PHYSICAL REVIEW E **67**, 025102(R) (2003)

Edwards-Wilkinson equation from lattice transition rules

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(Received 31 October 2002; published 26 February 2003)

Continuum equations of motion for the height fluctuations of lattice growth models are derived from their transition rules by regularizing and coarse-graining the associated discrete Langevin equations. For models with random deposition followed by instantaneous relaxation to a neighboring site based on identifying the local height minimum, our methodology yields the Edwards-Wilkinson equation. The application of this procedure to other growth models is discussed.

DOI: 10.1103/PhysRevE.67.025102 PACS number(s): 05.40.−a, 81.15.Aa

Driven lattice models are widely used to describe front fluctuations during surface growth. The statistical properties of such models are usually determined by kinetic Monte Carlo (KMC) simulations, from which a correspondence with particular continuum equations of motion can often be inferred from assignments to universality classes [1]. However, this is largely an empirical exercise and may require extensive simulations to eliminate crossover effects [2]. Proposals for establishing more direct associations between lattice models and continuum equations of motion have included phenomenological [3] and symmetry [4–6] arguments, mappings onto other models [4,7], real-space renormalization-group methods [8], and formal expansions of discrete equations of motion [7,9–12]. Despite these efforts, the connection between continuum equations and lattice models is seldom unequivocal.

In this paper, we present a method for deriving continuum equations of motion from the transition rules of lattice growth models. Our procedure is based on regularizing and coarse-graining discrete Langevin equations that are obtained from a Kramers-Moyal expansion of the master equation [13] and invoking a limit theorem due to Kurtz [14–16]. For models in which random deposition is followed by the instantaneous relaxation of the arriving particle to a neighboring site based on identifying the local height minimum [17,18], we obtain the Edwards-Wilkinson equation [19]. The coefficients in this equation are determined solely by the parameters of the lattice model. To our knowledge, this is the first time that a stochastic continuum equation of motion has been obtained directly from a lattice model with nonanalytic transition rules.

The method described below can be applied to growth on a d-dimensional lattice, but we focus here on one-dimensional substrates to simplify the calculations. We consider a lattice onto which particles are deposited at an average rate τ_0^{-1} per site. For each deposition event, a site is chosen at random and the deposition site is selected within a specified range of the chosen site according to some criterion based on the local height environment. Once deposited, the particles remain fixed at their positions. If the search range for the deposition site extends only to the nearest neighbors, the equation of motion for the height h_i at the ith site has the general form [10,20]

$$\frac{dh_i}{d\tau} = K_i^{(1)} + \eta_i , \tag{1}$$

where $K_i^{(1)}$, the first moment of the transition rate, is

$$K_i^{(1)} = \frac{1}{\tau_0}[w_i^{(1)} + w_{i+1}^{(2)} + w_{i-1}^{(3)}], \tag{2}$$

in which the $w_i^{(j)}$ embody the local relaxation rules, and the η_i are Gaussian noises that have zero mean, and covariance

$$\langle \eta_i(\tau)\,\eta_j(\tau')\rangle = K_i^{(1)}\delta_{ij}\delta(\tau-\tau'). \tag{3}$$

With the deposition of complete units replaced by units of size Ω^{-1}, where Ω is a ''largeness'' parameter that controls the magnitude of the fluctuations, and a corresponding transformation of the time to maintain the original deposition rate, the resulting equations of motion produce a morphological evolution that is statistically equivalent to that of KMC simulations [14–16,20].

In the first model we consider [17], a particle incident on a site remains there only if its height is less than or equal to that of both nearest neighbors. If only one nearest neighbor column is lower than that of the original site, deposition is onto that site. However, if both nearest neighbor columns are lower than that of the original site, the deposition site is chosen randomly between the two. These rules can be written in the following form for substitution into Eq. (2)

$$w_i^{(1)} = \theta_i^+\,\theta_i^- ,$$

$$w_i^{(2)} = \theta_i^+(1-\theta_i^-) + \frac{1}{2}(1-\theta_i^+)(1-\theta_i^-), \tag{4}$$

$$w_i^{(3)} = \theta_i^-(1-\theta_i^+) + \frac{1}{2}(1-\theta_i^+)(1-\theta_i^-),$$

where $\theta_i^{\pm} = \theta(h_{i\pm1} - h_i)$ and $\theta(x)$ is the unit step function, defined as

$$\theta(x) = \begin{cases} 1 & \text{if} \quad x \geqslant 0, \\ 0 & \text{if} \quad x < 0. \end{cases} \tag{5}$$

In Eq. (4), the $w_i^{(j)}$ express the conditions for a particle incident on site i to remain there ($j=1$), to relax to site $i-1$ ($j=2$), or to relax to site $i+1$ ($j=3$). Thus, $K_i^{(1)}$ is the total arrival rate of particles at site i. The identity

