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Controlled instability and multiscaling in models of epitaxial growth

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We show that discretized versions of commonly studied nonlinear growth equations have a generic instability in which isolated pillars (or grooves) on an otherwise flat interface grow in time when their height (or depth) exceeds a critical value. Controlling this instability by the introduction of higher-order nonlinear terms leads to intermittent behavior characterized by multiexponent scaling of height fluctuations, similar to the ''turbulent'' behavior found in recent simulations of one-dimensional atomistic models of epitaxial growth. [S1063-651X(96)51011-1]

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In recent years, much attention has been focused on the nonequilibrium dynamics of growing interfaces. A number of simple models of epitaxial growth have been proposed and studied [1–7] analytically and numerically, revealing a rich variety of interesting phenomena. One such phenomenon for which no explanation is available at present is the multiexponent scaling [6] of height fluctuations found in recent simulations [6,7] of a class of one-dimensional (1D) limited-mobility models of epitaxial growth. This phenomenon is particularly interesting because it exhibits a striking similarity [6] to the intermittent multiscaling of velocity fluctuations in fully developed fluid turbulence [8]. In this paper, we propose an explanation of this phenomenon. We first show that discretized versions of simple nonlinear growth equations, such as the Kardar-Parisi-Zhang (KPZ) equation [1] and the Lai–Das Sarma (LD) equation [2,3], exhibit an instability in which isolated pillars or grooves on an otherwise flat interface tend to grow in time. Instabilities in direct numerical integration of discretized KPZ and LD equations have been noted earlier [9,10]: our results show that these instabilities are *generic* to discretized nonlinear growth equations if the bare coupling constant (determined by the details of the model) exceeds a critical value (which may equal zero). In contrast to previous studies [9] that attributed the instability in the discretized KPZ equation to ''numerical artifacts,'' our work shows that this instability is an *intrinsic* property of the discretized equation with or without noise. Since the 1D continuum KPZ equation without noise *does not* have any instability, our results lead to the important conclusion that the behavior of discretized nonlinear growth equations may be very different from that of their truly continuum versions. Our second important finding is that the recently discovered multiexponent scaling phenomena [6] are closely connected to this nonlinear growth instability. Models in which this instability is controlled by introducing higher-order nonlinear terms exhibit deviations from simple scaling over the time interval during which the instability is operative. The behavior in this regime is found to be very similar to the multiexponent scaling observed in simulations [6,7] of atomistic growth models if the coefficients of the higher-order nonlinear terms are chosen appropriately. In particular, our results indicate that the multiscaling behavior observed [6] in the 1D Das Sarma–Tamborenea (DT) model [4] is described by the discretized LD equation or an atomistic version of it, supplemented by a set of higher-order nonlinear terms with appropriate coefficients. Our explanation of multiexponent scaling in growth models is conceptually similar to a recent proposal [11] that suggests that the multiscaling of structure functions in turbulence may be caused by singularities occurring on a dense set of space-time points.

Our conclusions are based on detailed studies of discretized versions of the LD and KPZ equations using direct numerical integration. The LD equation has the form

$$\partial h'(\mathbf{r},t)/\partial t = -\nu\nabla^4 h' + \lambda_1 \nabla^2 |\nabla h'|^2 + \eta(\mathbf{r},t), \qquad (1)$$

where $h'(\mathbf{r},t)$ represents the ''height'' variable at the point $\mathbf{r}$ at time t and η is a Gaussian random noise with correlations

