Kinetic roughening in deposition with suppressed screening

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Models of irreversible surface deposition of k-mers on a linear lattice, with screening suppressed by allowing only those overhangs that fully block small gaps, are studied by extensive Monte Carlo simulations of the temporal and size dependence of the growing interface width. Despite earlier findings that for such models the deposit density tends to increase away from the substrate, our numerical results place them within the standard Kardar-Parisi-Zhang universality class.

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The standard, KPZ (Kardar-Parisi-Zhang) [1] model of kinetic roughening of growing surfaces (reviewed, e.g., in [2,3]) yields the scaling prediction for the interfacial width W as a function of time, T, and substrate size, L,

$$W \simeq L^{\zeta} F\left(TL^{-z}\right) \ , \tag{1}$$

where for one-dimensional (1D) surfaces the exponent values are

$$\zeta_{\rm KPZ} = \frac{1}{2} \ , \tag{2}$$

$$z_{\rm KPZ} = \frac{3}{2} \ . \tag{3}$$

In fact, the value $\zeta = 1/2$ is common to many one-dimensional (1D) models of fluctuating interfaces, stationary or growing. However, Eq. (3) is characteristic of the KPZ universality class. For instance, for stationary, thermally fluctuating interfaces, Eq. (3) is replaced by $z = 2$. These values have been well established by numerical simulations and are believed to be exact (in 1D). The generic behavior of the scaling function F in (1) for small arguments is power law as will be further discussed later: see Eqs. (7) and (8), etc. For large arguments, the function F approaches a constant.

In deposition, the KPZ approach focuses on fluctuations of the growing surface which are determined by the evolving structure of the uppermost deposit layers, which are in the process of being formed due to arrival and adhesion of particles according to the rules of a particular model at hand. However, once the advancing surface has passed each fixed height h (measured from the substrate which is at $h = 0$), and once all the transient rearrangement of particles (if allowed in the model) ran its course, the remaining asymptotic (large-time), "saturated" deposit density $\rho(h)$ will be a function of h only. [We only consider infinite-size substrates when discussing $\rho(h)$ here.]

A natural question to pose is to what extent does the h dependence of $\rho(h)$ keep "memory" of the interfacial fluctuations from the time when the interface passed at height h? In an interesting study [4], Krug and Meakin argued that to the leading order, the KPZ fluctuations affect the growth rate by introducing, in the average deposit density $\rho(h)$ at the height h away from the substrate, the contribution,

$$\Delta\rho_{\rm KPZ} \simeq \lambda h^{-2(1-\zeta)/z} \ . \tag{4}$$

This expression applies for times T large enough so that the density has reached its limiting value at h, and assuming no finite-L effects, i.e., for infinite substrates. The coefficient $\lambda > 0$ is related to the nonlinear growth term in the KPZ theory [1–3]. Specifically, in 1D, this contribution suggests the coverage *decreasing* to the limiting large-h value according to the power law $\Delta\rho = \rho(h) - \rho(\infty) \sim h^{-2/3}$. The prediction Eq. (4) has been verified for several ballistic deposition models in 1D and 2D [4,5].

A recent study [6] of certain 1D models [7] with screening suppressed by disallowing overhangs in a manner to be defined shortly, yielded a surprising conclusion that in these models the density actually *increases* away from the substrate according to the power law,

$$\Delta\rho = \rho(h) - \rho(\infty) \simeq -Ch^{-\phi} \ , \tag{5}$$

where $C > 0$ and $\phi \simeq 0.3$. An interesting question, thus, arises: are these models in a universality class different from KPZ? An alternative is that the KPZ contribution to the density, Eq. (4), is possibly not seen because the added mechanism of "compactification" due to suppression of screening, elucidated in [6], yields the density term Eq. (5) with negative exponent ϕ *smaller* in absolute value than the KPZ-contribution exponent. Essentially, this amounts to allowing for both terms: the one displayed in Eq. (5), and also $\Delta\rho_{\rm KPZ}(h)$ from Eq. (4) added up to the right-hand side of Eq. (5). However, in the 1D models of interest the KPZ contribution has a larger-magnitude negative exponent, which makes it a subleading correction difficult to detect by numerical means.

