

## Stochastic equations for simple discrete models of epitaxial growth

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We derive continuous stochastic equations governing the asymptotic behavior of growth from a master equation for discrete growth models with local relaxation. We consider several simple models of epitaxial growth (the Family, the Wolf-Villain, and the Das Sarma–Tamborenea models and their modifications). In 1+1 dimensions, we derive, for each model, the corresponding Langevin equation and identify leading terms that determine the universality class. Our results for models with local relaxation are in agreement with recent computer simulations. The applicability of the method in 2+1 dimensions is demonstrated in the case of the Family model. Problems of the procedure, in particular regularization in the continuous limit, are discussed. [S1063-651X(96)00710-6]

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### I. INTRODUCTION

In recent years several simple discrete growth models for molecular-beam epitaxy (MBE) growth have been proposed and investigated [1–6]. The main purpose of their study was measuring scaling exponents for kinetic roughening, which determine the asymptotic behavior of growth on a large length scale and in a long time limit. The most important result of kinetic roughening studies [7] is that a large variety of different growth models can be divided into only a few universality classes, each class being characterized by specific values of two scaling exponents [7]. The question whether discrete models for MBE belong to a different universality class was only recently resolved by extensive numerical simulations [8].

In the coarse-grained picture, evolution of the growing surface is usually described by a stochastic Langevin equation with additive noise for the height variable  $h(\mathbf{x}, t)$  as a function of the lateral surface coordinate  $\mathbf{x}$  and time  $t$ . In the context of MBE growth several equations were suggested and studied [4,9,10]. It is generally believed that there is a correspondence between discrete growth models and continuous stochastic equations. The most common way of establishing the link between these two approaches is a simple comparison of critical exponents received from computer simulations of the discrete model and exponents for the continuous equation obtained by a Flory-type argument, renormalization-group analysis, or a direct numerical integration [7]. There are also attempts to reveal this relation in an explicit way. When the equation can be written in the form

$$\frac{\partial h(\mathbf{x}, t)}{\partial t} = \nabla^2 K(h, \nabla^2 h, (\nabla h)^2, \dots) + \eta(\mathbf{x}, t),$$

where  $K$  is a function of scalars such as  $h$ ,  $\nabla^2 h$ , and

$(\nabla h)^2$  and  $\eta$  represents noise, a way to construct the corresponding discrete model was proposed [11]. On the other hand, a (nonrigorous) procedure for establishing a continuous equation corresponding to a discrete model, starting from the master equation in discrete space, was suggested by Plischke and co-workers [12,13]. A similar procedure has been also introduced, and used for various models with Arrhenius-type dynamics, by Zangwill and co-workers [14,15]. The formal procedure was clearly explained in a paper by Vvedensky *et al.* [16] and in a different context by Fox and Keizer [17]. Recently, a relation between the Kardar-Parisi-Zhang (KPZ) equation [18] and the restricted solid-on-solid (SOS) model was explicitly clarified by employing this procedure [19]. However, there are several difficulties with this procedure [13]; in particular, it has been found that it fails for a full diffusion model with random deposition and diffusion with Glauber-type dynamics [20].

In this paper, we apply the procedure of Ref. [16] to a set of simple growth models with local relaxation just after deposition, thus fulfilling the following conditions.

- (a) The SOS condition is satisfied.
- (b) The deposition rate is constant and uniform for all sites.
- (c) A particle incident to a randomly selected site  $\mathbf{x}$  can jump to a nearest-neighbor site and stick there. Each model is further characterized by specific growth rules, which determine when and in what direction a jump occurs depending on a local configuration (cf. Sec. II).
- (d) Evaporation or migration of already stuck particles is not allowed.

The simplest example of a model of this kind is the model introduced by Family [21]. Conditions (a)–(d) are also fulfilled by toy models for MBE growth; several such models have been formulated in literature [1–6]. Although the rules of particular models are often very similar, the asymptotic properties can be quite different. Due to the ostensible similarity, very long simulations are needed to see the differences. Therefore, an alternative approach to study these models is of particular interest. Two of the most frequently

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studied models are the Wolf-Villain (WV) model [1] and the Das Sarma–Tamborenea (DT) model [2]. While computer simulations of the Family model are unambiguous and in accord with analytical solution of the Edwards-Wilkinson equation [22], which is believed to correspond to this model, for a long time the situation was not so clear in the case of the WV and DT models.

We explain in detail the procedure for finding Langevin equation for the set of above specified models. We show that, as expected, the corresponding equation is a conservation equation. We establish explicitly the form of Langevin equations corresponding to the Family model, the WV model, the DT model, and two modifications of the WV model. Analyzing coefficients in front of various space derivatives in these equations, we discuss their asymptotic behavior. We concentrate on models in 1+1 dimensions, but the applicability of our method in 2+1 dimensions is also documented for the Family model.

In Sec. II we define the models studied. The method for obtaining the Langevin equation from the master equation is recalled in Sec. III. In Sec. IV the structure of transition moments is discussed and an easy and clear way of calculating first transition moments in the case of relaxation models is described. The results of the most difficult work are contained in Sec. V, where all possible local configurations for the three models selected are analyzed and jump probabilities are explicitly calculated. Section VI is devoted to the problem of passage from discrete to continuous expressions. Quantitative results are presented in Sec. VII. Finally, a conclusion is given in Sec. VIII.

## II. MODELS STUDIED

Here we explain growth rules in models that will be explicitly studied below. Since most of our results (excluding Sec. VII E) are for one-dimensional substrates (i.e., for growth in 1+1 dimensions) we describe models, for the sake of clarity, in 1+1 dimensions. The configuration of a discrete SOS model is given by a surface height function  $h_i(t)$ , which sets the height of the surface above a lattice site with a horizontal coordinate  $i$  at time  $t$ . The actual horizontal coordinate  $x$  of site  $i$  is  $x=ia_{\parallel}$ ,  $a_{\parallel}$  being the lattice constant in the horizontal direction (parallel to the average surface orientation). For further purposes we explicitly distinguish the lattice spacing in the vertical and horizontal directions.

