Height and roughness distributions in thin films with Kardar-Parisi-Zhang scaling

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Abstract

We study height and roughness distributions of films grown with discrete Kardar-Parisi-Zhang (KPZ) models in a small time regime \((t/L^z \ll 1)\) which is expected to parallel the typical experimental conditions. Those distributions are measured with square windows of sizes \(8 \leq r \leq 128\) gliding through a much larger surface. Results for models with weak finite-size corrections indicate that the absolute value of the skewness and the value of the kurtosis of height distributions converge to \(0.2 \leq |S| \leq 0.3\) and \(0 \leq Q \leq 0.5\), respectively. Despite the low accuracy of these results, they give additional support to a recent claim of KPZ scaling in oligomer films. However, there are significant finite-size effects in the scaled height distributions of models with large local slopes, such as ballistic deposition, which suggests that comparison of height distributions must not be used to rule out KPZ scaling. On the other hand, roughness distributions of the same models show good data collapse, with negligible dependence on time and window size. The estimates of skewness and kurtosis for roughness distributions are \(1.7 \leq S \leq 2\) and \(3 \leq Q \leq 7\). A stretched exponential tail was found, which seems to be a particular feature of KPZ systems in \(2+1\) dimensions. Moreover, the KPZ roughness distributions cannot be fitted by those of \(1/f^\alpha\) noise. This study suggests that the roughness distribution is the best option to test KPZ scaling in the growth regime, and provides quantitative data for future comparison with other models or experiments.

Key words: computer simulations; models of surface kinetics; surface roughness; height distributions; roughness distributions; Kardar-Parisi-Zhang scaling

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1 Introduction

In order to understand the basic mechanisms of thin films or multilayer growth, it is helpful to compare the scaling properties of their surfaces with those of statistical growth models, which are able to represent such features without considering all details of the microscopic interactions [1,2,3]. The usual starting point for this comparison is to measure the surface roughness and the associated scaling exponents. The local roughness \( w(r, t) \) is defined as the rms fluctuation of the interface height averaged over windows of linear size \( r \) spanning the surface at time \( t \). For fixed \( t \), it scales as \( w \sim r^\alpha \) for \( r \ll L \), where \( \alpha \) is the roughness exponent and \( L \) is the total surface length. On the other hand, the global roughness \( \xi(t) \) is defined as the rms height fluctuation over the whole surface \( [w(r, t) \text{ for } r \to L] \), and scales as \( \xi \sim t^\beta \), where \( \beta \) is called the growth exponent. Instead of the local roughness \( w \), one may use height-height correlation functions, which have similar scaling properties.

A large number of experimental works have already obtained scaling exponents consistent with those of the Kardar-Parisi-Zhang (KPZ) theory [4] - see e.g. Refs. [5,6,7,8,9,10,11,12]. However, the available scaling region of experimental data is usually very small, including less than one order of magnitude of length or time. In some cases, a crossover from another dynamics to KPZ is suggested [13,14,15,16]. The difficulties to find accurate scaling laws for the local roughness are also present in the study of growth models [17], thus the main limitation is the method and not the nature (experimental or theoretical) of the data. At this point, the methods that provide accurate estimates of exponents for theoretical models are not helpful because they usually consider steady state data, where film thicknesses are very large and the full system is highly correlated \( (t/L^z \gg 1, \text{ where } z = \alpha/\beta \text{ is the dynamic exponent}) \). However, this regime is not typical of experiments, where the thickness and the lateral correlation length are much smaller than the lateral size of the deposit \( (t/L^z \ll 1) \).

This scenario motivates the proposal of alternative or complementary approaches to compare results of theoretical models and experimental data in the growth regime. Two alternatives are suggested by recent theoretical work: the study of the full height distributions [18,19,20], and the study of the full roughness distributions [21,22,23,24,25,26]. For instance, steady state roughness distributions of Gaussian interfaces were already helpful in the analysis of some controversial systems [27,28,29] and in the fit of experimental distributions of depinning interfaces [30]. Moreover, height distributions for KPZ

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systems in $1+1$ dimensions [31] were observed to fit those of combustion fronts propagating in sheets of paper [7], in the growth and in the steady state regimes. However, as far as we know, for three-dimensional (2+1-dimensional) KPZ systems, the currently available numerical results are limited to steady state distributions [19][20][26]. On the other hand, experience in $1+1$ dimensions shows that roughness distributions of EW interfaces in the growth regime are very different from the steady state ones [23], and that KPZ scaling is also very different in these regimes [32][33].

