Eur. Phys. J. B **52**, 557–562 (2006)
DOI: 10.1140/epjb/e2006-00331-6

THE EUROPEAN PHYSICAL JOURNAL B

Determination of cross over effects in lattice models from the local height difference distribution

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Received 5 September 2005 / Received in final form 1 May 2006
Published online 21 August 2006 –

Abstract. 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 cross over 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 determines the presence of cross over 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.

PACS. 68.55.-a Thin film structure and morphology – 81.15.Aa Theory and models of film growth – 82.20.Fd Collision theories; trajectory models

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 [1,2], then obtain a growth equation based on various symmetries of the problem under consideration [1]. Other way is to construct the growth terms from the given growth rules for a lattice model at the coarse-grained time and length scales [3]. The KPZ equation was introduced to include lateral growth in growth equation [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 [5–11]. In (1+1) dimensions, exponents can be exactly obtained [1]. However, in higher dimensions exact values are not obtained. Various lattice models and numerical solutions predict a range of values due to the cross over and finite size effects. In the following we develop a method to determine the existence of cross over effect in a model. We will apply the method to models belonging to Edward-Wilkinson (EW) [12] and KPZ universality. This will help us to identify those models that converge early to their respective universality and hence determine the corresponding growth exponents with better accuracy.

Growth equation representing EW universality is,

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

where, ν_0 explicitly depends upon F, and η is the noise due to the randomness in the deposition flux. It has the correlation given by $\langle \eta(\mathbf{x},t)\eta(\mathbf{x}',t')\rangle = 2D\delta(\mathbf{x}-\mathbf{x}')\delta(t-t')$. The angular brackets denote the ensemble average of the contents. The lowest ordered non-linear correction to EW equation was introduced by Kardar et al. [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 defining the KPZ universality. These growth equations are characterized by roughness exponent α and z, determining the evolution correlations in time. One can measure α from the height-height (h–h) correlations,

$$G(x,t) = \frac{1}{N}\sum_{x'}(h(x+x',t)-h(x',t))^2 = x^{2\alpha} f\left(\frac{x}{\xi(t)}\right) \tag{3}$$

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. We elucidate this point in the

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case of models believed to represent EW and KPZ equations. Time exponent β, where $z = \alpha/\beta$ can be obtained by measuring the width over a substrate of length L as,

$$w_2 = \frac{1}{N}\sum_x (h(x,t) - \bar{h}(t))^2 = L^{2\alpha} g\left(\frac{L}{\xi(t)}\right). \quad (4)$$

It can be shown that [1] for small times $w_2 \sim t^{2\beta}$.

We obtain our method by discretization of growth equations. Consider a one dimensional scalable lattice with a lattice constant a. We define step at site i as

$$\delta x_i(t) = h_i(t) - h_{i+1}(t). \quad (5)$$

Here, $h_i(t) = H_i(t) - \bar{H}(t)$, where $H_i(t)$ and $\bar{H}(t)$ are values of height and average height measured from the substrate so that $h_i(t)$ has a zero mean. The local slope is then $-\delta x_i/a$. Consider linear growth equation (1) in (1+1) dimensions. $\frac{\partial h}{\partial t} \to (h_i(t+\Delta t) - h_i(t))/\Delta t$ 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 change in h_i 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 $\langle \Delta h_i \rangle = 0$. On the r.h.s. of the discrete linear equation, $\langle \delta x_{i-1}(t) - \delta x_i(t) \rangle = 0$ and $\langle \eta_i(t) \rangle = 0$. 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 [13]. For KPZ equation r.h.s. is proportional to $(\delta x_{i-1}(t) - \delta x_i(t) + \delta x_i^2(t) + \eta_i(t))$. Between the terms $(\delta x_{i-1}(t) - \delta x_i(t))$ and $(\delta x_i^2(t))$, the latter term is b^α times stronger where b is scaling parameter. Hence for large b, Δh_i will be determined by $(\delta x_i^2(t))$ although the Laplacian is needed for the stable growth.

