Kinetics of Interface Growth in Driven Systems

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We study growing interfaces by the numerical simulation of several three-dimensional systems: the Kardar-Parisi-Zhang equation, a discrete variant of that model, and a solid-on-solid model with asymmetric rates of evaporation and condensation. Growth exponents in the rough phase are calculated, and we estimate the kinetic roughening transition temperature, its dependence on driving force, and analyze the transition by finite-size scaling. We find the transition depends strongly on driving force, which could be investigated experimentally.

Roughening transitions play an important role in three-dimensional crystal growth.[1-5] Nevertheless, while the roughening transition is reasonably well understood in equilibrium, its nature in systems which are far from equilibrium is not. In experiments on epitaxy,[6] where an interface grows at a constant rate, it is of interest to determine how a constant driving force affects the transition. For example, one would like to know the roughness of the interface above the transition temperature T_R, as well as the conditions, if any, under which an interface can be grown in the smooth faceted phase which exists below T_R. Experiments on crystal growth[7] find that one can go from a smooth to a rough phase by increasing the driving force beyond a particular strength, at a fixed temperature $T < T_R$. It should also be noted that the dynamics of a growing interface separating two phases is a fundamental problem in condensed-matter physics.

An important model for driven interface growth has been introduced by Kardar, Parisi, and Zhang (KPZ).[8] It is a nonlinear differential equation [Eq. (1) below] which can be used to study the universal long-time, long-wavelength properties of the width W of a driven interface. The width typically obeys[9] $W(L,t) \sim L^{\chi} \times f(tL^{-z})$, where L is the linear size of the growing substrate, t is time, and f is a scaling function. For dimension $d = 2$, a fluctuation-dissipation theorem allows one to calculate the interface exponents, $\chi = \frac{1}{2}$ and $z = \frac{3}{2}$. These are consistent with numerical simulations,[9,10] and are different from the equilibrium roughening exponents $\chi = (3-d)/2$ and $z = 2$.

The situation in the more experimentally interesting case of $d = 3$ is more problematic. Three dimensions is the critical dimension d_c of this system, above which nonlinearities are naively irrelevant. However, at d_c, the KPZ equation does not have a stable fixed point, and growth information can only be inferred indirectly, although it should be noted that the KPZ equation satisfies the scaling relation $\chi + z = 2$, when the nonlinear term is relevant. This is unfortunate, since the KPZ model provides a description of the driven interface growth in three dimensions. Given this unclear situation, there have

been several conjectures[11] for the value of the growth exponents as a function of d.

Hence we felt it worthwhile to study driven growth in three-dimensional systems. We report numerical studies of three models which we expect to be in the same dynamical universality class in the rough phase. First, we have numerically integrated the KPZ equations of motion directly at the critical dimension to determine growth exponents. Second, the possibility of a kinetic roughening transition was investigated through the study of variants of two important models used to study it in the past: the discrete Gaussian model and the solid-on-solid (SOS) model.[1-5,12-15] Our results are consistent with $\chi/z \approx 0.13$, and $\chi + z \approx 2$, for the KPZ equation and the SOS model in the rough phase.[16] We find that our data for both a discrete KPZ model and an asymmetric SOS model can be interpreted in terms of a roughening transition occurring at a nonzero T_R, which appears to be stronger than the usual Kosterlitz-Thouless transition. We characterize it with a simple finite-size scaling *Ansatz*, as is used for second-order phase transitions. The transition here corresponds to a nonequilibrium phase transition such as has been studied for driven diffusive systems.[17]

The KPZ equation is

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

where $h(\mathbf{x}, t)$ is the height of the interface from a reference plane, and is assumed to be a single-valued function of position $\mathbf{x}$, and ν and λ are constants. The random noise η satisfies Gaussian statistics with the second moment given by

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

where angular brackets denote an ensemble average and D is a constant. It provides the most simple model of driven growth. The nonlinear term is crucial, since it breaks the symmetry of positive and negative h. This piece cannot be derived from a free energy, and has a kinetic origin. Amongst other effects, it causes the average

position of the interface to grow at a constant rate at late times. Therefore, while the system approaches steady-state growth, it never equilibrates. If the nonlinear coupling constant $\lambda \equiv 0$, Eq. (1) describes the dynamics of roughening;[1,13-15] the fluctuation-dissipation relation implies that the ratio $D/v = T$, where T is the temperature in units of Boltzmann's constant divided by the surface tension.

