Slow crossover to Kardar-Parisi-Zhang scaling

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The Kardar-Parisi-Zhang (KPZ) equation is accepted as a generic description of interfacial growth. In several recent studies, however, values of the roughness exponent α have been reported that are significantly less than that associated with the KPZ equation. A feature common to these studies is the presence of holes (bubbles and overhangs) in the bulk and an interface that is smeared out. We study a model of this type in which the density of the bulk and sharpness of the interface can be adjusted by a single parameter. Through theoretical considerations and the study of a simplified model we determine that the presence of holes does not affect the asymptotic KPZ scaling. Moreover, based on our numerics, we propose a simple form for the crossover to the KPZ regime.

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Since its inception over 15 years ago, the Kardar-Parisi-Zhang (KPZ) equation [1] has proved itself as a generic stochastic description of a roughening interface. Such interfaces arise in a vast range of physical situations ranging from colloidal aggregation through bacterial growth to forest fires [2]. Typically, one describes such systems in terms of a d-dimensional plane (substrate) above each point $\mathbf{r}$ of which one associates an interfacial *height* function $h(\mathbf{r})$. The time evolution of the surface described by the height function is given by the $(d+1)$-dimensional KPZ equation thus:

$$\frac{\partial}{\partial t}h(\mathbf{r},t)=v_0+\nu\nabla^2 h+\frac{\lambda}{2}(\nabla h)^2+\eta(\mathbf{r},t). \qquad (1)$$

Here $\eta(\mathbf{r},t)$ is a Gaussian white noise of zero mean and correlator $\langle \eta(\mathbf{r},t)\eta(\mathbf{r}',t')\rangle=\Gamma\,\delta^d(|\mathbf{r}-\mathbf{r}'|)\,\delta(t-t')$.

Only for a small number of microscopic growth models—such as restricted solid-on-solid (RSOS) models [3,4]—has Eq. (1) been obtained from first principles [5]. Nevertheless, the appropriateness of Eq. (1) as a coarse-grained description is easily justified using phenomonological arguments as follows. First, the constant v_0 is simply the mean rate at which a flat interface would proceed in the absence of noise; the Laplacian represents a tendency of the interface to smoothen through surface tension and the nonlinear term expresses the fact that one generally expects growth to occur normal to an interface. The noise term models fluctuations superposed on deterministic growth rules.

Kinetic roughening is conveniently studied through examination of the interfacial width $W(t)$:

$$W^2(t)=\langle \Delta h(t)^2\rangle, \quad \Delta h(t)^2=\overline{h(t)^2}-\overline{h(t)}^2. \qquad (2)$$

The angular brackets represent an average over different realizations of the noise (an ensemble average) whereas the overbar denotes a spatial average in a given realization at a given time t. It has long been known [6] that the behavior can be summarized as a dynamic scaling relation $W(t)\sim t^{\beta}f(t/L^z)$ where $f(u)=$const for small u, giving β as the early time growth exponent; for large times $t\gg L^z$, the width saturates as $W\sim L^{\alpha}$ and $f(u)\sim u^{-\beta}$ implying that $\alpha=\beta z$. For the $(1+1)$-dimensional KPZ universality class the exponents are known exactly (via a range of methods, see [2]) as $\alpha=\frac{1}{2}$, $\beta=\frac{1}{3}$, and $z=\frac{3}{2}$.

The robustness of the KPZ description is due to a very important property: the derivatives of h that appear in Eq. (1) are the only ones whose contribution does not diminish under a rescaling transformation. The consequence of this is that any interface whose rate of growth depends only its local shape will be adequately described by Eq. (1) *on sufficiently large length and time scales*. Known ways of changing the asymptotic scaling are to alter the nature of the noise—e.g., to power-law distributed or correlated noise [7]—or to introduce nonlocal dynamics. By nonlocal dynamics it is meant that the velocity of the interface at a point depends on quantities other than the gradient of the height function there.

One origin of nonlocal contributions to surface growth is a bulk structure that is not compact. To understand this, consider first the case where the structure is compact, i.e., the surface grows by absorption of particles in such a way that no holes (bubbles or overhangs) are created. RSOS models [3,4] are examples of such a system. In this instance it is clear that the interface is *sharp* on the microscopic scale and the entire system can be completely described by the height function $h(\mathbf{r})$. Furthermore, the interfacial dynamics are entirely local and Eq. (1) should apply. Indeed, it is found that RSOS models exhibit KPZ scaling even at small system sizes [2].

