

Probing universality classes in solid-on-solid deposition

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We consider several stochastic processes corresponding to the same physical solid-on-solid deposition problem. Simplified models presenting the same (conditional) mean and variance for each process are also introduced as well as generalizations in terms of the deposition of blobs and probabilistic deposition rules. We compare the evolution of the roughness as a function of time for a three-parameter family that includes as limit cases the Family model and the Edwards-Wilkinson equation, showing that in all cases the derived models with the same mean and variance are indistinguishable from the originating models in terms of the evolution of the roughness. Finally, we show that although all the models studied belong to the same universality class, some relevant features such as the final surface roughness are reproduced only for models within a restricted class determined by sharing the same (conditional) mean and variance.

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I. INTRODUCTION

The increased technological requirements of high-quality solid films (atomically smooth), in particular in the rapidly developing field of nanotechnology, has stimulated interest in the understanding of the physical processes that determine interface dynamics and surface morphology.

Consequently, a renewed interest in models of surface growth has reemerged encompassing old (traditional) models as well as the development of new ones for more complex situations (substrate nanotrenches, nanocavities) and promoting an intense experimental work to understand the physical processes involved in chemical vapor deposition (CVD), physical vapor deposition (PVD), sputtering, molecular beam epitaxy (MBE), electrochemistry, etc. [1].

Surface growth phenomena involve randomness not only as a result of external sources of noise but also as an intrinsic property of surface growing, making stochastic dynamical systems the natural framework for modeling attempts.

The search for the most relevant factors organizing the behavior of stochastic dynamical systems—emerging in the simulation of solid-on-solid (SOS) deposition as well as in other areas of physics—has been largely focused on the emergence of asymptotic features partially characterized by scaling exponents and scaling laws.

Systems presenting the same scaling exponents are said to belong to the same *universality class* [2–8], producing in this form a taxonomy of stochastic dynamical systems. Furthermore, quite often such classes are named after particularly simple models (a partial differential equation with an additive noise source in most cases) that pertain to the class.

Certainly, any attempt to classify any taxonomy is an attempt to find key characteristics of the systems that will allow one to infer other common features shared by all the members of a class. Furthermore, one expects that after assessing the universality class to which our system pertains,

one would be capable of roughly determining other properties which might or might not be relevant to our particular interest; this is to say we shall *a priori* know whether determining the universality class will be a useful step to take or not.

So far, most of the effort referring to universality classes has focused on asserting the class of universality for different models. A few works have tried to relate solid-on-solid deposition models to the simplest differential equation with additive (white, Gaussian, density independent) noise relying in mathematical manipulations that, at one time or another, expand in Taylor series nondifferentiable functions [9,10]. The meaning and relevance of universality classes is a matter that claims elucidation. The present work is an attempt to advance towards this goal.

In our probing of the Edwards-Wilkinson [11] universality class we will study a three-parameter family of stochastic dynamical systems that includes as limit systems the Edwards-Wilkinson and the Family [3] model of surface growth and, according to the numerical simulations, belongs completely to the Edwards-Wilkinson class.

We shall further show that each element of our three-parameter family can be replaced by a denso-dependent stochastic model which only has in common the conditional flux and dispersion, without modifying the observed properties of the surface in terms the standard roughness characterization.

The work is organized as follows: In Sec. II we introduce basic definitions and some relevant aspects of stochastic models; in Sec. III we introduce the parametric families of stochastic processes that are our main tool to explore the Edwards-Wilkinson universality class. In Sec. IV we present selected numerical results, ending the work with a discussion of results Sec. V.

II. PRELIMINARY RESULTS

A. Basic definitions

We shall confine our attention to one-dimensional substrates subject to periodic boundary conditions, although most of our results can be easily extended to other dimensions and boundary conditions.

One of the most relevant statistics associated to material growth processes is the interface roughness, defined as the root mean square (rms) of the deviations of the substrate height from the average height.

Let L be the number of sites in the substrate (then, if a is the distance between sites, the substrate length will be La), and consider h_i the height at the site i ; the interface roughness is defined as

$$W(t,L) = \sqrt{\frac{1}{L} \sum_i (h_i - \bar{h})^2}, \quad (1)$$

where $\bar{h} = 1/L \sum_i h_i$ is the spatial mean of the interface. Often along this work we will consider for simplicity the squared roughness W^2 rather than with W .

In order to show the application of the methods proposed in the present work, we need to refer to some particular discrete models previously studied in the literature [6,7]. We shall now proceed to review the defining rules of these models:

(i) Random deposition model (RDM): A site, say i , is randomly chosen. The deposit occurs on the chosen site; i.e., the height at the site i increases by one unit ($h_i \rightarrow h_i + 1$).