For any given growth equation, in the time interval of Δt, a distribution of Δh_i is generated. The distribution of Δh_i in the case of KPZ equation is determined by fluctuations in $\delta x_{i-1}(t) - \delta x_i(t) + (\delta x_i(t))^2 + \eta_i(t)$ and in the case of EW equation by fluctuations in $\delta x_{i-1}(t) - \delta x_i(t) + \eta_i(t)$. Since we are assuming a growth in the scaling regime, it is required that for the given time interval Δt, the distribution of Δh_i must be independent of time. The time independence indicates that the random force as represented by the noise term in the growth equation 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 scalable growth* is not obtained. Normally one identifies scaling region by inspecting w vs. t on logarithmic scale. The beginning of linear region on this plot is considered as the onset of scaling region.

In the following we define a measure of Δh_i useful for any type of growth equation or a lattice model. Local configuration defining growth term is directly related to Δh_i. This suggests that a measure of Δh_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 Δh_i. We define such a height as a height measured from average height of neighbors. $(h_i(t))_{local} = h_i(t) - (h_{i-1}(t) + h_{i+1}(t))/2 = (\delta x_i(t) - \delta x_{i-1}(t))/2$, from equation (5), proportional to the difference between the local steps. Incidentally, the expression is similar to the Laplacian, hence $(h_i(t))_{local}$ can also be referred as Laplacian without losing the generality. Although Laplacian represents EW growth term, for any growth term it can be used to define a measure of Δh_i. The generality of $(h_i(t))_{local}$ can be established if it is related to some general property of the surface and not to the specific term in a growth equation. Consider the (h–h) correlations in (1+1) dimensions,

$$G(n,t) = \left\langle (h_i(t) - h_{i+n}(t))^2 \right\rangle. \quad (6)$$

We assume that *the correlation length ξ is very large compared to the lattice constant a*. Using the definition of steps equation (5),

$$G(2,t) = \langle \delta x_i^2(t) + \delta x_{i+1}^2(t) + 2\delta x_i(t)\delta x_{i+1}(t) \rangle. \quad (7)$$

Let $\langle \delta x_i(t)^2 \rangle = \langle \delta x_{i+1}(t)^2 \rangle = \delta^2$ and, $\langle \delta x_i(t)\delta x_{i-1}(t) \rangle = s\delta^2$ where s is the average coupling between the consecutive steps. The distribution for $\delta x_i(t)$ is *always* symmetric around zero for a rough surface that follows $x \to -x$ symmetry, and time independent for an ensemble average.

In the limit $\xi \to \infty$ equation (3) reduces to $G(x) = cx^{2\alpha}$ where constant $c = G(1)$. Hence equation (7) can be written as

$$2^{2\alpha} = 2 + 2s \quad (8)$$

where $G(1) = \delta^2$ in the discretized case. Coupling s uniquely determines α. Thus, for $s = -1/2$, 0, and 1, α is 0, 0.5, and 1 respectively. This analysis can be easily extended to higher dimensions. The relation, equation (8), between α and s remains unchanged over a square, cubic or hypercube lattice in higher dimension. We have independently verified it for the EW model. Note that s seems to be a local parameter whereas α is defined over all the ranges of space variable. However, as is mentioned in the beginning of this derivation, both α and s are defined over a scalable lattice. This allows us to compare them on the same footing. However, in the lattice models growth rules are applied on a physical lattice so that length scale is not reducible below this physical lattice. Effect of this finite length scale is expected to affect the initial growth in the transient region. How long this transient can be? In the following we suggest a method to determine the relative time scales for convergence of different models. Thus a growth model is expected to converge earlier to the asymptotic universality if it follows the growth equation closely even at this physical scale. We elaborate this fact and use it to compare the convergence of different lattice models in EW and KPZ universality. A rough surface will be characterized by some value of s. Using the definition of $(h_i(t))_{local}$ in terms of steps it can be shown that

$$4\langle (h_i(t))_{local}^2 \rangle = (2 - 2s)\delta^2. \quad (9)$$

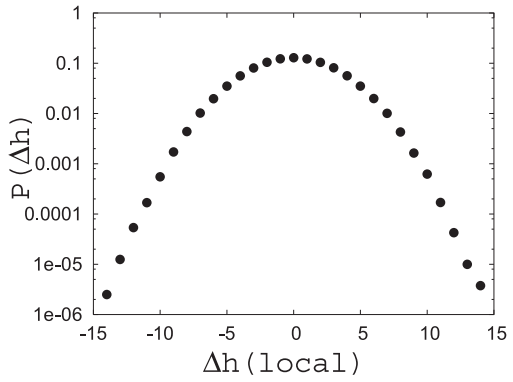

Fig. 1. Plot of distribution of $\Delta h(t)_{local}$ for the (1+1) dimensional SC model described in the text, on semi log scale. $P(\Delta h)$ represents relative probability of occurence of Δh. The distribution is for $t = 5000$ MLs, with $\sigma = 1.7$. The distribution is obtained by collecting the data over 3000 runs.

