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Numerical solution of a continuum equation for interface growth in 2+1 dimensions

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We present the results of extensive large-scale numerical integrations of the Kardar-Parisi-Zhang equation for stochastic interface growth in 1+1 and 2+1 dimensions as a function of the nonlinearity parameter ϵ. We find results for the growth exponents α and β close to those obtained for discrete models. In particular, we find that for large values of ϵ, the values of the exponents are close to the conjecture of Kim and Kosterlitz, indicating that the smaller values obtained previously are due to crossover effects. In contrast to recent studies of discrete models, our results do not show evidence of a phase transition in 2+1 dimensions for $\epsilon \gtrsim 1$.

Recently, there has been considerable interest in the study of rough surfaces[1] and stochastically growing interfaces in the context of ballistic deposition,[2-4] the Eden model,[5-7] and the continuum stochastic equation of Kardar, Parisi, and Zhang[8-10] (KPZ). Much of this interest stems from the fact that in addition to their connection to processes of fundamental practical importance such as thin-film growth and interface dynamics in random media, these models exhibit nontrivial scaling behavior. In particular, the scaling of the interface width is expected to be of the form[2]

$$W_L(t) \sim L^{\alpha} f(t/L^{\alpha/\beta}) , \tag{1}$$

where $W_L(t)$ is the interface width on length scale L at time t, and the scaling function $f(x) \sim x^{\beta}$ for $x \ll 1$ and $f(x) \rightarrow$ const for $x \gg 1$. The dynamics of the interface in these models has also been shown[8,10] to be intimately related to a variety of other problems, including directed polymers in random media, the large-time behavior of randomly stirred fluids, and the evolution of Sivashinski flame fronts. In particular, Kardar, Parisi, and Zhang have proposed[9] that all these problems lie in the same universality class as the KPZ equation.

For spatial dimension $d=2$ (substrate dimension $d-1$), the results for ballistic deposition,[2-4] the Eden model,[5-7] and the KPZ equation[9-11] agree giving $\alpha=\frac{1}{2}$ and $\beta=\frac{1}{3}$. However, for $d>2$, there is still controversy over the values of the exponents as well as the universality of the various surface-growth models.[12] In particular, the perturbative renormalization-group approach[9,10] to the KPZ equation has not been successful in predicting precise numerical exponents for $d>2$. In addition, previous attempts to solve the KPZ equation numerically[13,14] in 2+1 dimensions yielded exponent values ($\alpha \approx 0.18$, $\beta \approx 0.09$–0.15), which were much smaller than those obtained for the discrete microscopic models ($\alpha \approx 0.33$–0.40, $\beta \approx 0.20$–0.25). Therefore, a more extensive study of the continuum KPZ equation in 2+1 dimensions is needed to clarify the apparent disagreement between the results for microscopic models and the continuum equation. This study may also help to resolve the question of whether the existence of a phase transition in 2+1 dimensions, recently observed in discrete models,[14-17] implies a similar transition in the KPZ equation.

In this Rapid Communication we present the results of extensive numerical simulations of the KPZ equation as a function of the nonlinearity parameter $\epsilon=\lambda^2 D/2\nu^3$ [see Eqs. (2) and (4) below]. First, as a test of our integration technique, we consider simulations in $d=1+1$. We find that we recover the known exponents $\alpha=\frac{1}{2}$, $\beta=\frac{1}{3}$. In $d=2+1$ dimensions, we find exponents which are in the range of those found for discrete models, in contrast to previous studies of the KPZ equation.[13,14] In particular, for large enough ϵ, the asymptotic exponents appear to be close to those conjectured by Kim and Kosterlitz[12] (KK) in 2+1 dimensions. Finally, we discuss the evidence for a phase transition from the strong-coupling limit to the weak-coupling limit in 2+1 dimensions.

The KPZ equation for interface growth may be written[9] as

$$\partial h(\mathbf{r},t)/\partial t = \nu \nabla^2 h(\mathbf{r},t) + \lambda/2 \, |\nabla h|^2 + \eta(\mathbf{r},t) , \tag{2}$$

where $h(\mathbf{r},t)$ is the height of the interface at $\mathbf{r}$ at time t, and the noise term $\eta(\mathbf{r},t)$ is assumed to be Gaussian with delta-function correlation,

$$\langle \eta(\mathbf{r},t)\eta(\mathbf{r}',t')\rangle = 2D\delta(\mathbf{r}-\mathbf{r}')\delta(t-t') . \tag{3}$$

The parameter ν corresponds to the effects of surface diffusion, λ to sideways growth, and $\eta(\mathbf{r},t)$ to the effects of randomness. In the limit $\epsilon \rightarrow 0$ (weak-coupling limit) we recover the Edwards-Wilkinson equation,[18] which has been shown to exhibit logarithmic growth in 2+1 dimensions.