An example of the contrasting situation of a noncompact bulk structure is the Fisher wave [8]. To realize a Fisher wave microscopically, one must include particle removal processes in a growth model. As a result, (i) the bulk contains holes; (ii) the interface is *smeared out*: by this we mean that there is a finite interfacial region in which a coarse-grained density field decays to zero due to the presence of holes; and (iii) the interfacial motion could, in principle, be affected by fluctuations within the density field away from the interface (nonlocal dynamics). Consequently, the height function $h(\mathbf{r})$ does not uniquely specify a configuration of the density field and thus it is possible that its evolution may not be adequately described by the KPZ equation (1), which contains only $h(\mathbf{r})$. Numerical evidence for this scenario has recently been presented in the context of Fisher waves: most notably through a roughness exponent of $\alpha \approx 0.4$ for $d=1$ [8].

Even when the interfacial dynamics are local, numerical studies have suggested that α is reduced when the bulk structure contains holes: for the ballistic deposition (BD) model values of $\alpha = 0.42(3)$ [6] and 0.47(1) [4] were reported in early work on $(1+1)$-dimensional BD, whereas more recent very large-scale simulations [9] yielded an estimate of $\alpha = 0.45$. Although BD is generally accepted as being a realization of KPZ growth, the possibility that a noncompact bulk structure implies a new non-KPZ university class has been raised [9,10].

In this work we introduce a model of interfacial growth in which a parameter k allows us to vary the density of the bulk and hence the sharpness of the interface, and in turn any nonlocality in the interfacial dynamics. When $k=0$, the bulk is essentially compact and the interface nearly sharp—i.e., the density decays rapidly to zero across the interface. Here, we expect, and indeed observe, KPZ interfacial scaling. For nonzero k (a more smeared-out interface) our preliminary studies give an estimate of α close to 0.4, consistent with [8]. Thus the model apparently gives two different scaling behaviors depending on whether the interface is smeared out or not. However, we argue, through consideration of how the KPZ equation might be modified to incorporate the effect of holes in the interfacial region, that after sufficient coarse graining the KPZ equation is in fact the correct description for all values of k. In order to demonstrate this quantatively we study a simplified model that allows us to push the numerics to larger systems. We find that our data can be well fitted by a crossover scaling form to the KPZ scaling. The considerations that lead us to conclude that the KPZ equation is the correct description are generic and not model specific. Thus we conclude that values of a roughness exponent close to 0.4, as reported elsewhere for different models [8], are very likely the result of not having reached the asymptotic scaling regime.

We now define our interfacial growth model, which we shall call the wetting model. It comprises a d-dimensional substrate at $z=0$ where z is the growth direction. Periodic boundary conditions (with periodicity L) are imposed in the directions perpendicular to z. In order to sustain growth, the substrate is kept fully occupied (wet) at all times. Wetting events, where an occupied site causes its neighbor above (in the $+z$ direction) to become occupied, occur at a rate r. Additionally, a site at $z>0$ can dry out (become empty) with rate k. Particles (occupied sites) can move to a neighboring site with the same z coordinate, each at rate $D/(2d)$ and subject to the condition that the receiving site is empty. We define the height h of the interface between the wet and dry regions as the z coordinate of the uppermost occupied site above substrate position $\mathbf{r}$ [11]. We consider henceforth only the case $d=1$ (see Fig. 1) and thus replace $\mathbf{r}$ with x.

Before concentrating on the interfacial scaling behavior, we note some other interesting properties of the wetting model. First, if the ratio r/k of the wetting rate to the drying-out rate is too small, there will be no interfacial growth: as r/k is increased past some critical value (dependent on D) there is a wetting transition [12] to a regime where the wet region invades the dry part of the lattice. This transition is related to the directed percolation universality class [13]. Under these conditions one has a moving interface and interfacial growth. The limit $D=0$ reduces the model to a set of L noninteracting one-dimensional (1D) stochastic processes, namely asymmetric contact processes. The opposite limit $D \to \infty$, $L \to \infty$ renders the dynamics equivalent to a *deterministic* version of the same 1D process. Indeed, this case constitutes a microscopic realization of deterministic growth processes of the type studied in [14]. A fuller discussion of all the regimes will be presented elsewhere [15]; for the present study of interfacial scaling, we use intermediate values of D and r.

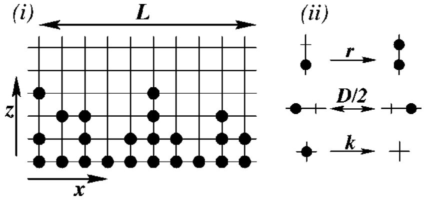

FIG. 1. (i) Realization of the $(1+1)$-dimensional wetting model for $L=10$. (ii) The rates defining the model dynamics.

