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Dynamics of rough surfaces with an arbitrary topology

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A model for kinetic growth is presented that allows for overhangs and arbitrary topologies of the growing interface. Numerical studies of the model show that with a choice of the aggregation mechanism equivalent to the one leading to the Kardar-Parisi-Zhang (KPZ) equation [Phys. Rev. Lett. **56**, 889 (1986)], we indeed obtain the KPZ results. On changing the aggregation mechanism, different dynamics of the growth are observed.

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The study of the dynamics of growth processes has received considerable attention recently [1–5]. The simplest of these involve physics at a local scale with the growth occurring *without* any overhanging configurations. A simple continuum model that is believed to capture the physics of these processes is the Kardar-Parisi-Zhang (KPZ) equation [3]:

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

where the height $h(\mathbf{x},t)$ is a single-valued function of the spatial coordinate $\mathbf{x}$, ν is a surface-tension term that relaxes the interface, the λ term describes normal growth, and η is a Gaussian noise with zero mean and

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

The principal theme of this paper is to present a simple local model of growth that allows for overhangs and arbitrary topologies of the growing interface. Our equations consist of two parts—the deterministic term and the noise term. The deterministic part builds in the correct physics and conservation law and is responsible for the growth. The noise term causes roughening at the interface. The deposition occurs on the interface, and islands disconnected from the interface do not form.

Our model is

$$\frac{\partial f(\mathbf{r},t)}{\partial t}=\nabla^2\frac{\partial F}{\delta f(\mathbf{r},t)}+I \qquad (3a)$$

with

$$F=\int\left[-\frac{f^2}{2}+\frac{f^4}{4}+a(\nabla f)^2\right]dv\ . \qquad (3b)$$

In order to maintain stability, we restrict the value of a to be non-negative. The field $f(\mathbf{r},t)$ describes a system with two phases having one of two values $f=\pm1$ in equilibrium, analogous to an up-down spin system. In $d=1+1$, the vector $\mathbf{r}$ has components (x,z), whereas in $d=2+1$, it is described by (x,y,z)—the z direction is perpendicular to the initially flat interface. The interface at time t is located at $\mathbf{r}_i$ such that $f(\mathbf{r}_i,t)\equiv0$. Indeed, other criteria for identifying the position of the interface such as the maximum value of $|\nabla f|$ lead to the same result. The initial condition is assumed to be an equilibrium profile that satisfies the equation $\partial F/\partial f=0$ with the boundary conditions $\lim_{z\to\pm\infty} f=\pm 1$. These boundary conditions are maintained during the growth process. I is a term allowing for growth at the interface. We have studied two different growth mechanisms

$$I_1=|\nabla f|C_1+D_1\sqrt{|\nabla f|}\eta(r,t) , \quad (4a)$$

$$I_2=|\nabla f|^2[C_2+D_2\eta(r,t)] , \quad (4b)$$

where $\eta(r,t)$ is a noise term that is uncorrelated in space and time and is chosen from a Gaussian distribution of width 1 and mean value 0. The ∇f factor in both the growth and noise terms ensures that the growth and fluctuations occur at the interface—the interface corresponds to the maximum value of ∇f and away from the interface, $\nabla f=0$.

We will present numerical results of the model that suggest that with the I_1 growth term, the model is in the same universality class as the KPZ equation. On the other hand, with the I_2 growth mechanism, the model exhibits different dynamical scaling behavior.

