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Kinetic roughening of interfaces in driven systems

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We study the dynamics of an interface driven far from equilibrium in three dimensions. First we derive the Kardar-Parisi-Zhang equation from the Langevin equation for a system with a nonconserved scalar order parameter, for the cases where an external field is present, and where an asymmetric coupling to a conserved variable exists. The relationship of the phenomena to self-organized critical phenomena is discussed. Numerical results are then obtained for three models that simulate the growth of an interface: the Kardar-Parisi-Zhang equation, a discrete version of that model, and a solid-on-solid model with asymmetric rates of evaporation and condensation. We first make a study of crossover effects. In particular, we propose a crossover scaling ansatz and verify it numerically. We then estimate the dynamical scaling exponents. Within the precision of our study, the Kardar-Parisi-Zhang equation and the solid-on-solid model have the same asymptotic behavior, indicating that the models share a dynamical universality class. Furthermore, the discrete models exhibit a kinetic roughening transition. We study this by monitoring the surface step energy, which shows a dramatic jump at a finite temperature for a given driving force. At the same temperature, a finite-size-scaling analysis of the bond-energy fluctuation shows a diverging peak.

I. INTRODUCTION

Systems that are far from equilibrium can have properties qualitatively different from those close to their equilibrium states. In this work we address a well-defined problem of this kind, the nature of interface roughening during crystal growth. We are most concerned with the relationship of this problem to self-organized criticality, the nature of roughening in driven growth, and the possibility of a nonequilibrium roughening transition.

The first suggestion of the existence of a roughening transition in equilibrium interfaces separating two coexisting phases was made by Burton, Cabrera, and Frank.[1] They argued that below a certain temperature T_R, thermal fluctuations could not overcome the barrier provided by surface energy, so that the interface remained microscopically flat. However, above T_R, the interface could wander freely, becoming rough. The argument is most transparent for the (100) facet separating phases of the three-dimensional simple-cubic Ising model. See Fig. 1. The low-temperature excitations of the facet correspond to one-block fluctuations either up or down. However, on looking "down" at the facet and its excitations, one recognizes that it is equivalent to the one-phase state of the *two-dimensional* Ising model with low-temperature excitations. One can also consider a ledge in the three-dimensional system, which is equivalent to coexisting phases in two dimensions. This low-temperature mapping shows the stability of the smooth facet, and suggests that T_R of that facet is approximately the critical temperature of the second-order phase transition in the two-dimensional Ising model.

Since that original study, much theoretical and experimental work has been done.[2-6] It is now understood that the Burton-Cabrera-Frank idea was incomplete since it did not take into account the possibility of clusters growing on other clusters as T approaches T_R from below. These give rise to capillary-wave excitations of the surface. As a consequence, the roughening transition, rather than being a second-order transition, is a Kosterlitz-Thouless transition.[7,8] Despite the fact that the transition is therefore of infinite order, signs of it have been observed experimentally.[9] Furthermore, renormalization-group techniques, in particular that used by Kosterlitz and Thouless to analyze the two-dimensional Coulomb gas system, have been successfully applied to the problem.[8] Also, many computer simulations of interface models have been performed to confirm the presence of the transition and quantitative results have been obtained.[10,11,2] Consequently, the roughening transition occurring in equilibrium interfaces is now well understood.

The nature of the roughening transition in systems that are far from equilibrium has received less attention.[4] This is unfortunate since roughening transitions play an important role in three-dimensional crystal growth.[2,3,5,12] In experiments on epitaxy and sputtering,[13,14] 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[15] 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 $T < T_R$. The effect of interface roughening on the process of crystal growth is that below T_R the growth occurs layer by layer, whereas above T_R the growth is continuous.[4,12,16] A more dramatic indication of this is that, when a crystal grows into a metastable supercooled liquid, the shape of the dendrite tip formed after a Mullins-Sekerka instability (which is important in crystal growth if the length scale over which heat diffuses is small compared to the edge length of the system) can be faceted or rounded depending on the supercooling strength.[15] Furthermore, in sputtering experiments, the interface is usually rough, and columnar growth can be observed,[14] while in epitaxial growth, very smooth interfaces can be produced.[13] Thus at a fixed temperature, rough or smooth interfaces can be grown by adjusting the external driving force.[13–15] Given the experimental and technological relevance of these systems, it is important to understand the basic physics of interface dynamics far from equilibrium. It should also be noted that the dynamics of a growing interface separating two phases is a fundamental problem in condensed-matter physics.

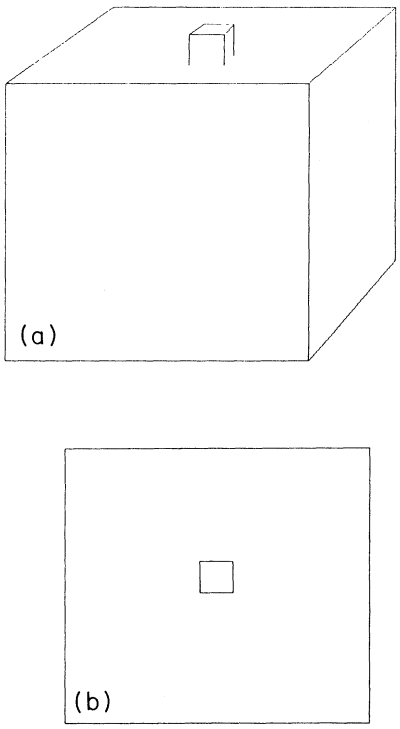

FIG. 1. (a) Side view of (100) facet with thermal fluctuation. (b) Top view.

An important step in this direction was made by the work of Kardar, Parisi, and Zhang (KPZ).[17] They proposed a nonlinear differential equation, given below, to model a growing interface driven by an external flux of particles. By applying a dynamical renormalization-group technique, a scaling form of the interface correlation is obtained along with the scaling exponents for a two-dimensional system. The width W obeys[18]

$$W(L,t) \sim L^{\chi} f(tL^{-z}), \tag{1}$$

where L is the linear size of the growing substrate, t is time, and f is a scaling function. For dimension $d = 2$ [the interface grows on a $(d-1)$-dimensional substrate], 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,[19–23] and are different from the equilibrium roughening exponents $\chi_0 = (3-d)/2$ and $z_0 = 2$, where the subscript 0 implies no driving force. In three dimensions, the critical dimension d_c of the model, no direct result was found due to the failure of perturbation theory for $d < d_c$, although a hyperscaling relation enforces $\chi + z = 2$ when the nonlinear driving force is relevant. Given this unclear situation, in the experimentally most important dimension, there have been several conjectures[24] for the values of the growth exponents as a function of d.

Like all interface models with translational invariance, in the KPZ equation there is a capillary-wave Goldstone mode due to the broken translational invariance normal to the interface. This causes the poles of response functions to be massless, and the frequency-dependent fluctuations around equilibrium to be $1/f$-like, where f is frequency. One novelty of the nonlinear Kardar-Parisi-Zhang equation is the appearance of anomalous dimensions in correlation functions (although we reemphasize that power-law correlations exist even for the linear case). However, a more important aspect of the equation is its relationship to self-organized criticality, which involves states with power-law correlations reached *without* tuning; driven interfaces provide an example of self-organized criticality where the limits of this concept are particularly transparent.

Recently, Bak, Tang, and Wiesenfeld[25] introduced the idea of self-organized criticality in a study of dynamical models that evolved automatically to a critical state without tuning any parameter. Such a self-organized critical state is characterized by the absence of length and time scales, and was argued to be responsible for long-range temporal correlations in many dissipative dynamical systems. There is thus a close relationship between the notion of self-organized critical phenomena, and earlier ideas concerning dissipative cellular automata.[26,27] These new critical phenomena are fundamentally differ-

ent from that near a second-order phase transition, or that due to the equilibrium capillary-wave fluctuations on an interface.[28] For example, the critical point can only be reached by tuning parameters such as pressure and temperature in the phase diagram, while interface equations describe a system's behavior *after* tuning onto, say, a line of liquid-vapor or solid-liquid coexistence in the phase diagram of a pure substance: Gibbs's phase rule forbids an inhomogeneous state in thermal equilibrium, except on, say, lines and points in a two-dimensional phase diagram.

Driven interfaces in crystal growth *do not* correspond to equilibrium or close-to-equilibrium states. Instead, for a solid growing into a supercooled liquid melt, one can supercool the liquid to a range of different temperatures below the melting temperature, for a given pressure. If one insists on identifying these states within an *equilibrium* phase diagram, the far-from-equilibrium states correspond to the limits to which one can, say, supercool a liquid or superheat a solid. In this sense, the critical state is reached without tuning, since it involves a nonzero fraction of the equilibrium phase diagram. However, this point of view concerning self-organized criticality implies strong bounds on the nature of the nonequilibrium state, since, in the example above, the liquid is only metastable. The eventual decay of this state by droplet nucleation implies limits on interface models which we shall discuss below, where we present a derivation of the driven interface equation from the Langevin equation for full space. We should also note that there are potentially important differences between self-organized critical systems and driven interfaces; for example, while the spectrum of noise is found to be irrelevant to the former, it is of crucial importance to the latter.