(ii) Symmetric Family model (SFM): A site, i , is randomly chosen. The surface is modified according to the following rules:

(I) If $h_i \leq h_{i\pm 1}$ the deposit occurs on the i site.

(II) If $h_i > h_{i+1}$ and $h_i \leq h_{i-1}$ the deposit occurs on the $i + 1$ site.

(III) If $h_i > h_{i-1}$ and $h_i \leq h_{i+1}$ the deposit occurs on the $i - 1$ site.

(IV) If both $h_i > h_{i+1}$ and $h_i > h_{i-1}$ the deposit occurs on the $i + 1$ or $i - 1$ sites with the same probability.

This model represents a small variation from the original Family model [3] in which at the step IV reads “if $h_{i+1} > (<) h_{i-1}$, the deposit occurs on the $i - 1 (i + 1)$ site.”

B. Discrete evolution equation

Solid-on-solid deposition models defined by rules such as those in the previous subsection are directly implemented into computer codes producing “Monte Carlo simulations” simply by selecting the site i with a pseudo random variable ψ uniformly distributed in the interval $[0, 1)$; then, $i = [L\psi]$ (where $[\dots]$ means integer value) is a uniformly distributed integer random number that takes values in $\{0, \dots, (L-1)\}$.

The particle is deposited according to the rules of the model, completing the cycle. Deposition models are defined directly in terms of the simulation algorithm, a fact that anticipates the preferred method of analysis: extensive numerical simulations.

We shall call the rules defining a model the “microscopic rules” and the Monte Carlo implementation describing the

“original model” to distinguish the direct implementation from other possible implementations.

In this picture the time between two successive deposition events is not defined and it becomes natural to measure time just in terms of the particles deposited or steps performed in the algorithm. In real deposition processes, the number of particles deposited per unit time is proportional to the system size L ; therefore, in the computational simulation context, it is sensible to measure the time in “Monte Carlo steps” ($t_{MC} \propto (\text{depositions})/L$).

The rules defining solid-on-solid deposition models might not be the model descriptions most suitable for nonnumerical studies. A useful rewriting is to consider the original model as the embedded process resulting from a denso-dependent (or state-dependent) jump process, of which the Monte Carlo simulations are just the associated Feller process [12,13]. In more common terms, a Markov chain in which the time between events is stochastic as well as the events, having transition probabilities that depend on the state of the system (in this case the state of the surface). Such a definition would be the natural starting point if use of the machinery of Markov processes was intended. The interested reader can see [14] for a solid-on-solid deposition model defined along these lines.

For our present purposes we can stop short of this setting, not planning to worry about the statistical characterization of the time intervals between depositions.

An alternative approach to the original implementation presenting equivalent statistical properties consists in defining a local growth rate $R_i = CLJ_i$ proportional to the probability for a particle to be deposited in the site i , J_i , in a fixed (and sufficiently small) time interval. J_i is the conditional probability of the embedded Markov chain associated with the transition $(h_1, \dots, h_i, \dots, h_L) \rightarrow (h_1, \dots, h_i + 1, \dots, h_L)$, which will characterize the different growing processes.

Consider the following stochastic process evolving in terms of a discrete time n that we will later relate with t_{MC} :

$$h_i(n+1) = \Theta(R_i(n) - X_i(n)) + h_i(n), \quad (2)$$

where $\{X_i\}$ are L independent random variables each one uniformly distributed on $[0, 1)$ and Θ is the step function, which we define as

$$\Theta(x) = \begin{cases} 1 & \text{if } x > 0, \\ 0 & \text{if } x \leq 0. \end{cases} \quad (3)$$

Notice that in this process the average number of sites with its height modified is $N = \sum_{i=1}^L R_i(n) = LC \sum_i J_i = LC$, corresponding to a time interval of C in Monte Carlo units of time. The process represents the simultaneous update of all sites based in the transition probabilities computed at the time n .

The conditions for the stochastic process (2) to be roughly equivalent to the corresponding original model are two: the first one is that both processes should have the same transition probabilities J_i for the same states of the surface; the second requirement is that the probability for depositions occurring at neighboring sites that imply changing the com-

puted transition rate (and consequently make improper the simultaneous update strategy) must be negligible.

The second condition can always be achieved making $R_i \ll 1$ or, what is the same, choosing C small enough.