We first check the growth of the interface in the case $k=0$ which is the situation where no holes may be spontaneously created in the bulk. Thus the bulk density is 1, and the only holes present are in a small zone (numbering a few lattice sites) near the interface and which have their origin in the sideways diffusion process. We consider the interface therefore effectively sharp and thus expect to find KPZ behavior. This is tested by performing a scaling collapse of the width [$W(t)/L^{\alpha}$ against t/L^{z}] which is shown in Fig. 2(i) for a range of system sizes and representative values of D,r. Good data collapse was achieved using exponents consistent with KPZ scaling: $z=1.50(5)$, $\alpha=0.49(2)$ where the figure in parentheses indicates the change in the last quoted digit required before the collapse becomes noticeably worse.

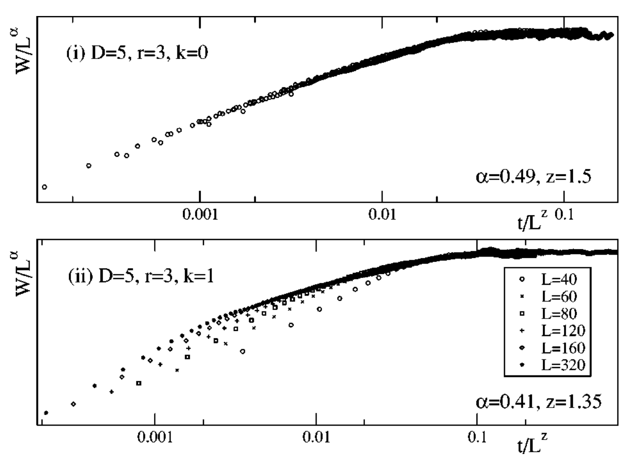

FIG. 2. The width function $W(t)$ in the wetting model with the drying-out process (i) inactive and (ii) active. Data from different system sizes L were made to collapse (at least at late times) by scaling W with L^{α} and t with L^{z}. The values of α, z used in each case are shown on the plots.

The second plot in Fig. 2 shows the corresponding collapse for the case where $k=1$, i.e., wet sites can dry out leaving holes in the bulk. We found we had to change the scaling exponents to $z=1.35(5)$, $\alpha=0.41(2)$ in order to obtain collapse of the saturation width. Note that in comparison to Fig. 2(i) the collapse is far less convincing. Therefore, although we appear at first sight to have obtained a value of the roughness exponent α consistent with [8,9], it is not clear that we were able to probe the true asymptotic scaling regime before simulation run times rendered increases in L impractical.

To assess whether the true scaling regime had been accessed, i.e., whether one truly has asymptotic scaling different from KPZ scaling in Fig. 2(ii), we consider how a smeared-out interface might be described through a modifed version of Eq. (1). In order to incorporate a generic coupling of the interface to holes in the bulk we introduce an additional term into Eq. (1) as follows:

$$\frac{\partial}{\partial t}h(x,t)=v_0+\nu\nabla^2 h+\frac{\lambda}{2}(\nabla h)^2-kg(x)+\eta, \qquad (3)$$

in which we have included an explicit dependence on k, so that when $k=0$ this equation reduces to Eq. (1) as required. The function $g(x)$ is intended to capture any nonlocal dynamics present. In the case of the wetting model, $-kg(x)$ is the rate at which $h(x)$ decreases when a particles at the interface disappears, implying that $g(x)$ is the size of the gap behind the interface, defined as the distance between the uppermost and second uppermost particle at position x. We have checked explicitly that decreases in $h(x)$ follow closely the profile of the gap size $g(x)$ and so we believe that Eq. (3) describes the wetting model adequately, at least on a coarse-grained level.

We now proceed to show that the presence of the extra term in Eq. (3) does *not* affect the long-wavelength properties of the interface. To this end we studied the statistics of $g(x)$ in the wetting model. We found first that the distribution of gap sizes became stationary rather quickly, at times when the interface was still roughening. In Fig. 3(i) we plot the stationary gap size distribution for three different system sizes. We note that the distribution is system-size independent and decays exponentially. Thus the finite length scale associated with the gap remains constant as the substrate length is increased, and is irrelevant once L is sufficiently large. Of course, at smaller L, $g(x)$ will play some role.

Now we argue that unless $g(x)$ exhibits scale-invariant correlations in the x direction, it will be rescaled into the noise term already present in Eq. (1). Specifically, g can be replaced with $g_0+\tilde{\eta}$ where g_0 is a constant that can be absorbed into v_0 and $\tilde{\eta}$ is a noise term with irrelevant short-range correlations that can be absorbed into the noise term η in Eq. (1). To exclude the possibility of long-range correlations, we plot the correlation function $c(\delta)=\langle g(0)g(\delta)\rangle/\langle g(0)^2\rangle-1$ in Fig. 3(ii). It is clear that for $L=100,200,400$ the correlation length retains the same (finite) value. The small anticorrelation for large δ vanishes with increased L and is a consequence of finite system sizes.