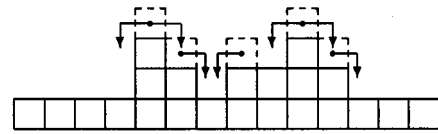
The *Family model* [21] describes deposition of particles that minimize their height, i.e., physically the behavior of particles that minimize their energy in the gravitational field (see Fig. 1). A particle sticks at the site of incidence  $i$  only when it is a local minimum of height, i.e.,

$$h_i \leq h_{i+1}, \quad h_i \leq h_{i-1}.$$

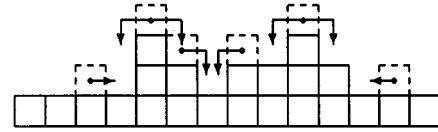
When only one of these conditions does not hold (tilted surface), the particle sticks at the neighboring site with lower height. In the case of incidence to a local maximum of height

$$h_i > h_{i+1}, \quad h_i > h_{i-1},$$

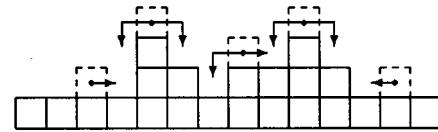
we distinguish two variants of the Family model. In the first, which we denote *F1*, a new particle jumps with equal probability (1/2) to any of the neighboring sites  $i-1$  or  $i+1$ ,



Family model



Wolf-Villain model



Das Sarma–Tamborenea model

FIG. 1. Comparison of the Family, the WV, and the DT models. Arrows indicate all possible jumps that can happen after the incidence of a new particle (dashed box).

regardless of their relative height. In the second variant (*F2*) a new particle jumps always to the lowest site. We shall consider these two variants of this model in order to ascertain how much a slight modification of the model rules effects the resulting equation.

In the *Wolf-Villain model* [1], as well as in other relaxation models for MBE growth, the relaxation is controlled by the number of bonds between nearest neighbors. A newly arriving particle maximizes the number of bonds with nearest neighbors. The algorithm is very similar to that of the *F2* model if we replace the height  $h_i$  by  $-n_i$ , where  $n_i$  represents the number of lateral neighbors at site  $i$  (cf. Fig. 1).

We also studied two modifications of the WV model, which we call *WV $\uparrow$*  and *WV $\downarrow$*  (cf. Refs. [3] and [23]). Both differ from the WV model only in the case of a tie, i.e., when both an incidence site and one of the neighboring sites offer one lateral bond to create and the other neighbor does not offer more (two) bonds to create. While in the case of the standard WV model no jump occurs in such a situation, in the case of the *WV $\uparrow$*  model a jump to a higher site offering one bond happens with a probability  $p$ , if such a site exists. Similarly, in the *WV $\downarrow$*  model a jump to a lower site offering one bond happens with a probability  $q$ . The *Das Sarma–Tamborenea model* [2] (to be precise, the DT1 variant of this model as defined by Krug in Ref. [24]) is very similar to the WV model, but it makes no distinction between states with one or two lateral neighbors (see Fig. 1).

## III. DERIVATION OF STOCHASTIC EQUATIONS

The method used in [16,14,19] basically consists of two steps: first, the derivation of the Langevin equation for a

discrete set of height variables from a master equation using the Kramers-Moyal expansion [25], and second, the transition from the equation system for a discrete set of heights to an equation for a continuous function  $h(x)$  of a continuous spatial variable  $x$ . We recall both steps here.

The evolution of a surface is given by the master equation (see, e.g., Ref. [25])

$$\frac{\partial P(H,t)}{\partial t} = \sum_{H'} W(H',H)P(H',t) - \sum_{H'} W(H,H')P(H,t), \quad (1)$$

where  $W(H,H')$  denotes the transition matrix from a configuration  $H$  (a configuration  $H \equiv \{h_i\}_{i=1}^N$  represents a set of heights  $h_i$  at every lattice site and  $N$  denotes the total number of sites on substrate) to a subsequent configuration  $H'$  and  $P(H,t)$  is the probability that the system is in the configuration  $H$  at time  $t$ .

In the case of relaxation models two subsequent configurations differ just by the addition of a new particle to one column. This leads to the following form of the transition matrix:

$$W_{\text{relax}}(H,H') = \frac{1}{\tau} \sum_i \left[ w_i^{(1)} \delta(h'_i, h_i + a_\perp) \prod_{j \neq i} \delta(h'_j, h_j) \right. \\ \left. + w_i^{(2)} \delta(h'_{i-1}, h_{i-1} + a_\perp) \prod_{j \neq i-1} \delta(h'_j, h_j) \right. \\ \left. + w_i^{(3)} \delta(h'_{i+1}, h_{i+1} + a_\perp) \prod_{j \neq i+1} \delta(h'_j, h_j) \right], \quad (2)$$

where  $w_i^{(1)}$  denotes the configuration-dependent probability of sticking at incidence site  $i$ ,  $w_i^{(2)}$  denotes the probability of a jump to the left after incidence at site  $i$ , and  $w_i^{(3)}$  denotes the probability of a jump to the right after incidence at site  $i$ . The constant  $\tau$  denotes the average time of deposition of a layer, given by the flux of incoming particles, and  $a_\perp$  is the vertical (perpendicular to the surface) lattice spacing.

In order to demonstrate the difference between the models with local relaxation and models with full surface diffusion, we present also the form of the transition matrix for diffusion models, although we are not going to study these models here. In this case we have two processes: random deposition and diffusion. In deposition a particle is deposited at a randomly selected site (no relaxation). The transition matrix is

$$W_{\text{dep}}(H,H') = \frac{1}{\tau} \sum_i \left[ \delta(h'_i, h_i + a_\perp) \prod_{j \neq i} \delta(h'_j, h_j) \right]. \quad (3)$$

During diffusion any surface particle  $i$  can jump to site  $j$  with a probability  $\omega_{i \rightarrow j} \in \langle 0,1 \rangle$  depending on the local configuration according to model rules. The transition matrix has the form

$$W_{\text{diff}}(H,H') = D \sum_{ij} \omega_{i \rightarrow j} \delta(h'_i, h_i - a_\perp) \delta(h'_j, h_j + a_\perp) \\ \times \prod_{k \neq i,j} \delta(h'_k, h_k), \quad (4)$$

where  $\omega_{i \rightarrow j}$  is the configuration-dependent probability of a jump from site  $i$  to site  $j$ . Usually one is restricted to models where only diffusion between nearest neighbors is allowed. The average time of deposition of a layer  $\tau$  and diffusion constant  $D$  sets the frequency of deposition and diffusion, respectively. The total transition matrix is the sum of contributions from deposition and diffusion.

