GENERALIZED DISCRETIZATION OF THE KARDAR-PARISI-ZHANG EQUATION

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Abstract

We introduce the generalized spatial discretization of the Kardar-Parisi-Zhang (KPZ) equation in 1+1 dimensions. We solve exactly the steady state probability density function for the discrete heights of the interface, for any discretization scheme. We show that the discretization prescription is a consequence of each particular model. From the ballistic deposition model we derive the discretization prescription of the corresponding KPZ equation.

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The interface growth models has attracted much attention during the two last decades due to its widespread application to many systems, such as film growth by vapor or chemical deposition, bacterial growth, evolution of forest fire fronts, etc. For such systems, the major effort has been concentrated in the identification of the scaling regimes and their classification into universality classes through Monte Carlo simulation of the discrete models or renormalization-group analysis of the continuous equations that describe the evolution of the interfaces in the coarse-grained approximation. This powerful tool allows a correspondence between the discrete models and the continuous equations. Another useful method is to derive continuous evolution equations from the transition rules of the discrete growth models based on a regularizing scheme and coarse-graining of the discrete Langevin equations. Phenomenological equations, selected according to symmetry principles and laws conservation, are often able to reproduce various experimental data. Between these phenomenological equations the introduced by Kardar, Parisi, and Zhang (KPZ) has been successful to describe the properties of rough interfaces, but is also related to Burgers equation of turbulence, and to directed polymers in random media. The KPZ equation describes the evolution of the profile $h(x, t)$ of the interface at position $x$ and time $t$:

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

where $\nu$ and $\lambda$ are the diffusion and nonlinear coefficients, respectively. The Gaussian thermal noise $\eta(x, t)$ has zero mean and covariance

$$\langle \eta(x, t)\eta(x', t') \rangle = 2 \epsilon \delta(x-x')\delta(t-t'),$$

where $\epsilon$ is the noise intensity. Here and elsewhere $\langle \rangle$ denotes average over the noise realizations. The KPZ equation differs from the Edwards-Wilkinson (EW) equation, that describe interfaces growing under the effect of random deposition and surface tension, in a nonlinear term due to microscopic lateral growth. The direct numerical integration is a powerful and simple tool to compute the exponents that characterize the universality class of a given continuous equation. In this context, the KPZ equation has been integrated using an unusual discretization method with exact steady state probability density function, a pseudospectral discretization method, and a least-square error method from experimental data. Several direct numerical integration methods has been used in various growing models, although the theoretical justification is not clear.
The main goal of this Communication is to introduce the generalized spatial discretization of the KPZ equation in $1 + 1$ dimensions. We show that exists the steady state probability density function of the discrete interface heights compatible with the continuous ones, after coarse grained approximation, independent of the discretization scheme. Finally, we find the discretization prescription for the KPZ equation derived from the ballistic model.

**Generalized discretization.** We propose as generic spatial discretization of the KPZ equation the following Langevin equation

$$\frac{dh_i}{dt} = \nu L_i + \frac{\lambda}{2} N_i^{(\gamma)} + \eta_i(t),$$

where $h_i(t) = h(ia, t)$ is the interface height at the $i$th-lattice point ($i = 1, \ldots, N$), $a$ is the horizontal lattice spacing, and $L = aN$ is the lattice size. Periodic boundary conditions are assumed, i.e. $h_0 \equiv h_N$. Without loss of generality we take the horizontal and vertical lattice spacing to be equal. Introducing in Eq. (3) the addimensional difference of heights

$$H_{i+k}^\ell = \frac{1}{a} (h_{i+k} - h_{i+k}) ,$$

where $\ell, k = -1, 0, 1$ ($\ell \neq k$), the standard discretized diffusive term is given by

$$L_i = \frac{1}{a} (H_{i+1}^i - H_{i-1}^i) .$$

Our discretized nonlinear term (with $0 \leq \gamma \leq 1$) in Eq. (3) is defined as

$$N_i^{(\gamma)} = \frac{1}{2(\gamma+1)} [(H_{i+1}^i)^2 + 2\gamma H_{i+1}^i H_i^{i+1} + (H_i^{i+1})^2].$$

The noise $\eta_i$ has zero mean and covariance

$$\langle \eta_i(t) \eta_j(t') \rangle = \frac{2\epsilon}{a} \delta_{ij} \delta(t-t') .$$

