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Dynamics of driven interfaces with a conservation law

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The dynamics of a growing interface with conservation of total volume under the interface is investigated using both dynamic renormalization-group and computer simulation. The conservation law leads to a new universality class from that discussed by Kardar, Parisi, and Zhang [Phys. Rev. Lett. **56**, 889 (1986)]. The growth exponents are calculated and compared with those from the simulation of a conserved restricted solid-on-solid model. Excellent agreement between theory and simulation is found.

Understanding the dynamics of a growing interface separating two phases is a challenging problem of both theoretical and practical interest.[1-12] Much work has been devoted to situations where the system is near equilibrium.[1] Far from equilibrium, however, these problems become exceedingly difficult due to the nonlinear collective interaction of many degrees of freedom. Examples include crystal growth into a supercooled melt,[2] layered growth by molecular-beam epitaxy or chemical vapor deposition,[3] development of ordered phases by spinodal decomposition,[4] propagation of flame fronts,[5] and cluster growth in diffusion-limited aggregation and Eden models.[6] Common to these problems is the existence of thin interfaces where active growth occurs. Although complicated patterns appear during the growth, there exist late-time regimes when a dominant large length develops and the growth shows scale invariance. As in critical phenomena, the "universality class" of the growth dynamics can be defined. Within a universality class, features such as growth exponents and shapes of scaling functions are independent of short-wavelength details. The concepts of scaling and universality classes greatly simplify the description of a dynamic system and much useful information can be obtained.

Recently, Kardar, Parisi, and Zhang[7] (KPZ) proposed an extremely interesting nonlinear differential equation which gives interfacial growth exponents consistent with numerical simulations of ballistic aggregation and Eden growth in the substrate dimension $d=1$ (the dimension of the system is $d+1$). The critical dimension d_c of the KPZ equation is two, above which the nonlinear coupling of the modes is irrelevant and one recovers the usual dynamical roughening results. At d_c, the KPZ equation does not have a stable fixed point, and growth information can only be inferred indirectly. However, KPZ argued that it is possible to have superuniversality, such that the growth exponents are independent of dimension. At $d=1$, a fluctuation-dissipation theorem holds which allows one to calculate the exponents $\chi=\frac{1}{2}$ and $z=\frac{3}{2}$ defined by the growth of the width of the interface: $W(L,t) \sim L^{\chi}f(tL^{-z})$, where L is the linear size of the growing substrate, t is time, and f is the scaling function (this scaling form was introduced by Family and Vicsek[9]). Furthermore, the KPZ equation satisfies a "Galilean" transformation which leads to a scaling relation $\chi+z=2$.

Many computer simulations in $d=1$ (Refs. 8-12) give results consistent with those obtained from the KPZ equation; notable are ballistic growth models,[9] Eden models,[10] and variants of solid-on-solid models.[8,11,12] While some simulations do not give the superuniversal exponents conjectured by KPZ, all agree with $\chi+z=2$.

It is thus natural to ask two questions: What features determine universality classes (beside possibly the spatial dimension) for interfacial growth? Are there growth models which do not obey $\chi+z=2$? In this Rapid Communication we propose a model which has $\chi+z\neq2$, and where χ and z differ from those of KPZ. Our model is simple enough that a renormalization-group analysis can be carried out. We have also performed extensive numerical simulations on a restricted solid-on-solid model in one substrate dimension, which generalizes a model introduced by Kim and Kosterlitz.[8] Excellent agreement between simulation and analytic results is obtained.

In critical dynamics,[13] it is known that universality classes in nonequilibrium are determined not only by the symmetry of the order parameter and the dimension of space, but also by the presence or absence of conservation laws, mode-coupling terms, and Poisson-bracket relations. We are thus motivated to generalize the nonconserved KPZ equation to the following conserved model:

$$\frac{\partial h}{\partial t}=-\nabla^2[\nu\nabla^2 h+\tfrac{1}{2}\lambda(\nabla h)^2]+\eta(\mathbf{x},t)\,, \tag{1}$$