Computer simulations of lattice-based models, such as deposition models,[21] Eden models,[20] solid-on-solid (SOS) models,[22] and directed polymer models,[23] agree with the results for the KPZ equation in two dimensions, suggesting that all these models belong to the same universality class. In three dimensions, however, the lattice models do not give consistent results.[29–32]

In this paper we report contributions to the issues discussed above.[33–35] First, we investigate the relationship between self-organized criticality and driven growth. Second, we numerically determine the roughening exponents at the critical dimension, $d_c = 3$. Third, we study the nature of the roughening transition in the driven system.

In Sec. II we introduce and discuss the origin of the KPZ equation. We derive that equation from the Langevin equation for a system with a nonconserved scalar order parameter, when an external field is present and when an asymmetric coupling to a conserved variable exists. The relationship of the phenomena to self-organized critical phenomena is discussed. The eventual decay of this state by droplet nucleation implies limits on the long-time and long-length-scale applicability of the KPZ equation to this class of problems, which we examine.

In Sec. III, we present the results of a numerical integration of the KPZ equation at $d_c = 3$; we also performed a study of crossover phenomena in this model, where the system crosses over from the zero-driving-force case to a finite-driving-force situation.[35] We report numerical studies of models which we expect to be in the same dynamical universality class in the rough phase. In particular, the growth and crossover exponents were numerically determined for the KPZ equation and via Monte Carlo simulation on the solid-on-solid model with asymmetric rates of evaporation and condensation, which we expect to be in the same universality class. Our results for both models 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.[34,36]

Section IV studies the possibility of a kinetic roughening transition. This was investigated through the study of variants of two important models used to study it in the past: the discrete Gaussian model and the SOS model.[2,3,5,7,10,12,37,38] 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.[39] Furthermore, we present results from a simulation of the nonequilibrium SOS model in which we compute the surface step energy[40] as a function of temperature at a given driving force, for different system sizes. For the equilibrium roughening transition, the step energy has been shown to be a useful indication of the transition.[40,10,11] In our study, a strong jump in the value of the step energy at a nonzero temperature T_R is observed. The value of T_R agrees with that of a finite-size scaling analysis of the bond-energy fluctuations of the model. We also give arguments in parallel to the original Burton-Cabrera-Frank work to discuss the nature of the transition. We conclude in Sec. V.

II. ORIGIN OF THE KARDAR-PARISI-ZHANG EQUATION

A. Introduction to the equation of motion and summary of exact results

The KPZ equation was first introduced to model the dynamical behavior of the lateral growth of an interface.[17] It is a nonlinear stochastic differential equation for the time evolution of the interface height variable $h(\mathbf{x},t)$,

$$\frac{\partial h}{\partial t} = \nu \frac{\partial^2 h}{\partial \mathbf{x}^2} + \frac{\lambda}{2}\left(\frac{\partial h}{\partial \mathbf{x}}\right)^2 + \eta, \tag{2}$$

where ν and λ are constants, and η is a random noise $\langle\eta\rangle = 0$, which is assumed to satisfy Gaussian statistics with

$$\langle \eta(\mathbf{x},t)\eta(\mathbf{x}',t')\rangle = 2D\delta^{d-1}(\mathbf{x}-\mathbf{x}')\delta(t-t'), \quad (3)$$

where D is a constant. The vector $\mathbf{x}$ determines positions in a $(d-1)$-dimensional plane of a full space $\mathbf{r}=(\mathbf{x},y)$. Since it has been assumed that h is a single-valued function of $\mathbf{x}$, overhangs and bubbles are not considered. We will argue below that bubbles are relevant, for very late times, for some important experimental representations of the KPZ equation. The nonlinear term cannot be obtained from a simple Hamiltonian and has a kinetic origin;[17] a derivation will be presented below. This term breaks the symmetry of positive and negative h and provides a driving force, which causes the interface to grow in time. Without the stochastic term, it can be transformed into the well-known Burger's equation, a simplified version of the Navier-Stokes equation, where h becomes the velocity potential.[41] With $\lambda = 0$, the equation describes the dynamics of interface roughening near equilibrium, where many investigations have been performed.[37,38,42-44]

The dynamics of the growing interface can be studied by monitoring the interface width $W(L,t)$ as a function of time and edge length of the system. A convenient definition is $W(L,t) \equiv \langle (h-\langle h\rangle)^2\rangle^{1/2}$, where W exhibits the scaling form[18] of Eq. (1), $W(L,t) \sim L^{\chi} f(tL^{-z})$. It is useful to write this in the equivalent way

$$W(L,t) \sim t^{\beta} g(tL^{-z}) \ , \quad (4)$$

where the exponent $\beta = \chi/z$ describes growth. Although no exact solution exists for Eq. (2), a renormalization-group analysis can be performed in the same manner as that for Burger's equation by Forster, Nelson, and Stephen.[45] The exact results derived by them apply to the KPZ equation in two dimensions,[17] $\chi = \frac{1}{2}$ and $z = \frac{3}{2}$ are obtained as a consequence of a fluctuation-dissipation theorem. As mentioned above, these values are consistent with many lattice-based growth models, and differ from those of dynamical roughening where $\lambda = 0$: $\chi_0 = (3-d)/2$ and $z_0 = 2$.

In three dimensions, the renormalization-group analysis fails to find a stable fixed point.[17] Hence no results for the strong-coupling regime are known. Furthermore, the values obtained for the exponents from the various discrete models disagree, as do conjectures for the exponents as a function of dimension. Therefore, since the KPZ equation provides a framework to describe a class of interface-dynamics problems, we felt it worthwhile to numerically estimate scaling exponents for the KPZ equation in $d = 3$.

It should be emphasized that one does not necessarily expect a failure of perturbation theory. Instead, although the ϵ expansion down from $d_c = 3$ is infrared unstable, it is ultraviolet stable. In which case, three dimensions is properly interpreted as the lower-critical dimension for an infrared unstable fixed point.[17] In that case, for $d = 3+\epsilon$ in the continuum equation, we expect a transition from a smooth interface controlled by the trivial roughening fixed point for small values of the driving force, to a driven roughening fixed point at a large particular value of that force. This would not, however, be a roughening transition in the usual sense since there would be no stiffness in the low-driving force regime (although lattice effects would presumably be a relevant perturbation).

B. Derivation of the equation of motion, relationship to self-organized critical phenomena, and relevance of bubbles

To derive the KPZ interface equation of motion, we require an equation for the full space, where the interfaces correspond to regions of rapid variation of an order-parameter field. (Some of our remarks in this section are implicit in the original work of Kardar *et al.*[17]) A dynamical equation can be prescribed at low temperatures in an ordered state by assuming that the time dependence of a slowly varying nonconserved order parameter is due to the minimization of the local free energy. All other degrees of freedom are modeled by a random noise whose intensity is determined in part by the temperature. That equation is

$$\frac{\partial \psi(\mathbf{r},t)}{\partial t} = -\Gamma\left(H + \frac{\delta F[\psi(\mathbf{r},t)]}{\delta \psi}\right) + \mu, \quad (5)$$

where $F[\psi]$ is the free energy functional, Γ is the mobility, and H is the external field. The transport coefficient is related to the intensity of the random noise μ by a fluctuation-dissipation relation

$$\langle \mu(\mathbf{r},t)\mu(\mathbf{r}',t')\rangle = 2\Gamma T\delta(\mathbf{r}-\mathbf{r}')\delta(t-t'), \quad (6)$$

where Boltzmann's constant has been set to unity. The free-energy functional F is the sum of all the exchange interactions plus the sum of the local free energies f at all sites $\mathbf{r}$,

$$F[\psi] = \int d\mathbf{r}\left(\frac{c}{2}(\nabla\psi)^2 + f(\psi)\right), \quad (7)$$

where $f = -m\psi^2 + u\psi^4$, and c, m, and u are positive constants. The Langevin equation (5) is well known from critical dynamics,[46-48] where it corresponds to the universality class of model A, the nonconserved Ising model. It is straightforward to derive Eq. (5) from the microscopic spin-flip kinetic Ising model.[48]

One can also recover the Langevin equation above from a modification of model C of critical dynamics,[46,49-52] where a nonconserved order parameter ψ is coupled to a conserved field, called e. The field e must be coupled asymmetrically to ψ (so that e's equilibrium value differs in the two phases, say $\psi = \pm 1$) and, for our purposes, the length scale for diffusion of e, L_T, must be larger than all other lengths in the system. With an asymmetric coupling, this provides a model for the liquid-solid interface, which can be used to study the Mullins-Sekerka instability and dendritic growth. By requiring $L_T \gg L$, we consider length scales much smaller than those of that

instability, implying that our analysis is only valid near the tip of a large growing dendrite, where curvature is small.