As noted, the quantity $\rho(h)$ was already studied extensively in [6]. In this work, we report extensive numerical simulations of the growing interface width. Our results place the models under consideration [6,7], to be defined in detail shortly, within the KPZ universality class. In fact, the exponent values and scaling form, Eqs. (1)–(3), are confirmed quite accurately. Thus, we favor the scenario whereby the suppression of screening does not change the universality class of the growing interface fluctuations even though it can dominate other aspects of the deposit structure such as variation of the saturated de-

posit density with height. In the latter, the KPZ fluctuation effects are manifested but as a subleading correction.

We consider multilayer deposition of k-mer "particles" on the linear lattice. The deposition attempts are "ballistic;" particles arrive at a uniform rate per site. The group of those k lattice sites, which are targeted in each deposition attempt, is examined to find the lowest layer $n \geq 1$, such that all the k sites are empty in that layer (and all layers above it). The deposition rules are illustrated in Fig. 1. Note that initially the substrate is empty, in all the sites and layers $1, 2, 3, \ldots$. If the targeted group of sites is in the layer $n = 1$, then the particle is deposited: the k sites become occupied. However, if the targeted layer is $n > 1$, then the deposition attempt is accepted only provided no gaps are thereby *partially* covered in layer $n - 1$. Thus, successful deposition of a k-mer in layer $n > 1$ requires that it *fully covers* any gap underneath it in layer $n - 1$. This lower gap must therefore be of size $1, 2, \ldots, k - 1$; see Fig. 1. Otherwise the attempt is rejected.

In successful deposition, at least one of the lattice sites below one of the end coordinates of the arriving k-mer is already occupied in layer $n - 1$. The other end coordinate has an occupied nearest neighbor lattice site in layer $n - 1$, or is itself occupied (in layer $n - 1$). Note that this deposition rule for dimers is the same as in [7]. For all $k = 2, 3, \ldots$ this rule was also used in [6] although its explanation in [6] was unclear and in some places misleading.

Thus, we disallow all overhangs which would *partially* block (screen) gaps in lower layers. In particular, gaps which are large enough to accommodate future deposition events (in layers $n - 1$ or lower) are k site or larger.

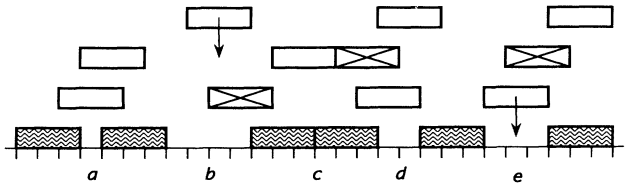

FIG. 1. Deposition of trimers on the 1D substrate. The shaded trimers illustrate a possible configuration in layer $n-1$. Lower layers ($n - 2$, $n - 3$, ...) are not shown. Instead, the underlying lattice structure is indicated. Possible locations of trimer arrival in a deposition attempt are illustrated. Gap a of size 1 will be successfully covered by any overlaying trimer (two out of the three possible locations are shown). Gap b of size 4, however, cannot be blocked in any of the possible arrival positions: in four "partial overhang" cases (one of which is shown) the deposition will be rejected (crossed trimer). Two other configurations (one of which is shown by an arrow-marked trimer) will result in deposition in a layer lower than n. Deposition over gaps of size 0, marked c, is always possible. For gaps of size 2, marked d, the successful deposition configurations are those that *fully* cover this gap. Both of them are shown, as is one of the two disallowed configurations. Finally, gap of size 3, marked e, cannot be fully covered. Therefore, the deposition will either be rejected (crossed trimer) or occur in a lower layer (arrow-marked). We note that head-on depositions (rightmost trimer), which involve no gaps, are allowed as well by our rules.

These gaps will not be blocked until they are filled up in lower layers: The final, large-time configuration in each layer contains gaps of at most $k - 1$ consecutive empty sites. In fact, deposition in lower layers $1, \ldots, N$ is unaffected by deposition in layers $N + 1$ on. For layer $n = 1$, exact solution for the fraction of occupied sites and for some correlation properties is known [8]; this problem corresponds to monolayer random sequential adsorption in 1D.

Motivation for considering simplified lattice models of deposition with various screening mechanisms is due to relevance to colloid deposition: see [12] and literature cited therein. Indeed, in colloid experiments the deposition process is largely irreversible (no relaxation), while a direct, experiment-based description of screening due to particle-particle interactions in multilayer formation is largely unavailable. One has to rely on phenomenological modeling instead. Therefore, identification of universality classes with various screening mechanisms is of interest. In our 1D model the screening is substantially suppressed; only small gaps survive in the final deposit morphology.