The selection of this stochastic process as an approximation of the original one is in part arbitrary. It has the advantage of being close to some simulation strategies introduced in the literature for cellular automata [15] and implementations of deposition models [16,17], being at the same time flexible enough for our discussion.

A numerical procedure implementing the stochastic system is as follows:

(i) A local deposition probability R_i for each site i is obtained from the microscopic rules of the model (as will be explained later in detail).

(ii) A pseudorandom variable is taken for each lattice site (all the lattice sites are visited sequentially). If the variable is lower than or equal to the local deposition probability at the site, then a particle will be deposited at this site, although that incorporation will be effective once all the lattice sites have been visited.

(iii) All the lattice sites are simultaneously updated.

The duration of a loop of this algorithm (an iteration) is C in Monte Carlo time. It must be stressed that, while in the standard algorithm the total number of deposited particles at a determined time is a deterministic quantity, in the present scheme this has (more realistically) a stochastic nature.

C. Expression of the local deposition rates

We have yet to find the probability of depositing the next particle in the site k in terms of the defining rules of the model.

Since the models are normally defined in two steps (Sec. II A), it is convenient to introduce first the conditional probability of depositing the particle at the site k given that the number i has been selected in the first step.

Let $Y_{i,k}\{\bar{h}\}$ be the conditional probability that the particle is deposited at k given that the site i has been selected. These quantities might depend on the entire configuration $\{\bar{h}\}$ (although in most cases it depends only on the heights within a given neighborhood of the site i), and they are often thought of as the contribution of two processes, one corresponding to moving $|k-i|$ sites to the left ($i > k$) or to the right ($k > i$) while the other contribution corresponds to moving $L-|k-i|$ sites to the right $i > k$ or to the left $k > i$, this latter contribution being due to the periodic boundary conditions.

The probability for the next deposit to happen at the site k (irrespective of the random number i) is obtained as a composition of a sum of independent events:

$$J_k = \left(\sum_{j=0}^{L-1} Y_{k+j,k}\{\bar{h}\} \right) / L \quad (4)$$

($1/L$ is the probability that the site i is chosen), and considering that $\sum_k Y_{i,k} = 1$, we can exclude of the sum the diagonal terms to produce

$$J_k = \left(1 + \sum_{j=1}^{L-1} Y_{k+j,k}\{\bar{h}\} - \sum_{j=1}^{L-1} Y_{k,k+j}\{\bar{h}\} \right) / L. \quad (5)$$

The subindex algebra must be understood as (mod L), due to the assumed periodic boundary conditions.

At this point it is worth noticing that since J_i defines the transition probabilities for the embedded Markov chain, the probabilities J_i define a density-dependent Markov chain. Using a time between events exponentially distributed with mean $1/L$ —i.e., measuring the time between events in units of t_{MC} —the total number of particles deposited responds to a Poisson process and an average of LC particles are deposited in a time interval C in correspondence with what is obtained for the process (2). This is arguably the most suitable definition for theoretical work in terms of particles but does not leave room for introducing blobs as proposed by Edwards-Wilkinson [11] while Eq. (2) does.

In many models studied in the literature [3,4,6,7,18] the transitions can only happen to first neighbors; in such a case, Eq. (5) takes a simpler form

$$J_i = (1 + Y_{i+1,i}\{\bar{h}\} + Y_{i-1,i}\{\bar{h}\} - Y_{i,i+1}\{\bar{h}\} - Y_{i,i-1}\{\bar{h}\})/L. \quad (6)$$

Thus, Eq. (6) for the local amplitudes, in conjunction with Eq. (2), permits us to find a discrete evolution equation for a broad class of SOS deposition models by selecting different transition probabilities Y .

At this point, we shall give an example of the application of this method to find the local amplitudes for the random deposition and symmetric Family models introduced in (Sec. II A).

(i) Random deposition model: For this model the transitions between sites are forbidden, all the conditional probabilities $Y_{i,k}$ are zero for $i \neq k$, i.e., $J_i^{(RDM)} = 1/L$.