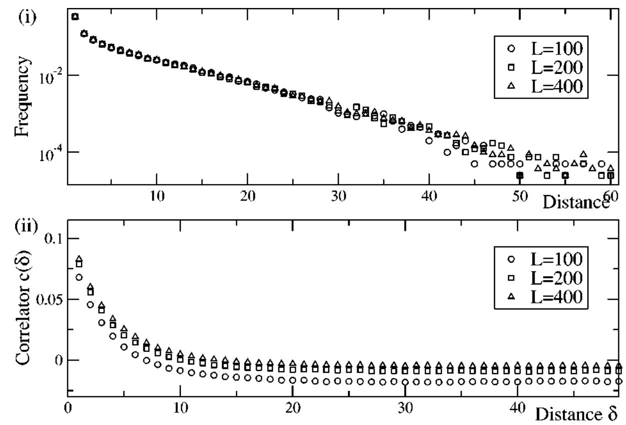

FIG. 3. (i) The gap size g probability distribution for the wetting model with $L=100,200,400$. (ii) The gap size correlation function in the x direction for the wetting model with $L=100,200,400$. In both cases $D=5$, $r=1.5$, and $k=1$.

Thus, our results strongly suggest that the term $g(x)$ modifying the KPZ equation from (1) to (3) is, for the wetting model, purely cosmetic. In short, we contest that if L were increased beyond the values used in Fig. 2 a crossover toward KPZ scaling would be observed. However, the system sizes that would be required to demonstrate quantitatively the crossover in the wetting model are unfeasible.

In order to examine the nature of such a crossover we study a simplified model which retains the important feature of the wetting model, namely, a parameter that allows us to go from a sharp to a smeared-out interface. The model is constructed by replacing the two-dimensional density field of the wetting model with an interface $h(x)$ coupled to a gap of size $g(x)$. Thus this model, which we will refer to as the ballistic deposition and desorption (BDD) model, should also be governed by Eq. (3).

The dynamics of the BDD model are defined as follows. At each time step, one chooses a substrate position x at random and then performs either a particle deposition move (at unit rate) or a desorption move (at rate κ). In the former case, a particle is ''dropped'' vertically downward in column x until it comes to rest at a site whose nearest neighbor is occupied. This increases the height $h(x)$ by an amount that defines the gap size $g(x)$. A desorption move is implemented by decreasing $h(x)$ by $g(x)$ and replacing $g(x)$ with one of the other gap sizes in the system, chosen at random (maintaining a self-consistency in the gap size distribution). The desorption move serves to smear out the interface, and thus the rate κ plays the same role as k in the wetting model (although no numerical equivalence between the two should be assumed).

With the desorption rate κ set to zero, one recovers the ballistic deposition model which is a widely accepted realization of Eq. (1) [16] and thus the interface should exhibit KPZ scaling behavior. With nonzero κ the height h can decrease by a random variable g. We have found that the statistics of g in the BDD model are very similar to those shown in Fig. 3 for the wetting model: both the gap distribution and correlation functions are stationary and have no dependence

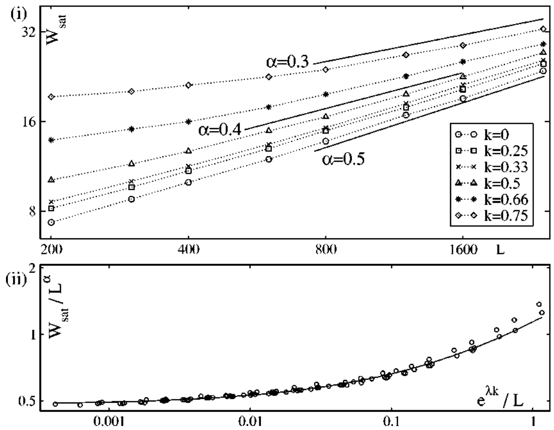

FIG. 4. (i) Log-log plot of saturation width W_{sat} for different L and κ in the BDD model. The solid lines correspond to $\alpha=0.5$ (KPZ), 0.4, and 0.3 and illustrate how underestimates in α arise if one has not taken care to reach the scaling regime. (ii) The same data scaled according to Eq. (4). The parameters $\alpha=0.5$ and $\lambda=7.4$ were used and the solid line corresponds to $A=0.47$, $B=0.66$, and $\gamma=0.55$ in Eq. (4).

on system size; the gap size distribution has an exponential tail and the correlation length in the x direction is almost zero. Thus we believe that the BDD model mimics the wetting model in all respects that may affect universal scaling behavior.

