Maximal and minimal height distributions of fluctuating interfaces

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Abstract

We study numerically the maximal and minimal height distributions (MAHD, MIHD) of the nonlinear interface growth equations of second and fourth order and of related lattice models in two dimensions. MAHD and MIHD are different due to the asymmetry of the local height distribution, so that, in each class, the sign of the relevant nonlinear term determines which one of two universal curves is the MAHD and the MIHD. The average maximal and minimal heights scale as the average roughness, in contrast to Edwards-Wilkinson (EW) growth. All extreme height distributions, including the EW ones, have tails that cannot be fit by generalized Gumbel distributions.

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Extreme value statistics (EVS) has already been applied in several fields of science and engineering [1, 2, 3]. It has recent important applications in surface science, e. g. for modeling the evolution of corrosion damage at time scales not easily accessible to experiment [4]. In uncorrelated random variable sets, the statistics of the $n$th extrema is described by the Gumbel’s first asymptotic distribution [1, 5] if the probability density functions (PDF) of those sets decrease faster than a power law. However, deviations from this statistics are expected in fluctuating interfaces if there are strong correlation of local heights. In one dimension, this is the case of Edwards-Wilkinson (EW) interfaces (Brownian curves) [6, 7] and other Gaussian interface models [8]. On the other hand, fluctuations of other global quantities in various physical systems follow generalized Gumbel distributions [9, 10, 11], i. e. the first asymptotic distribution with noninteger $n$ values. This is explained by the connections between the EVS of correlated variables and sums of independent variables drawn from exponential PDF [12], which shows that Gumbel statistics goes far beyond the description of uncorrelated variables sets.

The interface models where maximal height distributions (MAHD) were previously calculated [6, 7, 8] are symmetric with respect to the average height, consequently MAHD and minimum height distributions (MIHD) are the same. However, there is a large number of real interfaces where the up-down symmetry is broken [13], such as those described by the nonlinear growth models of Kardar-Parisi-Zhang (KPZ) [14] and of Villain-Lai-Das Sarma (VLDS) for molecular beam epitaxy [15], which raises the question whether MAHD and MIHD are the same in those systems. This is particularly important for two-dimensional interfaces due to the variety of real growth processes which show KPZ [16, 17] and VLDS scaling [18]. Recent works on persistence in VLDS growth also motivate such study, since different exponents for positive and negative height persistence were obtained [19]. Moreover, the above scenario raises additional (and not less important) questions for the nonlinear models. The first one is connected to the possibility of fitting their extreme height distributions (EHD) by generalized Gumbel distributions, similarly to other correlated systems. The second one is the scaling of the average maximal height, since EW interfaces showed an unanticipated scaling as the square of the average roughness [11], in contrast to several one-dimensional interfaces. This is essential to correlate surface roughness with the extreme events.

The aim of this letter is to address those questions by performing a numerical study of
the MAHD and MIHD in the steady states of the KPZ and VLDS equations and of various lattice models belonging to those classes in 2 + 1 dimensions. We will show that, for each growth class, two universal distributions are obtained, which may be a MAHD or a MIHD of a given model depending on the sign of the coefficient of the relevant nonlinear term. Combination of data collapse and extrapolation of amplitude ratios (e. g. skewness and kurtosis) of those distributions are used to separate systems with coefficients of different signs. In order to illustrate the drastic effects that asymmetric PDF (i. e. distributions of local heights) may have on MAHD and MIHD, we will discuss their differences in a random deposition-erosion model on an inert flat substrate. We will also show that average maximal and minimal heights is all those models scale as the average roughness, as usually expected, which shows that the EW scaling is an exception \[11\]. Finally, we will show that KPZ, VLDS and EW distributions cannot be fit by generalized Gumbel distributions.

