Determination of Finite Size Effects in Lattice Models from the Local Height Difference Distribution

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Growth of interfaces during vapor deposition is analyzed on a discrete lattice. It leads to finding distribution of local heights, measurable for any lattice model. Invariance in the change of this distribution in time is used to determine the finite size effects in various models. The analysis is applied to the discrete linear growth equation and Kardar-Parisi-Zhang (KPZ) equation. A new model is devised that shows early convergence to the KPZ dynamics. Various known conservative and non-conservative models are tested on a one dimensional substrate by comparing the growth results with the exact KPZ and linear growth equation results. The comparison helps in establishing the condition that helps in determining the presence of finite size effect for the given model. The new model is used in 2+1 dimensions to predict close to the true value of roughness constant for KPZ equation.

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Growth on a lattice from vapor can be represented in primarily two ways. It can be modeled as a lattice model where the atomic interactions are replaced by simple growth rules\cite{1, 2}, then obtain a growth equation based on various symmetries of the problem under consideration\cite{1}. Other way is to construct the growth terms from the given growth rules for a lattice model at the coarsen-grained time and length scales\cite{3}. The KPZ equation was introduced to include lateral growth in growth equation \cite{4}. It has attracted a lot of attention in the field of growth. There are many lattice models and numerical solutions claiming to belong to the same universality as KPZ equation\cite{5, 6, 7, 8, 9, 10, 11}. In 1+1 dimensions, exponents can be exactly obtained\cite{1}. However, in higher dimensions exact values are not obtained. Various lattice models and numerical solutions predict a range of values due to the finite size corrections. In the following we develop a method to determine the existence of finite size effect in a model. A model that converges to its representative universality can be identified and hence correct exponents can be determined.

A linear equation representing interface motion normal to the surface can be obtained in the frame of reference moving with the interface velocity by considering inter-planer hopping of ad atoms on the interface with a bias for downward or in-plane hopping toward step edge \cite{3}. It has the form

\[
\frac{\partial h}{\partial t} = \nu_0 \nabla^2 h + \eta \tag{1}
\]

where, \( \nu_0 \) explicitly depends upon \( F \), and \( \eta \) is the noise due to the randomness in the deposition flux. It has the correlation given by \(< \eta(\mathbf{x}, t)\eta(\mathbf{x}', t') > = 2D\delta(\mathbf{x} - \mathbf{x}')\delta(t - t') \). The angular brackets denote the ensemble average of the contents. Eq. (1) is known as Edward-Wilkinson (EW) equation \cite{12}. The lowest ordered non-linear correction to EW equation was introduced by Kardar, Parisi, and Zhang \cite{4}. The resulting equation,

\[
\frac{\partial h}{\partial t} = \nu_0 \nabla^2 h + \lambda(\nabla h)^2 + \eta \tag{2}
\]

is known as KPZ equation. This is a non-conservative equation.

The steady state growth is characterized by roughness exponent \( \alpha \) and \( z \), determining the evolution correlations in time. One can measure \( \alpha \) from the height-height (h-h) correlations,
\[ G(x, t) = \frac{1}{N} \sum_{x'} (h(x + x', t) - h(x', t))^2 \]

\[ = x^{2\alpha} f \left( \frac{x}{\xi(t)} \right) \quad (3) \]

where, correlation length \( \xi(t) \sim t^{1/z} \). In the limit \( x \to 0, f \to 1 \). Thus for a large \( \xi(t) \), the plot of \( G(x, t) \) vs. \( x \) on the log scale must be a straight line for small \( x \) on any scalable surface. Hence any lattice model should comply with this requirement for large enough length and time scales. Absence of straight region over large enough length and time scales for a lattice model indicates that the corresponding surface is not scalable and hence such a model cannot exactly follow the growth equation that it is supposed to represent. We elucidate this point in the case of models believed to represent EW and KPZ equations. Time exponent \( \beta \), where \( z = \alpha/\beta \) can be obtained by measuring the width over a substrate of length \( L \) as, \( w_2 = \frac{1}{N} \sum_x (h(x, t) - \bar{h})^2 = L^{2\alpha} g \left( \frac{L}{\xi(t)} \right) \). It can be shown that [1] for small times \( w_2 \sim t^{2\beta} \).