Using a particular transition matrix in the master equation (1), we obtain a full stochastic description of a given discrete growth model. However, finding the solution of such a master equation is possible only in exceptional cases. In the approach suggested by Vvedensky and co-workers [16,14,15] the master equation is approximated by the Fokker-Planck equation through the usual Kramers-Moyal expansion

$$\frac{\partial P(H,t)}{\partial t} = - \sum_i \frac{\partial}{\partial h_i} [K_i^{(1)} P(H,t)] \\ + \sum_{i,j} \frac{1}{2} \frac{\partial^2}{\partial h_i \partial h_j} [K_{i,j}^{(2)} P(H,t)], \quad (5)$$

where

$$K_i^{(1)}(H) = \sum_{H'} (h'_i - h_i) W(H,H') \quad (6)$$

is the first moment and

$$K_{ij}^{(2)}(H) = \sum_{H'} (h'_i - h_i)(h'_j - h_j) W(H,H'), \quad (7)$$

is the second moment of transition matrix.

Then the equivalent Langevin equation is written [25]

$$\frac{\partial h_i(t)}{\partial t} = K_i^{(1)}(H) + \eta_i(t). \quad (8)$$

Here  $\eta$  represents white Gaussian noise with zero mean and covariance given by the second transition moment

$$\langle \eta_i(t) \rangle = 0,$$

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

The set of equations (8) describes the evolution of heights  $h_i$  at site  $i$  as a function of heights at site  $i$  and discrete neighboring sites. To obtain the Langevin equation for the function  $h(x)$  of the continuous variable  $x$  one needs some smoothing procedure. The essence of the method of Vvedensky and co-workers is the assumption that there exists a smooth function  $h(x)$  that is obtained from a function interpolating through the points  $h_i(t)$  and then one expresses heights at neighboring sites using a Taylor expansion. This is

a crucial and highly nontrivial step. At the end one obtains a continuous Langevin equation with additive noise with zero mean

$$\frac{\partial h(x,t)}{\partial t} = K_i^{(1)}(h(x,t)) + \eta(x,t). \quad (9)$$

In practice this procedure is done by *regularization* in which nonanalytical quantities that enter the discrete Langevin equation are replaced by analytic functions. We will discuss this problem in detail below (see Sec. VI).

The procedure works in the case of diffusion models with Arrhenius dynamics [16,14] and also in the case of the far-from-equilibrium restricted SOS (RSOS) growth model [19]; however, there is also one case where it fails. Siegert [20] demonstrated that it does not work for the full diffusion model with the Hamiltonian  $H = \sum_i |h_{i+1} - h_i|^4$  and Glauber dynamics. Computer simulations show that this model is unstable, while direct application of the above method yields a positive Laplacian term, indicating stable behavior. It is not completely clear why the method fails. In this paper, we are not going to attack this problem; rather we explore results in the case of relaxation models that are simpler than diffusion models and close to the RSOS model for which the method works well [19]. Nevertheless, we would like to comment on possible reasons for this failure.

The conditions when the procedure is correct have not been clearly formulated. As far as the first step is concerned, the Fokker-Planck equation is obtained by the usual Kramers-Moyal expansion in the limit of a small parameter  $1/\Omega$ . It is supposed that only small jumps occur and that the solution and transition rates vary only slowly with the state [25], i.e., with heights  $h_i$  in our case; the change of variables (jump) in our case is vertical displacement given by  $a_\perp$ . Then, provided the intrinsic fluctuations are not too large [17], Eq. (8) is correct in the limit  $a_\perp \rightarrow 0$  and it is sufficient to know only the first and second moments.

In the case of models with local relaxation, the form of moments  $[K_i^{(n)} \propto (a_\perp)^n$ ; see below] suggests the choice  $1/\Omega = a_\perp$ . Transition rates  $w_i^{(1)}, w_i^{(2)}, w_i^{(3)}$  usually do not explicitly depend on the height increment associated with the deposition of a particle; it is true for all models studied below. The dependence of rates on  $h_i$  is often given by  $\theta$  functions or by a certain continuous function obtained after regularization (see below). Hence, in this case we expect that we can use the Fokker-Planck equation as an approximation to the master equation.

In the case of models with diffusion, rates  $\omega_{i \rightarrow j}$  may or may not explicitly depend on the changes of heights due to the diffusion jump. For example, in models studied by Vvedensky and co-workers [16,14]  $\omega_{i \rightarrow j}$  depends only on the number of nearest neighbors and is given, as in the relaxation models studied here, by  $\theta$  functions.

On the other hand, in the model considered by Siegert [20], the dependence both on the value of heights and on the changes of heights due to diffusion is nontrivial. We suspect that it is the primary reason why this method does not work here. There are also other factors that may conspire. As will be shown in Sec. IV, models with diffusion lead to a more complicated structure of higher moments than in the case of models with local relaxation. In particular the second mo-

ment, which determines the noise in the Langevin equation, contains off-diagonal terms. Finally, relaxation models are also simpler with respect to the type of noise appearing in the problem. Noise in a relaxation model is due only to random deposition, whereas in a nonequilibrium diffusion model two kinds of noise, nonconserved (rising from deposition) and conserved (from diffusion), have to be considered. It is not clear how to correctly incorporate this aspect into the derivation of a continuous equation.

#### IV. TRANSITION MOMENTS

In this section we first write down the expressions for transition moments for models with local relaxation and for full diffusion models; then we introduce a method for calculating the first transition moment of conserved models with local relaxation.

Substitution of (2) into (6) gives the following form of first transition moment [16]:

$$K_i^{(1)} = \frac{a_\perp}{\tau} [w_i^{(1)} + w_{i+1}^{(2)} + w_{i-1}^{(3)}]. \quad (10)$$

Henceforth we use such units that the prefactor  $a_\perp / \tau$  is equal to one. This is done by rescaling the vertical coordinate and time. The explicit expressions for jump probabilities  $w_i^{(1)}$ ,  $w_i^{(2)}$ , and  $w_i^{(3)}$  for the models considered will be constructed in Sec. V.