MAHD and MIHD were calculated for the KPZ equation \( \frac{\partial h}{\partial t} = \nu_2 \nabla^2 h + \lambda_2 (\nabla h)^2 + \eta(x,t) \) in dimension \( d = 2 \), with \( \nu_2 = 0.25 \), \( D = 5 \times 10^{-3} \) and \( \lambda_2 = \sqrt{75} \) (\( g \equiv \lambda_2^2 D/\nu_2^3 = 24 \)), in discretized boxes with spatial step \( \Delta x = 1 \), time increment \( \Delta t = 0.04 \) and linear sizes \( 8 \leq L \leq 64 \). A simple Euler integration method \[20\] and a scheme for suppression of instabilities \[21\] were adopted. We also simulated three discrete KPZ models in sizes \( 32 \leq L \leq 256 \): the restricted solid-on-solid (RSOS) model \[22\], the ballistic deposition (BD) \[23\] and the etching model of Mello et al \[24\]. From inspection of their growth rules \[25\] one knows that \( \lambda_2 > 0 \) for BD and the etching model and \( \lambda_2 < 0 \) for the RSOS model. The VLDS equation \( \frac{\partial h}{\partial t} = -\nu_4 \nabla^4 h + \lambda_4 \nabla^2 (\nabla h)^2 + \eta(x,t) \) was integrated with \( \nu_4 = 1 \), \( \lambda_4 = 1 \), \( D = 1/2 \), and \( \Delta t = 0.01 \), using the same methods, in sizes \( 8 \leq L \leq 32 \). We also simulated a generalized conserved RSOS model (CRSOS) \[26\], whose original version was proposed in Ref. \[27\]) and which belongs to the VLDS class, in sizes \( 16 \leq L \leq 128 \). The EW equation (KPZ with \( \lambda_2 = 0 \)) was integrated with \( \nu = 1.5 \), \( D = 1/2 \) and \( \Delta t = 0.01 \) in box sizes \( 8 \leq L \leq 64 \). For each model and each lattice size, distributions with at least \( 10^7 \) different configurations were obtained to ensure high accuracy, which is particularly important at their tails. The extremes were calculated relatively to the average height of each configuration, the minima being absolute values of the differences from the average.

In Fig. 1a we show the scaled MAHD and MIHD of the KPZ equation in box size \( L = 64 \). In these plots, \( P(m)dm \) is the probability that the extreme lies in the range \( [m, m + dm] \),
\[ x \equiv (m - \langle m \rangle) / \sigma \] and \[ \sigma \equiv \left( \langle m^2 \rangle - \langle m \rangle^2 \right)^{1/2}. \] The high accuracy in Fig. 1a allows us to distinguish those curves (log-linear plots also show discrepancies in the right tails). Results for smaller box sizes show that the finite-size effects are negligible, confirming that MAHD and MIDH are actually different.

Gumbel’s first asymptotic distribution used to compare our data is \( g(x; n) = \omega \exp \left( -n \left[ e^{-b(x+s)} + b(x+s) \right] \right), \) where \( b = \sqrt{\psi'(n)}, \) \( s = (\ln n - \psi(n))/b \) and \( \omega = n^n b / \Gamma(n), \) with \( \Gamma(x) \) the Gamma function and \( \psi(x) = \partial \ln \Gamma(x) / \partial x \) [9, 11]. In Fig. 1b, we show the MAHD of the KPZ equation and the Gumbel curve with the same skewness 0.79, which has \( n = 1.95. \) Although the fit near the peak is reasonable, there are significant differences in the tails. Data for different lattice sizes in Fig. 1b show that discrepancies are not consequence of finite-size effects. Similar disagreement is observed when we try to fit the MIHD with a Gumbel curve of skewness 0.65 \( (n = 2.75). \) However, the right tails of MAHD and MIHD of the KPZ class tend to simple exponential decays for large \( m, \) similarly to the Gumbel curves.

In Fig. 2a we show the scaled MAHD of the integrated KPZ equation and of BD, and the MIHD of the RSOS model. In Fig. 2b we show the MIHD of the KPZ equation and of the etching model, and the MAHD of the RSOS model. There is excellent data collapse in both plots, which confirm that MAHD (MIHD) of models with \( \lambda_2 > 0 \) are equal to MIHD (MAHD) of models with \( \lambda_2 < 0. \) This illustrates the possibility of using the MAHD and MIHD to identify the sign of the coefficient of the nonlinear term in cases where it is not known a priori. At this point, EVS is superior to the scaling of the local height distributions (the PDF), which might also reveal the sign of the nonlinear terms if distortion by huge finite-size effects were not so frequent [28].

