Kinetic roughening model with opposite KPZ nonlinearities

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Abstract

We introduce a model that simulates a kinetic roughening process with two kinds of particles: one follows the ballistic deposition (BD) kinetic and, the other, the restricted solid-on-solid (KK) kinetic. Both of these kinetics are in the universality class of the nonlinear KPZ equation, but the BD kinetic has a positive nonlinear constant while the KK kinetic has a negative one. In our model, called BD-KK model, we assign the probabilities $p$ and $(1-p)$ to the KK and BD kinetics, respectively. For a specific value of $p$, the system behaves as a quasi linear model and the up-down symmetry is recuperated. We show that nonlinearities of odd-order are relevant in these low nonlinear limit.

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The growth of interfaces by nonequilibrium kinetic roughening models is a very interesting topic of the far from equilibrium statistical mechanics [1-3]. In the two past decades, several models have been proposed, as ballistic deposition [4], Eden model [4], solid-on-solid (SOS) model with surface relaxation [7,8], and SOS model with refuse [8], SOS model with diffusion [3]. In computer simulations, interfaces are described by a discrete set \( \{ h_i(t) \} \) which represents the height of a site \( i \) at the time \( t \). Such interface has \( L^d \) sites, where \( L \) is the linear size and \( d \) is the dimensionality of the substrate. The roughness of the interface is defined by

\[
\omega^2(L, t) = \left\langle \frac{1}{L^d} \sum_{i=1}^{L^d} (h_i - \bar{h})^2 \right\rangle,
\]

where \( \bar{h} \) is the mean height at the time \( t \) and the symbols \( \langle \ldots \rangle \) means average over independent computational samples. In most of the kinetic roughening models, the roughness obeys the Family-Vicsek dynamic scaling [10]

\[
\omega(L, t) \sim L^\alpha f \left( \frac{t}{L^z} \right),
\]

where the function \( f(x) \) must be \( L \)-independent. The roughness behaves as \( \omega \sim t^\beta \), for short times \( (1 \ll t \ll L^z) \) and behaves as \( \omega_\infty(L) \sim L^\alpha \) in the steady state. The \( \beta \) and \( \alpha \) are the growth and roughness exponents, respectively, and are related with the dynamical exponent \( z \) through the relation \( z = \alpha/\beta \). For some systems, \( \alpha = \beta = 0 \) and \( z \neq 0 \) which means that the roughness does not obey Eq.2 and has a logarithmic behavior in space and time.

The kinetic growth models are also described by the continuum Langevin-like equations in the coarse-grained limit. These equations have terms which represents the main interactions among the incoming particles. Example of a linear equation is the EW equation [6],

\[
\frac{\partial h(x, t)}{\partial t} = v_0 + \eta(x, t) + \nu \nabla^2 h(x, t),
\]

that describes the fluctuations of the SOS model with surface relaxation [7]. In Eq.3, the first two terms of the right side are related to the deposition of particles. This deposition has a rate \( v_0 \) and a noise with zero mean and variance given by
\[ \langle \eta(x, t) \eta(x', t') \rangle = D \delta^d(x - x') \delta(t - t') \] . (4)

The third term represents the surface relaxation process.

The exponents of Eq.3, obtained by Fourier analysis \[3,11\], are \( \beta(d) = (2 - d)/4 \), \( \alpha(d) = (2 - d)/2 \) and \( z(d) = 2 \). For \( d = 1 \), these expressions gives \( \beta = 1/4 \) and \( \alpha = 1/2 \). For \( d = 2 \), the scaling exponents are \( \beta = \alpha = 0 \).