This shows that the distribution of $(h_i(t))_{local}$ can be used as a measure of α and the definition of $(h_i(t))_{local}$ is applicable to any growth equation which has $0 \leq \alpha \leq 1$.

However, distribution of $(h_i(t))_{local}$ cannot be used to represent that of Δh_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 Δh_i will be, uncorrelated fluctuations in $(h_i(t))_{local}$. Thus we measure the distribution of uncorrelated fluctuations $\Delta h(t)_{local}$ from the difference $\Delta h(t)_{local} = (h_i(t))_{local} - (h_i(t + \Delta t))_{local}$. Here we measure $(h_i(t + \Delta t))_{local}$ at a later time $(t + \Delta t)$, where $\Delta t > w(t)$. $w(t) = \sqrt{w}_2$ is the width of the interface at t, and the inequality ensures that the difference between local heights measured at t and $t + \Delta t$ are uncorrelated [14]. $w(t)$ represents correlation length in time [14]. Figure 1 shows such a distribution for the model SC described later in this paper representing KPZ universality. We obtain such distributions for a given model at two different times with an interval much larger than the Δt. In our case we have obtained distributions at $t = 500$ MLs and $t = 5000$ MLs for comparison, and $\Delta t = 100$ MLs in (1+1) dimensions. Since the counts at $\Delta h(t)_{local} = 0$ are largest in the distribution, the statistical error is minimum for zero fluctuation. We therefore use the parameter $P_0 = 100(\frac{I_{500} - I_{5000}}{I_{500}})$, where I_t is the count at $\Delta h(t)_{local} = 0$, to measure the time invariance of the distribution of $\Delta h(t)_{local}$ in (1+1) and (2+1) dimensions. Ideally P_0 should be zero. We have also calculated sum of absolute values of $P_i = 100(\frac{I_{i,500} - I_{i,5000}}{I_{i,500}})$ measured between $i = -4$ to $+4$ values of the $\Delta h(t)_{local}$ as an additional measure of the constancy of the distribution of $\Delta h(t)_{local}$. Here, $I_{i,500}$ and $I_{i,5000}$ are the counts at $\Delta h(t)_{local} = i$ 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 $\Delta h(t)_{local}$ only within this range. This sum is denoted by P_{sum}.

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 order to confirm the invariance of the distribution of $\Delta h(t)_{local}$, we compute this distribution by numerically integrating the EW equation. Being linear, this equation is ideally suited for numerical integration [15]. The discrete form of the equation is,

$$h_i^{n+1} = h_i^n + \delta t[\nu_0(h_{i+1}^n + h_{i-1}^n - 2h_i^n) + \sqrt{(D\delta t)}\psi_i^n \quad (10)$$

where, h_i^n approximates height variable $h(i\Delta x, n\delta t)$ and ψ_i^n is an independent Gaussian variable with zero mean and unit variance. We have chosen $\nu_0 = D = 1$ and $\delta t = 0.1$. The simulations are performed over $L = 8000$ for finding P_0 and P_{sum}. To obtain α, $L = 40000$ and 500 000 iterations are performed. After 5000 iterations, the width square $w_2 = 8.3$. To produce same amount of fluctuations in squared height, 35 iterations are required on an average. Thus we choose 100 iterations representing $\Delta t > w(t)$. We have measured P_0 and P_{sum} for the numerically integrated EW equation. The results are displayed in Table 1. Clearly $P_0 = 0.0085 \pm 0.01\%$ confirms the criterion of invariance proposed above. The α value is exact within statistical variance as expected. Thus the results show that smaller the values of P_0 and P_{sum} for a model, faster is the convergence to the underlying Universality.

In the following we apply this criterion of constancy to some of the models representing EW and KPZ universalities. Although above discussion was for growth on one dimensional substrate, the corresponding criterion can be easily extended to higher dimensions. We have chosen $\Delta t = 60$ MLs in (2+1) dimensions. 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 scaling region for the growth. In (2+1) dimensions, two sets of $\Delta h(t)_{local}$ are generated, one corresponding to x and other y direction, and added. The representative models are briefly described below.