The visual agreement between those distributions and the small finite-size effects are quantitatively confirmed by estimates of their skewnesses and kurtosis in various system sizes. Figs. 3a and 3b show the skewness of the same models of Figs. 2a and 2b, respectively, as a function of \( 1/L^{1/2} \) (BD data were not shown in Figs. 3a and 3b because they superimpose the etching model data). The small finite-size dependence of the data for the KPZ equation, BD and the etching models leads to \( S \approx 0.79 \) for \( (\lambda_2 > 0)\)-MAHD and \( (\lambda_2 < 0)\)-MIHD, and \( S \approx 0.65 \) for \( (\lambda_2 > 0)\)-MIHD and \( (\lambda_2 < 0)\)-MAHD. Surprisingly, the largest finite-size effects are observed in the RSOS data, which uses to be the best discrete KPZ model for numerical
The MAHD and MIHD for the VLDS equation in box size $L = 32$ are plotted in Fig. 4a. Differences in the peaks are tiny, but discrepancies in the tails are clearly observed. Finite-size effects are also negligible in this case. The MAHD has skewness $S \approx 0.63$ and the MIHD has $S \approx 0.55$. In contrast to the KPZ models, those distributions have Gaussian-shaped right tails [$\exp (-m^2)$]. For this reason, fits with generalized Gumbel distributions (which tend to simple exponentials as $m \to \infty$) are not possible. This is confirmed for MAHD in Fig. 4a by comparison with Gumbel’s curve with $n = 2.90$, which has skewness 0.63.

For the CRSOS model, MAHD and MIHD show significant finite-size effects, similarly to the RSOS model. However, extrapolation of the skewness of distributions in finite-size lattices, shown in Fig. 4b, suggest that MAHD and MIHD of both models are asymptotically the same. This means that $\lambda_4 > 0$ for the CRSOS model, similarly to its one-dimensional original version, which is exactly solvable [29].

The difference between MAHD and MIHD can be easily explained in a model of random deposition and erosion with an inert flat substrate in the erosion-dominated regime. Let $q > 1/2$ be the probability of single-particle erosion and $1-q$ of deposition, and assume that erosion is possible only if $h > 0$. A steady state is attained with average height (relatively to the substrate) $\langle h \rangle = q/(2q - 1)$ and PDF $P(h) \propto \exp (-h/\langle h \rangle)$ (for $q$ close to 1/2). Now consider that one measures the extremes in a set of $L$ (independent) columns. With that PDF, MAHD is given by Gumbel’s first asymptotic distribution with $n = 1$. For large $L$, the minimum absolute height is typically at the substrate, thus fluctuations of the relative minima are dominated by fluctuations of the average height, which are Gaussian [$\propto \exp \left(-m^2/a\sqrt{L}\right)$, $a \equiv \frac{2^{q-1}}{\sqrt{q(1-q)}}$], and so it is the MIHD. The difference between MAHD and MIHD is easily confirmed by visual inspection of the plots of these functions. It is related to the highly asymmetric local height distribution of this model (skewness of PDF is $S_{PDF} = 2$), in contrast to the slight asymmetry of KPZ ($S_{PDF} \approx 0.26$ [28]) and VLDS ($S_{PDF} \approx 0.20$ [26]).

Now we analyze the average values of extremes of KPZ and VLDS interfaces. They are assumed to scale as $\langle m \rangle \sim L^{\alpha_m}$, while the average roughness scales with the roughness exponent $\alpha$. We estimate $\alpha_m$ by extrapolation of effective exponents $\alpha_m(L) \equiv \frac{\ln \langle (m)(L)/\langle m \rangle / (L/2) \rangle}{\ln 2}$, as shown in Figs. 5a (KPZ) and 5b (VLDS). The estimates of $\alpha_m$ are consistent with the best known estimates of the roughness exponents $\alpha \approx 0.39$ (KPZ) [28] and $\alpha \approx 0.67$ (VLDS).
Consequently, the average values of extremes scale as the average roughness in the KPZ and VLDS classes in 2 + 1 dimensions. This contrasts with the scaling as the squared roughness in the EW class, which we also confirmed by simulation.

