Generalized discretization of the Kardar-Parisi-Zhang equation

R. C. Buceta
Departamento de Física, Facultad de Ciencias Exactas y Naturales, Universidad Nacional de Mar del Plata Funes 3350, B7602AYL Mar del Plata, Argentina
(Received 21 October 2004; published 12 July 2005)

We report 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. We derive the discretization prescription of the KPZ equation for the ballistic deposition model.

DOI: 10.1103/PhysRevE.72.017701 PACS number(s): 05.10.Gg, 02.60.Lj, 68.35.Ct, 68.35.Rh

The interface growth model has attracted much attention during the two last decades due to its widespread application to many systems [1–3], 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. Another powerful tool to characterize the scaling regimes is the renormalization-group analysis of the continuous equations in the hydrodynamic limit. These tools allow us to make a correspondence between the discrete models and the continuous equations. A useful method to make this connection 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 [4–6]. Phenomenological equations, selected according to symmetry principles and conservation laws, are often able to reproduce many experimental data. A widely studied phenomenological equation representing the irreversible growth of such interfaces is the Kardar-Parisi-Zhang (KPZ) equation [7]. The KPZ equation is also related to the Burgers equation of turbulence and to directed polymers in random media [2]. The KPZ describes the evolution of the profile $h(x,t)$ of the interface at position x and time t

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

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

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

where ϵ is the strength of the noise. Here and elsewhere $\langle\ \rangle$ denotes the average over noise realizations. The KPZ equation differs from the Edwards-Wilkinson (EW) equation [8] in the nonlinear term due to microscopic lateral growth. The later equation is succesful in describing interfaces growing under the effect of random deposition and surface tension. A powerful and simple tool to compute the exponents that characterize the universality class of a given continuous equation is the numerical integration [9–12]. The KPZ was integrated using a peculiar discretization method with exact steady state probability density function [13], a pseudospectral discretization method [14], and a least-square error method from experimental data [15]. The most common method is the direct numerical integration that was used in various models of growth [9–13] although their theoretical justification is not clear.

The main goal of this Brief Report is to introduce a generalized spatial discretization of the KPZ equation in 1+1 dimensions, i.e., a discrete Langevin equation for the local interface height. We find the steady state probability density function of the discrete interface heights for all discretization prescription. Finally, we establish the discretization prescription associated to the KPZ equation for the ballistic model and show that the Langevin equation with a nonlinear lateral growth term, obtained via regularization of the transition rules of the discrete models, depends on the discretization of the nonlinearity.

Generalized discretization. We propose the following Langevin equations as a general spatial discretization of the KPZ equation:

$$\frac{dh_i}{dt} = \nu\, L_i + \frac{\lambda}{2} N_i^{(\gamma)} + \eta_i(t), \tag{3}$$

where $h_i(t)=h(ia,t)$ is the interface height at the site i of the lattice $(i=1,\ldots,N)$, a is the horizontal lattice spacing, and $L=a\,N$ is the lateral 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 the addimensional difference of heights

$$H_{i+k}^{i+\ell} = \frac{1}{a}(h_{i+\ell} - h_{i+k}), \tag{4}$$

where $\ell,k=-1,0,1$ $(\ell \neq k)$, the standard discretized diffusive term of Eq. (3) is given by

$$L_i = \frac{1}{a}(H_i^{i+1} - H_{i-1}^{i}). \tag{5}$$

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

$$N_i^{(\gamma)} = \frac{1}{2(\gamma+1)}[(H_i^{i+1})^2 + 2\gamma\, H_i^{i+1} H_{i-1}^i + (H_{i-1}^i)^2]. \quad (6)$$

The noise η_i has zero mean and covariance

$$\langle \eta_i(t)\, \eta_j(t')\rangle = \frac{2}{a}\epsilon \delta_{ij}\delta(t-t'). \quad (7)$$

Expanding Eq. (5) and Eq. (6) around the ith site, the discretized diffusive term and the nonlinear term in the γ discretization are given by

$$L_i = \left.\frac{\partial^2 h}{\partial x^2} + \frac{1}{12}\frac{\partial^4 h}{\partial x^4}a^2 + O(a^4)\right|_{x=ia}, \quad (8)$$