Expanding Eq. (5) and Eq. (6) around the $i$th-site, the discretized diffusive term and the nonlinear term in the $\gamma$-discretization are

$$L_i = \frac{\partial^2 h}{\partial x^2} + \frac{1}{12} \frac{\partial^4 h}{\partial x^4} a^2 + \mathcal{O}(a^4) \bigg|_{x=ia} ,$$

$$N_i^{(\gamma)} = \left( \frac{\partial h}{\partial x} \right)^2 + \frac{1}{4} \left( \frac{1-\gamma}{1+\gamma} \right) \left( \frac{\partial^2 h}{\partial x^2} \right)^2 a^2 + \mathcal{O}(a^4) \bigg|_{x=ia} ,$$

respectively. Several discretizations will produce different results in the roughness even though the difference in numerical accuracy of the height profile are small [13]. Most numerical studies are done with the discrete spatial version of the KPZ equation corresponding
to the usual choice $\gamma = 1$ in Eq. (6) called standard or post-point discretization. The nonlinear term $N_i^{(1)} = \frac{1}{4}(H_{i+1} - H_{i-1})^2$ only depends on the nearest neighbor sites height and minimizes the error in approximating $\partial^2 h/\partial x^2$ [see Eq. (8)]. Moreover, the choice $\gamma = 0$ in Eq. (6), called anti-standard or pre-point discretization, used here afterwards, corresponds to the arithmetic mean of the squared slopes around any interface site. On the other hand, Lam and Shin [13] introduced the spatial discretization corresponding to the choice $\gamma = 1/2$ in Eq. (6) that enables an elegant analytical treatment. However, this choice is unusual and is only supported by the existence of a steady state probability density function equal to those of the linear case $\lambda = 0$. We explain this special choice and show, through a general calculus of the steady state solution, that the generalized discretization has an unambiguous limit in the continuous.

**Steady state density.** The main feature of the generalized discretization of the KPZ equation is that the corresponding steady state probability density function $\tilde{P}(h)$ of the discrete heights $h \equiv \{h_i\}$ exists. This density function gives rise to the known steady state probability density functional $\tilde{P}[h]$ of the continuous interface height $h(x,t)$ related to the KPZ equation [2]. Conversely, $\tilde{P}(h)$ is not a direct consequence of the $\tilde{P}[h]$ as we show below. The probability density function $P(h,t)$ of the discrete interface evolves according to the following Fokker-Planck equation

$$\frac{\partial P}{\partial t} = - \sum_{i=1}^{N} \frac{\partial J_i^{(\gamma)}}{\partial h_i},$$

$$J_i^{(\gamma)} = \left( \nu L_i + \frac{\lambda}{2} N_i^{(\gamma)} \right) P - \frac{\epsilon}{a} \frac{\partial P}{\partial h_i},$$

where $J_i^{(\gamma)}(h,t)$ is the probability current density. Replacing in Eq. (9) the general

$$\tilde{P}(h) = \exp \left( -\frac{\nu}{\epsilon} \sum_{i=1}^{N} a U_i^{(\gamma)} \right),$$

where $U_i^{(\gamma)}$ is a “potential” function to be derived below, we obtain the steady state probability current density function

$$\tilde{J}_i^{(\gamma)}(h) = \left( \nu L_i + \frac{\lambda}{2} N_i^{(\gamma)} + \nu \frac{\partial U_i^{(\gamma)}}{\partial h_i} \right) \tilde{P}.$$  

Lam and Shin [13] showed that $\tilde{P}(h)$ for the linear case ($\lambda = 0$) is also solution of the nonlinear one in the midpoint discretization. We explain their result setting $U_i^{(\gamma)} = N_i^{(0)}$ in
Eq. (11), i.e. the solution corresponding to \( \lambda = 0 \). It is easy to show that, under periodic boundary conditions, the current \( \tilde{J}^{(\gamma)}_i = (\lambda/2) N^{(\gamma)}_i \tilde{P} \) is conserved only if \( \gamma = 1/2 \) for \( \lambda \neq 0 \) (i.e. \( \sum_{i=1}^{N} \partial \tilde{J}^{(1/2)}_i / \partial h_i = 0 \)). Our goal is to find a steady state solution, independent of the choice of the discretization and therefore for any nonlinear coefficient \( \lambda \), with constant \( \tilde{J}^{(\gamma)}_i(h) \). It is easy to show, using Eq. (5) and Eq. (6), that

\[
N^{(\gamma)}_i = N^{(1/2)}_i + \frac{1}{6} \left( \frac{1 - 2\gamma}{1 + \gamma} \right) L_i^2 a^2,
\]

\[
\frac{dL_i}{dh_i} = -\frac{2}{a^2},
\]

\[
\frac{dN^{(\gamma)}_i}{dh_i} = -\left( \frac{1 - \gamma}{1 + \gamma} \right) L_i.
\]