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

This equation is numerically integrated using a simple Euler scheme [10,12]. To this end, we first define dimensionless variables x, τ, and h by choosing appropriate units of length, time, and height, respectively, and then discretize in space and time by defining the dimensionless discretization scale Δx and the integration time step $\Delta\tau$. This leads to a set of ''update equations'' [10] for the variables $\{h_i(\tau)\}$ representing the dimensionless height variables at the computational mesh points at dimensionless time τ. We use the standard three-point definition of the lattice derivatives in most of our calculations, but have explicitly verified that a more refined five-point definition does not change our results. The behavior of the discretized equation is governed by a single dimensionless parameter $\lambda = \sqrt{2\lambda_1^2 D/\nu^3}a_0^{(4-d)/2}$ (d is the substrate dimension and a_0 is the spacing between adjacent mesh points), which appears [10] as the coefficient of the nonlinear term. The KPZ equation can also be cast in a similar form with $\lambda = \sqrt{2\lambda_1^2 D/\nu^3}a_0^{(2-d)/2}$, where ν and λ_1 are, respectively, the coefficients of the linear and quadratic terms in the

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original continuum equation [1]. Note that in both LD and KPZ equations in one dimension, the value of λ can be made small by choosing a small value for a_0. However, the smallest value (λ_{min}) that λ can have for a physical system is obtained by replacing a_0 by a_{min}, the short-distance cutoff of the system, in the expressions for λ. We have also studied by simulation an atomistic version [5] of the LD equation in which the height variables $\{h_i\}$ are integers and ''time'' is measured by the number of layers deposited. This model also involves only one dimensionless parameter λ. We call this model the Kim–Das Sarma (KD) model below.

The possibility of multiexponent scaling was investigated in our simulations by monitoring different moments of the nearest-neighbor height difference and the height difference correlation function. Following Ref. [6], we define

$$\sigma_q(\tau)\equiv\langle[s_i(\tau)]^q\rangle^{1/q}, \quad s_i(\tau)=|h_{i+1}(\tau)-h_i(\tau)| \tag{3}$$

and

$$G_q(l,\tau)\equiv\langle|h_{i+l}(\tau)-h_i(\tau)|^q\rangle^{1/q}. \tag{4}$$

Multiexponent scaling, as observed in Refs. [6,7], is characterized by a q dependence of the exponents (denoted by α_q/z in Ref. [6], where z is the dynamical exponent) that describe the power-law growth of the quantities $\{\sigma_q(\tau)\}$ in time before saturation is reached, i.e., for $\tau\ll L^z$ where L is the lateral size of the system. The height difference correlation functions G_q are expected to behave as

$$G_q(l,\tau)\approx|l|^{\zeta_q}, \quad 1\ll l\ll\tau^{1/z}. \tag{5}$$

Again, multiexponent scaling is characterized by a dependence of the exponents ζ_q on q.

Results of integrating the 1D LD equation for small values of λ ($\lambda\leq 2.0$) show good agreement with the predictions of dynamical renormalization-group calculations [2] and no evidence of multiscaling. For higher values of λ, the system exhibits conventional scaling behavior at short times. However, an instability, indicated by a rapid growth and apparent divergence of the height variable, is found at longer times. A similar instability is found in simulations of the 1D KD model, where it shows up as a rapid increase of the rms interface width, manifested as a changeover from a power-law growth with an exponent close to 1/3 to a linear growth in time. This instability was reported by Tu [10] for the LD equation and by Kim and Das Sarma [5] for the KD model. Our results are concerned with the origin of this instability and its relation to multiscaling behavior.

Our study shows that this instability is caused by the growth of isolated pillars or grooves. Either pillars or grooves are unstable in a particular system; which one is unstable is determined by the sign of λ. We find that pillars (represented by the initial configuration $h_i=h_0>0$ at the central site, $h_i=0$ at all other sites) grow in time in the LD equation with positive λ if h_0 is sufficiently large. It is easy to show analytically that in the absence of noise ($\eta=0$), isolated pillars of height h_0 initially grow in time if $h_0>10/\lambda$. Our numerical studies of the equation with noise show that for values of h_0 slightly higher than $10/\lambda$, the height of the pillar eventually decreases after an initial increase. The apparent divergence mentioned above is encountered if h_0 is greater than a ''critical'' value $h_c\simeq 20/\lambda$. We find that the values of h_c obtained for $\Delta\tau=0.01$, 0.001, and 0.0001 are very close to one another, indicating that this instability is not a numerical artifact of not using a sufficiently small value of $\Delta\tau$. It is virtually impossible to determine numerically whether this behavior represents a true finite-time singularity or not (i.e., whether the height of the pillar would eventually decrease after reaching a very large but finite value). As described below, this issue is not crucial to our main results because these results are derived from models in which the growth of the height is cut off at a finite value.