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

respectively. Different discretizations will produce unequal results in the roughness even though the difference in the numerical accuracy of the height profile is small [13]. Most numerical studies are done with the discrete spatial version of the KPZ equation corresponding to the usual choice $\gamma = 1$ [see Eq. (6)] called standard or post-point discretization. The nonlinear term $N_i^{(1)} = \frac{1}{4}(H_{i-1}^{i+1})^2$ only depends on the height of the nearest-neighbor sites and thus the error in approximating $\partial^2 h/\partial x^2$ is minimized [see Eq. (8)]. Oppositely, the choice $\gamma = 0$, called antistandard or prepoint discretization, 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 $\gamma = 1/2$ 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 the one obtained for the linear case ($\lambda = 0$). Below we explain this special choice and we also show, through a general calculus of the steady state solution, that the generalized discretization has an unambiguous limit in the continuous independent of the γ value.

Steady state density. The main feature of the generalized discretization of the KPZ equation is that there is a steady state probability density function $\tilde{P}(\mathbf{h})$ of the discrete heights $\mathbf{h} \equiv \{h_i\}$. This 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, $\tilde{P}(\mathbf{h})$ cannot be derived from $\tilde{P}[h]$ as we show below. The probability density function $P(\mathbf{h},t)$ evolves according to the following Fokker-Planck equation

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

$$J_i^{(\gamma)} = \left(\nu\, L_i + \frac{\lambda}{2} N_i^{(\gamma)}\right) P - \frac{\epsilon}{a}\frac{\partial P}{\partial h_i}, \quad (9)$$

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

$$\tilde{P}(\mathbf{h}) = \exp\left(-\frac{\nu}{\epsilon}\sum_{i=1}^{N} a U_i^{(\gamma)}\right), \quad (10)$$

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

$$\tilde{J}_i^{(\gamma)}(\mathbf{h}) = \left(\nu\, L_i + \frac{\lambda}{2} N_i^{(\gamma)} + \nu \frac{\partial U_i^{(\gamma)}}{\partial h_i}\right)\tilde{P}. \quad (11)$$

Lam and Shin [13] showed that $\tilde{P}(\mathbf{h})$ 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 $\tilde{J}_i^{(\gamma)} = (\lambda/2) N_i^{(\gamma)} \tilde{P}$ is conserved only if $\gamma = 1/2$ for $\lambda \neq 0$ (i.e., $\Sigma_{i=1}^{N} \partial \tilde{J}_i^{(1/2)}/\partial h_i = 0$). Our goal is to find a steady state solution, independent of the choice of the discretization and therefore for any value of the nonlinear coefficient λ, with constant current $\tilde{J}_i^{(\gamma)}(\mathbf{h})$. Using Eq. (5) and Eq. (6) it is easy to show that

$$N_i^{(\gamma)} = N_i^{(1/2)} + \frac{1}{6}\left(\frac{1-2\gamma}{1+\gamma}\right) L_i^2 a^2,$$

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

$$\frac{dN_i^{(\gamma)}}{dh_i} = -\left(\frac{1-\gamma}{1+\gamma}\right) L_i. \quad (12)$$

Replacing Eqs. (12) in Eq. (11) we get

$$U_i^{(\gamma)} = N_i^{(0)} + \sigma\, L_i^3, \quad (13)$$

where

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

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

$$\tilde{J}_i^{(\gamma)} \equiv \tilde{J}_i^{(1/2)} = \frac{\lambda}{2} N_i^{(1/2)} \tilde{P}.$$

A dimensional analysis shows that ϵ/ν and ν/λ are proportional to a, and therefore σ is proportional to a^3. Moreover, notice from Eq. (8) that the errors of $N_i^{(\gamma)}$ 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 $U_i^{(\gamma)}$ in approximating $(\partial h/\partial x)^2$ is proportional to a^2 [see Eq. (13)]. The midpoint solution $U_i^{(1/2)} = N_i^{(0)}$ is symmetric under the interchange $H_i^{i+1} \leftrightarrow H_{i-1}^i$, but the term σL_i^3 breaks weakly the symmetry of Eq. (13). Notice that the limits $\lambda = 0$ (EW equation), $\gamma = 1/2$ (midpoint discretization), and $a = 0$ (coarse-grained approximation) are equivalent between them.