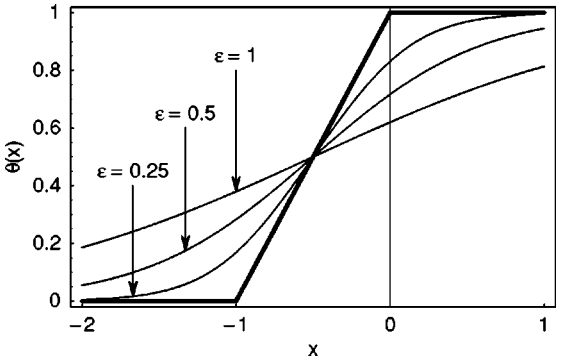

FIG. 1. The step function in Eq. (8) with $a=1$ (bold line) and the regularization in Eq. (9) for the indicated values of ϵ.

$$w_i^{(1)}+w_i^{(2)}+w_i^{(3)}=1 \tag{6}$$

mandates that deposition is always onto one of these sites and thereby ensures that the average deposition rate per site is τ_0^{-1}.

The step functions in Eq. (4) reflect the threshold character of the transition rules. Their presence is typical in models whose transition probabilities depend on the local height environment [10–12], but their nonanalyticity presents a major obstacle for coarse-graining the discrete equations of motion (1)-(3). One way of bypassing this problem is to use an analytic expression that reproduces the step function in some limit but is otherwise amenable to a Taylor expansion. Several such regularizations have been suggested, including expressions based on trigonometric [11,21] and hyperbolic [9,11,22] tangent functions, and the error function [23]. Here, we begin by observing that θ is required only at the discrete values $h_{i\pm1}-h_i$ [24], so we can choose an interpolation between these points at our convenience. Thus, from the following representation of the maximum function [25]

$$\max(x,y)=\lim_{\epsilon\to0^+}[\epsilon\ln(e^{x/\epsilon}+e^{y/\epsilon})], \tag{7}$$

we construct a corresponding representation of $\theta(x)$,

$$\theta(x)=\max(x+a,0)-\max(x,0) \tag{8}$$

$$=\lim_{\epsilon\to0^+}\left\{\frac{\epsilon}{a}\ln\left[\frac{e^{(x+a)/\epsilon}+1}{e^{x/\epsilon}+1}\right]\right\}, \tag{9}$$

where a is any constant in the interval $(0,1]$. In what follows, we will set $a=1$. This step function and its regularization are shown in Fig. 1. Expanding the right-hand side of Eq. (9) as a Taylor series in x yields

$$\theta_\epsilon(x)=A+\frac{Bx}{2}-\frac{B^2x^2}{8\epsilon}+\cdots, \tag{10}$$

where

$$A\equiv\epsilon\ln\left[\frac{1}{2}(1+e^{1/\epsilon})\right],\quad B\equiv\frac{e^{1/\epsilon}-1}{e^{1/\epsilon}+1} \tag{11}$$

have the property that

$$\lim_{\epsilon\to0^+}A=\lim_{\epsilon\to0^+}B=1 \tag{12}$$

and A has the asymptotic form

$$A=1-\epsilon\ln2+\cdots. \tag{13}$$

The suitability of this regularization will be discussed below.

By using the expansion in Eq. (10) for each term in Eq. (4), $K_i^{(1)}$ can be written as

$$K_i^{(1)}=\frac{1}{\tau_0}\left\{1+B\Delta^2h_i+\frac{1}{4}B(1-A)\Delta^4h_i-\frac{B^2(1-A)}{16\epsilon}\Delta^2[(\Delta^+h_i)^2+(\Delta^-h_i)^2]+\frac{1}{8}B^2\Delta^2[(\Delta^+h_i)(\Delta^-h_i)]+\cdots\right\}, \tag{14}$$

where we have defined the difference operators $\Delta^\pm h_i=\mp h_i\pm h_{i\pm1}$, $\Delta^2h_i=\Delta^+(\Delta^-h_i)=\Delta^-(\Delta^+h_i)$, and $\Delta^4h_i=\Delta^2(\Delta^2h_i)$. The expansion in Eq. (10) preserves the identity in Eq. (6) at each order.

We now introduce coarse-grained space and time variables x and t,

$$x=i\epsilon a_\parallel,\quad t=\epsilon^z\tau, \tag{15}$$

where $a_\parallel$ is the lateral lattice spacing, z is to be determined, and ϵ parametrizes the extent of the coarse graining, with $\epsilon\to0$ corresponding to the continuum limit. This parameter is the same as the regularization parameter for θ, so the continuum limit will be taken *together* with the limit in Eq. (9) [25]. The corresponding coarse-grained height function u is

$$u(x,t)=\epsilon^\alpha a_\perp\left(h_i-\frac{\tau}{\tau_0}\right), \tag{16}$$

where $a_\perp$ is the vertical lattice spacing, $a_\perp\tau/\tau_0$ is the average growth rate, and α is to be determined.