We first analyze the \( G(x, t) \) for some of the models representing KPZ and EW type growth. Finite size effects enter due to both, the substrate size \( L \) and the cutoff length \( a \). The rules in a lattice model are sensitive to both these lengths. This results in deviation of the growth dynamics from that of the growth equation, that the model is representing. Signature of this deviation is obtained in the non linear behavior of \( G(x, t) \) in the limit \( x \ll \xi \) where \( \xi \) is correlation length, from a log-log plot of \( G(x, t) \) Vs. \( x \). We have measured this deviation by fitting straight lines on log-log plot of \( G(x, t) \) Vs. \( x \) for every interval of \( \Delta x = 10 \). From these straight line fits \( y = m x + c_0 \), we obtain \( c_0 \) as a function of average \( x \). In the absence of a curvature in the log-log plot of \( G(x, t) \) Vs. \( x \), one must obtain \( c_0 \) to be independent of average \( x \).

The models are briefly described below. In most of the known models[1], finite size effects are present. We have chosen the model introduced in reference [5] along with a new model. This new model, we believe, converges to the KPZ dynamics during early growth as will be seen from the results ahead.

a) KK model [5]: In this model growth proceeds by selecting a site randomly (this is the first step in all the models described here.). A particle is
accommodated at the site if the absolute height difference between the selected site after deposition and for each of the nearest neighbors is less than or equal to a number $N$.

b) SC model: We introduce another SOS model which provides limited tunability with respect to the spread in the distribution. This helps in identifying exponent values close to the true values in 2+1 dimensions. The deposition rules for the model are as follows. In 1+1 dimensions the deposited atom is accommodated if both its neighbors have at least same height as the deposited one. Otherwise, largest of the step differences at the site , $s_d$, is obtained and accommodation is allowed according to the probability factor $e^{-s_d^2/(2\sigma^2)}$. Here $\sigma$ can be varied as a tunable parameter. In 2+1 dimensions the deposited atom is accommodated if three or more neighbors have at least same height as its own. For other depositions the accommodation is decided from the largest of the four steps around the site using above exponential probability factor. Details of this model are described elsewhere [13]

c) NN1 model [3] : This is a conservative SOS model. A particle after deposition is allowed to relax by hopping to a nearest neighbor site if it can lower its height. The hop is not allowed if the height of one or more of its nearest neighbors is equal or larger.

d) HM model [14]: This conservative model is based on the models proposed in ref [14]. Here, in a growth equation that involves terms of the form $\nabla^2 f(x)$, the growth proceeds by allowing the particle to hop to the nearest site that has minimum value for $f(x)$. Thus, $f(x)$ is like a potential. For $\nabla^2 h$, $f(x) = h(x)$. For, $\nabla^4 h$, $f(x) = -\nabla^2 h$.

Models (a),(b) are assumed to belong to KPZ universality and models (d) and (e) to EW universality.

Fig. 1 shows the log-log plots of $G(x, t)$ Vs. $x$ for various models. The substrate lengths and the number of MLs is large enough to provide saturation of $G(x, t)$ around $x = 1000$. $c_0$ is measured between $x = 10$ to 100. Fig. 2 shows plot of $c_0$ for various models as a function of average $x$. As can be seen, KK and NN1 models do not show straight line behaviour in this length scales. SC and HM models are straight lines within the statistical error bars. Deviation from straight line behavior is the indication of non scalable dynamics of the growth due to finite size effects in these models. Clearly, exponents derived from models like HM or SC are reliable in the respective universality classes in 1+1 dimensions since , from the straight line behavior, these models follow the dynamics of the growth equation that
they represent.