(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 σ 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

Table 1. α 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	α	P_0 in %	P_{sum} in %
KPZ and EW Equation Numerical solution to EW equation	0.4993 ± 0.0022	0.0085 ± 0.01	0.42 ± 0.4
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

decided from the largest of the four steps around the site using above exponential probability factor. Details of this model are described elsewhere [16]. We have computed the coefficient of nonlinear term $\lambda = -0.22$, for this model using tilted substrate method [17]. This model provides exact exponents within statistical error using structure factor $S(q)$ calculations [16]. It is seen that over a relatively larger range of q values, $S(q)$ falls on a straight line of slope -2.0 on the log-log plot giving $\alpha = 0.5$.

(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 [18]: this conservative model is based on the models proposed in reference [18]. 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.

In Table 1 we present the results from the measurement of distribution of $\Delta h(t)_{local}$ for different models in (1+1) dimensions. The error bars are obtained by performing the simulations with different sets of random numbers. Thus, to obtain P_0 for a model, 2000 runs are performed ones. Such 2000 runs are performed 5 to 10 times to obtain average P_0 and the standard deviation which is reported in the Table 1. Same procedure is followed for P_{sum}.

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 σ, spread is larger. The advantage of this model is that it shows comparatively smaller cross over effects. By varying σ it is possible to get faster convergence to the KPZ dynamics.

We have performed simulations between 200 MLs to 2000 MLs, 2000 MLs to 20 000 MLs. Corresponding results have same trends i.e. for SC model the P_0 and P_{sum} are less than 0.1% and 1.5% respectively while for KK model the absolute value is larger than 0.5% and 6%. These results when compared to the results of the numerical solution of EW equation indicate that SC model will converge earlier than KK model to the KPZ universality. The accuracy of the exponent values obtained from these models is discussed later. It has been shown in reference [19] that the two well known models, NNBD and NNNBD [1], both belonging to KPZ the universality have very different height distribution. Since our method is dependent on the local measure for height it is expected to show this difference. We have measured P_0 and P_{sum} for these models. The values are $(0.09 \pm 0.08\%,\ 1.4 \pm 1.1\%)$ and $(1.3 \pm 0.07\%,\ 3.4 \pm 1.1\%)$ for NNBD and NNNBD models respectively. As expected, P_0 and P_{sum} for the two models differ sufficiently to reflect the difference in the local height distributions. These results indicate that the NNNBD model will converge later than the NNBD model.

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} indicating late convergence to the EW universality compared to HM model.

Regarding α values, it will be seen that for SC model and HM model, the values do not overlap the exact value of 0.5 within statistical error bars, but KK and NN1 models do. This apparent contradiction is a result of curved nature of the plots on the log-log scale for $G(x,t)$ vs. x for these models. In order to bring out the curved nature of these plots for different models, we fit straight line $y = mx + c_0$ on the log-log plot for each model at an interval of $\Delta x = 10$. For a plot with no curvature, the values of c_0 should be independent of x. Figure 2 shows the log-log plots of $G(x,t)$ vs. x for different models. Figure 3 shows the plot of c_0 vs. average x for different models. As is evident from the results, KK and NN1 models show distinct

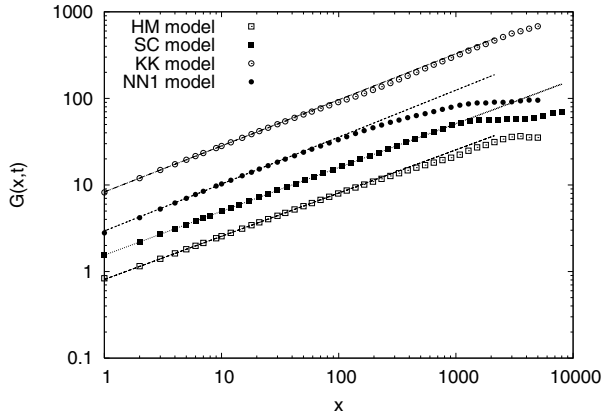

Fig. 2. Plot of $G(x,t)$ vs. x for KK model ($N = 1$) (open circles), for HM model (open squares), for NN1 model (filled circles), and for SC model (filled squares) in (1+1) dimensions. The curves are shifted along y-axis to avoid overlapping data. The growth is over 5×10^5 MLs with $L = 80\,000$.