As a consequence of the fact that subsequent configurations differ only in height at one site, all higher moments are diagonal and proportional to  $K_i^{(1)}$ ,

$$K_{i_1 i_2 i_3 \dots i_n}^{(n)} = (a_\perp)^{n-1} \delta_{i_1 i_2} \delta_{i_1 i_3} \dots \delta_{i_1 i_n} K_i^{(1)}.$$

In the case of diffusion models the first moment is given by [20]

$$K_i^{(1)} = a_\perp D [\omega_{i-1 \rightarrow i} + \omega_{i+1 \rightarrow i} - \omega_{i \rightarrow i-1} - \omega_{i \rightarrow i+1}] + \frac{a_\perp}{\tau'}.$$

Contrary to models with local relaxation, higher transition moments are *not* diagonal, e.g., the second moment reads

$$K_{ij}^{(2)} = a_\perp^2 D \delta_{ij} [\omega_{i-1 \rightarrow i} + \omega_{i+1 \rightarrow i} + \omega_{i \rightarrow i-1} + \omega_{i \rightarrow i+1}] - a_\perp^2 D (\delta_{i,j+1} + \delta_{i,j-1}) [\omega_{i \rightarrow j} + \omega_{j \rightarrow i}] + \frac{a_\perp^2}{\tau'} \delta_{ij}.$$

In the rest of this section we show how one can effectively calculate the first moment in the case of relaxation models. Equation (10) can be modified to a more convenient form. We will show that employing left-right symmetry and conserving the condition

$$w_i^{(1)} + w_i^{(2)} + w_i^{(3)} = 1, \quad (11)$$

it is sufficient to determine only  $w_i^{(2)}$  (or  $w_i^{(3)}$ ) in order to obtain  $K^{(1)}$  and hence the Langevin equation.

Due to local growth rules,  $w_i^{(2)}$  depends only on height differences of neighboring sites

$$h_+ \equiv h_{i+1} - h_i, \quad h_- \equiv h_{i-1} - h_i \quad (12)$$

and (in the case of rules depending on number of bonds) also on

$$h_{++} \equiv h_{i+2} - h_{i+1}, \quad h_{--} \equiv h_{i-2} - h_{i-1}.$$

Now, we suppose that  $h_i(t)$  can be replaced by a smooth function such that the expansions

$$\begin{aligned} h_+ &= \sum_{k=1}^{\infty} \frac{\partial^k h(x)}{\partial x^k} \frac{a_{\parallel}^k}{k!}, & h_- &= \sum_{k=1}^{\infty} \frac{\partial^k h(x)}{\partial x^k} \frac{(-a_{\parallel})^k}{k!}, \\ h_{++} &= \sum_{k=1}^{\infty} \frac{\partial^k h(x)}{\partial x^k} \frac{a_{\parallel}^k}{k!} (2^k - 1), \\ h_{--} &= \sum_{k=1}^{\infty} \frac{\partial^k h(x)}{\partial x^k} \frac{(-a_{\parallel})^k}{k!} (2^k - 1) \end{aligned} \quad (13)$$

are valid.

Assuming further that  $w_i^{(2)}$  is a continuous function of height differences, we can express  $w_i^{(2)}$  as a sum of products of various space derivatives of  $h(x)$ . It is convenient to arrange individual terms according to the total number of derivatives. Because every space derivative in (13) is associated with multiplication by lattice spacing  $a_{\parallel}$  (recall that  $x = ia_{\parallel}$ ), we can write  $w_i^{(2)}$  in the form

$$w_i^{(2)} = \sum_{n=0}^{\infty} C_n(x) a_{\parallel}^n, \quad (14)$$

where  $C_n(x)$  denotes a combination of terms, each with a total of  $n$  space derivatives.

Since the growth rules considered are symmetric with respect to left-right reflection, the probability  $w_i^{(3)}$  can be obtained from  $w_i^{(2)}$  simply by changing the orientation of the horizontal axis  $x$ . Explicitly for  $h_+$  and  $h_-$  we have the correspondence

$$h_+ \leftrightarrow h_-, \quad \frac{\partial^k h(x)}{\partial x^k} a_{\parallel}^k \leftrightarrow \frac{\partial^k h(x)}{\partial (-x)^k} a_{\parallel}^k = \frac{\partial^k h(x)}{\partial x^k} (-a_{\parallel})^k,$$

which shows that the change of orientation can be formally carried out by replacing  $a_{\parallel}$  by  $-a_{\parallel}$ . Hence

$$w_i^{(3)} = \sum_{n=0}^{\infty} C_n(x) (-a_{\parallel})^n. \quad (15)$$

Functions with shifted indices  $i \pm 1$ , which are needed in (10), are obtained by the Taylor expansion

$$\begin{aligned} w_{i+1}^{(2)} &= \sum_{k=0, n=0}^{\infty} \frac{\partial^k C_n(x)}{\partial x^k} \frac{a_{\parallel}^{k+n}}{k!}, \\ w_{i-1}^{(3)} &= \sum_{k=0, n=0}^{\infty} \frac{\partial^k C_n(x)}{\partial x^k} \frac{(-a_{\parallel})^{k+n}}{k!}. \end{aligned} \quad (16)$$

Finally, condition (11) yields

$$w_i^{(1)} = 1 - 2 \sum_{\substack{n=0 \\ n \text{ even}}}^{\infty} C_n(x) a_{\parallel}^n. \quad (17)$$

After insertion of (16) and (17) into (10), we have

$$\begin{aligned} K_i^{(1)} &= 1 - 2 \sum_{\substack{n=0 \\ n \text{ even}}}^{\infty} C_n(x) a_{\parallel}^n + 2 \sum_{\substack{k=0, n=0 \\ n+k \text{ even}}}^{\infty} \frac{\partial^k C_n(x)}{\partial x^k} \frac{a_{\parallel}^{k+n}}{k!} \\ &= 1 + 2 \frac{\partial}{\partial x} \left( \sum_{\substack{n=2 \\ n \text{ even}}}^{\infty} \sum_{k=1}^{n-1} \frac{\partial^{k-1} C_{n-k}(x)}{\partial x^{k-1}} \frac{a_{\parallel}^n}{k!} \right). \end{aligned} \quad (18)$$

If we identify

$$J(x) \equiv 2 \sum_{\substack{n=2 \\ n \text{ even}}}^{\infty} \sum_{k=1}^{n-1} \frac{\partial^k C_{n-k}(x)}{\partial x^{k-1}} \frac{a_{\parallel}^n}{k!}$$

as a horizontal current, we receive, according to (9), the conserving equation

$$\frac{\partial h(x, t)}{\partial t} = 1 + \frac{\partial J(x)}{\partial x} + \eta(x, t). \quad (19)$$

The first term corresponds to a constant flux of incoming particles and the second term represents the contribution of the configuration-dependent horizontal current. Note that we obtain a conservation equation for any SOS model with local relaxation (within nearest neighbors). Particularly, we can see that the so-called KPZ term [18]  $(\nabla h)^2$  cannot be present in the resulting Langevin equation.