This method requires measurement of $G(x, t)$ over large substrate length and large times. In higher dimensions it is increasingly difficult to perform such measurements. In order to facilitate the determination of finite size effects in higher dimensions, we introduce another measurement based upon the time invariance of distribution of height fluctuations.

Consider a one dimensional scalable lattice with a lattice constant $a$. We define step at site $i$ as 

$$\delta x_i = h_i - h_{i+1}$$

(4)

The local slope is then $-\delta x_i/a$. Consider linear growth equation Eq. (1) in 1+1 dimensions. $\frac{dh}{dt} \rightarrow (h_i(t + \Delta t) - h_i(t))/\Delta t$ on discretization. The r.h.s. is $(\delta x_{i-1}(t) - \delta x_i(t))/a + \eta_i(t)$. This relation predicts the value of $h$ at $(t + \Delta t)$ dependent on the discrete differences in steps at $t$. Let $\Delta h_i = h_i(t + \Delta t) - h_i(t)$. From the nature of the equation $<\Delta h_i> = 0$. Further, function $h_i(t) = H_i(t) - \bar{H}(t)$, where $H_i(t)$ and $\bar{H}(t)$ are values of height and average height measured from the substrate. On the r.h.s. of the discrete linear equation, $<\delta x_{i-1} - \delta x_i> = 0$ and $<\eta_i> = 0$. Thus the differential term and the noise term can be averaged to zero independently. In fact this is true for any conservative differential term. This observation is related to the fact that noise does not couple to conservative differential terms except with $q = 0$ mode [15]. For KPZ equation r.h.s. is proportional to $(\delta x_{i-1} + \delta x_i + \delta x_i^2 + \eta_i)$. Between the terms $(\delta x_{i-1} - \delta x_i)$ and $(\delta x_i^2)\; ,$ the latter term is $b^a$ times stronger where $b$ is scaling parameter. Hence for large $b$, $\Delta h_i$ will be determined by $(\delta x_i^2)$. We will therefore consider only non linear term contributing to $\Delta h_i$ in KPZ equation. The difference between the conservative terms and the KPZ term is that, on the r.h.s. of the equation, $<(\delta x_i)^2> \neq 0$. Since average over l.h.s. is zero, we must have $<(\delta x_i)^2 + \eta_i> = 0$. For a conservative term, the average over the term and the noise are independently zero. Hence, in the case of KPZ equation, the KPZ term couples with noise [2]. In order that the average on r.h.s. be zero, evaporation or vacancy addition is associated with the growth process.

The distribution of $\Delta h_i$ in the case of KPZ equation is determined by $(\delta x_i)^2 + \eta_i$. Since we are assuming a steady state growth, it is required that for the given time interval $\Delta t$, the distribution of $\Delta h_i$, which is same as that of $(\delta x_i)^2 + \eta_i$, must be independent of time. The time independence indicates that the random force as represented by the noise term is adequately
compensated for by the stabilizing growth term. The time dependence for
the distribution will indicate that on the growing surface 1) the weightages
of configurations are changing in time, and/or 2) new configurations are
generated as growth proceeds affecting the morphology on given scale. This
will imply that the true steady state is not obtained. Normally one identifies
steady state region by inspecting \( w \) vs. \( t \) on logarithmic scale. The beginning
of linear region on this plot is considered as the onset of steady state region.

In general, \( \Delta h_i \) is a result of all the terms on the r.h.s. of a growth equation.
Hence, cross over regions will not be discriminated with respect to the
distribution of \( \Delta h_i \). The distribution of \( \Delta h_i \) at small and large length scales
may differ. However, in either case it must be time independent irrespective
of the dominant term at the given scale.

