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Numerical study of a model for interface growth

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We present the first numerical study of the nonlinear stochastic differential equation characterizing interface growth, originally proposed by Kardar, Parisi, and Zhang [Phys. Rev. Lett. **56**, 889 (1986)]. Our studies are carried out in two dimensions which would correspond to three-dimensional studies of microscopic models such as the Eden or ballistic-deposition models. We find that the interface width satisfies the proposed scaling relations. The exponents associated with this scaling relation are calculated for different strengths of the effective coupling in the model and seem to be different from previous calculations on microscopic models.

The dynamical behavior associated with various different types of growth processes has received considerable attention in recent years.[1] One class of growth problems, which we study in this paper, includes the Eden[2] and the ballistic-deposition models[3] both of which produce compact clusters with a rough interface. Despite their simple appearance, the details of the growth processes of these models are not completely understood. It is realized, though, that the growth process occurs mainly at an "active zone" on the surface and that the width or thickness of the rough interface shows interesting scaling behavior.[4,5] Additional interest in the scaling behavior of the interface width developed when Kardar, Parisi, and Zhang[6] proposed a nonlinear stochastic differential equation (hereafter referred to as the KPZ equation) which is supposed to govern the growth of profiles for the second class of processes mentioned above. It was also realized by these authors that the KPZ equation is related to other physical problems such as randomly stirred fluids (Burger's equation[7]) and directed polymers in a random media.[8] Hence the KPZ equation received added attention, since the solutions of one problem can be directly used to elucidate the other problems as well.

Since the scaling exponents for the interface width calculated from recent three-dimensional ($d=3$) simulations[9-12] of microscopic models (Eden, etc.) neither agree with each other nor with studies of the KPZ equation[6,13] (or with the equivalent directed polymer problem[8,14]), we try to clarify the issue by carrying out a novel numerical study. In this paper, we present the results of a detailed *numerical study of the KPZ equation* on a square lattice (which being a model for the interface profile would correspond to the three-dimensional microscopic models, i.e., $d=3$). It turns out that the numerical solution of the KPZ equation is computationally very demanding since a large number of runs is necessary in order to extract statistically reliable information. However, we have been able to carry out the simulations to a reasonably good precision for several values of the sample size and the effective coupling in the model. We find that the interface width satisfies scaling relations.[4-6,13] The exponents associated with this scaling relation are calculated for different strengths of the effective coupling and seem to be different from previous calculations on microscopic models.

The KPZ equation for the interface profile is written in terms of a time-dependent coarse-grained height variable $\tilde{h}(\mathbf{r},\tau)$ as

$$\frac{\partial \tilde{h}}{\partial \tau} = \nu \nabla^2 \tilde{h} + \frac{\lambda}{2}(\nabla \tilde{h})^2 + \eta , \quad (1)$$

where ν and λ are constants, τ is the time, and the noise η is a Gaussian distributed stochastic variable of mean $\langle \eta(\mathbf{r},\tau)\rangle = 0$ and correlations

$$\langle \eta(\mathbf{r},\tau)\eta(\mathbf{r}',\tau')\rangle = 2D\delta(\mathbf{r}-\mathbf{r}')\delta(\tau-\tau') . \quad (2)$$

The vectors $\mathbf{r}$ define the $(d-1)$-dimensional space of the "substrate." Equation (1), then, corresponds to growth processes in d spatial dimensions. The addition of the nonlinear term $(\nabla \tilde{h})^2$ to the surface tension term $\nabla^2 \tilde{h}$ distinguishes the KPZ equation from similar equations previously studied by Edwards and Wilkinson.[15] The nonlinear term is expected to be present in all situations allowing lateral growth. The asymptotic behavior of the interface width $w(L,\tau)$ for a substrate of linear size L is found to obey the scaling relation

$$w = L^{\chi} f(\tau/L^{z}) , \quad (3)$$

where the exponents χ and z are related by[13]

$$\chi + z = 2 . \quad (4)$$

Equation (3) leads to two interesting limits: if $L \to \infty$, then for finite but sufficiently large τ, $w(\tau) \approx \tau^{\chi/z} \equiv \tau^{\beta}$; for finite L and $\tau \to \infty$, the equilibrium values of the interface width satisfy $w^{\mathrm{eq}}(L) \approx L^{\chi}$. In two spatial dimensions ($d=2$) the exponents found by Kardar, Parisi, and Zhang[6] from a perturbation expansion are actually exact and are given by $\chi = \frac{1}{2}$ and $z = \frac{3}{2}$ (i.e., $\beta = \frac{1}{3}$). In three dimensions ($d=3$) the effective coupling $\bar{\lambda} = \lambda^2 D/\nu^3$ is marginally relevant and the situation is not clear. The strong coupling behavior in three dimensions is probed by Kardar and Zhang[8] by mapping the problem of growth to a problem of directed polymers. Numerical simulations of the latter model at a temperature $T=0$ (which corresponds to $\bar{\lambda} \to \infty$ from the mapping) are claimed to be consistent with $\beta = \frac{1}{3}$ and thus a conjecture of superuniversality of the exponents was suggested. Subsequently, the superuniversal conjecture was supported[16] by an analytic argument based on replica methods. In higher dimensions both trivial values ($\chi=0$, $z=2$ corresponding to asymptotically smooth surfaces) and nontrivial values ($\chi>0$, $z<2$) of the exponents are possible[13] depending on the relative strengths of the surface tension and nonlinear terms.