(ii) Symmetric Family model: From the microscopic rules of this model it is clear that the jumps can only land at first neighbors; the result is

$$Y_{i,i+1} = \Theta(h_i - h_{i+1})[1 - 0.5\Theta(h_i - h_{i-1})], \quad (7)$$

$$Y_{i,i-1} = \Theta(h_i - h_{i-1})[1 - 0.5\Theta(h_i - h_{i+1})]. \quad (8)$$

Using Eqs. (7) and (8) with Eq. (6) we obtain the expression for the local amplitudes in the SFM:

$$\begin{aligned} L J_i^{SFM} = & 1 + \Theta(h_{i+1} - h_i) + \Theta(h_{i-1} - h_i) - \Theta(h_i - h_{i+1}) \\ & - \Theta(h_i - h_{i-1}) + 0.5[2\Theta(h_i - h_{i+1})\Theta(h_i - h_{i-1}) \\ & - \Theta(h_{i+1} - h_i)\Theta(h_{i+1} - h_{i+2}) - \Theta(h_{i-1} - h_i)\Theta(h_{i-1} \\ & - h_{i-2})]. \end{aligned} \quad (9)$$

Models such as the random deposition and symmetric Family models in their usual implementation do not have free parameters; just one particle is deposited in each iteration contrary to what happens with the evolution dictated by Eq. (2) where one has a free parameter C , representing the time interval.

The “optimal” value for C to get the closest approximation to the usual implementation would appear to be $C = 1/L$; however, this choice is not computationally efficient.

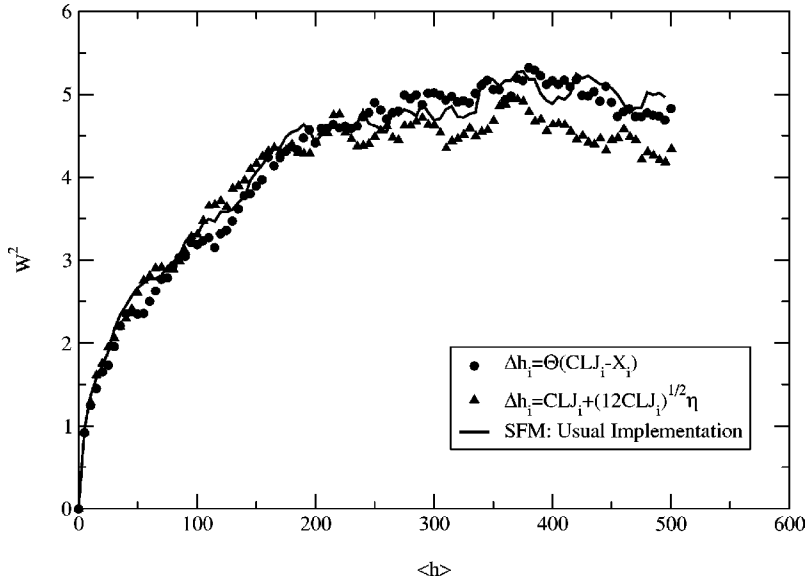


FIG. 1. W^2 as a function of the average height $\langle h \rangle$ for three different evolution mechanisms: the symmetric Family model (SFM) (standard implementation), the implementation of Eq. (2), and the flux +variance model for small values of C (11). The simulation was made with $L=100$ and $C=0.01$, while an average over 100 independent runs was performed.

Varying C modifies the time scale but does not substantially change the system. Values smaller than $1/L$ will simply mean that in most steps of the algorithm no particle is deposited leaving the surface unchanged. Values of C larger than $1/L$ appear to be convenient in terms of the efficiency of the algorithm. For example, for a lattice with $L=10\,000$ sites, the choice $C=10^{-4}$ requires an average of 10 000 iterations for depositing a monolayer of particles, resulting in a very inefficient procedure. A choice such as $C=0.1$ means that an average of just 10 iterations is required to deposit a monolayer of particles. For such value of C the effects of the neglected correlation introduced by multiple depositions still cause a small contribution which does not modify statistical indicators such as the scaling exponents.

III. RELATED MODELS

We shall now introduce two families of models related to the solid-on-solid deposition models and, in particular, to the symmetric Family model. The new models are introduced using three well-defined procedures:

(i) Substitute a given model by a new one that shares the same local average deposition rate and variance but uses a random variable with simpler statistics than the originating model (we will use uniformly distributed variables).

(ii) Allow for blobs—i.e., let h_i take real values and not just integer values. We call this procedure smoothing.

(iii) Soften the defining rules of the deposition model by allowing other probability values for $Y_{i,j}$ different from $\{0, \frac{1}{2}, 1\}$.

Note that the three procedures to obtain related models can be applied simultaneously as will be shown later.

A. Flux and variance models

Consider the stochastic system (2); the term $\Theta(R_i - X_i)$ is a stochastic variable with mean CLJ_i and variance $CLJ_i(1 - CLJ_i)$.

We can ask the question for any given statistics of the process such as the roughness or the scaling exponents: is this statistics sensitive only to the conditional mean and variance at each step and insensitive to any other characteristic of the random process?