The first two terms of Eq. (3a) arise simply from the Langevin equation for the dynamics of model B, the Ising model with conserved magnetization [6]. The choice of the signs of the coefficients of f^2 and f^4 corresponds to a temperature less than the critical temperature allowing for the coexistence of two equilibrium phases. These first two terms incorporate surface diffusion, inhibit the formation of islands, and allow for a well-defined interface even in the rough regime. The last term in Eq. (3a) allows for growth and noise. The positive coefficients C_1, D_1, C_2, and D_2 allow for the growth and fluctuations at the interface. We have restricted the growth and noise terms to be operative in the region where $|f|<b$, where in the majority of the runs we used $b=0.9$. The particular choice of b is not important as long as b is close to but below 1 (the equilibrium value of f). Otherwise the positive contribution from the growth term, especially for long runs, produces an unrestricted increase of f above the equilibrium value. The I_1 growth mechanism gives effectively a constant growth rate per unit length of the interface ($f\equiv 0$) equal to $C_1\int_{s_{\min}}^{s_{\max}}|\nabla f|ds=2bC_1$, where the integral is performed normal to the interface, independent of the shape of the ∇f contours and $s_{\min}$ and $s_{\max}$ are defined by $f(s_{\min})\equiv -b$ and $f(s_{\max})\equiv b$, respectively. (Note that $|\nabla f|=|df/ds|=df/ds$, since f is a monotonically increasing function from $s_{\min}$ to $s_{\max}$.) This feature would be expected to, and as we shall see, does lead to a KPZ-like behavior. The I_1 growth mechanism may be visualized to a continuum version of the Eden growth model (in which growth occurs randomly at the interface and the behavior is known to be in the KPZ universality class [3]) with a redistribution of the deposited particles via surface diffusion. The I_2 growth mechanism does not have these properties and, as we will show, the effective growth rate is a function of the curvature at the interface and is overall nonuniform.

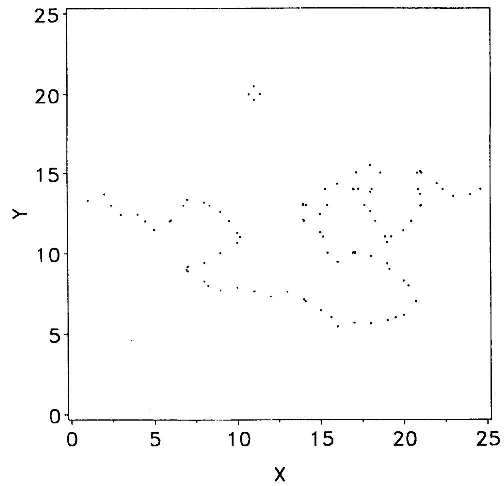

FIG. 1. Snapshot of interface, $f=0$, for dynamics with nonconserved order parameter in $d=1+1$.

The necessity for conserved dynamics may be argued by revisiting a model first introduced by Kim and Kosterlitz (KK) [4] to obtain the KPZ [3] exponents numerically. The KK model is a growth model of the restricted solid-on-solid type where particles are *added* one at a time on lattice sites with a *constraint* that neighboring columns do *not* differ in height by more than 1 unit. KK found that at long times the roughness width W scales [2] with the lateral size L as $W\sim L^{\alpha}$ whereas at early times t, $W\sim t^{\beta}$.

In $1+1$ dimensions, due to the restriction, any configuration of the growing interface may be considered to be made up of three kinds of basic segments (the interface is assumed, here, to go from the left to the right): a flat segment (denoted by 0), a downward step L (-1), and an upward step Γ $(+1)$. The growth dynamics of KK is such that the numerical sum of the segments is a locally *conserved* quantity.

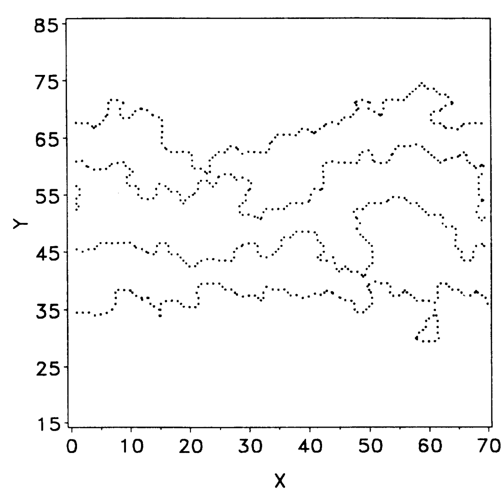

FIG. 2. Sequence of interfaces generated from Eq. (2) every 15 time units with I_2 growth mechanism and $a=\frac{1}{4}$ in $d=1+1$. The location of the interface was determined by solving for $f\equiv 0$. The third contour from the bottom has a hole at the boundary, where periodic boundary conditions are applied.