From the transformations in Eqs. (15) and (16), we obtain

$$\frac{dh_i}{d\tau}=\frac{1}{\tau_0}+\frac{\epsilon^{z-\alpha}}{a_\perp}\frac{\partial u}{\partial t}+O(\epsilon^{2z-\alpha}) \tag{17}$$

and

$$K^{(1)}(u)=\frac{1}{\tau_0}+\frac{\epsilon^{2-\alpha}a_\parallel^2B}{\tau_0a_\perp}\left[\frac{\partial^2u}{\partial x^2}+\frac{1}{12}\epsilon^2(4-3A)a_\parallel^2\frac{\partial^4u}{\partial x^4}-\frac{1}{8}\epsilon^{1-\alpha}B(1-A)a_\parallel^2\frac{\partial^2}{\partial x^2}\left(\frac{\partial u}{\partial x}\right)^2+\frac{1}{8}\epsilon^{2-\alpha}Ba_\parallel^2\frac{\partial^2}{\partial x^2}\left(\frac{\partial u}{\partial x}\right)^2+\cdots\right]. \tag{18}$$

The passage from Eqs. (14) to (18) relies on the presumption that all derivatives of u are well defined, i.e., that the discrete

morphology of steps and terraces described by h_i can be replaced by an analytic function. This can be justified for an interface that has been set into motion in the presence of fluctuations of whatever nature (e.g., kinetic or thermal), in which case asymptotic roughness is guaranteed.

The transformations in Eq. (15) imply that

$$\delta_{ij}=\epsilon a_{\parallel}\delta(x-x'), \quad \delta(\tau-\tau')=\epsilon^{z}\delta(t-t'), \tag{19}$$

which, together with Eq. (18), yield the corresponding transformation of the noise covariance

$$\begin{aligned}\langle \eta_i(\tau)\eta_j(\tau')\rangle &= \epsilon^{1+z}a_{\parallel}K^{(1)}(u)\delta(x-x')\delta(t-t')\\ &= \epsilon^{1+z}\frac{a_{\parallel}}{\tau_0}\delta(x-x')\delta(t-t')+O(\epsilon^{3+z-\alpha}).\end{aligned} \tag{20}$$

Thus, to leading order in ϵ, the coarse-grained noise ξ is given by

$$\xi(x,t)=a_{\perp}\epsilon^{-(1+z)/2}\eta_i(\tau). \tag{21}$$

By combining Eqs. (17)–(21), we obtain

$$\begin{aligned}\epsilon^{z-\alpha}\frac{\partial u}{\partial t}+O(\epsilon^{2z-\alpha}) &= \epsilon^{2-\alpha}\frac{Ba_{\parallel}^2}{\tau_0}\frac{\partial^2 u}{\partial x^2}+O(\epsilon^{4-2\alpha})+\epsilon^{(1+z)/2}\xi\\ &\quad +O(\epsilon^{(3-\alpha+z)/2}).\end{aligned} \tag{22}$$

The leading terms in the time derivative, $K_i^{(1)}$, and the noise can be made to scale with the same power of ϵ by setting $z=2$ and $\alpha=\frac{1}{2}$. The corrections to these terms then all scale with higher powers of ϵ. Thus, by taking the limit $\epsilon\to 0$, and invoking Eqs. (12) and (13), we obtain the Edwards-Wilkinson equation [19]:

$$\frac{\partial u}{\partial t}=\frac{a_{\parallel}^2}{\tau_0}\frac{\partial^2 u}{\partial x^2}+\xi, \tag{23}$$

where the ξ are Gaussian noises with zero mean, $\langle\xi(x,t)\rangle=0$, and covariance

$$\langle\xi(x,t)\xi(x',t')\rangle=\frac{a_{\perp}^2 a_{\parallel}}{\tau_0}\delta(x-x')\delta(t-t'). \tag{24}$$

We now consider a modification of the deposition scenario in Eq. (4) [18]. A particle incident on a site remains there if its height is less than or equal to that of both nearest neighbors *or* if there is no *unique* nearest neighbor site with a lower height. If one nearest neighbor column is lower than that of the original site, deposition is onto that site. If both nearest neighbor columns are lower than that of the original site, then deposition is onto the lowest of these columns. However, if both neighboring column heights are both equal and lower than that of the original site, the particle remains on the original site. The analytic expression of these rules is

$$w_i^{(1)}=\theta_i^{+}\theta_i^{-}+(1-\theta_i^{-})(1-\theta_i^{+})(\theta_{k+1,2}^{-}+\theta_{k-1,2}^{+}-1),$$