We studied the growth of the interfacial width in this deposition process. Specifically, we define L as the number of sites in the lattice (and we use periodic boundary conditions). The Monte Carlo (MC) time variable T is conveniently defined to have one deposition attempt per lattice site per unit time. The heights of the deposit, h_j, at sites $j = 1, \ldots, L$, were defined as the number of layers from the substrate to the last occupied layer, at each lattice site j. The rms width was defined as

$$W = \left\langle \left[\frac{1}{L} \sum_{j=1}^{L} h_j^2 - \left(\frac{1}{L} \sum_{j=1}^{L} h_j \right)^2 \right]^{1/2} \right\rangle , \qquad (6)$$

where the average $\langle\,\rangle$ over independent MC runs was taken after calculating the square root.

Figure 2 presents results for large substrates, $L = 2000$. These data, for $T \leq 200$, were typically averaged over 1000 independent MC runs. There is no visible size effect for $L = 2000$. Thus, Eq. (1) is replaced by

$$W \simeq T^{\zeta/z} \qquad (L \to \infty) , \qquad (7)$$

which corresponds to assuming that the scaling function $F(t)$ behaves according to $\sim t^{\zeta/z}$ for small arguments,

$$t = TL^{-z} . \qquad (8)$$

Least-squares fits of the data indicate that the exponent in Eq. (7) tends to 1/3. For instance, for the largest-T data, in the range $150 \leq T \leq 200$, we get 0.383, 0.345, 0.316, 0.304, 0.324, for $k = 2, 3, 5, 8, 10$, respectively. Our analyses were based on considering not just the values thus obtained for several T ranges, but also the trend as the time was increased (i.e., the least-squares fits were done for time intervals with both limits increasing). The trend is generally towards 1/3. We propose a conservative exponent estimate,

$$\zeta/z = 0.34 \pm 0.04 . \qquad (9)$$

Admittedly this range is quite wide. However, it is comparable to the error limits in other similar large-scale numerical studies and it comfortably excludes values such

as 1/2 or 1/4, favoring the KPZ [1–3] prediction 1/3. We also checked this estimate for several data sets taken at $L = 1000$ and 1500. The results were unchanged. For larger k, e.g., 10, the onset of the finite-L saturation can be seen for $L =$O(1000).

Analysis of the finite-L properties was complicated by two facts. First, to see finite-L saturation, simulations had to be done for large times. Second, we found that the statistical noise in the data became significant at saturation. Thus averages over many independent runs were required. We restricted our extensive MC runs to one k value, $k = 3$. This value was favored because generally, other conditions being equal, the observed statistical noise became larger as k increased. On the other hand, the $k = 3$ large-L data in Fig. 2 yield an exponent closer to 1/3 than the $k = 2$ data, suggesting, possibly, smaller corrections to the leading scaling behavior.

Figure 3 shows well saturated data for $k = 3$ and lattice sizes $L = 20$, 40, 60, 80, 100. These were averaged over typically 10 000 MC runs. Shown are also data for $L = 300$, averaged over 2000 MC runs, which have not attained saturation for the largest times reached in the simulation. The $L = 2000$ data from Fig. 2 are also included for comparison.

The spread of the saturation values at larger T selected to have only the statistical noise, is shown for $L = 20$, 40, 60, 80, 100 in Fig. 4. For large times, one assumes $F(t \to \infty) \simeq$ const in Eq. (1), so that the width behaves according to $L^{1/2}$. From least-squares fits to various data subsets for $L = 40$, 60, 80, 100, i.e., excluding the data for $L = 20$, which seem to be too small to reach the true asymptotic behavior, we propose the estimate,

$$\zeta = 0.49 \pm 0.03 \ . \tag{10}$$

As mentioned earlier, this exponent is the same for various 1D universality classes and it cannot be used to identify the KPZ behavior. However, accurate verification of the value 1/2 suggests that our data are generally well within the asymptotic regime for lattice sizes above O(40).

Thus, we also attempted the full scaling data collapse, i.e., we checked that the quantity,

$$w = WL^{-1/2} \ , \tag{11}$$

when plotted as a function of t defined in Eq. (8), is represented by a unique function $F(t)$; see Eq. (1). Of course the data collapse is exact only in the limit $L \to \infty$ and $T \to \infty$, with fixed t. Figure 5 illustrates the "collapse" for $k = 3$, where we used data for $L = 80$, 100, 300, 2000, described earlier. We also included data for $L = 1000$ which, together with the $L = 2000$ data, yield the dense portion of the plot for $w \lesssim 0.3$ (see Fig. 5): panel (a). This region was further enlarged on the log-log plot: panel (b).