In this work, we will analyze numerical data of height and roughness distributions of discrete KPZ models in the growth regime ($t/L^2 \ll 1$) in $2+1$ dimensions. Our aims are to test the reliability of those distributions to determine the KPZ universality class and to provide a set of quantitative data for comparison with other systems. In order that these results can be compared with experimental data, we will calculate distributions in narrow windows gliding through a much larger substrate. In other words, we will adopt the so-called window boundary conditions (WBC) [24].

First we will show discrepancies in the scaled height distributions of three discrete KPZ models, although the estimates of the absolute value of the skewness and of the kurtosis are not very different when two of them are compared. Despite having a large error bar, the estimate of the skewness for these models agrees with that of Refs. [9][10] for oligomer films. However, the data for the third model (ballistic deposition) exhibit strong finite-size corrections, which suggests that the height distribution cannot be used to rule out KPZ growth. On the other hand, we will show that roughness distributions in WBC show weak finite-size and finite-time corrections, providing a good data collapse for all KPZ models analyzed here. Estimates of the skewness and kurtosis of the universal distribution in the growth regime will be provided here, which we expect to be helpful for future identification of the KPZ universality class in experiments.

The rest of this work is organized as follows. In Sec. 2, we will present the theoretical models considered here and details of the simulation procedure. In Sec. 3, we will present the results for the heights distributions. In Sec. 4, we will present the results for the roughness distributions. In Sec. 5 we summarize our results and present our conclusions.

2 The KPZ equation and the lattice models

The Kardar-Parisi-Zhang equation [4]

$$\frac{\partial h}{\partial t} = \nu \nabla^2 h + \frac{\lambda}{2} (\nabla h)^2 + \eta(\vec{x}, t),$$

(1)
was proposed as a hydrodynamic description of processes where the local slope of the surface has significant effects on the growth velocity. In Eq. 1, $\nu$ is a surface tension, $\lambda$ represents the excess velocity (due e. g. to lateral growth) and $\eta$ is a Gaussian white noise. For growth in two-dimensional substrates, no exact solution is currently available, and the best known estimates of KPZ exponents, $\alpha \approx 0.39$ and $\beta \approx 0.23$, were obtained numerically \[19\[20].

Several stochastic lattice models, which are designed to represent microscopic aggregation processes, belong to the KPZ class, i. e. in the limit of large lengths and long times they are described by the KPZ equation. In this work, we will consider four models in this class: two restricted solid-on-solid (RSOS) models \[34], the etching model of Mello et al \[35] and ballistic deposition (BD). In the RSOS model, the incident particle may stick at the top of the column of incidence if the differences of heights between neighboring columns do not exceed a certain value $\Delta h_{\text{MAX}}$. Otherwise, the aggregation attempt is rejected. Here, we will consider the cases $\Delta h_{\text{MAX}} = 1$ and $\Delta h_{\text{MAX}} = 2$, hereafter called RSOS and RSOS2, respectively. The etching model of Mello et al \[35] is considered in its growth version: at each growth attempt, a column $(x, y)$, with current height $h(x, y) \equiv h_0$, is randomly chosen; subsequently, its height is increased by one unit ($h(x, y) \rightarrow h_0 + 1$), and any neighboring column whose height is smaller than $h_0$ grows until its height becomes $h_0$. Finally, in BD, each incident particle is released from a randomly chosen position far above the substrate, follows a trajectory perpendicular to the surface and sticks upon first contact with a nearest neighbor occupied site \[36\[37].