We have integrated the KPZ dynamical equation in both $d = 2$ and the critical dimension $d_c = 3$. We choose units such that $D = 1$, but let both v and λ vary in anticipation of our study of the discrete KPZ model below (one may choose $v = 1$ also[18]). It is convenient to estimate χ and β, where $W(L,t) \sim t^\beta g(tL^{-z})$, so that $\beta = \chi/z$. The growth is monitored through $W(L,t) \equiv [\langle (h - \langle h \rangle)^2 \rangle]^{1/2}$ to give β before saturation occurs, while χ is obtained by waiting until the width has reached its steady-state value, since $W \sim L^\chi$ as $t \to \infty$. Large numbers of independent runs were done to obtain good statistics. In $d = 2$, we find $\beta = 0.33$ for nonzero λ, and $\beta = 0.25$ for $\lambda = 0$, while $\chi = 0.5$ for all λ with very high numerical precision. These are consistent with the known exponents, mentioned above.

In the critical dimension, $d = 3$, the integration of the KPZ equation is hampered by large fluctuations and crossover effects. Besides a large number of independent runs for average, one must study sufficiently large system sizes so that the growth of the width persists until the nonlinear term becomes important. We studied systems of edge length $L = 128$, and integrated over times up to 40 000 time steps with a time mesh of 0.001. We obtain $\beta = 0.13 \pm 0.02$ for late times with fifty independent runs (see Fig. 1). Note that the effective exponent drops to that value from $\beta \sim 0.5$ for early times (due to the noise η). The steady-state exponent χ is much more difficult to estimate. To obtain reasonable statistics with a large number of independent runs, we are limited with rather
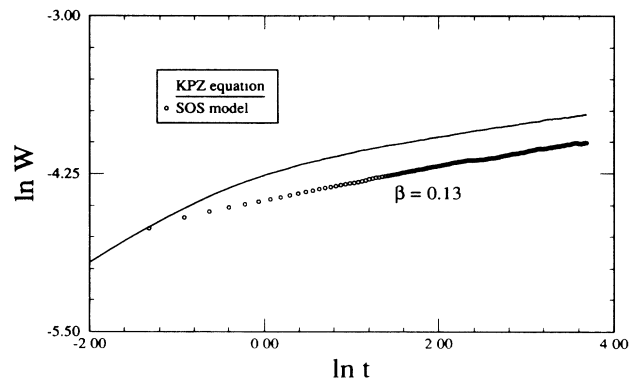
small systems. With $L < 30$, χ is found to be 0.24 ± 0.04. In these runs, we let $v = 1$ and $\lambda = 200$. The independent measurements of β and χ give $\chi + z \approx 2.1$. Other values of v and λ were studied, and give values of the exponents consistent with those quoted above.[16] The results are different from the usual roughening exponents which give both β and χ to be 0, since W has only a logarithmic divergence. Below, we discuss our results for β and χ further.

The possibility of a kinetic roughening transition cannot be studied with the continuum KPZ equation. Therefore, we introduce a generalized model, motivated by the discrete Gaussian model of Chui and Weeks,[12] which has been used to study the equilibrium roughening transition. This corresponds to Eq. (1) on a lattice, with the height variable h restricted to integer values of the lattice constant. We call this the discrete KPZ model, since choosing $\lambda \equiv 0$ gives the discrete Gaussian model. Figure 2 shows the typical growth of the average height in a given run as a function of time. Different curves are for different driving forces λ with the temperature $T = 1/v < T_R(\lambda = 0)$ fixed. For small values of λ, the growth is one layer at a time (curves a and b), suggesting that the system is in faceted phase. For large values of λ, the growth becomes continuous (curve e), signaling that the rough phase is reached. Unfortunately, the discrete KPZ model is numerically a difficult problem, so our observations are only qualitative. To undertake a quantitative study, we consider a nonequilibrium SOS model with asymmetric rates of evaporation and condensation.