Much effort has been devoted to the determination of the exponents χ and z from simulations of microscopic models. The values of the exponents in two dimensions are generally accepted to be[4,5,9,17–19] $\chi=\frac{1}{2}$ and $z=\frac{3}{2}$. On the other hand, the situation in higher dimensions is not clear at all. The simulations of Zabolitzky and Stauffer[18] on the Eden model do not provide a reliable estimate for the growth exponents in three dimensions. The simulations of Meakin and co-workers[9,10] suggest $\chi\approx\frac{1}{3}$. On the other hand, Wolf and Kertesz[11] conjectured $\chi=1/d$ (i.e., $\beta=\frac{1}{5}$ in three dimensions) and Kim and Kosterlitz[12] claimed that $\beta=1/(d+1)$ on the basis of their investigation on the Eden model and the restricted solid-on-solid model, respectively.

We start by writing the KPZ equation [Eq. (1)] in a simpler form by defining rescaled variables $h=\tilde{h}/(2\nu/\lambda)$ and $t=\nu\tau$. The resulting equation is

$$\frac{\partial h}{\partial t}=\nabla^2 h+(\nabla h)^2+\sqrt{\varepsilon}\xi\,, \tag{5}$$

which contains only one parameter[20] $\varepsilon=\lambda^2 D/2\nu^3$ (which is essentially the effective coupling parameter $\bar{\lambda}$) and the new noise term $\xi(\mathbf{r},t)$ satisfies

$$\langle\xi(\mathbf{r},t)\xi(\mathbf{r}',t')\rangle=\delta(\mathbf{r}-\mathbf{r}')\delta(t-t')\,. \tag{6}$$

We have studied Eq. (5) on a square lattice of side L with periodic boundary conditions for system sides $16\leq L\leq 128$ and for $\varepsilon=1$, 2, 5, and 10. We have performed the numerical integrations by using a simple Euler scheme. We have chosen the mesh size for the spatial derivatives to be $\Delta r=1$ always, and time steps $\delta t=0.01$ for $\varepsilon=1$ and $\varepsilon=2$, $\delta t=0.001$ for $\varepsilon=5$, and $\delta t=0.0001$ for $\varepsilon=10$. We have checked that smaller values of δt do not change the values of the measured quantities by any appreciable amount. For example, even after reducing δt by a factor of 2 from the above mentioned values the width is still found to be within the statistical error bars [which is about (1-2)%]. We always start from a smooth interface as the initial configuration [i.e., $h(\mathbf{r},0)=0$ everywhere] and measure width as

$$w(L,t)=[\langle h(\mathbf{r},t)^2\rangle-\langle h(\mathbf{r},t)\rangle^2]^{1/2}\,.$$

The measurements are then averaged over 500 realizations of the noise term (when $\varepsilon=10$, however, we have averaged only over 100 realizations due to the very small time step needed for convergence).

In Figs. 1 and 2 we show two typical plots for the width $w(L,t)$ vs t for two different values of ε and different L values. When ε is small systems with small L reach equilibrium quickly and one needs to consider large system sizes to find the exponent β directly from a logarithmic plot. In the above figures it is shown that the data for two different L values agree with each other reasonably well, indicating that the finite-size effects are negligible for these system sizes. Nevertheless, we calculate the exponent β for different ε's from the slope of the log-log plot of the width for the *largest value of L* considered in each case. We find that the exponent values as calculated are $\beta=0.09(2)$ for $\varepsilon=1$, $\beta=0.10(2)$ for $\varepsilon=2$, $\beta=0.11(2)$ for $\varepsilon=5$, and $\beta=0.15(3)$ for $\varepsilon=10$. Also, in order to check the relationship $\chi+z=2$, we ran the systems to equilibrium in the case of $\varepsilon=2$. The resulting equilibrium widths are plotted in Fig. 3 in a log-log plot. The slope of the curve yields $\chi=0.18(1)$ which together with $\beta\equiv\chi/z=0.10(2)$ satisfies Eq. (4) in this case within the statistical errors. We note that for $\varepsilon=10$, the value of β is slightly larger than those found for smaller ε's. Since our numerical accuracy is comparably smaller for $\varepsilon=10$ (in this case we could make only 100 runs compared to 500 runs made for smaller ε's, due to the very small δt required for