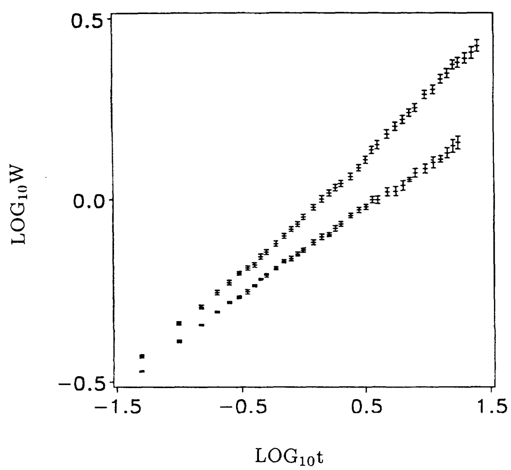

FIG. 3. Interface width as a function of time for $a=1$, I_1 growth mechanism. Upper data correspond to $d=1+1$, and the lower to $d=2+1$. Data are for lateral size 100 in $d=1$ and 40×40 in $d=2+1$.

A standard model with no conservation law (model A) [6] has been used by Grossman, Guo, and Grant [5] as a starting point for the derivation of the KPZ equation. In this case, the system is governed by the equation

$$\frac{\partial f(\mathbf{r},t)}{\partial t}=-\Gamma\frac{\partial F}{\partial f}+\eta(\mathbf{r},t)$$

with

$$F=-Af^2+Bf^4+C(\nabla f)^2-h_1 f\ ,$$

where η is an uncorrelated Gaussian noise and h_1 is a magnetic field responsible for the growth. We have found, by numerically solving the above equation, that when the interface is significantly rough, it is not well defined with islands of the growing component within a sea of the other component (Fig. 1). These undesirable features may be suppressed by decreasing the noise amplitude and the magnitude of the growth term h, but then the interface is virtually flat and the roughness is essentially zero.

The results of our numerical studies of the model are summarized in Figs. 2–4. Figure 2 shows typical interfacial profiles of the model with the I_2 growth mechanism with $a=\frac{1}{4}$. The interface is well defined and the topology of the contour is richer than that obtained in a numerical integration of the KPZ equation. Overhangs are present—they occasionally merge leaving holes behind. Such holes are filled up due to the growth mechanism and do not play any role in further growth. Similar topological properties can be observed using the I_1 growth term. In all cases where overhangs were present, the highest value of the interface was chosen in order to calculate the measure of roughness. In practice, we began all calculations with an equilibrated f profile (in the absence of the growth and noise terms) by imposing antiperiodic boundary conditions in the growth direction z. This resulted in the edges of the system, in the z direction, having the values $f=+1$ and -1 with a flat interface located in the middle of the system. Periodic boundary conditions were imposed in the transverse directions. Typical values of D_1 (the noise term) and C_1 (the growth term) and D_2 and C_2 were of order 1. Smaller values of these parameters lead to essentially flat interfaces while much larger values produce an instability in the numerical integration of Eq. (2). Our calculations were carried out with an integration time step of 0.01 units—statistically similar results were obtained with a time step reduced by a factor of 2. A square grid with lattice constant 1 was used. An interpolation scheme to locate the zeros of f, however, leads to a resolution an order of magnitude finer than the lattice constant. Figure 3 shows a calculation of the dynamical exponent in $d=1+1$ and $2+1$ for the I_1 growth mechanism for $a=1$. The best fits yield values of the dynamical exponent β of 0.34 ± 0.02 and 0.24 ± 0.03 in $d=1+1$ and $2+1$, respectively (the KK estimates [4] for β are 0.332 ± 0.005 and 0.248 ± 0.005) [7]. The estimate for the exponent α in $d=1+1$ is 0.51 ± 0.03, the value being