Using Eqs. (12) in Eq. (11) we obtain that

\[
U^{(\gamma)}_i = N^{(0)}_i + \sigma L^3_i,
\]

where

\[
\sigma = \frac{\lambda}{72} \nu \left( \frac{1 - 2\gamma}{1 + \gamma} \right) a^4.
\]

Eq. (13) gives a steady state solution of the Fokker-Planck equation [Eq. (10)] with conserved current

\[
\tilde{J}^{(\gamma)}_i \equiv \tilde{J}^{(1/2)}_i = \frac{\lambda}{2} N^{(1/2)}_i \tilde{P}.
\]

A dimensional analysis shows that \( \epsilon/\nu \) and \( \nu/\lambda \) are proportional to \( a \), and therefore \( \sigma \) is proportional to \( a^3 \). Besides, note from Eq. (8) that the errors of \( N^{(\gamma)}_i \) and \( L_i \) in approximating \( (\partial h/\partial x)^2 \) and \( \partial^2 h/\partial x^2 \), respectively, are at most proportional to \( a^2 \). Thus, we conclude that the error of \( U^{(\gamma)}_i \) in approximating \( (\partial h/\partial x)^2 \) is proportional to \( a^2 \) [see Eq. (13)]. The midpoint solution \( U^{(1/2)}_i = N^{(0)}_i \) is symmetric under the interchange \( H_{i+1} \leftrightarrow H_{i-1} \), but the term \( \sigma L^3_i \) breaks weakly this symmetry in Eq. (13). Notice that the limits \( \lambda = 0 \) (EW equation), \( \gamma = 1/2 \) (midpoint discretization), and \( a = 0 \) (coarse grained approximation) in Eq. (13) are equivalent between them.

If we denote by \( P([h], t) \) the probability density functional of the interface position function \( h(x, t) \) in 1 + 1 dimensions, the corresponding Fokker-Planck equation is

\[
\frac{\partial P([h], t)}{\partial t} = - \int_0^L dx \frac{\delta}{\delta h} \left\{ \left[ \nu \frac{\partial^2 h}{\partial x^2} + \frac{\lambda}{2} \left( \frac{\partial h}{\partial x} \right)^2 \right] P \right\}
+ \epsilon \int_0^L dx \frac{\delta^2 P}{\delta h^2},
\]
from which we can obtain the well-known steady state solution

$$\tilde{P}[h] = \exp \left[ -\frac{\nu}{\epsilon} \int_0^L dx \left( \frac{\partial h}{\partial x} \right)^2 \right].$$

Incidentally, this is the solution in absence of the nonlinearities. Moreover,

$$\tilde{J}[h] = \frac{\lambda}{2} \left( \frac{\partial h}{\partial x} \right)^2 \tilde{P} = \text{const}$$

for the nonlinear case. A special feature of our discretization is that $\tilde{P}(h)$ is a steady state solution for all values of the $\lambda$. While the nonlinear coefficient is present in $\tilde{P}(h)$, it is absent in $\tilde{P}[h]$, because $\lim_{a \to 0} \sum_{i=1}^N a \, U_i^{(\gamma)} = \int_0^L (\partial h / \partial x)^2 \, dx$. This means that the coarse grained approximation erase in $\tilde{P}[h]$ our knowledge on the discrete model and the nonlinearity. Again, for any discretization, the coarse grained approximation preserves the nonlinear dominant term of the steady state current, since $\lim_{a \to 0} \tilde{J}_i^{(\gamma)} = \tilde{J}[h]$.

**Ballistic deposition model.** The KPZ equation is tractable by direct numerical integration when we specify its associate spatial discretization. In order to verify this fact, we derive the Langevin equation [Eq. (3)] for the ballistic deposition (BD) model. The procedure used here is based on regularizing the step functions included in the growth rules of the microscopic model, in order to obtain the discrete Langevin equation and, afterward coarse graining, the KPZ equation. Let us first introduce the general treatment. The discrete interface growth at an average rate $\tau$ and the interface height at an $i$th-site increase in $h_i(t+\tau) - h_i(t) = a \sum_{j=1}^m r_i^{(j)}$, where $r_i^{(j)}$ are the rules of the deposition processes. Expanding $h_i(t+\tau)$ up to second order in Taylor series around $\tau$, we obtain $h_i(t+\tau) - h_i(t) \approx \tau \frac{dh_i}{dt}$. Thus, the height evolution equation of the $i$th-site is given by the Langevin equation

$$\frac{dh_i}{dt} = K_i^{(1)} + \eta_i(t),$$

where the Gaussian thermal noise $\eta_i$ has zero mean and covariance

$$\langle \eta_i(t) \eta_j(t') \rangle = K_{ij}^{(2)} \delta(t - t').$$

The first and second moments of the transition rate, in terms of growth rules, are given by