We obtained very similar results for the 1D KD model. A little algebra shows that in this model, an attempt to deposit a ''particle'' at the site of a pillar of initial height h_0 or at one of its nearest-neighbor sites leads to an increase in the height of the pillar if $h_0>12/\lambda$. Our simulations (which are exact because all the variables in this model are discrete) show that the height of a pillar continues to grow linearly in time if its initial value is somewhat larger than $12/\lambda$.

The instability described above appears to be *generic* to all discretized growth equations containing nonlinear terms. In particular, we have found very similar results for the 2D LD equation and for the 1D KPZ equation. All the qualitative features of the instability found in these two systems appear to be the same as those found for the 1D LD equation [13]. However, the behavior of these two systems differs from that of the 1D LD equation in one very important aspect. During the evolution of the system from a flat initial state, the average nearest-neighbor height difference saturates quickly after an initial increase in both the 2D LD equation and the 1D KPZ equation. These systems, therefore, are expected to spontaneously exhibit the instability discussed above only if the value at which the maximum nearest-neighbor height difference s_{max} saturates is higher than (or at least close to) the critical value h_c defined above. Since h_c decreases while the saturation value of s_{max} generally increases with λ, we can define a nonzero critical value λ_c of λ at which these two quantities become equal. According to the discussion above, systems with values of λ substantially smaller than λ_c are not expected to show the instability during their time evolution from a flat initial state. However, as noted before, the value of λ cannot be made arbitrarily small and the instability cannot be avoided if the ''bare'' parameters are such that $\lambda_{\mathrm{min}}>\lambda_c$. In contrast, nearest-neighbor height differences in the 1D LD equation, which is believed to exhibit anomalous dynamic scaling [14], are expected to continue growing in time. This system, therefore, should always show the instability at sufficiently long times, implying λ_c to be zero for this system. Results of our simulations with flat initial conditions are fully consistent with this picture.

The instability described above would, in general, lead to deviations from single-exponent scaling for the quantities $\{\sigma_q\}$. When the instability sets in, the value of the nearest-neighbor height difference s at the point of instability becomes large and it grows rapidly in time. Since higher moments of s (i.e, σ_q for large q) are more sensitive to such large values of s, the growth of σ_q in time would be faster for larger values of q. The instability would also produce a long tail extending to large values in the distribution of s, leading to departures from single-exponent scaling for the correlation functions $\{G_q\}$. In fact, we do find approximate multiscaling in our simulations near the time of onset of the instability. The time interval over which such behavior is observed in the systems considered so far is, however, very short. This is due to the following reason. In the continuum equations, the time evolution of the system cannot be followed numerically beyond the instability time because the height variables become too large. In the atomistic KD model, the height variables increase so fast after the onset of the instability that global quantities such as the width of the interface begin to show deviations from scaling. In order to explain the numerical results obtained in Refs. [6,7], it is necessary to have a situation in which global quantities scale in a normal way, whereas the quantities $\{\sigma_q\}$ and $\{G_q\}$ show anomalous multiexponent scaling. The discussion above suggests that such a situation may be realized if the instability is ''controlled'' in some way. We have considered several different ways of controlling the instability. We describe here the results obtained from simulations of two 1D models in which the instability is controlled by replacing the $|\nabla h_i|^2$ term appearing in the discretized LD equation and in the KD model by $f(|\nabla h_i|^2)$, where $f(x) \equiv (1-e^{-cx})/c$, c being an adjustable parameter. Note that this replacement corresponds to the introduction of an infinite number of higher-order nonlinear terms of the form $|\nabla h_i|^{2n}$ with specific coefficients that depend on the value of c. Since the function $f(x)$ approaches a *constant value* $1/c$ in the limit $x \gg 1/c$, it is easy to show analytically that the growth instability of isolated pillars in both these models is completely suppressed if the value of c is higher than a critical value that depends on the value of λ. For values of c smaller than this critical value, the instability occurs for an isolated pillar if its height lies within a range $h_{\min}(\lambda,c) < h_0 < h_{\max}(\lambda,c)$.