## V. DETERMINATION OF JUMP PROBABILITIES

The jump probability  $w_i^{(2)}$  depends on a local configuration. In this section we shall find this dependence explicitly for several models with local relaxation. For each model we start with a complete classification of configuration types and then we determine for each particular configuration the probability of a jump to the left or right nearest-neighbor site.

### A. Family model

The considerations for this model are simple, but it is instructive to explain them in detail before studying more complex models for MBE. In the Family model, the incidence site  $i$  is more convenient for a particle than site  $i+1$  when  $h_i \leq h_{i+1} \Leftrightarrow \theta(h_+) = 1$ ; here the discrete  $\theta$  function is defined by

$$\theta(k) = \begin{cases} 1, & k \geq 0 \\ 0, & k < 0 \end{cases} \quad (20)$$

with  $k \in Z$  and  $Z$  being the set of integers. On the other hand, site  $i+1$  is more convenient than site  $i$  when

$$h_i > h_{i+1} \Leftrightarrow \theta(h_+) = 0 \Leftrightarrow 1 - \theta(h_+) = 1.$$

Analogous expressions are valid for site  $i-1$ . We use these expressions to divide all local configurations into four groups (see Fig. 2) according to possible jumps: no jump, a jump to the left, a jump to the right, a jump either to the left or to the

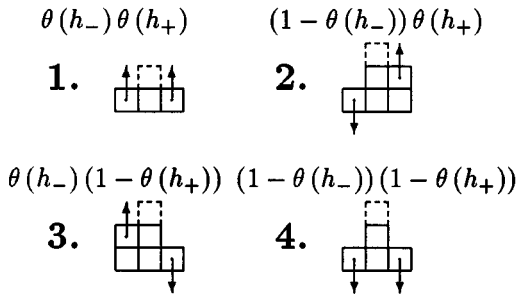


FIG. 2. Groups of local configurations in the Family model. The upward (downward) arrow indicates that the surface particle at a given column can occupy any higher (lower) site relative to the new particle (dashed box).

right. For any local configuration, exactly one of the expressions shown in Fig. 2 is equal to one and the remaining expressions are zero.

In the  $F1$  variant of the Family model, a new particle jumps to the left with certainty in configuration from the second group and with probability  $1/2$  in configuration from the fourth group. The probability  $w_{F1}^{(2)}$  is a sum of the probabilities of a jump to the left over all configurations [26],

$$w_{F1}^{(2)} = [1 - \theta(h_-)]\theta(h_+) + \frac{1}{2} [1 - \theta(h_-)][1 - \theta(h_+)] \\ = \frac{1}{2} [1 - \theta(h_-)][1 + \theta(h_+)], \quad (21)$$

(this expression was already found in Ref. [16]).

To obtain proper form of  $w_{F2}^{(2)}$ , the probability of a jump to the left in the  $F2$  model, we have to divide the fourth group into three subgroups according to relative heights at sites  $i-1$  and  $i+1$ .

(4a) A jump to the left occurs with certainty when

$$[1 - \theta(h_-)][1 - \theta(h_+)] = 1,$$

i.e., when the height at site  $i-1$  is lower than that at site  $i+1$ .

(4b) The case when heights at sites  $i \pm 1$  are equal can be expressed using the Kronecker  $\delta$  as

$$[1 - \theta(h_-)][1 - \theta(h_+)]\delta(h_- - h_+) = 1.$$

In this case a jump to the left is equally probable as a jump to the right.

(4c) If

$$[1 - \theta(h_-)][1 - \theta(h_+)] = 1,$$

a particle jumps to the right, lower site  $i+1$ .

These three expressions form a complete representation of group 4 since the Kronecker  $\delta$  and discrete  $\theta$  function satisfy

$$\theta(-k) + \theta(k) = 1 + \delta(k). \quad (22)$$

Having the division of local configurations, we can immediately write down the probability of a jump to the left in the  $F2$  model

$$w_{F2}^{(2)} = [1 - \theta(h_-)]\theta(h_+) + [1 - \theta(h_-)][1 - \theta(h_+)] \\ \times (1 - \theta(h_- - h_+) + \frac{1}{2} \delta(h_- - h_+)). \quad (23)$$

### B. Wolf-Villain, Das Sarma–Tamborenea, and modified models

The dependence on the number of bonds at sites within nearest neighbors of an incidence site  $i$  in growth rules can be transcribed into the dependence on height differences of neighboring sites within second nearest neighbors of an incidence site. There is a large number of different types of local configurations that have to be considered. In order to simplify their classification, we divide every local configuration into left and right parts, which we call semiconfigurations and at first classify separately. We determine different types of semiconfigurations according to the number of bonds before and after a jump. Then we determine when (for which combination of the left and the right semiconfigurations) this fictive jump actually happens.

We concentrate our interest again on jumps to the left and investigate the left semiconfigurations (this term stands for a part of the whole configuration given by columns at sites  $i-2$ ,  $i-1$ , and  $i$ ). Let us denote by  $n$  the number of left neighbors ( $n=0,1$ ) of a particle incident to site  $i$  and by  $m$  the total number of lateral neighbors ( $m=0,1,2$ ) that the same particle would have after jump to  $i-1$ . We denote a group of semiconfigurations corresponding to these numbers by  $L_n^m$ . All such possible groups are schematically figured, together with their representation using discrete functions, in Fig. 3.

This enumeration is again disjunctive and complete since

$$L_0^2 + L_0^{1(b)} = 1 - \theta(h_-), \quad L_0^{1(a)} + L_0^0 = \delta(h_-),$$

$$L_0^1 + L_1^1 = 1 - \theta(-h_-), \quad L_0^1 \equiv L_0^{1(a)} + L_0^{1(b)},$$

$$L_0^0 + L_0^1 + L_0^2 + L_1^0 + L_1^1 = 2 + \delta(h_-) - \theta(h_-) - \theta(-h_-) = 1. \quad (24)$$

Replacing  $h_- \leftrightarrow h_+$  and  $h_{--} \leftrightarrow h_{++}$ , we receive right semiconfigurations ( $R$ ) instead of left ones.