All the general expectations on the form of the scaling function $F(t)$ are qualitatively confirmed by our data. Specifically, it approaches a constant for large arguments. The power-law behavior with exponent 1/3 for small arguments is confirmed only semiquantitatively. Note that the leftmost data in panel (b) of Fig. 5 does not satisfy the condition T large, while the rightmost data fails the

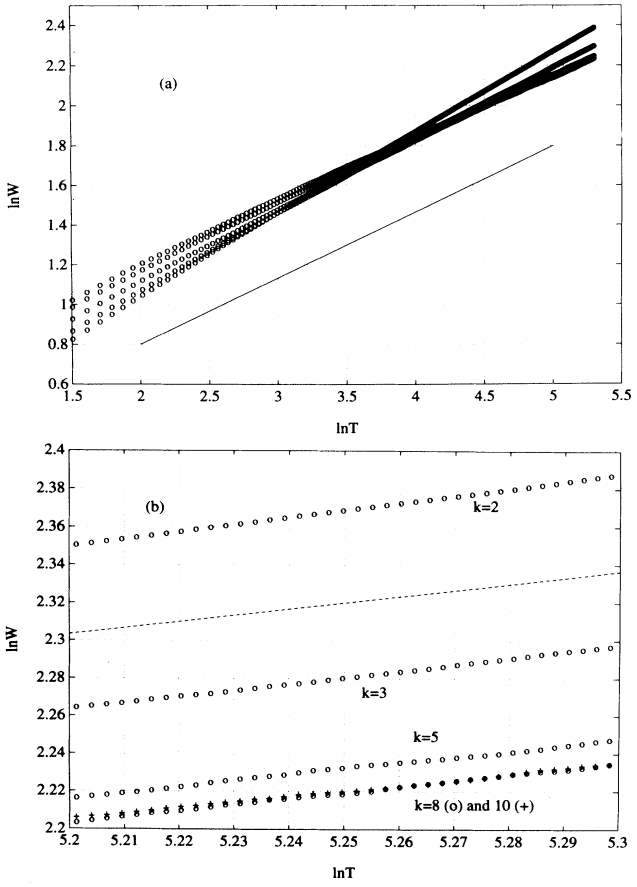

FIG. 2. (a) Data for $k = 2, 3, 5, 8, 10$ on substrates of size $L = 2000$. For small T, $W_{k=2} < W_{k=3} < \cdots < W_{k=10}$. For large T, the relation is reversed on the average, although the differences, especially for $k = 8$ and 10, are small and fluctuate in sign, due to statistical noise. The solid line illustrates slope 1/3. (b) To emphasize consistency with the slope 1/3 (illustrated by the dashed line), the largest-T data were replotted on a finer scale. Note that the data for $k = 10$ were marked by + symbols, while the data for other k values were marked by ○ symbols.

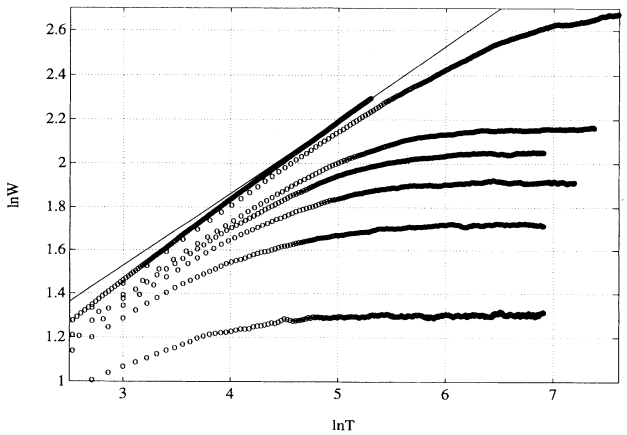

FIG. 3. Data for $k = 3$ on substrates of sizes $L = 20$, 40, 60, 80, 100, 300, 2000. For fixed T, $W(L)$ values monotonically increase with L. Solid line illustrates slope 1/3.