In equilibrium, the order parameter ψ will equal its time-independent value ψ_0. If equilibrium is characterized by coexisting phases separated by a flat diffuse interface located around $y = 0$, which requires $H = 0$, then

$$-c\frac{d^2\psi_0(y)}{dy^2} + \frac{\partial f}{\partial \psi_0} = 0. \tag{8}$$

The mean-field surface tension is given by

$$\sigma = c\int dy \left(\frac{d\psi_0}{dy}\right)^2. \tag{9}$$

Far from equilibrium, the interface may be convoluted and time dependent. Instead of being located at $y = 0$, it is useful to write it as the zeros of an auxiliary function

$$u = 0. \tag{10}$$

See Fig. 2. To determine the equation of motion for u, we impose the solvability condition

$$\psi(\mathbf{r}, t, H) \simeq \psi_0(u(\mathbf{r}, t, H)). \tag{11}$$

This is reasonable for a gently curved surface. Note that writing the interface as $u = 0$ implies that bubbles are not considered (although overhangs have not yet been excluded), since the interface does not interact with other surfaces. In the presence of a field, there can be many nucleated droplets, whose interfaces would eventually interact as the droplets grow to macroscopic size. Thus our analysis is restricted to the time regime when the interfaces can be considered independent. The implications of this will be discussed below.

Using Eq. (11), the Langevin equation transforms into

$$\frac{\partial u}{\partial t}\frac{\partial \psi_0(u)}{\partial u} = -\Gamma\left(H - c\nabla^2\psi_0(u) + \frac{\partial f}{\partial \psi_0}\right) + \mu. \tag{12}$$

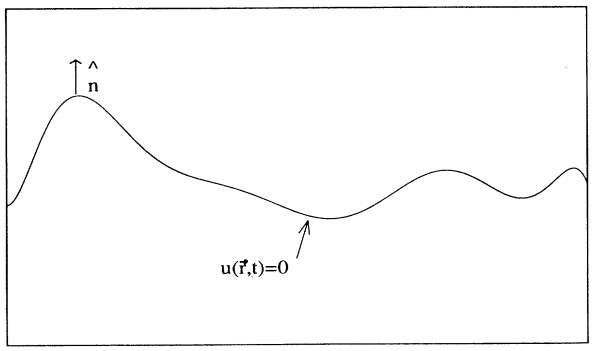

FIG. 2. Interface coordinate system. The interface position is $u(\mathbf{r}, t) = 0$; normal is $\hat{\mathbf{n}}$.

But from Eq. (8), one can eliminate $\partial f/\partial\psi_0$ in terms of second derivatives of ψ_0,

$$\frac{\partial u}{\partial t}\frac{d\psi_0(u)}{du} = -\Gamma\left(H - c\nabla^2\psi_0(u) + c\frac{d^2\psi_0(u)}{(\ell du)^2}\right) + \mu, \tag{13}$$

where $\ell = |\nabla u|^{-1}$ is the differential length in the u direction. Decomposing the Laplacian on the right-hand side of the equation gives

$$\frac{\partial u}{\partial t}\frac{d\psi_0(u)}{du} = -\Gamma\left(H + cK\frac{d\psi_0(u)}{\ell du}\right) + \mu, \tag{14}$$

where $K = -\nabla\cdot\hat{\mathbf{n}}$ is the differential curvature, and $\hat{\mathbf{n}} = \ell\nabla u$ is the normal unit vector to the interface. Let us now project the equation onto the interface with the operator

$$\mathcal{P}(\cdots) = \frac{1}{\Delta\psi_0}\int \ell du \frac{d\psi_0}{\ell du}(\cdots), \tag{15}$$

where $\Delta\psi_0$ is the miscibility gap. We obtain

$$-\ell\frac{\partial u}{\partial t} = \frac{\Gamma c H \Delta\psi_0}{\sigma} + \Gamma c K + \eta, \tag{16}$$

where $\eta = -(c/\sigma)\int \ell du\, d\psi_0/(\ell du)\mu$ is the noise at the interface. Finally, since the velocity normal to the interface at $u = 0$ is given by $v = -\ell\partial u/\partial t$, from continuity of flux at $u = 0$, we obtain

$$v = \lambda + \nu K + \eta, \tag{17}$$

where

$$\lambda = \nu\frac{H\Delta\psi_0}{\sigma}, \tag{18}$$

$$\nu = \Gamma c, \tag{19}$$

the noise satisfies

$$\langle\eta(\mathbf{s}, t)\eta(\mathbf{s}', t')\rangle = 2D\delta^{d-1}(\mathbf{s} - \mathbf{s}')\delta(t - t'), \tag{20}$$

where $\mathbf{s}$ is a vector determining positions on the $u = 0$ surface, and

$$D = \nu\frac{T}{\sigma}. \tag{21}$$

This equation can be written in terms of a free energy:

$$v = -\frac{\nu}{\sigma}\frac{\delta F_s}{\ell\delta u} + \eta, \tag{22}$$

where

$$F_s = \int d\mathbf{r}\left(-H\psi_0(u) + \sigma\frac{\delta(u)}{\ell}\right). \tag{23}$$

The first term is essentially a step function on the interface, and gives the volume energy, while the second is a δ function on the interface, giving the surface energy. Equations of this kind are well known in other contexts.[52–56] For example, the equation of motion for the case where the field H is a random quenched variable was derived several years ago.[57,58]

The form of Eq. (17) can also be obtained from a simple phenomenological argument.[59] A similar approach has been given by Krug and Spohn.[60] In the presence of a field, a flat interface will translate at a constant velocity $v = \lambda$, since velocity is proportional to thermodynamic force. If the interface is curved, the velocity should be a function of the natural thermodynamic variables of the system. An interface is best described, if it is very thin, by asking how curved it is, i.e., what is its local curvature K. Thus we have $v = v(K)$, in the most simple case. Now, if in addition the interface is only gently curved, so that K is small, to leading order in a Taylor-series expansion, one obtains $v = \lambda + \nu K$ as above, and ν must be positive if the motion is so as to reduce curvature.

To recover the KPZ equation, we consider an interface which is almost flat, without overhangs, i.e., $u(\mathbf{r},t) = y - h(\mathbf{x},t) = 0$. One then obtains

$$\frac{\partial h}{\partial t} = \frac{1}{\ell}\left(\lambda + \nu\ell^3 \frac{\partial^2 h}{\partial \mathbf{x}^2} + \eta\right), \tag{24}$$

where $1/\ell(h) = [1 + (\partial h/\partial \mathbf{x})^2]^{1/2}$. Thus to leading order in $(\partial h/\partial \mathbf{x})^2$, letting $h \to h - \lambda t$ for convenience, one obtains the KPZ equation

$$\frac{\partial h}{\partial t} = \nu \frac{\partial^2 h}{\partial \mathbf{x}^2} + \frac{\lambda}{2}\left(\frac{\partial h}{\partial \mathbf{x}}\right)^2 + \eta, \tag{25}$$

where the noise satisfies Eq. (3) to this order.

This derivation implies that the KPZ equation can be used to describe a flat growing interface in the nonconserved Ising universality class in the presence of a field, or a solid growing into a supercooled liquid, subject to the restrictions mentioned above.[61] We should also note that there are many experimental representations of models A and C. (It may be that derivations can be given of the KPZ equation for other situations, without these restrictions.[60]) This clarifies the notion of self-organized critical phenomena for these systems: the far-from-equilibrium states described by the KPZ equation are regions in an equilibrium phase diagram corresponding to the limits to which one can, say, supercool a liquid or superheat a solid. In this sense, the critical state is reached without tuning, since it involves a nonzero fraction of the equilibrium phase diagram.

However, this scenario implies strong bounds on the nature of the nonequilibrium state, since, in the example above, the liquid is only metastable. The state eventually decays by droplet nucleation, which implies limits on driven interface models, since there is a time regime for which bubbles are relevant. Nucleation is a subtle problem in nonequilibrium theory, involving the nature of metastable states in the hydrodynamic limit. (By hydrodynamic limit, we mean the late-time, large-system-size analog of the thermodynamic limit for nonequilibrium systems). However, the nucleation rate is easy to obtain within the classical approach of Becker and Döring.[48,62] Nucleation occurs when droplets of a stable phase form by spontaneous thermal fluctuations from a metastable matrix. Small nucleated droplets disappear, thus the metastability, while large droplets grow. The rate-limiting process for the formation of the stable phase involves droplets that barely grow, called critical droplets. Classical nucleation theory has two main parts, a quasiequilibrium theory of the critical droplet, and a kinetic theory of its growth.

Assume the system is ordered with spins up, and an infinitesimal uniform external field is applied that favors spins down. The free energy of a domain of down spins is assumed to be

$$F_s(R) \approx -HR^d + \sigma R^{d-1}, \tag{26}$$

where R is the size of the domain and factors of 2 and π have been ignored for convenience. The first term corresponds to the volume energy of a droplet, while the second to its surface area, so that $F_s(R)$ is a simplified form of Eq. (23). The free energy has a maximum $R^* = [(d-1)/d]\sigma/H$. Domains with radii $R > (<)R^*$ grow (shrink), respectively, where R^* is the critical droplet radius. The rate of nucleation I is proportional to the probability of such a droplet appearing by a fluctuation, i.e., $I \propto \exp[-F_s(R^*)/T]$ or

$$I = \frac{L^d}{t^*} e^{-F_s(R^*)/T}, \tag{27}$$

where L^d is the volume of phase space accessible for such a fluctuation, and the time scale is given by

$$t^* \equiv \left(\frac{\partial \ln R^*}{\partial t}\right)^{-1}, \tag{28}$$

so that $1/t^*$ is the linearized growth rate of the critical droplet. The characteristic time scale for a droplet fluctuation is $\tau \sim I^{-1}$, or

$$\tau \propto \exp\left(\frac{\sigma}{H^{d-1}} + \ln L^d\right), \tag{29}$$

where some numerical factors have been ignored. Note that τ is only weakly dependent on system size and dimension of space for $d > 1$, e.g., $\tau_{d=2} \approx \exp(\ln \tau_{d=3})^{1/2}$.