In all models, one time unit corresponds to $L^2$ random selections of columns of incidence in a lattice of linear size $L$, independently of the average height increase. Simulations were done in lattices with $L = 1024$, up to times $t_{\text{max}} = 8 \times 10^3$ for the RSOS, RSOS2 and BD models and $t_{\text{max}} = 6 \times 10^3$ for the etching model. Nearly 100 different deposits were generated for each model, starting from flat substrates. Our previous experience with simulation of those models \[20\[26] show that these times are sufficiently small compared to the relaxation times to the steady states, so that the deposits are certainly in the growth regime. Periodic boundary conditions were considered, but they are not expected to affect our conclusions because we have analyzed results from windows sizes much smaller than $L$ and the lateral correlation lengths are also much smaller than $L$.

At time intervals typically $\Delta t = 1000$, the local roughness and height distributions were collected for various window sizes $r$, with square windows. To be more precise, we calculated $P_h(\Delta h)$ and $P_w(w_2)$, so that $P_h(\Delta h) dh$ is the probability that the height relative to the window average ($\Delta h = h - \bar{h}$) is in the interval $[\Delta h, \Delta h + dh]$, and $P_w(w_2) dw_2$ is the probability that the squared roughness $w_2$ is in the interval $[w_2, w_2 + dw_2]$. For each $r$, the center of the window was allowed to occupy all columns of the substrate, and height
fluctuations inside that window were measured. For small $r$, a large number of different microscopic environments is present in a large lattice and, consequently, accurate results are obtained with a small number of realizations of the growth process.

3 Height distributions

In the analysis of the height distributions of KPZ models, one should care about the consequences of the symmetry of the KPZ equation (1) under the transformation $h \rightarrow -h$, $\lambda \rightarrow -\lambda$ [20]. While RSOS models are represented by KPZ equations with negative $\lambda$, BD and the etching model have positive $\lambda$ [20,33]. Thus the transformation $h \rightarrow -h$ should be applied to one of these sets of models for the comparison of their height distributions.

In Fig. 1 we show a log-linear plot of the height distributions for the RSOS, the etching and the BD models at $t = 4000$ and window size $r = 128$. $P_h(\Delta h)$ is shown for models with $\lambda > 0$ (etching and BD) and $P_h(-\Delta h)$ is shown for the model with $\lambda < 0$ (RSOS). We do not observe a very good data collapse between the data for these models, but only a reasonable agreement near the peaks. Deviations of the BD distribution are particularly large in its tails. Discrepancies are found in other window sizes, and they are larger for BD.

A quantitative characterization of each distribution can be done by estimating the skewness

$$S \equiv \frac{\langle (\Delta h)^3 \rangle}{\langle (\Delta h)^2 \rangle^{3/2}} \quad (2)$$

and kurtosis

$$Q \equiv \frac{\langle (\Delta h)^4 \rangle}{\langle (\Delta h)^2 \rangle^2} - 3. \quad (3)$$

The former is a measure of the asymmetry of the distribution, while the latter is a measure of the weight of its tails when compared to a Gaussian.

In Fig. 2a we plot $\pm S$ for those models ($+S$ for models with $\lambda > 0$ and $-S$ for models with $\lambda < 0$), obtained in $t = 4000$. The values for the RSOS and the etching models do not show a significant size dependence for $1 \ll r \ll L$ (simulations in $L = 1024$). Extrapolation to large $r$ ($1/r \rightarrow \infty$) suggests $|S| \approx 0.2$. However, there is a large difference between those models and BD, whose skewness has a remarkable dependence on the window size. Such behavior was
Fig. 1. Normalized height distributions $\sigma_h P_h(\pm \Delta h)$ as a function of $\pm \Delta h / \sigma_h$ for $r = 128$ and $t = 4000$, where $\Delta h \equiv h - \langle h \rangle$ and $\sigma_h$ is the rms fluctuation of $\Delta h$. Plus signs for etching model (empty squares) and BD (full triangles), minus signs for RSOS model (solid curve).

also observed in steady state data for BD [20], thus this discrepancy must not be viewed as a failure of universality, but an expected feature for a model with typically large corrections to scaling.