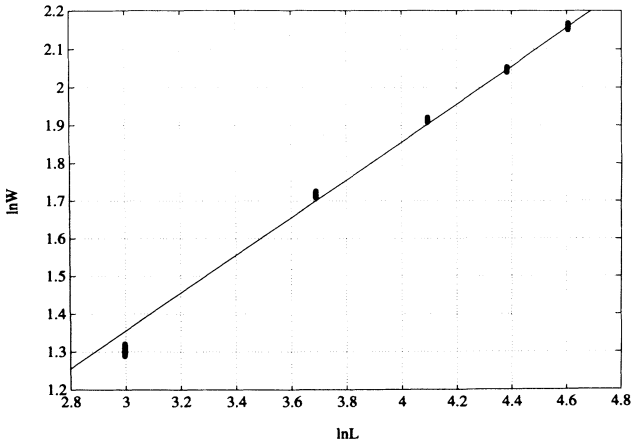

FIG. 4. Large-T data for $k = 3$ on substrates of sizes $L = 20$, 40, 60, 80, 100, illustrating the L dependence of the saturation values (with the statistical noise). Solid line illustrates slope 1/2.

condition t small. Thus, only the central region, dense data for $L = 1000$ and $L = 2000$, show the appropriate asymptotic slope 1/3.

There are several extensive numerical studies of the KPZ and other growth-universality classes by scaling data collapse and tests of universality of quantities derived from scaling functions similar to $F(t)$; see, for instance, [9–11]. The quality of our data is comparable to other accurate verifications of the scaling predictions in 1D, though we found no results in the literature to allow direct comparison with the scaling-function data such as Fig. 5.

In summary, we found that, by extensive MC simulations measuring directly the growing interface width, the models with suppressed screening, which show unusual density variation [6] are, in fact, described quite accurately by the KPZ scaling form [1–3] typical of growing interfaces, with the appropriate 1D exponent values. After this work was completed, we learned of a new MC study by Ko and Seno [13], of ballistic and other deposition processes. Specifically, these authors question the KPZ universality class identification for ordinary ballistic deposition in 1D. While the details of the models are different, we note that our central exponent values are closer to KPZ than those reported in [13], while the error limits are comparable.

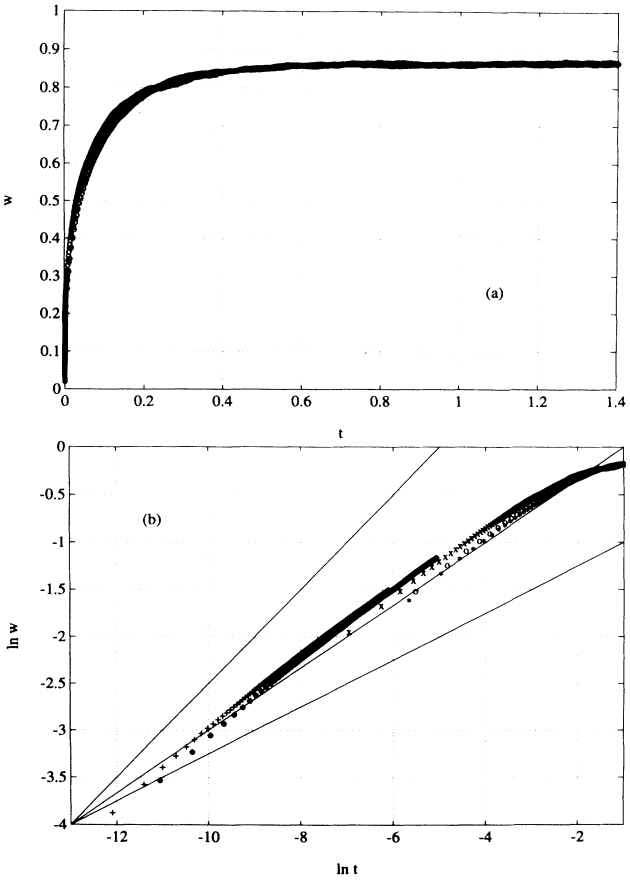

FIG. 5. (a) Scaling data collapse according to Eq. (1), for $k = 3$. The scaled width w is plotted as a function of the scaled time t, for substrate sizes $L = 80$, 100, 300, 1000, 2000. (b) The region of small-w and small-t explored on the log-log plot. The data sets for $L = 80$, 100, 300, 1000, 2000, are marked, respectively, by $*$, $\circ$, $\times$, $\oplus$, $+$. The solid lines indicate slopes 1/2, 1/3, 1/4.

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