Finally, in Fig. 6 we show the MAHD of the EW equation and the generalized Gumbel distribution with $n = 2.6$, which has the same skewness. Despite the good agreement in almost three decades of the scaled $P(m)$, the discrepancy in the tails is clear. Again, data for two box sizes ($L = 64$ and $L = 32$) show that this is not caused by finite-size effects nor to low accuracy of the data. On the other hand, the analytical prediction by Lee of a Gaussian-shaped tail [$\sim \exp(-m^2)$] of the MAHD is confirmed by the trend of our data for large $m$. Together with the above results for KPZ and VLDS classes, it shows that EVS of important interface growth models in two dimensions are not connected to the EVS of independent variables, despite the wide applicability of Gumbel statistics to correlated systems.

In summary, we showed that interface growth models with asymmetric local height distributions have different maximal and minimal height distributions, the most important examples being the KPZ and the VLDS classes in two dimensions. In each class, a pair of universal curves may be maximal of minimal height distributions depending on the sign of the relevant nonlinear term. The average maximal and minimal heights of KPZ and VLDS models scale as the average roughness, in contrast to the EW class. All extreme height distributions, including the EW ones, cannot be fit by generalized Gumbel distributions. Although most works on statistical properties of interfaces focus on features of height distributions and/or roughness scaling, recent studies show that the statistics of global quantities are very useful to characterize real growth processes. The EVS has the same advantages of roughness distribution scaling for this task, such as weak finite-size effects, and also reveals the sign of the nonlinear terms. Information on rare events is also essential in systems where drastic changes in the dynamics occur if the global minima or maxima attain certain values, such as in corrosion damage. On the other hand, for some applications (from friction to parallel computing) the distributions of local extremes may be important, and the present study certainly motivates additional studies of those quantities.
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FIG. 1: (Color online) a) Scaled MAHD (solid curve) and MIHD (dashed curve) of the KPZ equation in box size $L = 64$. b) Scaled MAHD of the KPZ equation (solid curve for $L = 64$, squares for $L = 32$) and generalized Gumbel distribution with $n = 1.95$ (dashed curve).
FIG. 2: (Color online) a) Scaled MAHD of the KPZ equation (solid curve) and BD (triangles), and MIHD of the RSOS model (squares). b) Scaled MIHD of the KPZ equation (solid curve) and etching model (triangles), and MAHD of the RSOS model (squares). For KPZ equation, box size is $L = 64$, and for discrete models $L = 256$. 
FIG. 3: a) Finite-size dependence of the skewness $S$ of MAHD of the KPZ equation (squares) and etching model (triangles), and of MIHD of the RSOS model (crosses). b) Finite-size dependence of $S$ of MIHD of the KPZ equation (squares) and etching model (triangles), and of MAHD of the RSOS model (crosses). In both plots, the variable in the abscissa was chosen to make clearer the evolution of the data as $L \to \infty$. 
FIG. 4: (Color online) a) Scaled MAHD (solid curve) and MIHD (dashed curve) of the VLDS equation in $L = 32$ and generalized Gumbel distribution with $n = 2.90$ (dotted curve). b) Finite-size dependence of the skewness $S$ of EHD of the VLDS equation (crosses for MAHD, circles for MIHD) and of the CRSOS model (squares for MAHD, triangles for MIHD). The variable $1/L^{2/3}$ provides the best linear fits of the data (dashed lines).
FIG. 5: Finite-size dependence of effective exponents $\alpha_m(L)$ of discrete models: a) KPZ class (BD: crosses; etching: triangles; RSOS: squares) and b) VLDS class (CRSOS model). $\overline{L}$ is the average size among $L$ and $L/2$. The variables in the abscissa provide the best linear fits (dashed lines) with exponents $\Delta = 1/2$ (a) and $\Delta = 2/3$ (b).

FIG. 6: (Color online) Scaled MAHD of the EW equation in $L = 64$ (solid curve) and $L = 32$ (squares) and the generalized Gumbel distribution with $n = 2.6$ (dashed curve).