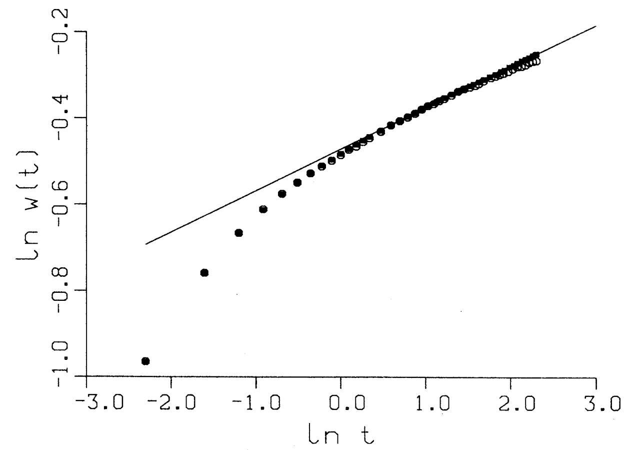

FIG. 1. Log-log plot of width $w(L,t)$ vs t for $\varepsilon=2$. The symbols correspond to different values of L as follows: ○ for $L=64$ and ■ for $L=128$. After an initial transient time, the width varies as a power law of time. The slope of the straight line then yields $\beta=0.10(2)$. Here, and in other figures, the statistical errors are smaller than the symbol sizes.

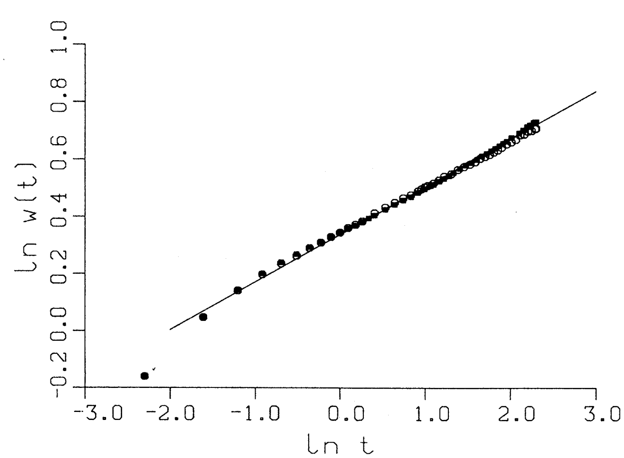

FIG. 2. Log-log plot of width $w(L,t)$ vs t for $\varepsilon=10$ and $L=32$ (○) and $L=64$ (■). The slope of the straight line yields $\beta=0.15(3)$.

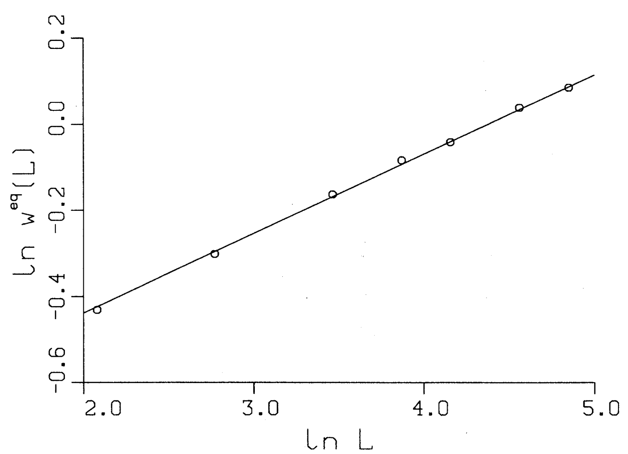

FIG. 3. Log-log plot of the equilibrium width $w^{eq}(L)$ vs L for $\varepsilon=2$. The slope of the straight line yields $\chi=0.18(1)$.

accurate numerical integration), we tend to believe that this discrepancy will go away with better statistical accuracy. Also, the independent direct measure of χ from the equilibrium values of the width for $\varepsilon=2$ provides added weight that $\beta\approx 0.1$.

Although, the relationship between the KPZ model and the microscopic models has not yet been rigorously established, it is generally accepted that these models are intimately related and probably belong to the same universality class. The exponent β calculated in our study is clearly different from the superuniversality conjecture[6] and from the results of several other analytical studies.[14] The β values are also different from those obtained in simulations of the Eden and the restricted solid-on-solid models. However, we refrain from making any quick comment about the true value of β and the corresponding relations between the microscopic and the coarse-grained models for several reasons. The calculation of β in our simulation, as well as in the Eden and other models, are carried out from a log-log plot covering not too large time interval and one cannot rule out the possibility that all these studies may be providing just different "effective" values for the exponent β. We also note that the parameter ε is marginally relevant[6] in $d=3$ and the crossover from the smooth interface behavior to the rough interface behavior is probably very slow for small values of ε. Thus for small values of ε the transient time is very large and the exponents calculated from the log-log plot could be different from the "true" values. Finally, ε being a marginally relevant variable in three dimensions, the scaling relations might contain some strong correction terms associated with them which, although not easy to detect numerically, could easily produce systematic errors in the calculation of the scaling exponents. This could also explain the dispersity in the values of the exponents found in different numerical studies. Whether our results have been affected by all these effects remains to be seen, since we could not carry out simulations for larger values of L, t, and ε's due to limitations of computer times (the present study used more than 200 hours of central processing unit time in a Cray YMP).

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[20]Note that in general dimensions $d\neq 3$, one can rescale $\tilde{h}$, τ, *and* the space variable **r** such that the resulting equation is *parameterless.* This rescaling, however, breaks down in $d=3$ and one is left with one parameter in the equation.