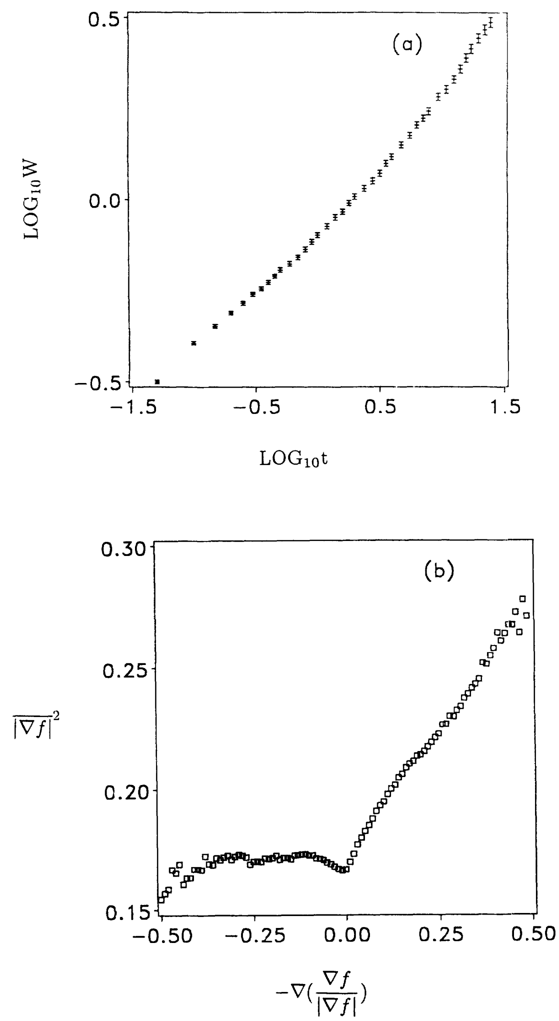

FIG. 4. (a) Log-log plot of width vs time for the I_2 growth mechanism with $a=1$ in $d=1+1$; the lateral size is 100. (b) Average value of $(\nabla f)^2$ vs curvature of interface ($-\nabla\cdot\nabla f/|\nabla f|$), data are averages for 30 samples, all other parameters are the same as in (a).

consistent with the expected value [3] of $\frac{1}{2}$. The data are averages over 100 systems in $d=1+1$ and 10 systems in $d=2+1$.

Figure 4(a) shows a $\log_{10}W$ vs $\log_{10}t$ plot for the I_2 growth mechanism (data are averages over 100 systems). We estimate that the scaling behavior of the roughness with lateral size is, within the statistical error, the same as for the I_1 growth mechanism. α is equal 0.53 ± 0.03. But the dynamical behavior is different. The exponent β is found to constantly increase from a value of 0.3 to 0.5. To understand the origin of this behavior we study the correlation between $(\nabla f)^2$ and the curvature of the interface

$$\left[-\nabla\cdot\left[\frac{\nabla f}{|\nabla f|}\right]\right]$$

(note that the ∇f vector is directed toward the $f=1$ region). Figure 4(b) shows a plot of the average value of $|\nabla f|^2$, over the region of $|f|<0.8$, versus curvature, showing that while for negative curvature the $\overline{|\nabla f|^2}$ is fairly constant, for positive curvatures it increases sharply with curvature. Since the growth rate per unit length of the interface of the I_2 mechanism is proportional to $\int_{s_{\min}}^{s_{\max}}|\nabla f|^2 ds$, one obtains nonuniform growth of the interface that is higher in regions of positive curvature. This is in contrast to the I_1 growth mechanism where the growth rate is *constant*.

In summary, the model described by Eq. (3a) provides a simple framework for describing the growth of interfaces having an arbitrary topology. Distinct universality classes of dynamical behavior may be obtained as special cases of the equations. A KPZ-type behavior is found when the I_1 growth term is used. On the other hand, when the other growth term is used, our numerical results suggest a new type of dynamical behavior.

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[7] It is interesting that the β exponent $(\frac{1}{4})$ in $d=2+1$ is equal to the spinodal decomposition growth exponent in the xy model. Note that in $d=2+1$, the high-temperature phase of the *Gaussian* solid-on-solid model is related to the low-temperature phase of a Coulomb gas (xy model) by duality.