Now, the construction of the total probability of a jump to the left for the WV model  $w_{WV}^{(2)}$  is straightforward: it is a sum of contributions from all combinations of left and right semiconfigurations

$$w_{WV}^{(2)} = L_0^2(R_0^0 + R_0^1 + R_1^1 + R_1^0 + \frac{1}{2} R_0^2) + L_0^1(R_0^0 + \frac{1}{2} R_0^1). \quad (25)$$

Jump probabilities for modifications of the WV model with additional jumps in the case of a tie are [cf. (25)]

$$w_{WV\uparrow}^{(2)} = L_0^2(R_0^0 + R_0^1 + R_1^1 + R_1^0 + \frac{1}{2} R_0^2) + L_0^1(R_0^0 + \frac{1}{2} R_0^1) \\ + L_1^1(R_0^0 + R_0^1)p, \quad (26)$$

$$w_{WV\downarrow}^{(2)} = L_0^2(R_0^0 + R_0^1 + R_1^1 + R_1^0 + \frac{1}{2} R_0^2) + L_0^1(R_0^0 + \frac{1}{2} R_0^1) \\ + L_0^{1(b)}(R_1^0 + R_1^1)q. \quad (27)$$

$$L_0^2 = (1 - \theta(h_-)) (1 - \theta(-h_{--})) \quad L_0^0 = \delta(h_-) \theta(-h_{--})$$



$$L_0^{1(a)} = \delta(h_-) (1 - \theta(-h_{--})) \quad L_0^{1(b)} = (1 - \theta(h_-)) \theta(-h_{--})$$



$$L_1^0 = (1 - \theta(-h_{--})) \theta(-h_{--}) \quad L_1^1 = (1 - \theta(-h_{--})) (1 - \theta(-h_{--}))$$

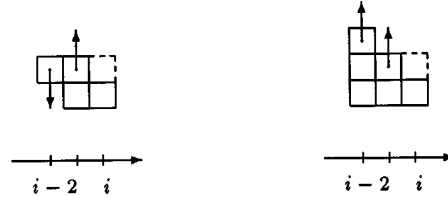


FIG. 3. Groups of semiconfigurations for models with growth rules depending on the number of bonds. The horizontal bar indicates the equality of heights and the meaning of arrows is the same as in Fig. 2.

The Das Sarma–Tamborenea model makes no distinction between a site with one or two lateral neighbors, which results in the following form of jump probability:

$$w_{\text{DT}}^{(2)} = (L_0^1 + L_0^2) (R_0^0 + \frac{1}{2} R_0^1 + \frac{1}{2} R_0^2). \quad (28)$$

## VI. PASSAGE TO CONTINUOUS EQUATIONS

In this section we describe how to combine particular results obtained in previous sections together and how to carry out the passage from a discrete to a continuous description. Our calculations start with a discrete-value set of heights  $h_i$  at discrete sites  $i$ . In this representation we classify different kinds of local configurations (as shown in Figs. 2 and 3) and we obtain a jump probability  $w_i^{(2)}$  for a particular model [Eqs. (21), (23), and (25)–(27)]. These expressions contain discrete  $\theta$  and  $\delta$  functions. However, the procedure described in Sec. III assumes that  $w^{(2)}$  is a continuous differentiable function of the space coordinate  $x$  obtained by some coarse-graining procedure. Here we describe a regularization procedure in which the step function  $\theta(k)$ , defined on the set of integers by (20), is replaced by a continuous function  $\tilde{\theta}(\xi)$ . There is uncertainty in the form of the regularization function  $\tilde{\theta}(\xi)$  and, as we will show below, different choices can lead to different results.

Some forms of regularization functions have been suggested in the literature [13,15,16,19], but to our knowledge the problem of a proper choice of regularization scheme has not been discussed. One suggested choice is

$$\tilde{\theta}(\xi) = [1 + \tanh(C\xi)]/2, \quad (29)$$

where  $C$  is an arbitrary positive parameter, with the exact  $\theta$  function being obtained in the limit  $C \rightarrow \infty$ .

In general, one can suppose that the regularization function is given by expansion

$$\tilde{\theta}(\xi) = \sum_{k=0}^{\infty} A_k \xi^k. \quad (30)$$

Some authors [16,19] considered this form with  $A_0 = 1$ ,

$$\tilde{\theta}(\xi) = 1 + \sum_{k=1}^{\infty} A_k \xi^k, \quad (31)$$

but we do not adhere to this restriction.

Our focus is on the properties of the surface on large length and time scales. Since the asymptotic scaling is determined by nonzero terms of lowest order in Eq. (9), we can restrict ourselves in the expansions considered in Sec. III to a finite order and neglect higher-order terms. In the calculation below, we shall consider terms only up to the fourth order. Since the argument of the  $\theta$  function is always a height difference of neighboring sites (which is of first order in space derivatives), it is sufficient to treat expansion (30) also only to fourth order

$$\tilde{\theta}(\xi) = A_0 + A_1 \xi + A_2 \xi^2 + A_3 \xi^3 + A_4 \xi^4. \quad (32)$$

The definition of the continuous  $\tilde{\delta}$  function by relation (22) yields the approximation up to fourth order

$$\tilde{\delta}(\xi) = 2A_0 - 1 + 2A_2 \xi^2 + 2A_4 \xi^4. \quad (33)$$

Instead of the form (29), we shall consider the ‘‘shifted’’ form [27]

$$\tilde{\theta}(\xi) = \{1 + \tanh[C(\xi + \alpha)]\}/2, \quad (34)$$

where  $\alpha$  is in the interval  $(0, 1/2)$ ; a preferable choice  $\alpha = 1/2$  gives a symmetric approximation to the discrete  $\theta$  function, the odd function with respect to the point  $x = -1/2$ . The reason for our choice is that with this choice, we can satisfy relation (22), whereas regularization (29) does not allow us to define the  $\delta$  function. Relation (22) is important in models for MBE and the  $F2$  model because we have to distinguish, in the classification of configurations, the situation where the argument of the discrete  $\theta$  function is zero. The regularization has to conserve this difference, i.e., relation (22). This problem is not encountered in the case of the single-step SOS or restricted SOS model [19], where regularization (29) can be used.

From the behavior of the approximative  $\tilde{\theta}$  function (34), we can see that coefficients  $A_k$  fulfill [27]

$$A_0 \in (1/2, 1), \quad A_1 > 0, \quad A_2 < 0. \quad (35)$$

In Sec. VII, we show that much information can be obtained without a detailed study of the coefficients  $A_k$ , assuming only the validity of (35).