$$\langle\eta(\mathbf{x},t)\rangle=0\,,$$

and

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

where $h(\mathbf{x},t)$ describes the height of the interface from some reference plane $h=0$, and is assumed to be a single-valued function of position $\mathbf{x}$. Angular brackets denote an ensemble average, where higher-order correlations of the noise η are determined by Gaussian statistics, and ν, λ, and D are constants. The conservation of total h is evident because the right-hand side of Eq. (1), including the noise, can be written as the divergence of a current. To motivate the conservation law, one can imagine atoms relocating on a damaged solid surface due to a driven flux so that the total number of atoms is conserved. Without the nonlinear term, Eq. (1) describes the dynamics of an interface involving surface diffusion with the diffusion constant proportional to ν. The nonlinear term is of kinetic origin and cannot be derived from any Hamiltonian, as was noted by KPZ. Dimensional analysis gives the upper critical dimension of this model, $d_c=2$.

We have applied a dynamic renormalization-group analysis[14] to Eq. (1), which is written in Fourier space as

$$h(\mathbf{k},\omega)=h_0(\mathbf{k},\omega)-\tfrac{1}{2}\lambda G_0(\mathbf{k},\omega)k^2\int_{\mathbf{q},\Omega}\mathbf{q}\cdot(\mathbf{k}-\mathbf{q})h(\mathbf{q},\Omega)h(\mathbf{k}-\mathbf{q},\omega-\Omega)\,, \tag{2}$$

where

$$h_0(\mathbf{k},\omega)=G_0(\mathbf{k},\omega)\eta(\mathbf{k},\omega)\,,$$

$$G_0(\mathbf{k},\omega)=(-i\omega+\nu k^4)^{-1}\,,$$

$$\langle\eta(\mathbf{k},\omega)\eta(\mathbf{q},\Omega)\rangle=2D(2\pi)^{d+1}k^2\delta^d(\mathbf{k}+\mathbf{q})\delta(\omega+\Omega)\,,$$

and $\int_{\mathbf{q},\Omega}\equiv\int d^dq\,d\Omega/(2\pi)^{d+1}$. We solved the equation iteratively in the vertex $-\frac{1}{2}\lambda k^2\mathbf{q}\cdot(\mathbf{k}-\mathbf{q})$. For convenience, Eq. (2) and the renormalizations of ν, D, and λ are schematically represented in Fig. 1. Following Forster, Nelson, and Stephen,[14] the intermediate values of ν, D, and λ were calculated by integrating out fast modes in the momentum shell $e^{-l}\Lambda\le|\mathbf{k}|\le\Lambda$. The remaining slow modes ($|\mathbf{k}|<\Lambda$) were restored to full momentum space by a rescaling of space and time: $\mathbf{k}'=e^l\mathbf{k}$, $\omega'=e^{zl}\omega$, $h'(\mathbf{k}',\omega')=e^{-zl-(d+\chi)l}h(\mathbf{k},\omega)$, and $\eta'(\mathbf{k}',\omega')=e^{-(d+\chi)l}\times\eta(\mathbf{k},\omega)$. The scaled variable h' satisfies the same equation as Eq. (2) provided the renormalized coefficients satisfy the flow equations which are given to lowest order by

$$\frac{d\nu(l)}{dl}=\left[z-4+\frac{4-d}{4d}K_d\bar{\lambda}^2\right]\nu(l)\,, \tag{3}$$

$$\frac{dD(l)}{dl}=(z-2-d-2\chi)D(l)\,, \tag{4}$$

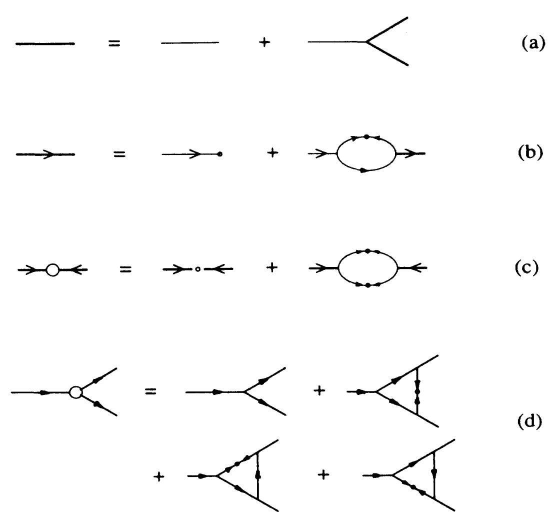

FIG. 1. (a) Diagrammatic representation of Eq. (2); (b) ν renormalization to leading order; (c) D renormalization; and (d) λ renormalization. Intermediate frequencies are summed from $-\infty$ to $+\infty$. Intermediate momenta are integrated over the shell $e^{-l}\Lambda<|\mathbf{q}|<\Lambda$. Light and heavy lines represent $h_0(k,\omega)$ and $h(k,\omega)$, respectively. Lines with arrows represent propagators $G_0(k,\omega)$ and $G(k,\omega)$, respectively.