$$K_i^{(1)} = \frac{a}{\tau} \sum_{j=1}^m r_i^{(j)}, \quad K_{ij}^{(2)} = a \delta_{ij} K_i^{(1)},$$

respectively. In the BD model, a particle is released from a randomly chosen lattice position $i$ above the interface, located at a distance larger than the maximum height of the interface.
The incident particle follows a vertical straight trajectory and sticks to the interface at time \( t \). The height in the column \( i \) is increased by \( \max[h_{i-1}, h_i + 1, h_{i+1}] \). For this model the rules can be summarized as:

\[
\begin{align*}
    r_i^{(1)} &= \Theta(H_{i+1}^i) \Theta(H_{i-1}^i), \\
    r_i^{(2)} &= H_{i+1}^i \left[ 1 - \Theta(H_{i+1}^i) \right] \left[ 1 - \Theta(H_{i-1}^i) \right], \\
    r_i^{(3)} &= H_{i-1}^i \left[ 1 - \Theta(H_{i-1}^i) \right] \left[ 1 - \Theta(H_{i+1}^i) \right], \\
    r_i^{(4)} &= \frac{1}{2} \delta(H_{i+1}^i, 0) \left\{ H_{i+1}^i \left[ 1 - \Theta(H_{i+1}^i) \right] \\
    &+ H_{i-1}^i \left[ 1 - \Theta(H_{i-1}^i) \right] \right\},
\end{align*}
\]

where \( \Theta(z) \) is the unit step function defined as \( \Theta(z) = 1 \) for \( z \geq 0 \) and \( \Theta(z) = 0 \) for \( z < 0 \), and \( \delta(z, 0) = \Theta(z) + \Theta(-z) - 1 \) is the Kronecker delta. The representation of the step function can be expanded as \( \Theta(z) = \sum_{k=0}^{\infty} c_k z^k \) providing that \( z \) is smooth. In any discrete model there is in principle an infinite number of nonlinearities, but at long wavelengths the higher order derivatives can be neglected using scaling arguments, since one expect affine interfaces over a long range of scales, and then one is usually concerned with the form of the relevant terms. Thus, keeping the expansion of the step function to first order in its argument and replacing the expansion in Eq. (17) and (16) the first moment is

\[
K_i^{(1)} = v_0 + \nu L_i + \frac{\lambda}{2} N_i^{(\gamma)}, \quad (18)
\]

where

\[
\begin{align*}
    v_0 &= c_0^2 \frac{a}{\tau}, \\
    \nu &= (1 - c_0 - 2c_0c_1) \frac{a^2}{\tau}, \\
    \lambda &= 2c_1 \left( 5 - 4c_0 - c_1 \right) \frac{a}{\tau}, \\
    \gamma &= \frac{1}{2} + \frac{1 - 2(c_0 + c_1)}{2(3 - 2c_0)}. 
\end{align*}
\]

The average driving velocity \( v_0 \) can be subtracted in the expression of the first moment given by Eq. (18), choosing adequately a moving reference frame. Retaining only the constant term in Eq. (18) we obtain \( K_{ij}^{(2)} \simeq a \delta_{ij} v_0 = \epsilon \delta_{ij}/a \). Replacing in Eq. (15) we recover Eq. (7) with noise intensity \( \epsilon = a^2 v_0 \). Notice that in order to integrate numerically the continuous equation, we need a continuous representation of the \( \Theta \)-function to numerically compute the
coefficients $c_0$ and $c_1$ related to the ones of the KPZ equation through Eq. (19), such as the shifted hyperbolic tangent representation [16]. Our parameter of discretization is related to the parameters of the microscopic model and the KPZ coefficients [see Eq. (19)]. Choosing $\gamma$, the KPZ coefficients $\lambda$, $\nu$ and $\epsilon$ depends only of one of the microscopic parameters, e.g. with $\gamma = 1/2$ the parameters $c_0$ and $c_1$ are related as $c_0 + c_1 = 1/2$.

In summary, we propose a finite difference discretization criterion for the numerical integration of the KPZ growth equation starting from the corresponding generalized discrete Langevin equation. We show that, for any discretization scheme, exists a steady state probability density function of the discrete interface heights compatible with the continuous ones, after coarse graining. Besides, we derived the KPZ coefficients of the BD model as an example of our generalized discretization. Finally, our results can be used as a new tool for the direct numerical integration of growing continuous equations with nonlinear terms due to lateral growth like the KPZ one.

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