In Fig. 2b, we show $Q$ for those models as a function of inverse window size. Fluctuations are larger, thus it is difficult to obtain a very accurate asymptotic estimate. Anyway, it is clear from Fig. 2b that $0 < Q < 0.5$ for these KPZ systems, which may be eventually used to test the possibility of this universality class in other models or experiments. The results obtained for other times ($t = 1000$ to $t = 6000$) show the same trends of those in Figs. 2a and 2b.

Tsamouras et al [10] obtained $0.2 \leq S \leq 0.5$ for the height distributions of oligomer films, and $\alpha \approx 0.45$ from the scaling of local roughness. This exponent is near the KPZ value, and the asymmetry of the height distribution was considered as further evidence of KPZ scaling, since no theoretical value of $S$ was known at that time. We believe that the claim of KPZ scaling is reinforced by our estimate of $S$, despite the large error bars and the discrepancies in the
values of $S$ for different models. On the other hand, the same uncertainties and discrepancies show that height distributions may not be considered reliable evidence against KPZ scaling.

It is also interesting to compare the above results with those for KPZ models in the steady states. There, $|S| = 0.26 \pm 0.01$ and $Q = 0.134 \pm 0.015$ were obtained [19,20]. Our estimates have much larger error bars as an effect of finite-time and finite-size corrections, which are much stronger than in the steady states. Thus, we are not able to decide whether there is some difference between the height distributions in the growth regime and in the steady state. Anyway, we recall that distributions in these regimes are different in $1 + 1$ dimensions [33], thus the present analysis of the growth regime is essential for a comparison with experimental data.

Fig. 2. Skewness $\pm S$ (a) and kurtosis $Q$ (b) of height distributions as a function of inverse window size at $t = 4000$ for RSOS (diamonds), etching (squares) and ballistic deposition (triangles). Minus sign of $S$ only for the RSOS model, whose data have been shifted horizontally by 0.001 for clarity. Error bars are of the same size of the data points, except where indicated.
4 Roughness distributions

In Fig. 3 we show the scaled squared roughness distributions for the RSOS, RSOS2, etching and BD models, obtained in window sizes $r = 64$ and $t = 4000$. Here, $\langle w_2 \rangle$ is the average squared roughness and $\sigma_w \equiv \sqrt{\langle w_2^2 \rangle - \langle w_2 \rangle^2}$ is the rms deviation. In this case, a good data collapse is observed in the peaks and in the tails of the distributions.

Fig. 3. Normalized squared roughness distribution $\sigma_w P_w (w_2)$ as a function of $(w_2 - \langle w_2 \rangle)/\sigma_w$ for window size $r = 64$ and $t = 4000$, for RSOS (line), RSOS2 (circles), etching (squares) and ballistic deposition (triangles) models.

This is confirmed by the values of the skewness and the kurtosis of those distributions, which are shown if Fig. 4a and 4b, respectively, as a function of inverse window size. Although the size dependences of $S$ and $Q$ are not negligible, the convergence of the results for different KPZ models as $r \to \infty$ is suggested, which gives universal values of $S$ and $Q$. The trend of the data for all models suggest $1.7 \leq S \leq 2.0$ and $3 \leq Q \leq 7$. 

The universal KPZ distribution in the growth regime is slightly different from that in the steady state. This is illustrated in Fig. 5, where we show the normalized distributions for the RSOS model and the BD model in the growth regime, with $r = 64$ and different times, and the distribution for the RSOS model in the steady state, for lattice size $L = 256$. The plot of Fig. 5 is also helpful to show that the dependence of the scaled roughness distribution on time is very small. Although visual inspection shows deviations in the tails of the distributions of different regimes, the above values of the skewness and kurtosis have large uncertainties and, consequently, they are not able to exclude the steady state values $S = 1.70 \pm 0.02$ and $Q = 5.4 \pm 0.3$ \cite{26}.