$$\begin{aligned}w_i^{(2)} &= \theta_i^{+}(1-\theta_i^{-})+(1-\theta_i^{-})(1-\theta_i^{+})(1-\theta_{k+1,2}^{-}),\\ w_i^{(3)} &= \theta_i^{-}(1-\theta_i^{+})+(1-\theta_i^{-})(1-\theta_i^{+})(1-\theta_{k-1,2}^{+}),\end{aligned} \tag{25}$$

where $\theta_{i,j}^{\pm}=\theta(h_{i\pm j}-h_i)$ and we have used the same labeling convention for the $w_i^{(j)}$ as in Eq. (4). By following the steps leading to Eq. (14), we obtain

$$\begin{aligned}K_i^{(1)}=\frac{1}{\tau_0}\Bigg\{ & 1+B[1+2(1-A)^2]\Delta^2 h_i+\frac{1}{2}B(1-A)\Delta^4 h_i\\ & -\frac{1}{4}B^2(1-A)\left[1-\frac{(1-2A)}{2\epsilon}\right]\Delta^2[(\Delta^{-}h_i)^2+(\Delta^{+}h_i)^2]\\ & +\frac{1}{4}B^2\left[A+\frac{(1-A)^2}{\epsilon}\right]\Delta^2[(\Delta^{-}h_i)(\Delta^{+}h_i)]\cdots\Bigg\}.\end{aligned} \tag{26}$$

Note that, although the coefficient of the second difference in this expression differs from that in Eq. (14) because of the modified transition rules, the difference is, according to Eq. (13), of order ϵ^2. Hence, when the coarse-graining transformations in Eqs. (15) and (16) are applied to this expression and the continuum limit taken, we again obtain the Edwards-Wilkinson equation (23) and (24). Thus, not only are the exponents the same in the two models, but the continuum equations of motion are identical.

There is an alternative method of deriving the Edwards-Wilkinson equation from the regularized Langevin equations that makes a more direct connection to the Van Kampen system size expansion [13]. In the spirit of the central limit theorem, we first write the coarse-grained height function as

$$a_{\perp}\left(h_i-\frac{\tau}{\tau_0}\right)=\epsilon^{-1}U(x,t)+\epsilon^{-1/2}u(x,t), \tag{27}$$

where x and t are defined in Eq. (15). The function U represents the macroscopic morphology of the system, while u corresponds to fluctuations of this morphology on a finer ''mesoscopic'' scale. By using the transformations in Eqs. (17)–(21), the leading terms, of order ϵ, yield a deterministic equation for U,

$$\frac{\partial U}{\partial t}=\frac{a_{\parallel}^2}{\tau_0}\frac{\partial^2 U}{\partial x^2}, \tag{28}$$

which is, of course, the heat equation. The fluctuation corrections to this deterministic evolution of the interface, of order $\epsilon^{3/2}$, are described by the Edwards-Wilkinson equation for u, as given in Eqs. (23) and (24). The equation for U states that, if the surface is initially macroscopically flat, then it remains so for all times. Moreover, any modulation of the surface profile decays with time. Because the Edwards-Wilkinson equation is linear, Eq. (28) is the same as that obtained by averaging Eq. (23) over the noise

We return now to our implementation of the step function and its regularization. The most apparent difference between the step function in Eq. (8) and the definition in Eq. (5) is

that the former is a *continuous* function. This results in finite values for the first *two* terms in the expansion in Eq. (10) as $\epsilon \to 0$, with

$$\lim_{\epsilon \to 0^+} A = \theta(0) \tag{29}$$

and

$$\frac{1}{2} \lim_{\epsilon \to 0^+} B = \frac{1}{2}\left[\lim_{x \to 0^-} \left(\frac{d\theta}{dx} \right) + \lim_{x \to 0^+} \left(\frac{d\theta}{dx} \right) \right] \tag{30}$$

corresponding to the average of the left- and right-hand derivatives of θ at $x=0$. In contrast, for other regularizations [9,11,21–23], B either diverges or vanishes, depending on whether the discontinuity of the step function is at the origin or shifted away. One consequence of our choice is that the exponents α and z required to obtain the Edwards-Wilkinson equation are the same as those derived from a scaling analysis of this equation [1]. Further discussion of different regularization schemes for step functions will be presented elsewhere.

Finally, we consider the applicability of our methodology to other lattice models. As the standard scaling analysis [1] of continuum models indicates, the scaling transformations we used in the passage from the discrete regularized equations of motion to the Edwards-Wilkinson equation cannot be expected to be valid for inherently nonlinear models in all spatial dimensions. In such cases, an expansion such as that in Eq. (18) provides initial conditions for the coefficients in an equation of motion to which a renormalization-group transformation is applied. But even this represents an advance because the presence or absence of particular terms, and their sign, can qualitatively influence the long-wavelength behavior of the growth front [11,26].

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