We have studied numerically the behavior of both these models for different values of λ and c. We describe below results obtained for the atomistic KD model because simulations of this model are easier, so that better statistics can be obtained. Very similar results, but with poorer statistics, were obtained for the modified version of the discretized LD equation.

For values of c that are so large that the instability is completely absent, we find conventional scaling with exponents close to the expected values. For very small values of c, we find deviations from scaling for global quantities such as the interface width. More interesting behavior is found in simulations with intermediate values of c for which the instability occurs for a limited range of values of h_0. For such values of c, the instability is expected to be operative over a limited time interval. At very early times, the values of the nearest-neighbor height difference s are small and no instability occurs. As time progresses, the instability sets in when the value of $s_{\max}$ crosses $h_{\min}$. The value of s at the point of instability then grows rapidly until the growth is cut off at $h_{\max}$. As time progresses, the instability occurs at more and more points in the system. The number of points at which a fresh instability can occur decreases in this process. Also, effects of this instability become less pronounced as the typical value of s, which grows in time, approaches $h_{\max}$. So the instability is expected to become ineffective at long times. If multiscaling arises due to the instability, then one expects to see multiscaling only during the finite time interval over which the instability is active. This is precisely the behavior

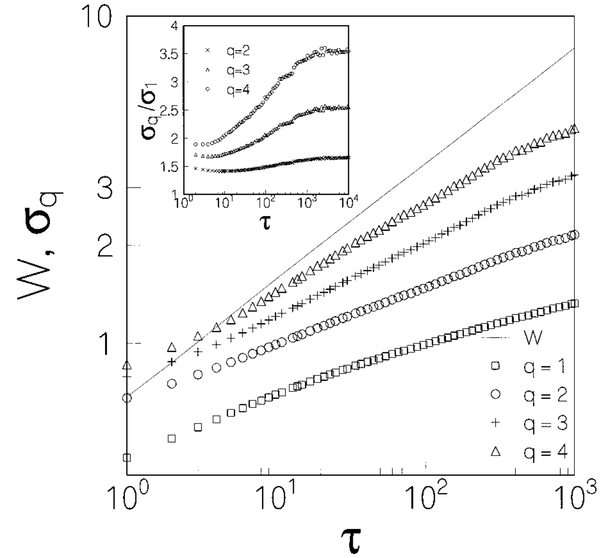

FIG. 1. rms interface width W and the moments σ_q, $q=1$–4, of the nearest-neighbor height difference (see the text) as functions of time τ for the 1D KD model with controlled instability ($\lambda=2$, $c=0.02$). Inset: ratios $\sigma_q(\tau)/\sigma_1(\tau)$, $q=2$, 3, and 4, as functions of time τ.

we find in the simulations. In Figs. 1 and 2, we show a representative set of simulation results obtained for $L=1000$, $\lambda=2.0$, and $c=0.02$, averaged over 2000 runs. For these parameter values, $h_{\min} \simeq 5.0$ and $h_{\max} \simeq 34.0$. As shown in Fig. 1, the rms interface width W shows excellent scaling with an exponent close to 1/3. The quantities $\{\sigma_q\}$, however, show clear evidence of multiscaling during the time interval between $\tau \approx 5$ and $\tau \approx 1000$. Power-law fits to the data over this time interval yield the following values for the effective