There are also some nonlinear equations that describes nonlinear kinetic roughening models. The more known nonlinear equation is the KPZ equation \[12\]

\[ \frac{\partial h(x, t)}{\partial t} = v_0 + \eta(x, t) + \nu \nabla^2 h(x, t) + \frac{\lambda}{2} (\nabla h(x, t))^2 . \] (5)

This equation is more complete than Eq.4 because the nonlinear term may represent the lateral growth, or the appearance of a driven force. In \( d = 1 \), the exponents of this equation \[12\] are \( \beta = 1/3 \), \( \alpha = 1/2 \) and \( z = 3/2 \). In \( d = 2 \), the analytical solution is not known. Examples of models in the universality class of KPZ equation are the ballistic deposition (BD) \[4\] and the SOS model with refuse (KK) \[8\]. In \( d = 1 \), numerical simulations \[13\] indicate \( \beta \approx 0.30 \), \( \alpha \approx 0.47 \) for the BD model and \( \beta \approx 0.332 \), \( \alpha \approx 0.489 \) for the KK model. In \( d = 2 \), these exponents are \( \beta \approx 0.24 \), \( \alpha \approx 0.40 \) (BD) and \( \beta \approx 0.25 \), \( \alpha \approx 0.40 \) (KK).

In this letter we report on results of computer simulation of a growth model with two kinds of particles. Both of them obeys the KPZ kinetic, but they have opposite signs of the nonlinear \( \lambda \) constant. The effort to understand the nonlinearity in stochastic systems out of equilibrium is due to the great influence of the nonlinearities in the scaling analysis, as pointed by Binder et al \[14\]. The anisotropic KPZ equation, studied analytically in 1991 by Wolf \[15\], also contains two nonlinear terms with opposite signs that describes the distinguishable directions of the substrate in a vicinal surface. He has found, by renormalization group, a logarithmic behavior of the roughness \( \alpha = \beta = 0 \) for opposite signs of nonlinearity and power-law behavior when the nonlinearities have same signs. This results were confirmed by Kim et al. \[16\] by simulations of a discrete model with two different kinetics applied in each direction of the substrate.
The motivation of our work is the paper published by Bernardes et al [17]. They have studied the deposition of particles with different radii on a cold substrate by Monte Carlo simulation. The authors have found the growth exponent $\beta \approx 0.26$, for $d = 1$. So, they have concluded that the universality class of this model is next to the EW class [8]. However, there are two nonlinear characteristics in the morphology of the model of Bernardes et al: (i) existence of porosity in the bulk; (ii) the growth velocity, that is, $v = \langle d\bar{h}/dt \rangle$, is greater than the deposition rate. These characteristics can indicate that the up-down symmetry ($h \to -h$) is broken [4]. The break of this symmetry leads to appearance of the nonlinear term in the KPZ equation. Bernardes et al. also have checked the need of logarithmic correction in the behavior of roughness [14,18] that indicates the presence of odd nonlinear terms in the growth equation.

The aim to create a model with opposite KPZ nonlinearities is to verify the possibility of generating a linear process (when the effective nonlinearity vanishes) with a morphology of a nonlinear growth process. Our model is a probabilistic combination among the ballistic deposition model (BD) and the SOS model with refuse (KK). The KK model occurs with $p$-probability, and the BD model occurs with $(1 - p)$-probability.

Ballistic deposition is a process where particles are dropped vertically onto a smooth substrate. The incoming particles are automatically joined to the growing cluster when its first contact with the growing interface occurs. In the in-lattice version, we select at random a site $i$ of the lattice and its new height is evaluated by the algorithm [19]

$$h'_i = \max(h_i + 1; h_{\{j\}}),$$

where $\{j\}$ are the first neighbors of the site $i$. The BD kinetic does not generate a solid-on-solid deposition because it generates a structure with porosity. Therefore, we define the growing profile as the major height of an occupied site of each column.

The KK model is a SOS random deposition with the difference of height constraint $h_i - h_{\{j\}} < m$, where $m$ is the parameter that controls the roughness. If the height of the particle deposited on the site $i$ did not satisfy the height constraint, this particle is not
incorporated to the interface.

Both of them are in the same universality class of KPZ equation. We have chosen these two models because: (i) the BD model generates a bulk with porosity and has nonlinear parameter $\lambda_{BD} > 0$ because the growth velocity is bigger than the deposition rate $v_0$; (ii) the KK model has $\lambda_{KK} < 0$ because the kinetic of refuse makes the growth velocity smaller than the rate of deposition.