If we now perform a simple change of scale, $h = y\sqrt{2D/\nu}$ and $t=\tau/\nu$, Eq. (2) may be rewritten as

$$\partial y(\mathbf{r},\tau)/\partial \tau = \nabla^2 y(\mathbf{r},\tau) + \sqrt{\epsilon}\, |\nabla y|^2 + \xi(\mathbf{r},\tau) , \tag{4}$$

where $\epsilon = \lambda^2 D/2\nu^3$ and $\langle \xi(\mathbf{r},\tau)\xi(\mathbf{r}',\tau')\rangle = \delta(\mathbf{r}-\mathbf{r}')\delta(\tau-\tau')$. We note that this transformation reduces the KPZ equation to a function of a single parameter ϵ, with $\sqrt{\epsilon}$ multiplying the nonlinear term. In Ref. 13, a similar change of scale [$h=y(2\nu/\lambda)$ and $t=\tau/\nu$] was used and the parameter $\sqrt{\epsilon}$ was placed in front of the noise term. A comparison of the two transformations indicates that they are the same except for a factor of $\sqrt{\epsilon}$ in the height.

In our simulations, Eq. (4) was integrated on a discrete grid in one and two dimensions using a simple finite-difference scheme.[19] In one dimension our largest grid size was $L=16\,384$, while the largest grid size in two dimensions was $L=1024$. In discrete form, Eq. (4) can be rewritten in 2+1 dimensions as

$$y_{\tau+1}(i,j)=y_\tau(i,j)+\Delta\tau([y_\tau(i,j+1)+y_\tau(i+1,j)-y_\tau(i-1,j)-y_\tau(i,j-1)-4y_\tau(i,j)] \\ +(\sqrt{\epsilon}/4)\{[y_\tau(i,j+1)-y_\tau(i,j-1)]^2+[y_\tau(i+1,j)-y_\tau(i-1,j)]^2\})+\sqrt{\Delta\tau}\xi(i,j;\tau)\,, \quad (5)$$

where $\xi(i,j;\tau)$ corresponds to independent Gaussian noise, generated using the Box-Muller transformation,[19] and $\Delta\tau$ was varied to get good convergence.

For $\epsilon=1$ and 2, a time step $\Delta\tau=0.005$ was used, while for $\epsilon=5$, 10, and 25, the time steps used were, respectively, $\Delta\tau=0.005$, 0.001, and 0.000 25. We checked for convergence by verifying that smaller time steps did not change our results. In addition to runs with Gaussian noise, runs were also performed in which the Gaussian noise $\xi(\mathbf{r},t)$ was replaced by "white" noise $\xi_W(\mathbf{r},\tau)$, where $\xi_W(\mathbf{r},\tau)$ is an independent random variable between $-\sqrt{3}$ and $+\sqrt{3}$ such that $\langle\xi_W(\mathbf{r},\tau)\xi_W(\mathbf{r}',\tau')\rangle=\delta(\mathbf{r}-\mathbf{r}')\times\delta(\tau-\tau')$. This change in the noise distribution is not expected to change the exponents, and in fact, the results for the surface width for the cases of Gaussian noise, and white noise were essentially identical.

For each run, the width of the interface $W_L(\tau)$ at time τ was measured as

$$W_L^2(\tau)=\langle y^2(\mathbf{r},\tau)\rangle-\langle y(\mathbf{r},\tau)\rangle^2\,, \quad (6)$$

where $y(\mathbf{r},\tau)$ is the height of the surface at position $\mathbf{r}$ and time τ. The initial configuration was always $y(\mathbf{r},0)=0$ and averages were taken over several runs to get the growth exponents. Saturation data were obtained from averages over very long runs. We note that, for early times, the width is a self-averaging quantity, since, for example, if the correlation length at time τ has grown to a size λ, then there are $(L/\lambda)^{d-1}$ independent samples. Thus, one run on a system of size $L=1024$, for early times, is statistically equivalent to 64 runs on a 128×128 system. Furthermore, the simulation of a large system with $L=1024$ for the early-time data enabled us to sample the correct early-time behavior and avoid the effects of saturation.

Figure 1 shows results for the early-time growth behavior (averaged over several runs) for five different values of ϵ ($\epsilon=1$, 2, 5, 10, and 25) for systems of size $L=1024$. For large ϵ, we find from fits to the late-time data (see Fig. 1): $\beta=0.24$ ($\epsilon=25$), 0.23 ($\epsilon=25$ white noise), 0.24 ($\epsilon=10$), and 0.25 ($\epsilon=10$ white noise). We note that these values appear to be close to the Kim-Kosterlitz value $\beta=0.25$. It is not clear whether the slight decrease in β from $\epsilon=10$ to 25 is due to numerical problems for large ϵ requiring the use of multigrid techniques or is a sign of a crossover to slightly lower exponents. However, the data for the exponent α (see below) seem to indicate the former.