Another important feature of the KPZ roughness distribution is the stretched exponential tail, as suggested by a careful inspection of the log-linear plots of Figs. 3 and 5. In order to find a reliable fit of this tail, it is reasonable to assume
Fig. 5. Normalized squared roughness distributions for the RSOS model in the steady state with lattice size $L = 256$ (solid curve), and for RSOS and BD in the growth regime with $r = 64$ and different times ($t = 4000$ for BD - triangles - and $t = 6000$ for RSOS - squares).

that the scaling function decay has the general form $P_w(x) \sim \exp(-Ax^\gamma)$. Thus, at a given range of values of the variable $x \equiv (w_2 - \langle w_2 \rangle)/\sigma_w$, the estimate of the exponent $\gamma$ is given by

$$
\gamma(x) = \frac{\ln[\ln(\Psi(x))/\ln(\Psi(x-\Delta))]}{\ln[x/(x-\Delta)]},
$$

with constant $\Delta$, where $\Psi(x) = \sigma_w P_w(x)$. In Fig. 6 we show the effective exponents obtained from the data of the RSOS and the etching models in $r = 64$ as a function of $1/x^2$. The trend for large $x$ suggests $0.85 \leq \gamma \leq 0.9$.

In order to appreciate the relevance of this result, we recall that other systems which are represented by linear growth equations have roughness distributions with simple exponential decays\cite{22,26}, of the type $\exp(-Cx)$ ($\gamma = 1$). This also occurs in $1/f^\alpha$-noise interfaces \cite{24}. For the particular case of EW growth in $2 + 1$ dimensions, a sharply peaked roughness distribution is expected\cite{22}. These are examples of Gaussian interfaces. Moreover, a simple exponential tail
is also obtained in roughness distributions of models in the class of the fourth order nonlinear growth equation in 2 + 1 dimensions [26].

The comparison which these widely studied systems suggests that the stretched exponential tail in the roughness distribution may be a signature of KPZ scaling in 2 + 1 dimensions. It is also obtained in the steady state of KPZ systems, as expected from universality grounds [26]. Thus, if highly accurate experimental data eventually shows a stretched exponential tail, it may be viewed as strong evidence of KPZ scaling.

Unfortunately, current theoretical approaches could not to provide a clear and consistent picture of the KPZ scaling in 2 + 1 dimensions [38,39,40]. At some points, they lead to contradictory results and show discrepancies with highly accurate numerical data [19,20,25]. Consequently, we cannot provide a reliable explanation for this stretched exponential tail, but only to state that it is probably related to the non-Gaussian behavior of these KPZ interfaces [20,26].
A final important point is that the KPZ roughness distribution in the growth regime cannot be fitted by $1/f^\alpha$-noise distributions for any value of $\alpha$, similarly to the steady state distribution. The stretched exponential tail is a strong reason to expect that such fit is impossible. However, this conclusion also follows from our high value for the skewness: in $1/f^\alpha$-noise distributions in $2 + 1$ dimensions, the maximum possible value of the skewness is $\sqrt{2}$ \cite{24}, which is far below the lower bound of our estimate, $S = 1.7$.

5 Conclusion

We studied height and roughness distributions of discrete KPZ models in the growth regimes, i.e. in the regimes where correlations along the substrate directions are developed but the correlation length is still much smaller than the substrate size.

Even considering models with typically weak scaling corrections, the height distributions of those models show some deviations, thus we were not able to extract very accurate universal values of amplitude ratios to characterize them: the absolute value of the skewness is in the range $[0.2, 0.3]$ and the kurtosis is in the range $[0, 0.5]$. The value of the skewness agrees with that of oligomer films in Refs. \cite{9,10}, which provides additional support to their claim of KPZ scaling. However, the data for ballistic deposition shows large deviations from these values, which suggests that height distributions may be misleading for a test of KPZ scaling.

On the other hand, roughness distributions of different models show a good data collapse, and we estimate their skewness $1.7 \leq S \leq 2.0$ and kurtosis $3 \leq Q \leq 7$. A stretched exponential tail is found, which seems to be a particular feature of KPZ systems in $2 + 1$ dimensions. We conclude that roughness distributions are much superior than height distributions for tests of KPZ scaling. We expect that these results can be useful for a reliable quantitative comparison with available experimental data and that they motivate further analysis of scaling properties of thin films and/or multilayers surfaces.

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