Substituting continuous representations of  $\theta$  and  $\delta$  functions (32) and (33) into the expression for the jump probability

ity  $w^{(2)}$  and retaining terms up to fourth order, we obtain the continuous stochastic Langevin equation in the form

$$\begin{aligned} \frac{\partial h(x,t)}{\partial t} = & \nu \frac{\partial^2 h(x,t)}{\partial x^2} + \frac{\lambda_2}{3} \frac{\partial}{\partial x} \left( \frac{\partial h(x,t)}{\partial x} \right)^3 \\ & + \frac{\lambda_1}{2} \frac{\partial^2}{\partial x^2} \left( \frac{\partial h(x,t)}{\partial x} \right)^2 + K \frac{\partial^4 h(x,t)}{\partial x^4} + F + \eta(x,t), \end{aligned} \quad (36)$$

where coefficients  $\nu$ ,  $\lambda_1$ ,  $\lambda_2$ , and  $K$  depend on the growth rules of a model and on the regularization used and are expressed as a combination of coefficients  $A_k$ .

We carried out this substitution and the following simplifications using symbolic manipulations. Thus we not only avoided tedious work but also checked the completeness of the division into semiconfigurations. For each model, we also independently found an expression for  $w_i^{(1)}$ , i.e., the probability of sticking at an incidence site, we obtained the probability  $w_i^{(3)}$  from  $w_i^{(2)}$  using left-right symmetry, and we checked the validity of (11), which served as a test of the proper expression for  $w_i^{(2)}$ .

## VII. RESULTS

Here we present values of coefficients  $\nu$ ,  $\lambda_1$ ,  $\lambda_2$ , and  $K$  appearing in the general form of the Langevin equation (36) for all models studied.

### A. Family model

In the case of the  $F1$  model, we have

$$\begin{aligned} \nu = 2A_1, \quad \lambda_1 = 2A_2 - 2A_0A_2 + A_1^2, \\ \lambda_2 = 6A_3, \quad K = \frac{A_1}{6}(4 - 3A_0), \end{aligned}$$

whereas for the  $F2$  model, we obtain

$$\begin{aligned} \nu = 2A_1(3 - 4A_0 + 2A_0^2), \\ \lambda_1 = 4A_0A_1^2 - 3A_1^2 - 2A_0A_2 + 2A_2, \\ \lambda_2 = 6(-4A_1A_2 + 9A_3 - 2A_1^3 + 8A_3A_0^2 + 4A_0A_2A_1 \\ - 16A_3A_0), \\ K = \frac{A_1}{6}(12 - 19A_0 + 8A_0^2). \end{aligned}$$

When coefficients  $A_k$  satisfy relations (35) then, in both cases, the coefficient  $\nu$  is positive and the scaling is determined by the Laplacian term [29] (for the  $F1$  model the coefficient  $\nu$  is less than or equal to that for the  $F2$  model), i.e., both models belong to the Edwards-Wilkinson (EW) class as expected. When the form of regularization (31) with  $A_0=1$  is used there is no difference in coefficients  $\nu$ ,  $\lambda_1$ , and  $K$  for both variants  $F1$  and  $F2$ , which is also true for regularization (34), with a nonzero shift ( $\alpha>0$ ) in the limit  $C \rightarrow \infty$ .

### B. Wolf-Villain model

The coefficients for the WV model are

$$\begin{aligned} \nu = 2A_1(2A_0 - 1)(A_0 - 1)^2, \\ \lambda_1 = 2(4A_2 - 10A_0A_2 - 4A_0A_1^2 - 8A_0^3A_2 + 2A_0A_1^2 + 16A_2A_0^2 \\ + A_1^2), \\ \lambda_2 = 6(-A_3 + 4A_3A_0 + A_1^3 + 4A_1A_2 - 2A_0A_1^3 - 5A_3A_0^2 \\ + 6A_0^2A_2A_1 + 2A_0^3A_3 - 10A_0A_2A_1), \\ K = \frac{A_1}{6}(-19 + 64A_0 + 44A_0^3 - 95A_0^2). \end{aligned}$$

The coefficient  $\nu$  is positive in our regularization scheme (34) with  $\alpha>0$  and finite  $C$ . In contrast to the Family model, it goes to zero when  $C \rightarrow \infty$ . In the regularization schemes for which conditions (35) are not strictly satisfied, for example, in scheme (31) with  $A_0=1$  or in scheme (29) with  $A_0=1/2$ , we get identically  $\nu=0$ , which contradicts the results of the simulations [8].

### C. Modified models

The permission of upward jumps (with probability  $p$ ) in the  $WV\uparrow$  model tends to cause instability. From the expression for the Laplacian coefficient  $\nu$  in this case,

$$\nu = 2A_1(A_0 - 1)[2A_0^2 - 3A_0 + 1 - p(2A_0^2 - 5A_0 + 1)],$$

it can be seen that for any  $A_0 \in (1/2, 1)$  there exists a critical probability

$$p_c = \frac{(2A_0 - 1)(A_0 - 1)}{2A_0^2 - 5A_0 + 1},$$

at which  $\nu=0$ . The behavior is similar to that of the WV model, i.e., stable ( $\nu>0$ ), for  $p < p_c$ , whereas we obtain a negative value of  $\nu$  for  $p > p_c$ , which indicates unstable growth. Note again that for the scheme (31) we get identically  $\nu=0$ , in contradiction with results of simulations [3,23].

There is no such transition in the  $WV\downarrow$  model. The coefficient

$$\nu = 2A_1(A_0 - 1)[2A_0^2 - 3A_0 + 1 - q(A_0 + 1)]$$

increases with an increasing value of the probability  $q$ . This is in agreement with the intuitive expectation that the permission of additional downward jumps increases the stability of the model and also agrees with results of recent simulations [23].

### D. Das Sarma-Tamborenea model

The coefficients  $\nu$ ,  $\lambda_1$ ,  $\lambda_2$ , and  $K$  for this model are

$$\begin{aligned} \nu = 0, \lambda_2 = 0, \\ \lambda_1 = 2(12A_2A_0^2 - 4A_0A_1^2 + A_1^2 + 2A_0^2A_1^2 - 8A_0^3A_2 - 2A_0A_2), \end{aligned}$$



$$K = A_0 A_1 (3 + 6A_0^2 - 10A_0).$$

Note that the values of the coefficients  $\nu$  and  $\lambda_2$  are zero for any  $A_k$ , i.e., for any regularization of the  $\theta$  function. The coefficient  $K$  is strictly negative provided conditions (35) are satisfied. The absence of the Laplacian term implies pertinence to a different universality class than the EW class. The resulting equation has the form of the so-called conserved KPZ equation (see Ref. [7]).