Local configuration defining growth term is directly related to \( \Delta h_i \). This
suggests that a measure of \( \Delta h_i \) can be obtained by defining local height with
respect to a local reference. Such height will respond to local changes in
heights and help in providing a measure of \( \Delta h_i \). We define such a height as
a height measured from average height of neighbors. \( (h_i)_\text{local} = h_i - (h_i - 1 +
i + 1) / 2 \), proportional to the difference between the local steps. Incidentally,
the expression is similar to the second derivative of \( h(x) \) representing EW
term. However, for any growth term, same expression can be used in defining
a measure of \( \Delta h_i \). The definition \( (h_i)_\text{local} \) is more general. Note that
\( (h_i)_\text{local} = (\delta x_i - \delta x_i - 1) / 2 \). In 1+1- dimensions, the (h-h) correlations in the
discrete form are

\[
G(n) = \langle (h_i - h_i + n)^2 \rangle
\]  

We assume that the correlation length \( \xi \) is very large compared to the length
a. Using the definition of steps Eq.(4),

\[
G(2) = \langle \delta x_i^2 + \delta x_{i+1}^2 + 2\delta x_i \delta x_{i+1} \rangle .
\]  

Let \( \langle \delta x_i^2 \rangle = \langle \delta x_{i+1}^2 \rangle = \delta^2 \) and \( \langle \delta x_i \delta x_{i-1} \rangle = s \delta^2 \) where \( s \) is the coupling
between the steps around a given site \( i \). The distribution for \( \delta x_i \) is always
symmetric around zero and time independent for an ensemble average.

In the limit \( \xi \rightarrow \infty \) Eq. (3) reduces to \( G(x) = cx^{2\alpha} \) where constant
c = \( G(1) \). Hence Eq. (6) can be written as

\[
2^{2\alpha} = 2 + 2s
\]

where \( G(1) = \delta^2 \) in the discretized case. Coupling \( s \) uniquely determines \( \alpha \).
Thus, for \( s = -1/2, 0, \) and 1, \( \alpha \) is 0, 0.5, and 1 respectively. This analysis can be
easily extended to higher dimensions. The relation between $\alpha$ and $s$ remains unchanged over a square, cubic or hypercube lattice in higher dimension. We have independently verified it for the EW model. A rough surface will be characterized by some value of $s$. Expressing $(h_i)_{\text{local}}$ in terms of steps it can be shown that $4 < (h_i)^2_{\text{local}} >= (2 - 2s)\delta^2$. This shows that the distribution of $(h_i)_{\text{local}}$ can be used as a measure of $\alpha$ and the definition of $(h_i)_{\text{local}}$ is applicable to any growth equation which has $0 \leq \alpha \leq 1$. However, distribution of $(h_i)_{\text{local}}$ cannot be used to represent that of $\Delta h_i$. Latter quantity is a result of local configuration dependent term and the fluctuation due to the noise term. Thus the appropriate measure of the distribution of $\Delta h_i$ will be, uncorrelated fluctuations in $(h_i)_{\text{local}}$. Hence, we measure the distribution of change in $(h_i)_{\text{local}} = \delta(h_i)_{\text{local}}$ over a time interval $\Delta t > w(t)$, ensuring the uncorrelated fluctuations. For any model expected to follow the KPZ, EW or any other conservative or non conservative growth equation, it is required that this distribution must be constant in time.

In the following we apply this criterion of constancy to the same models described earlier. Although above discussion was for growth on one dimensional substrate, the corresponding criterion can be easily extended to higher dimensions. We have chosen $\Delta t = 100$ MLs in 1+1 dimensions and 60 MLs in 2+1 dimensions where $\Delta t$ is the time difference considered in the simulations. The time difference over which the constancy of distribution is tested is from 500 MLs to 5000 MLs in 1+1 as well as in 2+1 dimensions. In this time interval for all the models considered, $\ln(w)$ Vs $\ln(t)$ curve is linear implying a steady state growth region. In 2+1 dimensions, two sets of $\delta(h_i)_{\text{local}}$ are generated, one corresponding to $x$ and other $y$ direction, and added. The constancy of the distribution is checked by measuring the ratio of the values in the distribution at zero for 500 MLs and 5000 MLs i.e. $P_0 = 100(I_{500} - I_{5000}) / I_{500}$, where $I_t$ is the count of $\delta(h_i)_{\text{local}}$ at zero. The ratios $P_0$ are obtained by averaging over large enough runs so that values of $P_0$ are statistically discriminated. In 1+1 dimensions over 3000 runs are required for substrate size of $L = 8000$. We have also calculated sum of absolute values of $P_i = 100(|I_{i,500} - I_{i,5000}| / I_{i,500})$ measured between $i=-4$ to $+4$ values of the $\delta(h_i)_{\text{local}}$ as an additional measure of the constancy of the distribution of $\delta(h_i)_{\text{local}}$. Here, $I_{i,500}$ and $-I_{i,5000}$ are the counts at $i$th position in the distribution at 500 and 5000 MLs respectively. This range (-4 to +4) is chosen because one of the models used in the present work provides values of $\delta(h_i)_{\text{local}}$ only within this
range. This sum is denoted by $P_{sum}$.