Thus, for the systems mentioned above, the KPZ equation is useful on time scales $t \ll \tau$, since droplets (i.e., bubbles) are neglected by assuming that $h(\mathbf{x},\mathbf{t})$ is single-valued. It is known from the study of the kinetics of first-order transitions that droplet nucleation becomes appreciable at the cloud point in experimental systems,[47,48] when $\tau = O(1)$. For even larger field strengths, the system's state can become completely unstable; for example, in long-range-force systems (where the critical droplet is of the system size), this occurs at the spinodal curve $H = H_{sp}(T)$, which is a line of mean-field second-order transitions. It should be emphasized that the nature and formal definition of a metastable state in the hydrodynamic limit is as yet unresolved, except for the relatively uninteresting case of systems with long-range forces.

III. NUMERICAL STUDY OF DRIVEN INTERFACE DYNAMICS

Given the usefulness of the KPZ equation for the problems of experimental interest mentioned above, and the absence of results in the critical dimension $d_c = 3$, we have numerically integrated the KPZ equation of motion, as well as a simple model we expect to be in the same universality class. The KPZ equation was discretized[63] in three dimensions on a grid with substrate sites labeled (i,j),[64]

$$\frac{\partial h_{i,j}}{\partial t} = \nu(h_{i,j+1} + h_{i,j-1} + h_{i+1,j} + h_{i-1,j} - 4h_{i,j}) + \frac{\lambda}{2}[(h_{i,j+1} - h_{i,j-1})^2 + (h_{i+1,j} - h_{i-1,j})^2] + \eta_{i,j}, \tag{30}$$

where periodic boundary conditions were used, and a simple Euler scheme was applied to effect the time integration. We chose $2D/\Delta t = \nu = 1$, and varied the driving parameter λ, without loss of generality.

As an independent test of our results, we also undertook the Monte Carlo simulation of a model we expect to be in the same universality class as the KPZ equation: the solid-on-solid (SOS) model with asymmetric rates of evaporation and condensation. The SOS model has been extensively studied both theoretically and with the aid of computer simulations, and its equilibrium properties are well understood.[2] It belongs to a class of microscopic models devised to describe crystal surfaces in equilibrium. At sufficiently low temperatures, it is assumed that one can neglect the presence of crystal defects, such as vacancies, and particularly bubbles and overhangs. The surface of the crystal can then be represented by a set of discrete variables $h_{i,j}$ representing the height of the interface at a lattice position (i,j), with an appropriate energy assigned to different configurations. The Hamiltonian is defined as

$$\mathcal{H}[h_{i,j}] = \sum_{i,j}(|h_{i,j} - h_{i+1,j}| + |h_{i,j} - h_{i,j+1}|). \tag{31}$$

To study the nonequilibrium properties of a driven interface, we use $\mathcal{H}$ 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. Thus λ_a gives the asymmetry of rates of evaporation and condensation on the interface corresponding to λ in the KPZ equation, while the temperature T for Monte Carlo moves approximately corresponds to D/ν in the KPZ equation. This implies that $\lambda_a = 0$ represents the equilibrium case, while $\lambda_a > 0$ causes a constant velocity of the interface. We expect this asymmetry to allow terms even in $\partial h/\partial \mathbf{x}$ to appear in long-wavelength equations of motion, so that this model would be in the same universality class as the KPZ equation.

A. Results in two dimensions

To test our algorithms, we first studied[65] $d = 2$. On integrating the KPZ equation, we recovered the exact results of Kardar *et al.* for large values of the driving force. The equilibrium-roughening results were obtained when the driving force was zero. The equation was solved with systems of size $L = 4096$ and λ between 0 and 80, which we found was of sufficient size to avoid finite-size effects. A time mesh $\Delta t = 10^{-2}$ was used; smaller values gave essentially the same results. Results from over 100 independent integrations of the equation were averaged. The width of the interface W was monitored as a function of time t, where $W \sim t^{\beta}$. For $\lambda = 0$, we obtained $\beta = \frac{1}{4}$. For large values of λ, e.g., $\lambda > 40$, the driven growth result, $\beta = \frac{1}{3}$ was obtained. However, for values $0 < \lambda < 40$, effective exponents were observed, with values $\frac{1}{4} < \beta < \frac{1}{3}$, indicating the presence of crossover behavior.

To obtain the roughening exponent χ, the equation was integrated until a steady state was reached. We then estimated the steady-state exponent χ from $W \sim L^{\chi}$ as the system size was varied from $L = 32$ to 512. For all values of λ, $\chi = \frac{1}{2}$ was consistently found, in agreement with both the dynamic roughening and the driven growth results.

Monte Carlo simulations of the nonequilibrium SOS model were performed with the system temperature T set to a convenient value. The growth exponents were found to be independent of temperature. In $d = 2$, systems of size $L = 6000$ and times of up to 40 000 Monte Carlo steps were used to obtain the growth exponent β, and smaller system sizes were used to calculate the growth exponent χ. For any nonzero λ_a, we expected $\chi = \frac{1}{2}$ and $\beta = \frac{1}{3}$ in the hydrodynamic limit. Indeed, $\chi = \frac{1}{2}$ was obtained for all values of λ_a. For $\lambda_a = 1.0$, i.e., when there are only growth attempts, we found $\beta = \frac{1}{3}$, in agreement with the results for the two-dimensional KPZ equation. For smaller values of λ_a, crossover effects were again observed, while at $\lambda_a = 0$, we observed $\beta = \frac{1}{4}$ as expected.

B. Crossover scaling in two and three dimensions

As is clear from the above, to extract reliable asymptotic results a careful analysis of crossover effects is needed.[35] Since the presence or absence of the nonlinear driving force determines the dynamic universality class (driven or roughening), a natural analogy arises with critical phenomena. There, 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.[66] For the driven growth problem described above, a crossover regime is thus expected when the driving force is small, and either t or L is not asymptotically large. While the usual crossover phenomenon occurs 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.

Guided by experience in critical phenomena, it is natural to propose an ansatz to account for crossover. In two dimensions it is

$$W(L,t,\lambda) \sim t^{\beta_0} f_2(tL^{-z_0}, t\lambda^{\phi}), \tag{32}$$

where $\beta_0 = \frac{1}{4}$ and $z_0 = 2$ are the exponents for $\lambda = 0$, f_2 is the crossover scaling function, and the new exponent ϕ accounts for crossover to nonzero λ. Setting $\lambda = 0$, we recover the dynamical roughening results. When $t \ll L^{z_0}$ (or for $L = \infty$), the L dependence of f_2 can be dropped:

$$W \sim t^{\beta_0} f_2(t\lambda^{\phi}). \tag{33}$$

If $\lambda > 0$, the growth will eventually be controlled by the unknown strong-coupling fixed point which is characterized by the driven growth exponents β and z. Hence we must have $W \sim t^{\beta}$, so that $f_2(u) \sim u^{\beta-\beta_0}$ for large u. This gives

$$W \sim t^{\beta}\lambda^{\phi(\beta-\beta_0)} \approx t^{1/3}\lambda^{\phi/12}. \tag{34}$$

We expect Eqs. (33) and (34) to hold in the large L limit.

In $d = 3$, the above ansatz must be modified since dynamic roughening is marginal: $W^2 \sim A_0 \ln t$, where A_0 is a constant. Thus we propose the following crossover scaling ansatz:

$$W^2(L,t,\lambda) \approx A_0[f_3(t\lambda^{\phi}) - \phi \ln \lambda] \tag{35}$$

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. A logarithmic crossover has been suggested by Tang *et al.*[67] That argument was based on a fixed-dimension calculation to one-loop order of the KPZ equation,[17] which requires the effective nonlinear coupling constant $\bar{\lambda} \ll 1$. However, this is not the case for the numerical solutions of the KPZ equation performed to date, where typically $\bar{\lambda} > 1$. In that case, the fixed-dimension calculation does not give a controlled approximation. Indeed, if a logarithmic crossover form describes the large $\bar{\lambda}$ regime, the effective crossover exponent ϕ in the equation above should be exceedingly large, which we do not observe.