The SOS model has a roughening transition in equilibrium,[1,13] and its nonequilibrium properties have been previously studied by many authors, particularly Gilmer.[1] Analytic work, within linear response, has been done by Chui and Weeks[12] and by Saito.[14,15] We use

FIG. 1. ln-ln plot of interface width W vs time t in three dimensions. Edge length is $L = 128$ for the continuous KPZ model and $L = 100$ for the asymmetric SOS model. The slope gives the growth exponent $\beta = \chi/z \approx 0.13$. Data for the SOS model were shifted along both axes for convenience.
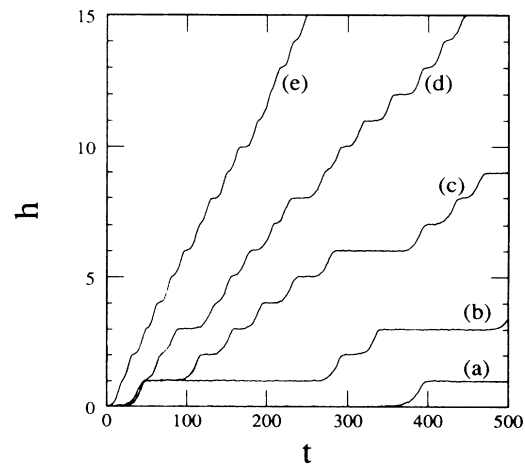

FIG. 2. The height of the interface for representative runs in the discrete KPZ model, as the nonlinear driving force is increased (labeled a-e). Note the change from layered to continous growth.

the SOS Hamiltonian, $H = \sum_{\langle i,j \rangle} |h_i - h_j|$, 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 $\lambda_a > 0$ causes a constant velocity of the interface. We expect this asymmetry allows terms even in ∇h to appear in long-wavelength equations of motion, so that this model would be in the same universality class as the KPZ equation.

To check this, we first calculated the growth exponents for the asymmetric SOS model. In $d = 2$, we obtained $\chi = 0.50$ for all λ_a. For any nonzero λ_a, we expect $\beta = \frac{1}{3}$, although transients were important for small values of λ_a: The effective exponents were $\beta(\lambda_a = 1.0) \approx 0.33$, $\beta(0.8) \approx 0.31$, $\beta(0.6) \approx 0.31$, $\beta(0.4) \approx 0.29$, and $\beta(0.2) \approx 0.29$, while $\beta(\lambda_a \equiv 0) \approx 0.25$ for runs in systems of edge lengths up to $L = 6000$ and times up to 40000 Monte Carlo steps. In the rough phase in $d = 3$ the asymmetric SOS model gives $\beta = 0.13 \pm 0.02$, and $\chi \approx 0.25$, which are in agreement with the results of integrating the KPZ equation (see Fig. 1). These results constitute our best estimates for the growth exponents. Our results are not consistent with conjectures in the literature.[11] Those conjectures were, however, motivated by the study of simple models which, although they share similar features to the KPZ equation, are not obviously in the same universality class. Nevertheless, we caution that crossover effects could play an important role in $d = 3$, because it is a marginal dimension, which may imply considerable systematic errors in our estimation of exponents. Further study is required to definitively determine the nature of growth in $d = 3$.

The possibility of a roughening transition was analyzed with C, which is the analog of specific heat defined by $C \equiv (\langle H^2 \rangle - \langle H \rangle^2)/L^{d-1}T^2$. Here C is a nonequilibrium quantity describing fluctuations of local bond ener-

gies in the steady state. There is no anomaly in the specific heat for roughening of an equilibrium interface,[1] although there is a bump close to T_R. In the driven system, however, we expect any roughening transition to be *stronger* than the usual Kosterlitz-Thouless-type transition for equilibrium, because $\chi > 0$ in the driven rough phase while $\chi = O(\log)$ in equilibrium. Indeed, we find that C is strongly peaked for nonzero λ (see Fig. 3), and from inspection of configurations, that its peak corresponds to the roughening transition. Thus we interpret the peak position as $T_R(\lambda, L)$, which shifts to lower temperatures as λ is increased. Motivated by the equation of motion, we fit this to $T_R(\lambda) \sim T_R(0)/[1 + O(\lambda)]$, in the inset to Fig. 3, where[1,19] $T_R(0) = 1.24$ is the equilibrium roughening transition temperature for the SOS model. This implies one can go from the smooth to the rough phase by increasing the driving force at a given temperature, as seen qualitatively for the discrete KPZ model mentioned above. This feature has also been observed experimentally.[7] To estimate the nature of possible singular behavior in C, in the absence of theory which includes the effect of the nonlinearity, we have followed standard treatments for *second-order* transitions. We make the finite-size scaling *Ansatz*, $C \sim L^{a/\nu} F(|T - T_R| \times L^{1/\nu})$, and fit to find a and ν. These are not equilibrium exponents since C could depend on the dynamical universality class.[20] We caution here that such a procedure is not appropriate for the equilibrium case ($\lambda_a = 0$) since, as mentioned above, the equilibrium roughening transition is of Kosterlitz-Thouless type. From the data collapse shown in Fig. 4 for $\lambda_a = 0.4$, we find that our *Ansatz* is self-consistent, and allows us to estimate $a/\nu \approx 0.5$ and $\nu \approx 1.5$. Finally, from ν we estimate $T_R(L \to \infty) \approx 0.54$ for $\lambda_a = 0.4$, using $T_R(L) = T_R(L \to \infty) + O(1/L^{1/\nu})$. We believe that an ultimate validation of this *Ansatz* can only come from further