If we denote by $P([h],t)$ the probability density functional of $h(x,t)$ 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

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

This steady state probability density is precisely the solution in absence of 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 $\tilde{P}(\mathbf{h})$ is a steady state solution for all the values of λ. While the nonlinear coefficient is present in $\tilde{P}(\mathbf{h})$, it is absent in $\tilde{P}[h]$, because $\lim_{a\to 0}\Sigma_{i=1}^{N} a\ U_i^{(\gamma)} = \int_0^L (\partial h/\partial x)^2 dx$. Thus the coarse-grained approximation wipes out our knowledge on the discrete model and the nonlinearity. Again, for any discretization, the coarse-grained approximation preserves the dominant nonlinear term of the steady state current, since $\lim_{a\to 0}\tilde{J}_i^{(\gamma)} = \tilde{J}[h]$.

Ballistic deposition model. The KPZ equation can be solved 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, after coarse graining, the KPZ equation. Let us first introduce the general treatment. In an average time interval τ, the discrete interface height at the site i increase in $h_i(t+\tau) - h_i(t) = a\Sigma_{j=1}^{m} r_i^{(j)}$, where $r_i^{(j)}$ are the rules of the deposition processes. Expanding $h_i(t+\tau)$ up to second order in the Taylor series around τ, we obtain $h_i(t+\tau) - h_i(t) \approx \tau\, dh_i/dt$. Thus, the evolution of the height on the site i is given by the Langevin equation

$$\frac{dh_i}{dt} = K_i^{(1)} + \eta_i(t), \tag{14}$$

where the Gaussian thermal noise η_i has zero mean and covariance

$$\langle \eta_i(t)\,\eta_j(t')\rangle = K_{ij}^{(2)}\delta(t-t'). \tag{15}$$

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

$$K_i^{(1)} = \frac{a}{\tau}\sum_{j=1}^{m} r_i^{(j)}, \quad K_{ij}^{(2)} = a\ \delta_{ij} K_1^{(1)}, \tag{16}$$

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

$$\begin{aligned} r_i^{(1)} &= \Theta(H_{i+1}^i)\Theta(H_{i-1}^i), \\ r_i^{(2)} &= H_i^{i+1}[1-\Theta(H_{i+1}^i)][1-\Theta(H_{i+1}^{i-1})], \\ r_i^{(3)} &= H_i^{i-1}[1-\Theta(H_{i-1}^i)][1-\Theta(H_{i-1}^{i+1})], \\ r_i^{(4)} &= \frac{1}{2}\delta(H_{i-1}^{i+1},0)\{H_i^{i+1}[1-\Theta(H_{i+1}^i)] + H_i^{i-1}[1-\Theta(H_{i-1}^i)]\}, \end{aligned} \tag{17}$$

where $\Theta(z)$ is the unit step function defined as $\Theta(z)=1$ for $z \geqslant 0$ 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 $\Theta(z) \doteq \Sigma_{k=0}^{\infty} c_k z^k$ 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 expects 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 the first order in its argument and replacing the expansion in Eq. (17) and Eq. (16), the first moment is

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

where

$$\begin{aligned} v_0 &= c_0^2 \frac{a}{\tau}, \\ \nu &= (1 - c_0 - 2c_0c_1)\frac{a^2}{\tau}, \\ \lambda &= 2\ c_1(5 - 4c_0 - c_1)\frac{a}{\tau}, \\ \gamma &= \frac{1}{2} + \frac{1-2(c_0+c_1)}{2(3-2\ c_0)}. \end{aligned} \tag{19}$$

The 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 strength $\epsilon = a^2 v_0$. Notice that in order to define the KPZ coefficients and the parameter γ [see Eq. (19)], we need a continuous representation of the Θ function (such as the shifted hyperbolic tangent representation [16]) to compute the coefficients c_0 and c_1 of this expansion. For a given γ, the KPZ coefficients λ, ν, and ϵ depend only on one of the microscopic parameters, e.g., for $\gamma = 1/2$ the coefficients c_0 and c_1 are related by $c_0 + c_1 = 1/2$.