In Table I we present the results from the measurement of distribution of $\delta(h_i)_{local}$ for different models in 1+1 dimensions. Along with $P_0$ and $P_{sum}$, we also measure $\alpha$ for each model. However, as is seen from Fig. 1, $G(x, t)$ for KK and NN1 models are curved on the log-log scale. Hence, the measured $\alpha$ values are not reliable. Fig.3 shows a plot of such a distribution for the model NN1 described above.

KK Model: It shows a deviation of $-0.5 \pm 0.06\%$ and $6.86 \pm 1.0\%$ in $P_0$ and $P_{sum}$ respectively. For KK model the distribution becomes narrower in time (-ve $P_0$) indicating that number of tilted regions are growing with time. We have used $N = 1$ for KK model as height limitation [5].

SC Model: With $\sigma = 1.7$ it shows significantly small spread compared to KK model in the distribution. We have observed that for other values of $\sigma$, spread is larger. The advantage of this model is that it does not suffer from cross over effects. By varying $\sigma$ it is possible to get faster convergence to the KPZ dynamics.

We have performed simulations between 200 MLs to 2000 MLs, 2000 MLs to 20000 MLs. Corresponding results have same trends i.e. for SC model the $P_0$ and $P_{sum}$ values are less than 0.1% and 1.5% respectively while for KK model the absolute value is larger than 0.5% and 6%. Our analysis is based on the spatial discretization of the growth equation. It is known that [16] the real space group renormalization leads to different results than the KK result. Also for the KK model, in reference [17] the $\alpha$ value for 1+1- dimensions is 0.489 although in [5] from saturation of width at larger $L$ values it is given as 0.5. Our results show that the pathology associated with KK model is manifested in the form of change in the distribution of $\delta(h_i)_{local}$ in time. This in turn indicates that the finite size effects are dominant over the time scales considered.

The results for conservative growth models also confirm to this behavior.

HM Model and NN1 Model: HM model is like solving linear second ordered growth equation locally. It is expected to follow the dynamics exactly. The $P_0$ and $P_{sum}$ values are indeed close to zero for this model. The NN1 model restricts the minimization of $h(x)$ due to the constraint that it is immobile if one or more nearest neighbors are present. This model has larger values of $P_0$ and $P_{sum}$.

Above comparison between HM and NN1 models show that finite size effects do not allow convergence to EW dynamics in NN1 model due to the
constraint over the time scale studied. We consider the deviation from zero for $P_0$ and $P_{\text{sum}}$ as the measure of convergence to the universality class that the model is belonging to. Larger the deviation farther is the model from the convergence. This convergence is with respect to the true dynamics of the growth equation, belonging to a particular universality class. Thus, SC model converged to the KPZ universality within the statistical error bar for the measurements of $P_0$ and $P_{\text{sum}}$, but KK model has not yet converged. Similarly, HM model has converged to EW universality but NN1 model has not. It is expected that asymptotically these convergences occur. However, within the time and length scales used for our measurements, scaling corrections do not allow true value measurements for KK and NN1 models in the KPZ and EW universality classes respectively.