Although no perturbable strong-coupling fixed point has been found for the KPZ equation in $d \leq 3$, it is still worthwhile to show how to find ϕ by simple scaling arguments, if such a fixed point existed. First, we perform a scale transformation in space and time of the KPZ equation using the exponents for $\lambda = 0$: $\mathbf{x}' = e^{-l}\mathbf{x}$, $t' = e^{-z_0 l}t$, $h' = e^{-\chi_0 l}h$. Next, 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 $h'(\mathbf{x}',t',\lambda') = e^{-\chi_0 l}h(\mathbf{x},t,\lambda)$ implies

$$W(L,t,\lambda) \sim t^{\beta_0} F(Lt^{-1/z_0}, t\lambda^{z_0/(\chi_0+z_0-2)}) , \tag{36}$$

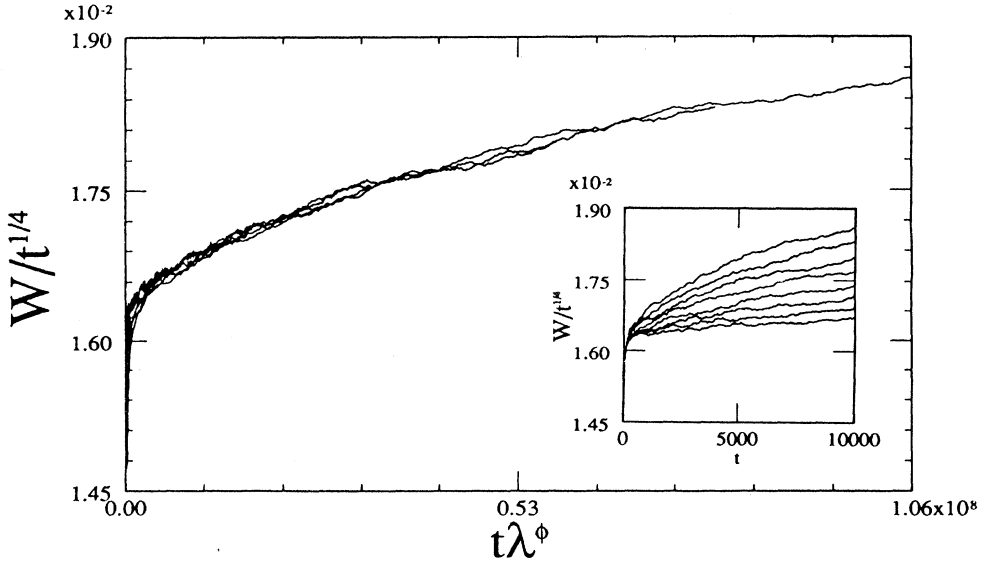

FIG. 3. Plot of the crossover scaling function $f_2 = W/t^{1/4}$ vs $t\lambda^{\phi}$ of the KPZ model in $d = 2$. Good data collapsing is achieved for $\phi = 3.0$. System size $L = 4096$. Data for $\lambda = 8$ to 22 in steps of 2 were used to get the scaling curve. The inset shows curves before data collapsing.

where a choice of l has been taken such that $e^l = t^{1/z_0}$. This implies that the crossover exponent $\phi = z_0/(\chi_0 + z_0 - 2)$. Thus, for $d = 2$, this gives $\phi = 4$. However, our numerical results of the KPZ equation below give $\phi \approx 3$. This discrepancy is related to the absence of a stable fixed point in the strong-coupling regime which is required for the scaling argument to work. 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.

To test the crossover scaling ansatz and obtain the exponent ϕ, the numerical results of Sec. III A were used. In $d = 2$, data for those values of λ which gave $\beta < \frac{1}{3}$ were analyzed. The inset to Fig. 3 shows $f_2 = W/t^{1/4}$ as a function of t for several values of λ. The curves, each representing an average of 100 independent runs, are well separated. If plotted as a function of $t\lambda^\phi$, as shown in Fig. 3, a good data collapse can be seen on using $\phi = 3.0$. This implies that our scaling ansatz is reasonable, with the curve of Fig. 3 corresponding to the crossover scaling function f_2.

An independent check on the value of ϕ was performed by taking large values of λ, so that $\beta = \frac{1}{3}$. We then monitored W versus λ for a fixed time. Our ansatz then predicts, as in Eq. (34), a power-law dependence, $W \sim \lambda^{\phi/12}$. Indeed, we found that $\ln W$ vs $\ln \lambda$ was well fitted by a straight line, as shown in Fig. 4, with a slope 0.23 ± 0.02, which is again consistent with $\phi \approx 3$. Combining the two independent calculations of ϕ, our best estimate for the crossover exponent is $\phi = 3.0 \pm 0.2$.

If the nonequilibrium SOS model shares a universality class with the KPZ model, we expect not only growth exponents, but also crossover behavior to be identical. Thus a crossover scaling analysis of our Monte Carlo data for small values of λ_a was performed. Keeping the system at a fixed temperature $T = 0.5$, we averaged results of 250 independent runs on systems of size $L = 2000$, each with 4000 Monte Carlo steps for different values of λ_a. Figure 5 shows the crossover scaling function defined in Eq. (33) for the SOS model after data collapsing. This analysis gave a crossover exponent $\phi \approx 3.0$, which indeed agrees with that of the two-dimensional KPZ model.

In three dimensions, we integrated the KPZ equation using parameters discussed in Sec. III C. Data with λ ranging from 120 to 240 by steps of 20 were used for the crossover analysis. For $\lambda < 120$, much longer runs were needed. Figure 6 plots $f_3 = w^2/A_0 + \phi \ln \lambda$ versus $t\lambda^\phi$, where A_0 is obtained from the fit $W^2 = A_0 \ln t$ when $\lambda = 0$. As shown in the plot, with $\phi = 4.5$ excellent data collapsing is achieved. The behavior of f_3 at large values for $t\lambda^\phi$ was consistent with our results for β in three dimensions in Sec. III C. Nevertheless, we caution that systematic errors could be present in our estimation of exponents in $d = 3$, because it is a marginal dimension. We did not perform a crossover scaling analysis on the three-dimensional SOS model due to the complications caused by the presence of a roughening transition.

C. Roughening exponents for the driven interface in three dimensions

The integration of the KPZ equation is hampered by large fluctuations and crossover effects. Besides large numbers of independent runs for averages, one must study sufficiently large system sizes so that the growth of

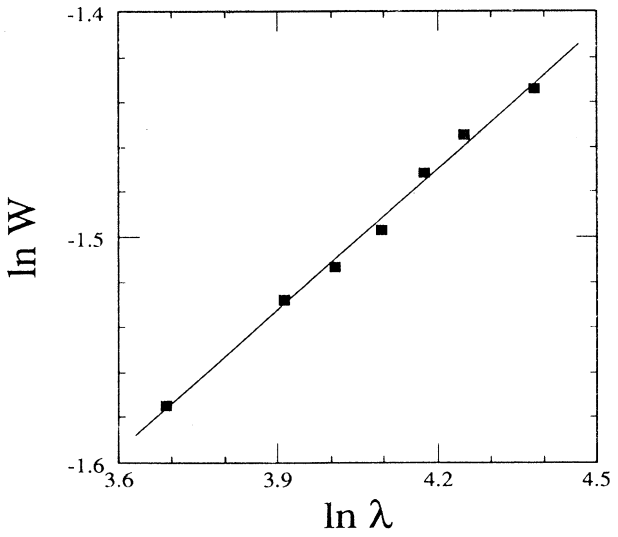

FIG. 4. Typical ln-ln plot of $W(t)$ vs λ at a given time t for the $d = 2$ KPZ model. The linear fit to data for all times gives a slope of 0.23 ± 0.02, consistent with $\phi \approx 3.0$.

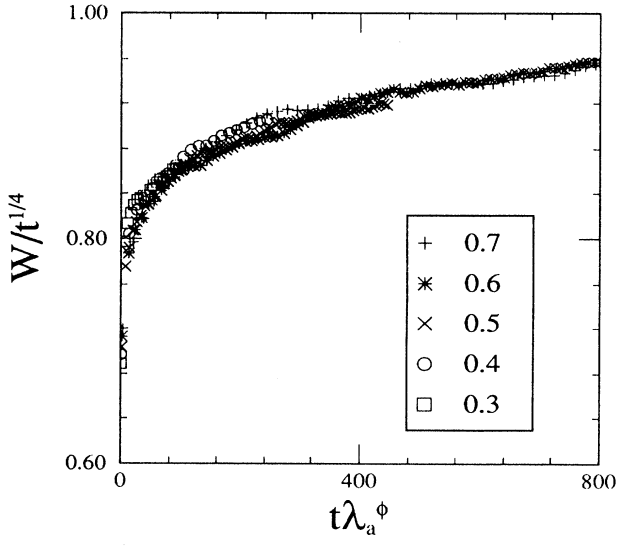

FIG. 5. Crossover scaling function for the $d = 2$ asymmetric SOS model. The system size $L = 2000$. Data from five different λ_a's were collapsed onto a single curve using $\phi \approx 3.0$.