The extension of the discretization prescription to $n+1$ dimensions is direct. Nevertheless, to clarify, notice that $(\nabla h)^2 = \Sigma_{i=1}^{n}(\partial h/\partial x_i)^2$, where x_i are the coordinates (i

$=1,\ldots,n$). The extension is direct since Eq. (6) is related to each one of the nonlinear terms of the previous sum. Thus, the generalized discretization depends on n parameters γ_i, one by each coordinate.

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, there is a steady state probability density function of the discrete interface heights. Besides, we derive the KPZ coefficients for the BD model as an example of our generalized discretization. We remark that all the discretization prescriptions are equivalent in the sense that the same continuous equation is obtained. Nevertheless, the numerical convergence of equivalent discretizations to the continuous is a pending task that goes beyond the aim of this paper. Finally, our results can be used as a tool for the direct numerical integration of growth continuous equations with nonlinear terms such as the KPZ one.

We wish to thank M. Bellini for valuable suggestions and L.A. Braunstein for a critical reading of the manuscript. This work was supported by UNMdP and ANPCyT (Grant No. PICT-O 2000/1-03-08974).

[1] A.-L. Barabási and H. E. Stanley, *Fractal Concepts in Surface Growth* (Cambridge University Press, New York, 1995).
[2] T. Halpin-Healy and Y.-C. Zhang, Phys. Rep. **254**, 215 (1995).
[3] P. Meakin, *Fractals, Scaling and Growth Far From Equilibrium* (Cambridge University Press, Cambridge, 1998).
[4] D. D. Vvedensky, A. Zangwill, C. N. Luse, and M. R. Wilby, Phys. Rev. E **48**, 852 (1993); D. D. Vvedensky, *ibid.* **67**, 025102(R) (2003); **68**, 010601(R) (2003).
[5] G. Costanza, Phys. Rev. E **55**, 6501 (1997); J. Phys. A **31**, 7211 (1998).
[6] L. A. Braunstein, R. C. Buceta, C. D. Archubi, and G. Costanza, Phys. Rev. E **62**, 3920 (2000); D. Muraca, L. A. Braunstein, and R. C. Buceta, *ibid.* **69**, 065103(R) (2004).
[7] M. Kardar, G. Parisi, and Y.-C. Zhang, Phys. Rev. Lett. **56**, 889 (1986).
[8] S. F. Edward and D. R. Wilkinson, Proc. R. Soc. London, Ser. A **381**, 17 (1982).
[9] J. G. Amar and F. Family, Phys. Rev. A **41**, 3399 (1990); Phys. Rev. E **47**, 1595 (1993).
[10] K. Moser, J. Kertész, and D. E. Wolf, Physica A **178**, 215 (1991); K. Moser and D. E. Wolf, J. Phys. A **27**, 4049 (1994).
[11] M. Beccaria and G. Curci, Phys. Rev. E **50**, 4560 (1994).
[12] C. Dasgupta, S. Das Sarma, and J. M. Kim, Phys. Rev. E **54**, R4552 (1996); C. Dasgupta, J. M. Kim, M. Dutta, and S. Das Sarma, *ibid.* **55**, 2235 (1997).
[13] C.-H. Lam and F. G. Shin, Phys. Rev. E **58**, 5592 (1998); **57**, 6506 (1998).
[14] L. Giada, A. Giacometti, and M. Rossi, Phys. Rev. E **65**, 036134 (2002); A. Giacometti and M. Rossi, *ibid.* **63**, 046102 (2001).
[15] A. Giacometti and M. Rossi, Phys. Rev. E **62**, 1716 (2000).
[16] M. Předota and M. Kotrla, Phys. Rev. E **54**, 3933 (1996).