Phys. Rev. B **38**, 4781 (1988); J. M. Kim and J. M. Kosterlitz, Phys. Rev. Lett. **62**, 2289 (1989).

[6]H. Guo, B. Grossmann, and M. Grant, Phys. Rev. Lett. **64**, 1262 (1990).

[7]A. Chakrabarti and R. Toral, Phys. Rev. B **40**, 11 419 (1989).

[8]E. Brezin, J. C. LeGuillou, and J. Zinn-Justin, Phys. Rev. B **10**, 892 (1974).

[9]In two recent studies of driven growth in lattice models [H. Yan, D. Kessler, and L. M. Sander, Phys. Rev. Lett. **64**, 926 (1990); J. Amar and F. Family, *ibid.* **64**, 543 (1990)] driving-force-dependent exponents have been reported, although no crossover scaling was investigated.

[10]T. Sun, H. Guo, and M. Grant, Phys. Rev. A **40**, 6763 (1989).

[11]G. H. Gilmer, in *Chemistry and Physics of Solid Surfaces,* edited by R. Vanjselow and R. Howe, Springer Series in Chemical Physics Vol. 35 (Springer-Verlag, Berlin, 1982).

[12]We found that the growth exponent was independent of temperature.