For smaller values of ϵ ($\epsilon=1$, 2, 5), the effective exponents are smaller than the KK value. However, for $\epsilon=5$ the slope is still increasing at $\tau=1000$, indicating the existence of strong crossover effects. We note that our data for $W_L(\tau)$ for $\epsilon=10$ is identical to that of Chakrabarti and Toral[13] over the time range studied by them ($0<\tau<10$), except for a trivial rescaling factor of $\sqrt{\epsilon}$. Clearly this range falls in the crossover region for $\epsilon=10$ (see Fig. 1) and this is the reason that they did not obtain the asymptotic values of the exponents.

Figure 2 shows data for the surface-roughness exponent α for different values of the nonlinearity parameter ϵ. In particular, the saturation width $W_L(\infty)$ as a function of system size L, for $L=8$, 16, 32, 64, and 128, is plotted for $\epsilon=5$, 10, and 25. For $\epsilon=25$, the slope (0.39 ± 0.01) is close to the Kim-Kosterlitz value $\alpha=0.4$. For $\epsilon=10$, the slope (0.37 ± 0.02) is somewhat below this value but appears to be increasing with L. This can also be seen in the data for $\epsilon=5$. Thus, it appears that the Kim-Kosterlitz exponents in $d=2+1$ are in fact the correct asymptotic exponents for the universality class of the KPZ equation in the strong-coupling limit.

Some additional support for these results is provided by the correlation function $G_L(r)$ which at late times is expected to scale as,

$$G_L(r)=\langle[y(\mathbf{r})-y(\mathbf{0})]^2\rangle\sim r^{2\alpha} \text{ for } r\ll L\,. \quad (7)$$

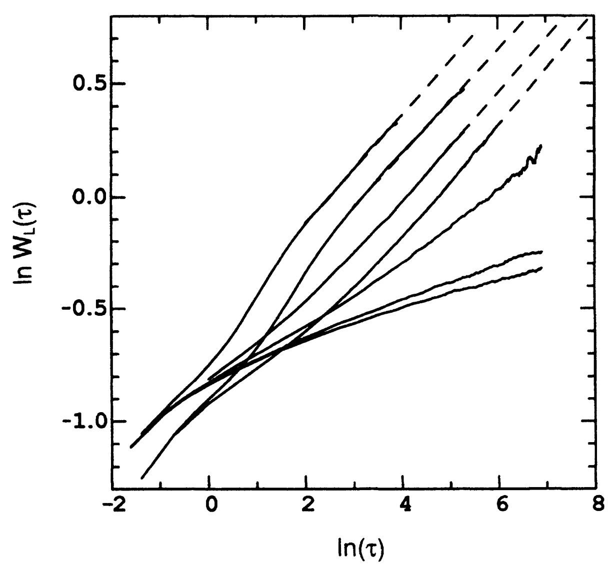

FIG. 1. Log-log plots of width $W_L(\tau)$ for $L=1024$ for $\epsilon=1$, 2, 5, 10, and 25. Curves are from top to bottom (on the right-hand side): $\epsilon=25$, $\epsilon=25$ (white noise), $\epsilon=10$, $\epsilon=10$ (white noise), $\epsilon=5$, $\epsilon=2$, $\epsilon=1$. [The white-noise data have been shifted by a constant ln(2) in order to distinguish from the Gaussian noise data.] Dashed lines are linear fits to late-time data with slopes (from top to bottom): 0.24 ($\epsilon=25$), 0.23 ($\epsilon=25$ white noise), 0.24 ($\epsilon=10$), 0.25 ($\epsilon=10$ white noise). Fit to late-time data for $\epsilon=5$ has slope 0.18.

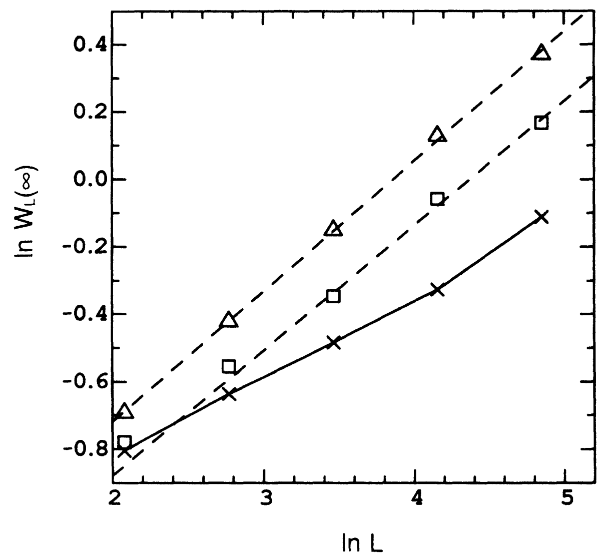

FIG. 2. Log-log plots of saturation width $W_L(\infty)$ for systems of size $L=8$, 16, 32, 64, and 128 for $\epsilon=25$ (△), 10 (□), and 5 (×). Slopes of dashed-line fits are ($\epsilon=25$) 0.39 ± 0.01 and $\alpha=0.37\pm0.02$ ($\epsilon=10$, fit to last three points).