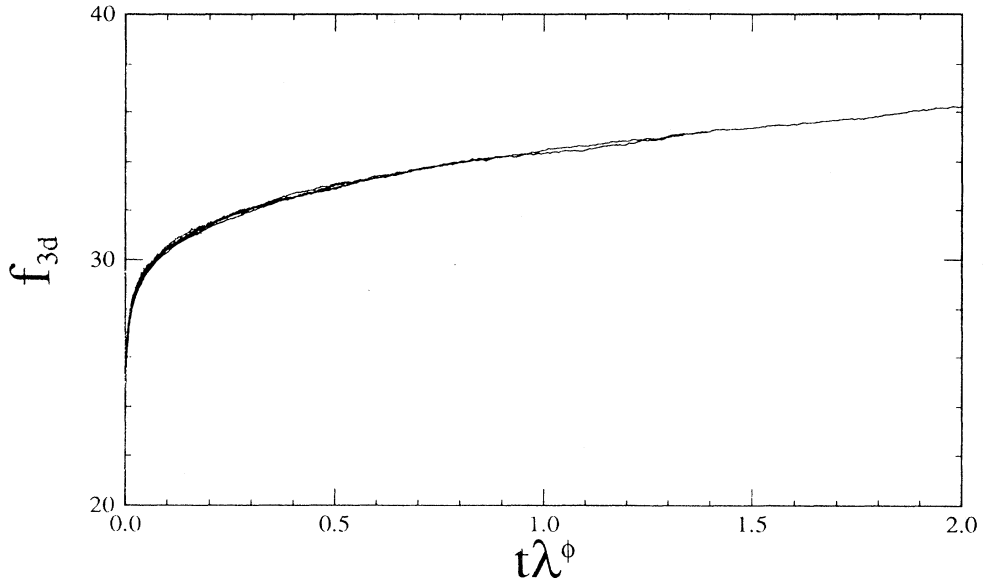

FIG. 6. Plot of the crossover scaling function $f_3 = W^2/A_0 + \phi \ln \lambda$ vs $t\lambda^{\phi}$ of the KPZ model in $d = 3$. Very good data collapsing is achieved with $\phi = 4.5$. The system size is 128^2. Data for $\lambda = 120$ to 240 in steps of 20 were used to get the scaling curve.

the width persists until the nonlinear term becomes important. Typically the following parameters were used: $\Delta t = 10^{-3}$, with 40 000 integration steps, and system sizes of 128^2 and 256^2. Test runs on 512^2 systems were also performed, which yielded the same value for β. Reducing the time mesh to $\Delta t = 2.5 \times 10^{-4}$ and integrating over 200 000 steps also gave the same results. As in the two-dimensional case, we varied λ to ensure that the system was in the driven growth regime. Figure 7 shows our results for W versus t with $\lambda = 240$, from averag-

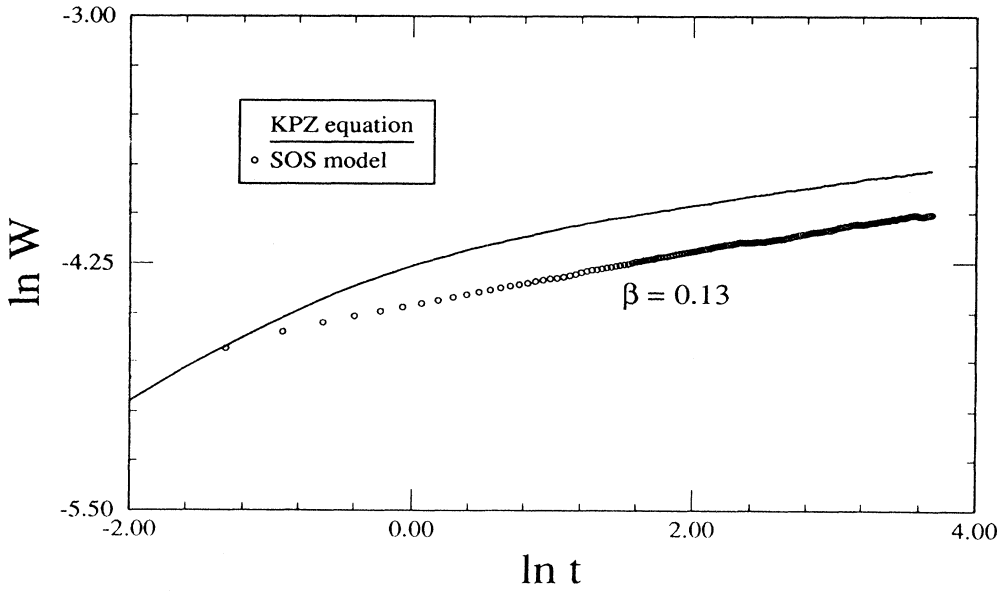

FIG. 7. ln-ln plot of interface width W vs time t in three dimensions. The edge length is $L = 128$ for the continuous KPZ model and $L = 100$ for the asymmetric SOS model. The slope gives a growth exponent $\beta = \chi/z \approx 0.13$. Data for the SOS model were shifted along both axes for convenience.

ing 50 independent runs. For late times, we estimate $\beta \approx 0.13 \pm 0.02$, in agreement with the value obtained by Chakrabarti and Toral.[34,36,68] Note that the effective exponent *drops* to that value from $\beta \sim 0.5$ for early times (due to the noise η). It is also worth mentioning that we have undertaken some selected analyses of larger systems, as well as larger values of coupling constants, and recover equivalent results. While for any nonzero λ we expect the dynamics in the asymptotic regime to be governed by the strong-coupling fixed point, for small values of λ crossover effects were important, as discussed above. Nevertheless, for $\lambda > 240$ we found the value quoted above. In units of other workers,[68] $\lambda = 240$ corresponds to $\epsilon = 14.5$.

The value for χ was more difficult to obtain because of large fluctuations, thus requiring a large amount of computing time. Nevertheless, data for $L \leq 30$ yielded $\chi = 0.24 \pm 0.04$. Noting that $z = \chi/\beta$, we thus verified numerically the hyperscaling relation[17] $\chi + z = 2$ in $d = 3$. Note that these exponents are distinctly different from those of dynamical roughening, $\beta_0 = 0$ and $\chi_0 = 0$, where W only diverges logarithmically.

As mentioned above, the interface dynamics represented by the KPZ equation is expected to account for that of a large universality class of lattice models, which we expect to include the asymmetric SOS model. In $d = 3$, Monte Carlo simulations of that model were done to extract the growth exponents β and χ. Systems of size 100^2 were used throughout, since they were found to be of sufficient size. In Fig. 7, the ln-ln plot of W versus t is shown along with that for the three-dimensional KPZ model. For $\lambda_a = 1$ and any reasonable T well above the roughening transition, we estimate $\beta \approx 0.13$ and $\chi \approx 0.25$, in agreement with the results obtained for the three-dimensional KPZ equation. As in the two-dimensional case, smaller λ_a showed strong crossover effects, as discussed above. Nevertheless, the good agreement between the various exponents obtained in $d = 2$ and $d = 3$ make us confident that the KPZ equation and the nonequilibrium SOS model are in the same dynamic universality class in *both* two and three dimensions.

Thus, in $d = 3$, our best estimates for the growth exponents for both the KPZ equation and the asymmetric SOS model are $\beta \approx 0.13$, and $\chi \approx 0.25$. These results are not consistent with conjectures in the literature.[24] 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 again caution that crossover effects could play an important and subtle 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 $d = 3$.

IV. ROUGHENING TRANSITION IN DRIVEN SYSTEMS

A. The discrete Kardar-Parisi-Zhang equation

To investigate the possibility of a kinetic roughening transition, we introduce a model, motivated by the discrete Gaussian model of Chui and Weeks,[7] which has

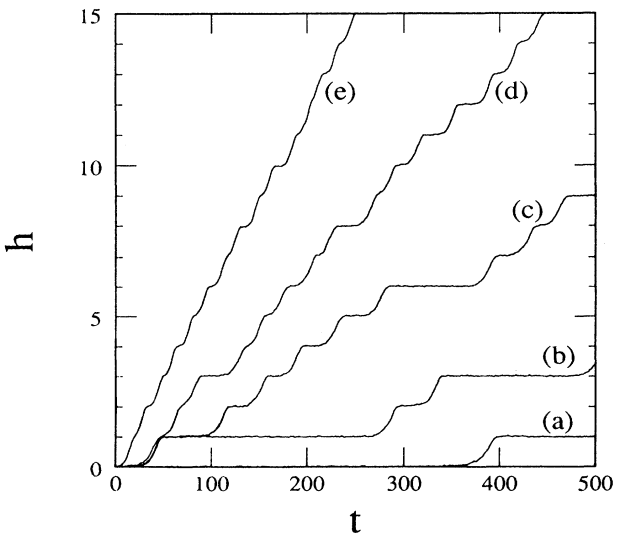

FIG. 8. Height of interface for representative runs in discrete KPZ model, as nonlinear driving force is increased [labeled (a)–(e)]. Note the change from layered to continuous growth.