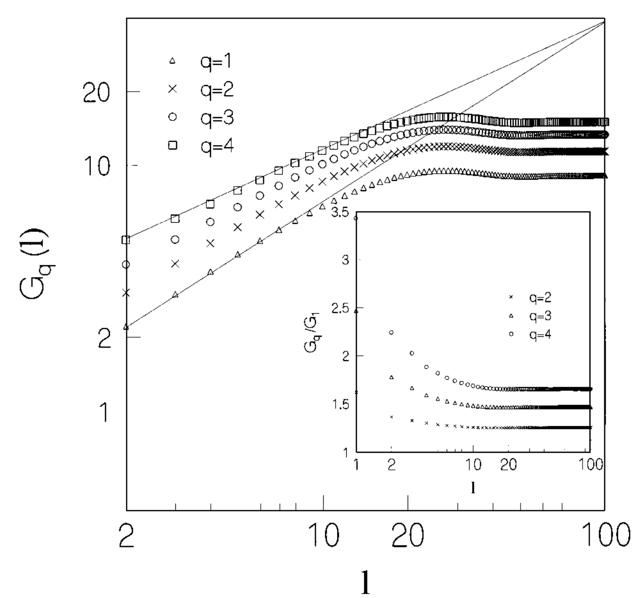

FIG. 2. Height-difference correlation functions $G_q(l)$, $q=1$–4, as functions of the separation l for the 1D KD model with controlled instability ($\lambda=2$, $c=0.02$, $\tau=1000$). The solid lines are power-law fits to the data for $l \leq 10$. Inset: ratios $G_q(l)/G_1(l)$, $q=2$, 3, and 4 as functions of l.

exponents: $\alpha_1/z=0.14\pm0.02$, $\alpha_2/z=0.17\pm0.02$, $\alpha_3/z=0.22\pm0.02$, and $\alpha_4/z=0.26\pm0.03$. These exponent values are similar to those found in Ref. [6] for the 1D DT model [4]. As shown in the inset of Fig. 1, where we have plotted the time dependence of the ratios σ_q/σ_1 for $q=2$, 3, and 4, the multiscaling is not present at very early times and also at times longer than about 1000. By monitoring the time development of the distribution of $\{s_i\}$, we find that $\tau\approx1000$ is precisely the time at which the instability begins to level off.

In Fig. 2, we have plotted the correlation functions $\{G_q\}$ for the same system at time $\tau=1000$. Multiscaling is clearly seen, with the following exponent values calculated from power-law fits to the data for $2\leqslant l\leqslant10$: $\zeta_{11}=0.74\pm0.03$, $\zeta_2=0.66\pm0.03$, $\zeta_3=0.58\pm0.03$, and $\zeta_4=0.50\pm0.03$. The multiscaling behavior for $l\leqslant$ 20 is also seen clearly in the inset, where we have plotted the ratios $G_q(l)/G_1(l)$ for $q=2$, 3, and 4 as functions of l. From the calculated value ($\simeq0.35$) of the exponent β (defined by $W\sim\tau^\beta$ before saturation), we estimate the value of $z=1/(1-2\beta)$ to be about 3.4. Also, the value of the exponent α (defined by $W\sim L^\alpha$ after saturation) is found to be about 1.25 from calculations of the sample-size dependence of the interface width after saturation. These exponent values satisfy the expected relation [6] $\zeta_q+\alpha_q=\alpha$ within error bars, although there appear to be systematic deviations from this relation for large q. Very similar results were obtained in Ref. [6] for the 1D DT model.

These results clearly show that multiscaling very similar to that observed in Refs. [6,7] can be generated by a controlled instability. It should, however, be noted that the multiscaling we find is approximate in the sense that it occurs only over a limited range of time. A careful look at the data of Refs. [6,7] indicates that the same is true for the atomistic models studied in these papers. The multiscaling we find is nonuniversal in the sense that the effective exponents α_q and ζ_q depend on the way in which the instability is controlled. Similar nonuniversality was also found in the models of Refs. [6,7]. To establish further the validity of the proposed mechanism of multiscaling, we have studied the evolution of isolated pillars and grooves in the 1D DT model and found the probability of growth of isolated grooves in this model to be very similar to that of pillars in some of the controlled instability models described above.

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