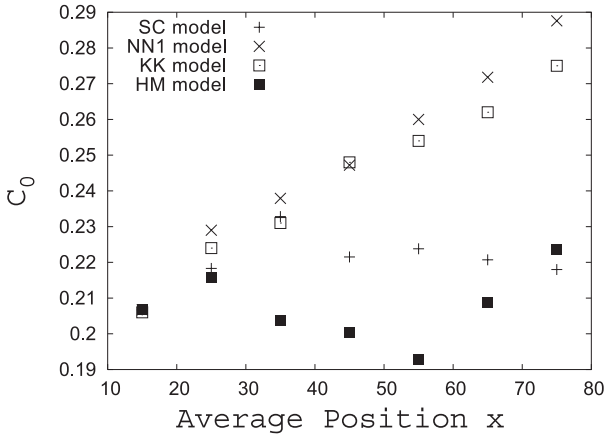

Fig. 3. Plot of c_0 the straight line intercept on y-axis, as a function of average x. The plots are for the models in (1+1) dimensions, KK ($N = 1$) (open squares), SC (+), NN1 (×) and, HM (filled squares). For the sake of comparison, values at $\bar{x} = 15$ are adjusted to the same value for all the models.

curvature for small values of x. This implies that scalable region is not generated for the time scales and lengths used for simulation of these models. In fact the statistical variation associated with the α values of KK and NN1 models is due to the curvature. It cannot be further reduced by increasing the number of simulations for averaging purpose. The P_0 and P_{sum} for SC and HM models are larger than those obtained for numerically integrated EW equation. Hence the convergence for these models is expected to be for longer times and lengths than those used in the simulations. The deviation in measured α values from the exact value for these models are consistent with these facts. The closeness of α values is true in nature. On the contrary, the apparent overlap through statistical variance with the exact α value for KK and NN1 models is misleading due to the curved nature of corresponding $G(x,t)$ vs. x plots on the log-log scale.

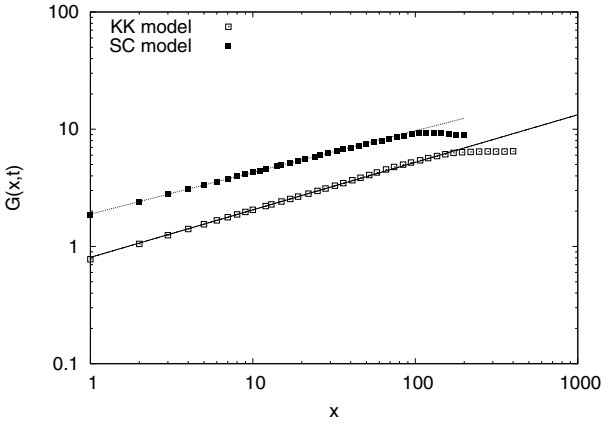

Fig. 4. Plot of $G(x,t)$ vs. x for KK model ($N = 1$) (open squares), and for SC model (filled squares) in (2+1) dimensions.

Above results assert that a model will converge earlier to its representative growth equation dynamics if the spread in its distribution of $\Delta h(t)_{local}$ 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 cross over effects in a model at an early stage.

We have applied this method to determine an accurate value of α for the KPZ equation in (2+1) dimensions. For KK ($N = 1$) model the P_0 is $0.29 \pm 0.02\%$ and $P_{sum} = 5.0 \pm 1.0\%$ with $\alpha = 0.402 \pm 0.016$. For SC model with $\sigma = 2.5$, P_0 is $0.02 \pm 0.05\%$ and $P_{sum} = 1.3 \pm 1.1\%$ with $\alpha = 0.355 \pm 0.001$. For KK model α is measured between $x = 5$ and 20 while for SC model it is between $x = 2$ and 50. We have plotted these results in Figure 4. From the comparison of the values of P_0 and P_{sum} for these two models, we conclude that the SC model is expected to converge earlier than the KK model. The α value obtained from SC model is expected to be closer to the true value. These results show that in (2+1) dimensions, true value of α for KPZ equation is close to 0.36.

In conclusion, we have established a new criterion that can be applied to check the cross over 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 converge earlier to the respective universality in terms of the underlying dynamics. We find that SC model is expected to converge to the universality much earlier compared to the KK model over the time and length scales used here. Similarly HM model is expected to converge earlier to EW universality compared to NN1. Hence, the exponent measurements based on earlier converging models are reliable.

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