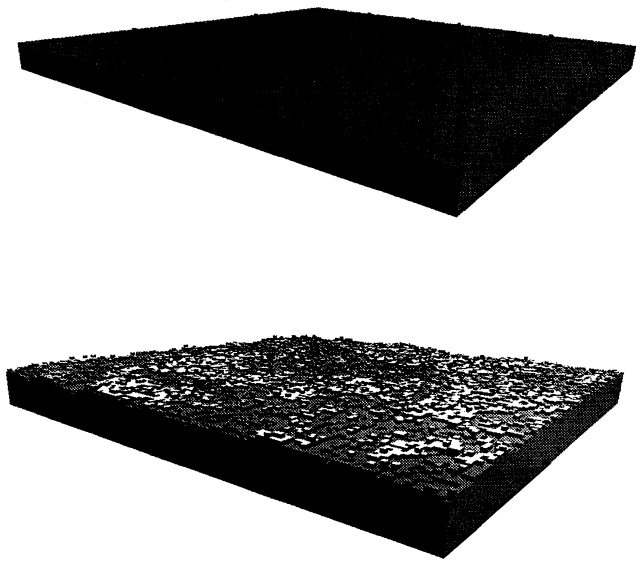

FIG. 9. Configurations for discrete KPZ equation showing (top) smooth phase with $\lambda = 0$ and (bottom) rough phase with $\lambda = 2$ at fixed temperature $T = 0.2$, and edge length $L = 128$.

been used to study the equilibrium roughening transition. It corresponds to Eq. (2) 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. Making h integer valued implies a nonzero energy gap at low temperatures, for small fluctuations on the interface, which is necessary for a roughening transition to take place. Thus translational invariance is not built into the model, and there can be a gap in the capillary-wave spectrum at low temperatures $T < T_R$. Above any roughening transition, the energy gap is irrelevant since the width diverges with system size. As a consequence, the asymptotic growth exponents in the rough phase of the discrete KPZ equation will be the same as those for the original model. The interest of the new model therefore lies in its low-temperature properties, where the discreteness of h could be relevant. It is worth noting that the transition here corresponds to a nonequilibrium phase transition such as has been studied for driven diffusive systems.[39]

We again performed numerical integrations of Eq. (2), now with integer-valued h and edge length $L = 128$, as λ varied, keeping D and ν constant; in essence fixing T. The plots of the average height of the interface for various λ versus time are shown in Fig. 8. Different curves are for varying driving forces λ with the temperature $T = D/\nu < T_R(\lambda = 0)$ fixed. For small values of λ, the growth is one layer at a time (curves a and b), suggesting that the system is in a faceted phase. Beyond a large particular value of λ, the growth becomes continuous (curve e) signaling that the rough phase is reached. Some configurations corresponding to these runs are shown in Fig. 9. We also verified that one could go from layer-by-layer growth to continuous growth by increasing temperature beyond a particular value, at fixed nonzero driving force. Unfortunately, the discrete KPZ model is numerically a difficult problem, so our observations are only qualitative. To undertake a quantitative study, we again considered the SOS model with asymmetric rates of evaporation and condensation.

B. Solid-on-solid model with asymmetric rates of evaporation and condensation

The SOS model has a roughening transition in equilibrium,[3,8,10] and its nonequilibrium properties have been previously studied by many authors, particularly Gilmer.[3] Analytic work, within linear response, has been done by Chui and Weeks,[7] Saito,[37] and Nozières and Gallet.[38] Here we wish to determine the conditions, if any, under which the interface can be grown layer by layer in the smooth faceted phase which exists below T_R. While signs of such a kinetic roughening transition have been observed in experiments,[15] there is little theoretical understanding of the phenomenon.

The properties of the equilibrium roughening transition, on the other hand, have been much more thoroughly investigated; many numerical studies of the SOS, Gaussian, and three-dimensional Ising models,[10,11,69] have been performed. A quantitative description of the roughening transition is difficult to obtain since the transition is of infinite order. One useful approach, due to Leamy and Gilmer,[40] is to determine the extra energy associated with the presence of a step on the interface, $E_{\rm step}$. This should vanish at the roughening temperature T_R in the thermodynamic limit. This idea, combined with finite-size scaling, can accurately determine T_R.[11,69]

Motivated by the success of that work for the equilibrium roughening transition, we have applied these ideas to the nonequilibrium asymmetric SOS model. We computed the step energy for a given driving force λ_a, at different temperatures for several system sizes. It exhibits a strong transition from a large value to a much smaller value at a given temperature. Another quantity that shows a strong transition is the bond-energy fluctuations, a quantity similar to the specific heat. We note here that the specific heat does not have any divergence in the *equilibrium* roughening transition, since that transition is of infinite order. However, in equilibrium the width of the interface diverges at T_R as $\ln L$ for $L \to \infty$, whereas in driven growth the width diverges as a power law in the steady state, $W \sim L^{\chi}$, as shown in Sec. IV A. Thus we expect the kinetic roughening transition to be stronger than its counterpart in equilibrium. Indeed, our finite-size-scaling analysis below finds that the bond-energy fluctuations show a diverging peak at $T_R > 0$. Moreover, the roughening transition temperature obtained from the step energy and the bond-energy fluctuation are in good agreement.

The step energy $E_{\rm step}$ can be defined as the energy difference between a surface with one step and the same surface without such a step,[10,40]

$$E_{\rm step} \equiv \frac{1}{L}[\langle \mathcal{H} \rangle (\text{one step}) - \langle \mathcal{H} \rangle (\text{no steps})] \ . \qquad (37)$$

In our simulations of the three-dimensional nonequilibrium SOS model, a step on the surface $\mathbf{x} = (x_1, x_2)$ can easily be created by maintaining a periodic boundary condition in, say, the x_1 direction, while applying a screw boundary condition in the x_2 direction (the growth is in the y direction). The height of the step can also be adjusted, although we chose it to be unity.

For $T < T_R$, one should obtain a nonzero value of $E_{\rm step}$ which increases with lattice size. On the other hand, for $T > T_R$, $E_{\rm step}$ should decrease and ultimately vanishes as $L \to \infty$. We have simulated systems of edge length $L = 10$ to 50 for various temperatures. The asymmetric growth rate λ_a was fixed at 0.4. The simulations were run with and without a step for 2×10^5 Monte Carlo steps. In Fig. 10, $E_{\rm step}$ for different temperatures as a function of L is shown. As anticipated, for different T, the curves bend upward or downward, showing a smooth phase at low temperatures and a rough phase at high temperatures. We find $T_R \approx 0.55$. Indeed, for all sizes a transition of $E_{\rm step}$ from a large value to a much smaller one is visible. Note also the sharpening of the transition as L increases, and the curves' common intersection point

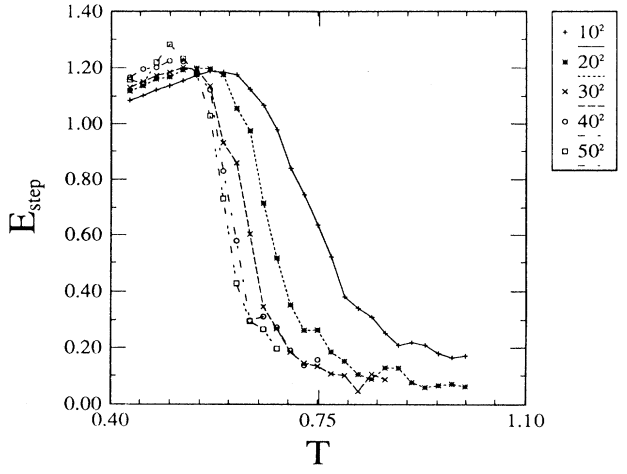

FIG. 10. Step energy E_{step} vs temperature for different system sizes $L = 10$ to 50 in the asymmetric SOS model, where $\lambda_a = 0.4$.

is at $T_R = 0.55$.

We also studied the bond-energy fluctuations defined as

$$C \equiv \frac{1}{L^2T^2}(\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2). \tag{38}$$

In equilibrium, this gives the specific heat. Figure 11 shows C as a function of the temperature for several driving forces λ_a. C is strongly peaked for nonzero λ_a at a finite T, and from inspection of configurations, 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. In contrast, there is no anomaly in the specific heat for roughening of an equilibrium interface,[3] although there is a small bump close to T_R.[10] Note that as λ_a increases, the peak position of C shifts to lower temperatures. This implies that 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 in Sec. IV A. This feature has also been observed experimentally.[15] The inset to Fig. 11 shows a fit to $T_R(\lambda) \sim T_R(0)/[1 + O(\lambda)]$, motivated by the equation of motion, where $T_R(0) = 1.24$ is the equilibrium roughening transition temperature for the SOS model.

An important issue is to determine if $T_R(\lambda, L)$ is nonzero as $L \to \infty$. 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,

$$C \sim L^{\alpha/\nu} F(|T - T_R| L^{1/\nu}) \tag{39}$$

and fit to find α and ν. These are not equilibrium exponents since C could depend on the dynamical universality class.[70] We also caution that such a procedure is not appropriate for the equilibrium case ($\lambda_a = 0$) since, as mentioned above, the equilibrium roughening transition is of infinite order. We believe that an ultimate validation of this ansatz can only come from further study of the nature of the nonequilibrium phase transition. In any case, from the data collapse shown in Fig. 12 for

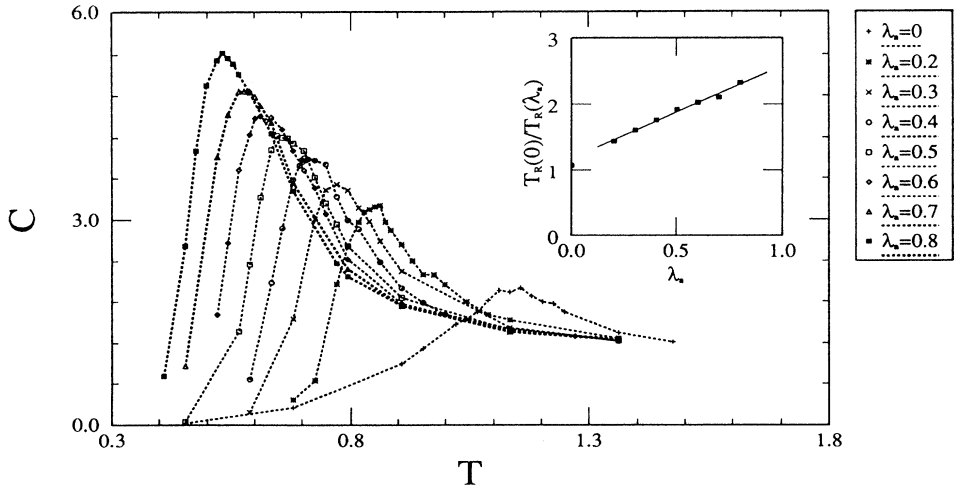

FIG. 11. Plot of fluctuations in local bond energy C for the asymmetric SOS model as a function of driving force $\lambda_a = 0$ to $\lambda_a = 0.8$, as indicated. The inset shows the position of the maximum for different driving forces (point at $\lambda_a = 0$ from Ref. 10). Normalizing $T_R(\lambda)$ with (Refs. 3 and 69) $T_R(0) = 1.24$ is only for convenience.