In our simulations, a unit of time means that we have done $L$ attempts of deposition. Moreover, all simulations were done with a one-dimensional substrate ($d=1$) and, in the KK model, the difference of height constraint $m = 1$.

Figure 1 shows the plot of the effective growth exponent $\beta_{eff}$ vs. the parameter $p$, for $L = 50,000$. The long dashed line is the exact value of $\beta$ obtained from KPZ equation by renormalization group. We have done 100 independent runs for each probability and we applied consecutive slopes method [2] in the log-log plots of $\omega$ vs. $t$ in the time interval $20 < t < 10000$, giving an ensemble of $\beta_{eff}$ exponents for each value of $p$. So, we have estimated the error bars around each value of $\beta_{eff}$. For $p^* = 0.83$, the model is near to the EW class, because the growth exponent is $\beta_{eff} \approx 0.27$. However, the error bars in this region has increased, indicating the need of more careful analysis of the scaling. These results can point that the effective KPZ term was removed in the probability $p^*$.

In order to make better characterization of the KPZ nonlinearity in our model, we do finite size analysis in the growth velocity. In 1990, Krug and Meakin [20] showed that the finite size correction, $\Delta v(L, t) = v(L, t) - v_\infty$, for a model in KPZ class behaves as

$$\Delta v(L) \sim -\lambda L^{-\alpha ||}, \quad \text{for } t \gg L^z,$$

where the $\alpha ||$ exponent depends on the roughness exponent. The $\Delta v$ correction goes to zero when the KPZ term vanishes. So, with Eq.7, we can obtain the sign of the KPZ nonlinearity and determine when the nonlinearity goes to zero in function of the tunning parameter $p$. Figure 2 shows the plot of $\Delta v = v(L = 10) - v(L = 1280)$ vs. $p$ for the BD-KK model. The finite size correction vanishes for $p \approx 0.81$ (see inset), very close to the value obtained in the
minimum of the $\beta$ vs. $p$ plot (see Figure 1).

We also check the need of multiplicative logarithmic corrections in the scaling for $p = p^*$. When the growth equation for a process has a sequence of odd nonlinear terms as

$$\frac{\partial h(x, t)}{\partial t} = \eta(x, t) + \nu \frac{\partial^2 h(x, t)}{\partial x^2} + \sum_{2n+1} \lambda_{2n+1} \left( \frac{\partial h(x, t)}{\partial x} \right)^{2n+1},$$  

for $n = 1, 2, \ldots$, the roughness behaves as

$$\omega(L, t) \sim t^{1/4} (\log t)^{1/8},$$  

for $t \ll L^z$. So, if logarithmic corrections are accepted for $p = p^*$, it means that the system is marginally in the EW class.

In order to show that Eq. 9 is really the better equation that describes the system near to $p^*$, we rewrite this equation as

$$\omega(L, t) \sim t^\delta (\log t)^\gamma,$$  

and we do small variations around the exact values $\delta = 1/4$ and $\gamma = 1/8$. We analyze the validation of the Eq. 10 by the evaluation of the deviations from the horizontal curve $Y(\delta, \gamma, t) = \omega(L, t)/t^\delta (\log t)^\gamma$ vs. $t$, because this emphasizes better the deviations of the behavior from this equation. So, we measure the relative error $\Delta Y/\langle Y \rangle$ of each curve $Y(\delta, \gamma, t)$ in function of the variations in $\delta$ and $\gamma$. Figure 3a shows the plots of $Y(t, \gamma)$ vs. $t$ with $\delta = 1/4$ and Figure 3b shows the plots of $Y(t, \delta)$ vs. $t$ with $\gamma = 1/8$. The insets shows the relative error $\Delta Y/\langle Y \rangle$ vs. the scaling exponent related to each case, $\gamma$ or $\delta$, respectively. The relative error, for the two cases, reaches a minimum when the exponents $\gamma = 1/8$ and $\delta = 1/4$, indicating that Eq. 9 is a good description for the temporal behavior of roughness. This is pointing out that odd-nonlinear terms are relevant.