### E. Family model in 2+1 dimensions

The procedure described above for the calculation of jump probabilities and determination of stochastic equation corresponding to the discrete relaxation model can be straightforwardly generalized into 2+1 dimensions introducing two horizontal coordinates  $x$  and  $y$  and considering all possible combinations of space derivatives [28]. Now we must investigate conditions at an incidence site and four nearest neighbors instead of at an incidence site and two nearest neighbors as in 1+1 dimensions.

In the case of the  $F1$  model, we identify five configuration types according to the number of nearest-neighbor sites lower than the incidence site. We found that the stochastic equation governing the asymptotic behavior of the  $F1$  model in 2+1 dimensions contains a positive Laplacian term

$$\begin{aligned} \frac{\partial h(x,y;t)}{\partial t} = & 1 + \frac{2}{3} A_1 (A_0^2 + A_0 + 1) \\ & \times \left( \frac{\partial^2}{\partial x^2} h(x,y) + \frac{\partial^2}{\partial y^2} h(x,y) \right) + \eta(x,y;t). \end{aligned}$$

Because of the increasing number of relevant sites that determine the sticking site of the incident particle (5 in 1+1 dimensions versus 13 in 2+1 dimensions) and the corresponding rapid increasing number of configuration types, we did not study models with growth rules dependent on the number of bonds in 2+1 dimensions, although it would be of great interest.

## VIII. CONCLUSION

In this paper we have derived Langevin equations for discrete growth models with local relaxation. We explicitly studied the asymptotic behavior of several models with local relaxation: the Family model, the Wolf-Villain model, and the Das Sarma–Tamborenea model. Our results can be summarized as follows.

In the case of the Family model, we reproduced previously known results [16], but in addition we have investigated the effects of the modification of growth rules on the resulting equations. We compared two variants of this model with slightly different rules. For both models  $F1$  and  $F2$ , we obtained a positive Laplacian term, which dominates the asymptotic behavior, i.e., the Family model belongs to the EW class as expected. Moreover, in the limit  $C \rightarrow \infty$  for the parameter of regularization scheme, the values of the Laplacian coefficient  $\nu$  for both models coincide. This confirms that the difference between both variants is slight and does not effect the asymptotic behavior. At the same time, we see that the

procedure we used is sensitive enough to distinguish both variants properly.

In the case of relaxation models for MBE-like growth, our results show that the asymptotic behavior is different for the WV model and the DT model. For the WV model, we found a positive Laplacian term in the corresponding stochastic equation (i.e., the WV model belongs to the EW class), in agreement with recent computer simulations of discrete models [8,23]. Conversely, in the case of the DT model, we obtain a zero Laplacian term, and also the coefficient in front of the term  $\nabla(\nabla h)^3$  is identically zero. The first asymptotically relevant term for the DT model is  $\nabla^2(\nabla h)^2$ ; the coefficient in front of the fourth-order derivative is negative. Hence we arrived at the conserved KPZ equation. However, the roughness exponent calculated from the height-height correlation function (the so-called exponent  $\zeta$ ) in the DT model [30,31] is different from results of renormalization-group calculations for the conserved KPZ equation [4,9], and also the exponent for the time dependence of the surface width (the so-called exponent  $\beta$ ) found in simulations of the DT model [30,31] is different from the exponent predicted by the renormalization-group calculation [4,9] or the exponent obtained by direct integration [32] of the conserved KPZ equation. Here we should note that there is one feature of these models that so far is not completely understood. It has been revealed in simulations [33,30] that both the WV model and the DT model exhibit, over a long time, the increase of an average step size that leads to anomalous scaling [33,30,24]. In the WV model, the average step size saturates and so it does not effect the asymptotic behavior that is fully described by the EW equation. However, in the case of the DT model, it seems that the average step size increases infinitely; moreover, the DT model displays another peculiarity: spatial multiscaling [31]. If these features are really characteristic for the asymptotic behavior of the DT model then they should be contained in the continuous description. On the other hand, properties of the conserved KPZ equation are only partially known [32,24]. Our result provides a link between the DT model and the conserved KPZ equation, but because of the approximative character of our procedure we cannot exclude that the continuous description of the DT model is more complicated.

In the study of the WV model, we encountered a problem connected with the approximation of the discrete theta function that was not mentioned in previous works. We have found that the regularization procedure is a delicate problem. There is no rigorous treatment of the regularization procedure and consequently there is an uncertainty in the choice of the regularization scheme. We have shown that the values of coefficients in the resulting Langevin equation can be quite different for different approximations of the  $\theta$  functions appearing in the discrete Langevin equation (some schemes lead to a zero Laplacian term in the equation corresponding to the WV model). We do believe that a proper choice is that conserving all symmetries present in a discrete model. This choice is supported by the agreement of our results with results of recent simulations. This problem does not affect the result for the DT model, where we obtain a zero Laplacian term independent of the approximation of the  $\theta$  function used.

Our procedure can be straightforwardly applied also to other relaxation models suggested in the literature [11,31,23]. An advantage of our procedure is the easy incor-

poration of variations in growth rules in comparison to costly, extensive numerical simulations. We illustrated this on two variations of the WV model. One of them, the  $WV\uparrow$  model (with upward jumps in the case of a tie), shows an interesting behavior: a transition between stable and unstable growth, which has been found in recent simulations as well [3,23].

On the other hand, the method based on the formal Kramers-Moyal expansion and the subsequent transition to a continuous equation is not applicable in general for models with dynamics controlled by a local energy function. A specific feature of the model for which the failure of the method was demonstrated [20] is that the functional contains an explicit dependence on the vertical size of a particle together

with a dependence on the surface height. We suspect that in this case the first step, i.e., the transition to a set of discrete Langevin equations, is not correct. Nevertheless, at the moment it is not completely clear why the method gives correct results in some cases while it breaks down in others. A mathematically rigorous formulation of the formal method is missing and more work is needed to clarify this problem, in particular to understand the role of noise in this approach.

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