and

$$\frac{d\lambda(l)}{dl}=(z+\chi-4)\lambda(l)\,, \tag{5}$$

where $\bar{\lambda}^2=\lambda^2D/\nu^3$ is the reduced coupling constant, and K_d is the geometric angular factor of the momentum integration. Note that diagrams contributing to $D(l)$ have prefactors proportional to k^4. Thus they correspond to higher derivatives in the original noise spectrum and are irrelevant. The three diagrams of $O(\lambda^3)$ in Fig. 1(d) cancel exactly so λ is not corrected. As we will discuss below, contributions to λ are zero to all orders of the perturbation expansion due to a transformation invariance of the original equation.

The recursion relation for the reduced coupling $\bar{\lambda}$ is

$$\frac{d\bar{\lambda}}{dl}=\frac{2-d}{2}\bar{\lambda}+\frac{3(d-4)}{8d}K_d\bar{\lambda}^3\,. \tag{6}$$

Above two substrate dimensions, $\bar{\lambda}$ is driven to zero as $l\to\infty$. At $d=2$, $\bar{\lambda}$ still goes to zero because the second term has a negative sign. Below $d=2$, a stable fixed point can be found: $K_2\bar{\lambda}^{*2}=\frac{4}{3}\epsilon$, where $\epsilon\equiv2-d$. The strong-coupling regime $d<2$ can be studied using an ϵ expansion. Scaling exponents χ and z were adjusted to keep ν and D invariant under the renormalization-group transformation as $l\to\infty$. In particular, the fixed-point values of χ and z below the critical dimension were found to be

$$z=\frac{12-\epsilon}{3},\quad \chi=\tfrac{1}{3}\epsilon\,. \tag{7}$$

The interface growth exponent β where $W(L,t)\sim t^\beta g(tL^{-z})$, is related to χ and z by $\beta=\chi/z$. Thus in one substrate dimension we have $z=\frac{11}{3}$, $\chi=\frac{1}{3}$, and $\beta=\frac{1}{11}$, with $\chi+z=4$. At and above $d=2$, the stable fixed point is $\bar{\lambda}^*=0$, which gives the "classical" exponent $z=4$.

The exponents obtained above are distinctly different from those of the KPZ equation, indicating that the conservation law changes the universality class, as anticipated. The hyperscaling relation between χ and z, $\chi+z=4$, is also novel. This is a direct consequence of the conservation law in Eq. (1) which breaks the Galilean invariance discussed by KPZ. Instead, Eq. (1) is invariant under the transformation

$$h\to h+\mathbf{a}\cdot\mathbf{x},\quad \mathbf{x}\to\mathbf{x}-\lambda t\mathbf{a}\nabla^2\,, \tag{8}$$

where $\mathbf{a}$ is any constant vector. The presence of λ in the transformation guarantees that diagrams correcting λ cancel to all order. Hence from Eq. (5), $\chi+z=4$ is an exact result. Furthermore, the noise spectrum D is not renormalized, because the diagrams generated correspond to irrelevant variables. Thus from Eq. (4) we have $z-2-d-2\chi=0$. Together with $\chi+z=4$, we have, quite generally, $z=\frac{1}{3}(10+d)$, $\chi=\frac{1}{3}(2-d)$. These results are expected to be exact. In particular, setting $d=1$, we re-