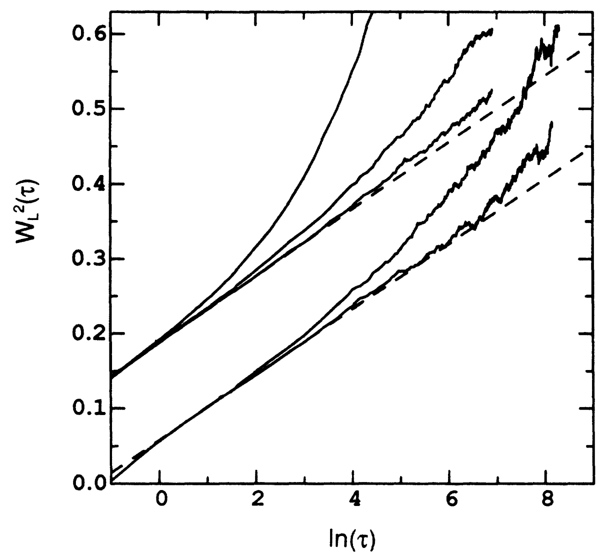

FIG. 3. Semi-log plots of $W_L^2(\tau)$ for $\epsilon=1$, 2, and 5. Curves are (from top to bottom): $\epsilon=5$, $\epsilon=2$, $\epsilon=1$ (Gaussian noise), and $\epsilon=2$ and 1 (white noise). The white-noise curves have been shifted down by 0.1 and to the right by ln(2) in order not to interfere with the Gaussian-noise data. Dashed lines show fits to early-time data.

For $\epsilon=25$ and for systems of size $L=128$ and 256, we find $\alpha\approx0.38$. For smaller values of ϵ, the exponent α is found to be smaller. However, this is due to crossover effects and for larger L and much longer times, the exponents are expected to crossover to the KK values.

Finally, we discuss the possibility of a phase transition from the strong-coupling to the weak-coupling limit. Figure 3 shows plots of $W_L^2(\tau)$ vs $\ln(\tau)$ for small values of the parameter ϵ ($\epsilon=1$, 2, 5), both with Gaussian noise and with white noise. At early times, all the curves appear to be straight and consistent with Edwards-Wilkinson[18] or "weak-coupling" behavior ($\epsilon=0$) corresponding to logarithmic growth of $W_L^2(\tau)$ with time. However, for much later times, even for $\epsilon=1$, the curves appear to bend upwards indicating a departure from weak-coupling behavior. Thus, we find no evidence for a phase transition, at least down to $\epsilon=1$, in the KPZ equation in 2+1 dimensions.

We note that this interpretation of our data is in contrast with the observations of a phase transition in *discrete* models in 2+1 dimensions reported by Guo, Grossmann, and Grant,[14] Amar and Family,[15] Derrida and Golinelli,[16] and Yan, Kessler, and Sander.[17] As pointed out in Ref. 15, there may not be a phase transition in the KPZ equation in 2+1 dimensions, due to the fact that this equation is continuous. The situation is perhaps analogous to that of the roughening transition: while the continuous Gaussian model has no transition in two dimensions, the discrete Gaussian model does. Given the obvious existence of strong crossover effects (especially for small ϵ), it would be most valuable to formulate general arguments which predict the existence or absence of a phase transition in 2+1 dimensions.

Our other main result, i.e., the striking agreement at large values of ϵ with the exponents found in the Kim-Kosterlitz model, indicates that the KK conjecture may be correct for models in the KPZ universality class in 2+1 dimensions. Thus, the intuitive suggestion by Kim and Kosterlitz that their model (because of the emphasis on sideways growth) corresponds to the large-ϵ limit of the KPZ equation, and thus exhibits asymptotic behavior at early times and small system sizes, appears to be in agreement with our numerical results. In this connection, recent simulations of the Eden model[6,20] and the ballistic-deposition model[21] show an increase in the exponents with increasing system size towards the KK values. The determination of the correct universality classes for these models, as well as *analytic* predictions of the strong-coupling exponents for the KPZ equation as a function of dimension, remain challenging open questions.

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