A clear insight into interfacial scaling as one approaches the scaling regime is obtained from Fig. 4(i) which shows the saturation width against system size for a range of desorption parameters κ. With both axes logarithmic, one can define an effective exponent $\alpha(L,\kappa)$ as the gradient of the function $\log W(\log L,\kappa)$. As is evident from the graph, there is a significant range of L,κ for which $\alpha(L,\kappa)\approx 0.4$–$0.45$ (similar to the values of [8]). However, the graph also gives evidence for a trend in which the limit $\lim_{L\to\infty}\alpha(L,\kappa)$ coincides for all values of κ. This limit would give the true scaling value for the roughness exponent α for all κ. We show this by collapsing all the data of Fig. 4(i) onto a single curve.

To effect the collapse we use the simple crossover scaling form

$$W_{\text{sat}}(L,\kappa)=L^{\alpha}\{A+B[\ell(\kappa)/L]^{\gamma}\} \tag{4}$$

where $\ell(\kappa)$ is some finite length induced by the nonlocal desorption process and γ is the crossover exponent. Remarkably, a reasonable collapse for all L,κ could be effected by taking A,B constant and $\ell(\kappa)=\exp\lambda\kappa$ with λ constant—see Fig. 4(ii). That is, all the κ dependence enters through $\ell(\kappa)$ in a very simple way.

The fit to Eq. (4) allows a precise estimate of $\alpha=0.50(1)$ (coincident with the KPZ value) for the BDD model for all κ. Without invoking Eq. (4) the estimation of α would be hampered by the slow power-law crossover to the asymptotic regime and underestimates of α would be obtained (as discussed above). This crossover would explain the discrepancies between previous estimates of α for BD ($\kappa=0$) and the KPZ value [6,4,9].

It is interesting to see how the crossover scaling form (4) generalizes the standard procedure of introducing an intrinsic width, first used for an Eden growth model [17,16]. In that approach one writes $W_{\text{sat}}^2=AL^{2\alpha}+w_i^2$, i.e., the scaling width and the intrinsic width w_i are added in quadrature. Our scaling form would coincide with this procedure for large L if $\gamma=2\alpha=1$. Moreover, $\gamma=\alpha=\frac{1}{2}$ would correspond to the distinct procedure of the linear addition of two widths. For the BDD model, we have found that data collapses, all of reasonable quality, can be achieved for values of $\gamma\approx 0.5$–0.7.

To summarize, we first studied a wetting model whose bulk phase contains holes if a parameter k is nonzero. In the case $k=0$, the expected KPZ scaling was observed, whereas for k nonzero simulations on small systems gave a value of the roughness exponent α reminiscent of values reported for a wide range of models with holes in the bulk phase [8,9]. Through theoretical considerations we concluded, in fact, that with k nonzero and in the true asymptotic scaling regime, KPZ exponents should return. To demonstrate and quantify the crossover to the KPZ regime we studied the BDD model for which more extensive data could be obtained. We identified a power-law crossover of the form (4). An interesting question concerns the applicability of this simple form to other models, and in particular whether the value of γ is universal.

To conclude we place our observations in the context of other work. Very recently, it has been suggested [10] that in the case of a stable phase invading an unstable phase (e.g., Fisher waves and our wetting model) one should observe not the $d+1$ KPZ exponents but instead those of the KPZ equation in $d+2$ dimensions. The essence of that work is that, in the situation where an interface is not sharp (e.g., due to the presence of holes), the correct surface to consider in terms of the scaling is (a suitable transformation of) the density field interpreted as a height variable. As the dimensionality of the density field over the smeared-out interfacial region is necessarily one greater than that of the interface, the d-dimensional interface should scale in the same way as a line across the $(d+1)$-dimensional density surface governed by the $d+2$ KPZ equation. However, as also pointed out in [10], the system does not scale isotropically: a rescaling transformation would affect only the size of the substrate. Thus if the interfacial region remains finite for increasing L the relative size of the extra dimension shrinks to zero and thus one returns to the $d+1$ KPZ equation, i.e., there is a crossover to KPZ scaling. For the models studied in the present work, our numerical evidence explicitly shows a finite interfacial region indicated by the typical gap size remaining constant as the system size L is increased. Furthermore, for the BDD model we could quantify the crossover. It would be interesting to confirm whether this crossover is also present in the model of [8].

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