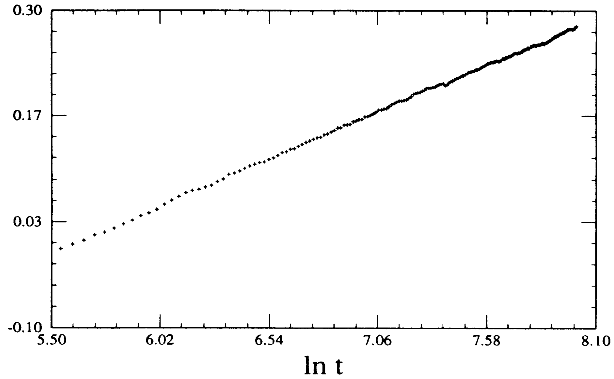

FIG. 2. Simulation results: ln-ln plot of interface width W vs time t. System size $L=2000$. Time measured as number of growth attempts. Slope gives growth exponent $\beta=\chi/z\approx 0.091$.

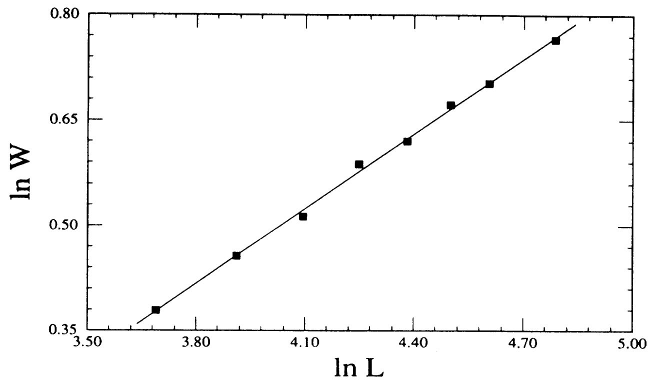

FIG. 3. Simulation results: ln-ln plot of saturated interface widths W vs system size L. Slope of the fitted straight line gives roughening exponent $\chi\approx 0.35$.

cover the ϵ expansion results given above.

To test the analytical results, we have performed extensive numerical simulations on a conserved restricted solid-on-solid model in one substrate dimension. The model is a natural extension of one proposed by Kim and Kosterlitz.[8] Briefly, the model is as follows. We randomly pick a site i on a one-dimensional substrate of length L, and increase its height h_i by one unit, provided the height difference Δh between h_i and its nearest neighbors remains $\Delta h \leq 1$ after the updating. During each attempt, conservation is enforced by decreasing a height h_j by one unit (subject to the same restriction) where site j is as close to site i as possible, but no further than a few lattice spacings. If such a jth site could not be found, the update on site i is canceled and the process is continued. This enforces a local conservation law which is consistent with Eq. (1). The growth of the interface is monitored by following the time evolution of the width W of the interface, where $W(L,t)\equiv[\langle h^2(\mathbf{x},t)\rangle]^{1/2}$. Large numbers of runs were required to obtain good statistics.

At early times and large L, W grows as a power law in time. Figure 2 shows our results for $\ln W$ vs $\ln t$. We obtain $\beta=0.091\pm 0.002$, which is in excellent agreement with the renormalization-group calculation $\beta=\frac{1}{11}$. The roughening exponent χ can be obtained by running the simulation until the width is saturated, since $W\sim L^{\chi}$ as $t\rightarrow\infty$. This is much more difficult to do because a great deal of computing time is required due to the large value of the exponent z ($t\gg L^z$ is required to get into the finite-size regime). We are thus limited to rather small systems and moderate numbers of runs for the average. Figure 3 shows $\ln W$ vs $\ln L$. The slope gives $\chi=0.35\pm 0.03$, which is again consistent with our analytical calculation $\chi=\frac{1}{3}$. The independent measurements of β and χ imply $\chi+z=4.2\pm 0.4$.

In summary, we have introduced a new model describing the dynamics of a growing interface where a conservation law is present. We have shown that it belongs to a different universality class from that studied by Kardar, Parisi, and Zhang. A stable nontrivial fixed point was shown to exist below the critical dimension, which allowed the study of the strong-coupling regime. A formal transformation invariance of the equation, similar to Galilean invariance, led to the hyperscaling relation $\chi+z=4$, which we expect to be exact. Numerical simulation of a conserved restricted solid-on-solid model confirmed the scaling relation and gave values of growth exponents in agreement with theory. We have also studied models for interfacial dynamics belonging to other universality classes. These and other results will be presented elsewhere.[15]

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