The nonlinear Eq. 8 preserves the up-down symmetry, but this is not obvious in BD-KK model at $p = p^*$, and also in the growth model of Bernardes et al.. Eq. 1 can be generalized for any moment $q$ of the height distribution, in $d = 1$, as

$$\omega^q(L, t) = \left\langle \frac{1}{L} \sum_{i=1}^L (h_i - \bar{h})^q \right\rangle,$$  

for $q = 1, 2, \ldots$.
and we concentrate on the behavior of odd-moments, especially the third moment \((q = 3)\) which is related to up-down symmetry. The skewness, defined by \(S = \omega^3/(\omega^2)^{3/2}\), can show us if the system has this symmetry. If the skewness is null, the system has up-down symmetry because all odd moments of the height distribution vanish. On the other hand, for systems without the up-down symmetry and in the KPZ class, some authors \([21,22]\) believe that the skewness has a universal value \(|S| \approx 0.28\). Figure 4 shows the skewness \(S\) as a function of the time \(t\) for the model with positive nonlinearity \((p = 0.0, \text{triangle up})\), with negative nonlinearity \((p = 1.0, \text{triangle down})\) and at the low nonlinear point \(p = p^*\) (filled circles). As illustration, we also show the curve for the model with surface relaxation \([7]\) which is a linear model and has the up-down symmetry (plus). We note that the skewness for \(p = 0\) tends to \(S = 0\) and, for \(p = 1.0\), to \(S = -0.28\). For \(p = p^*\), in the asymptotic limit, the skewness goes to zero, suggesting the presence of the up-down symmetry.

In conclusion, we have studied the scaling properties of a model with opposite signs of the KPZ nonlinearity through numerical simulations of a model with two kinds of particles. The Kim-Kosterlitz kinetic occurs with a probability \(p\) and the ballistic deposition model with a probability \((1 - p)\). For a specific value of the tuning parameter \(p\), we show that the KPZ nonlinearity goes to zero and the up-down symmetry is recuperated. We also show that odd-nonlinearities are relevant in this model.

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**Figure captions**

**Figure 1**

The growth exponent $\beta$ vs. the parameter $p$ plot of the BD-KK model for $L = 50,000$. The long-dashed line is the exact value of the $\beta$ exponent for the KPZ equation.

**Figure 2**

Plot of the difference between the steady state growth velocities for $L = 10$ and $L = 1280$ vs. the parameter $p$ which gives the amount of KPZ nonlinearity in the system. The inset is showing the behavior next to the crossover.

**Figure 3**

Plots of the function $Y(t, \gamma, \delta)$ vs. the time $t$: (a) $\delta = 1/4$ and small variations in $\gamma$ are performed, (b) $\gamma = 1/8$ and small variations in $\delta$ are performed. The bold curves are showing the behavior of the function $Y(t, 1/8, 1/4)$. The insets shows the relative error $\Delta Y/\langle Y \rangle$ vs. the scaling exponent related to each case.

**Figure 4**

Plots of the skewness $S$ as a function of the time $t$ for $p = 0.0$ (triangle up), $p = 1.0$ (triangle down) and $p = p^*$ (filled circles). The skewness for the EW linear model is represented by the symbol plus. The long dashed straight lines indicate the $\pm 0.28$ estimated values. All simulations were done with $L = 50,000$. 
$\beta_{eff}$ vs $p$

T. J. da Silva and J. G. Moreira - Figure 1
T. J. da Silva and J. G. Moreira - Figure 2
$Y(t, \delta) = \omega(L, t)/t^{1/8}$

$Y(t, \gamma) = \omega(L, t)/t^{1/4}$

$\Delta Y(\gamma)/<Y(\gamma)>$

$\Delta Y(\delta)/<Y(\delta)>$

T. J. da Silva and J. G. Moreira - Figure 3
T. J. da Silva and J. G. Moreira - Figure 4