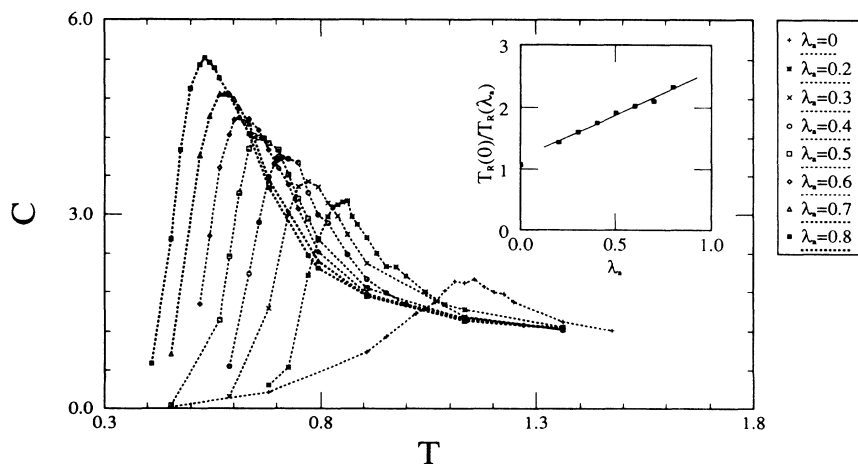FIG. 3. Plot of fluctuations in local bond energy C for the asymmetric SOS model as a function of driving force $\lambda_a = 0$ to $\lambda_a = 0.08$, as indicated. Inset: The position of the maximum for different driving forces (point at $\lambda_a = 0$ from Ref. 13). Normalizing $T_R(\lambda)$ with (Refs. 1 and 19) $T_R(0) = 1.24$ is only for convenience.
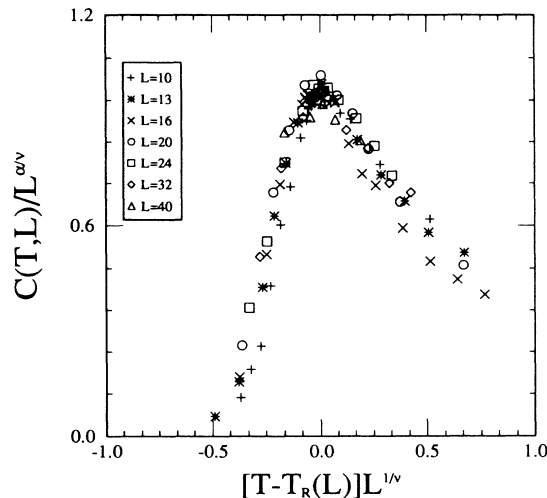
FIG. 4. Finite-size scaling plot of fluctuations in local bond energy for the asymmetric SOS model $C/L^{a/v}$ vs $|T - T_R| \times L^{1/v}$, with $a/v = 0.5$, $v = 1.5$, $L = 10$–40, as indicated, and $\lambda_a = 0.4$. $T_R(L)$ is the peak position of the bond energy fluctuations for system of size L.

study of the nature of this nonequilibrium phase transition. However, our results can be consistently, and we believe most naturally, interpreted in terms of a transition occurring at a nonzero temperature.

In summary, we have integrated the dynamical interface model for driven growth introduced by Kardar, Parisi, and Zhang, and generalized it to a discrete model. To the accuracy of our study, the KPZ equation belongs to the same universality class as the solid-on-solid model, with asymmetric rates of evaporation and condensation, in the rough phase. Numerical simulations suggest the possibility of a roughening transition at nonzero temperature in the two discrete models, which we characterized by a finite-size scaling *Ansatz*. These results, in particular the kinetic roughening transition in driven interfacial growth, are experimentally accessible by many methods. Such a study would be of considerable interest.

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