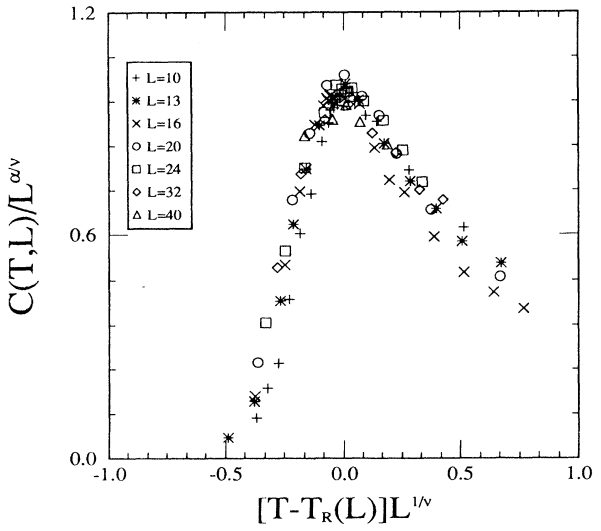

FIG. 12. Finite-size-scaling plot of fluctuations in local bond energy for the asymmetric SOS model $C/L^{\alpha/\nu}$ vs $|T - T_R|L^{1/\nu}$, with $\alpha/\nu = 0.5$, $\nu = 1.5$, $L = 10$ to 40, as indicated, and $\lambda_a = 0.4$. $T_R(L)$ is the peak position of the bond-energy fluctuations for system of size L.

$\lambda_a = 0.4$, our ansatz is self-consistent, and we estimate $\alpha/\nu \approx 0.5$, and $\nu \approx 1.5$. The transition temperature in the hydrodynamic limit is then estimated using

$$T_R(L) = T_R(L \to \infty) + O(1/L^{1/\nu}), \tag{40}$$

which gives $T_R(L \to \infty) \approx 0.54$. This value agrees very well with that from the step-energy data discussed above. Indeed, the consistency of the results for the step energy E_{step}, and the bond-energy fluctuations C, gives us confidence in interpreting our data in terms of a transition occurring at a nonzero temperature.

C. Discussion

To conclude this section, we give arguments to clarify the nature of the transition. Some of our remarks are implicit in the earlier work of Gilmer,[4] Weeks[3], and Saito.[37] We expect that, for a system of any large size, a kinetic roughening transition at nonzero temperature occurs, and that this nonzero temperature is intimately connected to the relevance of bubbles in the KPZ equation.

Layered growth in the smooth phase can occur, unless layers themselves are thermally unstable, or further ledges appear in an amount that contributes to the width of the interface in the hydrodynamic limit. At low T, one must determine the time scales for the speed at which a ledge grows, and for the appearance of a new nucleated ledge. For small fields (i.e., small driving forces) in systems of finite size, the time scale for growth is algebraic, while that for nucleation is exponentially small in the external field. Thus the ledge will sweep through the system before any appreciable nucleation event has the time to occur. Hence we expect that layer-by-layer growth is possible for a significant time regime in a finite-size system, at low T in a small field.

The question of the hydrodynamic limit, $t \to \infty$, $L \to \infty$ is more subtle. Consider Fig. 13, where we show an interface growing layer-by-layer in the smooth faceted phase (perhaps with screw boundary conditions as mentioned above). As we discussed in the Introduction, it can be useful to look down from the top of the facet. One then sees that the low-temperature one-block excitations of layered growth in three-dimensional driven growth are equivalent to the low-temperature fluctuations of *two-dimensional* driven growth, as described by the KPZ equation. Those fluctuations are not sufficient to destroy coexistence in the two-dimensional KPZ equation, since $W/L \to 0$ as $t, L \to \infty$. Therefore we do not expect them to destroy layer-by-layer growth at low tem-

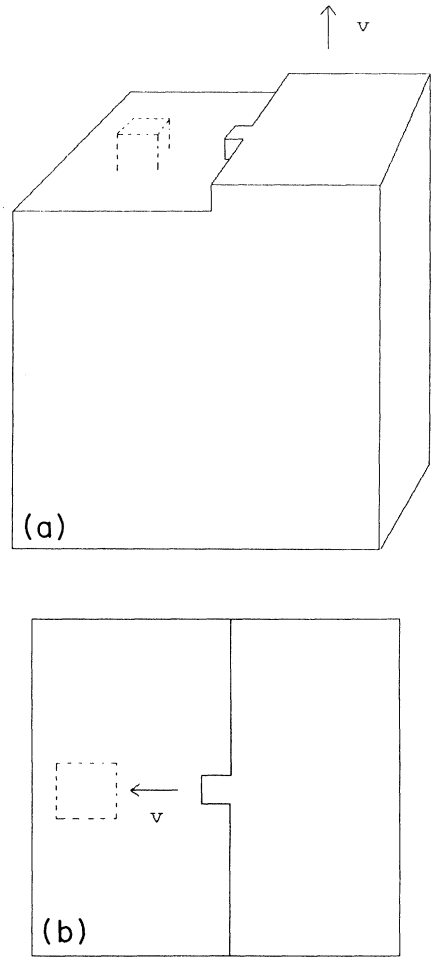

FIG. 13. (a) Side view of growing (100) facet with one ledge and thermal fluctuation (dotted lines show nucleated ledge, larger than critical size). (b) Top view.

peratures in the three-dimensional system.

Nevertheless, one must also consider the possibility of large nucleated ledges. Note that the rate of appearance of such ledges, which could destroy growth in the smooth phase, is essentially independent of dimension of space for $d > 2$. Thus the argument below applies to $d \geq 3$. In Fig. 13, the rate of appearance of new layers is independent of whether they appear on the top or bottom ledge. So consider only the bottom, as shown by the dotted lines. Then one sees that ledges on ledges correspond to the droplet fluctuations occurring on very long time scales τ, rendering the two-dimensional KPZ equation irrelevant, as discussed in Sec. II. [Note that the time scales for the two-dimensional droplet fluctuations are not well separated from the time scales for three-dimensional droplet fluctuations from Eq. (29).] Thus, we expect any definition of the hydrodynamic limit for the KPZ equation to also be consistent with a kinetic roughening transition at nonzero temperature, when a finite energy gap is introduced. To the best of our knowledge, it is unfortunately not known how to define a metastable state in the hydrodynamic limit. Finally, we note that the order of the transition is not clear. Although nucleation of ledges would be a signature of a first-order transition, if the hydrodynamic limit requires the presence of long-range forces to suppress dropletlike fluctuations, the transition could occur at the spinodal curve, a line of second-order phase transitions.

In any event, existing experiments,[15] as well as our simulation data, seem to suggest that the kinetic roughening transition occurs at a nonzero temperature for a given driving force, in the hydrodynamic limit. We expect that a consistent definition can therefore be found for that limit. It should also be noted that the existence of the hydrodynamic limit for the transition from smooth to rough, or rough to rough interfaces for $d > 3$ has been implicitly assumed in other studies[17,71] [our comments concerning nucleation on the $(d-1)$-dimensional substrate are essentially independent of dimension for $d > 2$].

V. CONCLUSIONS

We have studied the nature of interfaces during driven growth. The Kardar-Parisi-Zhang equation was derived from the Langevin equations for a system with a nonconserved scalar order parameter, for the cases where an external field is present, and where an asymmetric coupling to a conserved variable exists. The relationship of the phenomena to self-organized critical phenomena was discussed.

We then numerically integrated the nonlinear stochastic differential equation proposed by Kardar, Parisi and Zhang, and used Monte Carlo simulation to study a nonequilibrium solid-on-solid model. We established that these models share the same dynamic universality class, in both two and three dimensions, by analyzing crossover behavior and estimating asymptotic scaling exponents.

For the nonequilibrium SOS model, evidence of a kinetic roughening transition was found. In particular, our data can be naturally and self-consistently interpreted in terms of such a transition occurring at nonzero temperature. Moreover, this transition seems to be stronger than the equilibrium roughening which is of the Kosterlitz-Thouless type. In order to establish this, however, further study is required. Finally, the results of this paper, in particular the kinetic roughening transition in driven interfacial growth, are experimentally accessible by many methods. In our opinion, such a study would be of considerable interest.

Note added if proof. We have recently received papers by T. Hwa, M. Kardar, and M. Paczuski (unpublished) and by M. Paczuski (unpublished), which investigate theoretically the kinetic roughening transition, and are complementary to our numerical study.

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