Above results assert that a model can be considered to have converged to its representative growth equation dynamics if the spread in its distribution of $\delta(h_i)_{\text{local}}$ is minimum. The advantage of this measurement is that it can be performed over a relatively small amount of growth compared to the $G(x,t)$ measurement. Thus, even in higher dimensions the method can be used to determine the finite size effects in a model at an early stage.

We have applied this method to determine an accurate value of $\alpha$ for the KPZ equation in 2+1 dimensions. For KK (N=1) model the $P_0$ is $0.29 \pm 0.02\%$ and $P_{\text{sum}} = 5.0 \pm 1.0\%$ with $\alpha = 0.402 \pm 0.016$. For SC model with $\sigma = 2.5$, $P_0$ is $0.02 \pm 0.05\%$ and $P_{\text{sum}} = 1.3 \pm 1.1\%$ with $\alpha = 0.355 \pm 0.001$. For KK model $\alpha$ is measured between $x = 5$ and 20 while for SC model it is between $x = 2$ and 50. We have plotted these results in Fig. 4. These results show that in 2+1 dimensions, true value of $\alpha$ for KPZ equation is close to 0.36.

In conclusion, we have established a new criterion that can be applied to check the finite size effects at an early stage of growth. When applied to the models representing KPZ equation, it is seen that a new model , SC model in this connection can be adjusted to follow the KPZ dynamics accurately. This is true in both 1+1 and 2+1 dimensions. Based on this study it is seen that KK model predicts exponents that are away from the true values. Only those models that satisfy the condition of invariance of the distribution of $\Delta h(x)$ will follow the dynamics of the representative growth equation correctly. These are the models that have already converged to the respective universality in terms of the underlying dynamics. We find that SC model converge to the universality much earlier. The KK model is not converged over the time and length scales used here. The HM model converges to EW
universality but NN1 does not. Hence, the exponent measurements based on converged models are reliable.

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Figure 1: Plot of $G(x, t)$ vs. $x$ for KK model (N=1) (open circles), for HM model (open squares), for NN1 model (filled circles), and for SC model (filled squares) in 1+1 dimensions. The curves are shifted along y-axis to avoid overlapping data. The growth is over $5 \times 10^5$ MLs with $L=80000$.

Figure 2: Plot of $c_0$ the straight line intercept on y-axis, as a function of average $x$. The plots are for the models in (1+1) dimensions, KK(N=1) (open squares), SC (+), NN1 (x), and HM (filled squares). For the sake of comparison, values at $\bar{x} = 15$ are adjusted to the same value for all the models.

Figure 3: Plot of distribution of $\delta(h_i)_{local}$ for the model NN1 on semi log scale. The inner distribution (+) is for $t = 500$ MLs and the outer one (x) is for $t = 5000$ MLs.

Figure 4: Plot of $G(x, t)$ vs. $x$ for KK model (N=1) (open squares), and for SC model (filled squares) in 2+1 dimensions.

Table 1: $\alpha$ values as obtained from height-height correlations, $P_0$ the ratios of values, and sum of ratios $P_{sum}$ of $\delta(h_i)_{local}$ at 500 MLs and 5000 MLs for different models in 1+1 dimensions.

| Model/Parameter | $\alpha$ | $P_0$ in % | $P_{sum}$ in % |
|-----------------|----------|------------|----------------|
| KPZ and EW Equation | 0.5 | 0.0 | 0.0 |
| KK (N=1) | 0.5089 ± 0.012 | -0.5 ± 0.06 | 6.8 ± 1.0 |
| SC ($\sigma = 1.7$) | 0.5062 ± 0.0015 | 0.07 ± 0.02 | 1.1 ± 0.4 |
| NN1 | 0.514 ± 0.02 | 1.82 ± 0.12 | 14.3 ± 2.0 |
| HM | 0.496 ± 0.002 | 0.06 ± 0.05 | 1.5 ± 1.2 |