In order to explore answers for this question, we produce a “Langevin-like” equation from Eq. (2) with the same mean and variance:

$$h_i(n+1) - h_i(n) = CLJ_i + \sqrt{12CLJ_i(1 - CLJ_i)}\eta_i, \quad (10)$$

where η_i are independent stochastic variables with uniform distribution in $[-1/2, 1/2]$.

Although the limit $C \rightarrow 0$ is not attractive from a computational point of view, it is interesting to consider it. When $C \ll 1$ the term CLJ_i is negligible in front of 1 in Eq. (10)—i.e., $\sqrt{12CLJ_i(1 - CLJ_i)} \sim \sqrt{12CLJ_i}$ —and hence

$$h_i(n+1) - h_i(n) = CLJ_i + \sqrt{12CLJ_i}\eta_i. \quad (11)$$

The evolution of the interface roughness obtained from the usual implementation of the symmetric Family model (see Sec. II A), the simultaneous update implementation resulting from Eq. (2), and the approximate models (11) are compared in Fig. 1. The figure shows that the sensitivity of roughness to the details of the stochastic process is almost negligible provided the flux and variance are correct.

We further notice for future use that Eq. (11) can be considered as a discrete integration, with an integration step $\Delta t = C$, of the continuous time equation

$$\frac{\partial h_i}{\partial t} = LJ_i + \sqrt{LJ_i}\xi_i, \quad (12)$$

where ξ_i has zero mean and correlation properties given by

$$\langle \xi_i(t)\xi_j(t') \rangle = \delta_{ij}\delta(t - t'). \quad (13)$$

B. Smoothing procedure: Blobs

In most of the solid-on-solid (discrete) deposition models, local amplitudes are obtained from microscopic rules as

those described in Sec. II A that include step functions or even more complex nondifferentiable functions. For example, the local amplitudes given in Eq. (9) for the symmetric Family model contain several step functions.

In what follows we will consider the step functions as limits of sufficiently smooth functions. This smoothing procedure has been employed earlier [9,10,19,20] in contexts similar to the present one; nevertheless, our interpretation of the smoothing process will differ from previous approaches.

The choice of a proper smoothing family of functions for the step function is not unique. Because of this reason, we will not constrain our discussion to one particular family; instead, we will work using a few and not very restrictive hypotheses regarding the properties of this family of functions. We shall call $F_{K_0}(x)$ a one-parameter family of functions, where the real parameter K_0 labels the family members.

Throughout this work we will assume the following:

(I) $F_{K_0}(x)$ is a continuous, nondecreasing real function for each $K_0 > 0$ value such that (for fixed x)

$$\lim_{K_0 \rightarrow \infty} F_{K_0}(x) = \Theta(x). \quad (14)$$

(II) $F_{K_0}(x)$ is differentiable at the origin, being approximated at $x=0$ by

$$F_{K_0}(x) = \frac{1}{2} + K_0 x + o(K_0 x). \quad (15)$$

For example, we can consider

$$F_{K_0}(x) = \frac{1}{\pi} \arctan(\pi K_0 x) + \frac{1}{2}, \quad (16)$$

obtaining a smooth family. Another possible choice would be

$$F_{K_0}(x) = \begin{cases} 0 & \text{if } x < \frac{1}{2K_0}, \\ K_0 x + \frac{1}{2} & \text{if } -\frac{1}{2K_0} \leq x \leq \frac{1}{2K_0}, \\ 1 & \text{if } \frac{1}{2K_0} < x, \end{cases}$$

obtaining a family of piecewise linear functions which are not differentiable at $x = \pm 1/2K_0$.

Smoothing the step functions we extend the stochastic process (2) to a family of processes in the form

$$h_i(n+1) = F_{K_0}(R_i(n) - X_i(n)) + h_i(n). \quad (17)$$

This equation reproduces exactly the results of the Monte Carlo simulations only at the limit $K_0 \rightarrow \infty$. For finite values

of K_0 the equation will be only an approximation. We now allow for the deposition of blobs of height smaller than 1.

C. Smoothing procedure: Probabilities

We can think that we have a family of models, one for each K_0 value, and only the family member that corresponds to $K_0 = \infty$ coincides with the Monte Carlo model. The cost of introducing “smoothness” is then to lose the discretization in the heights of the deposit (i.e., the heights will not be increased in units of 1).

As has been already mentioned, in some cases the local amplitudes J_i will also have nonanalytical functions in their definitions. We will also smooth these functions using the same one-parameter family of smoothing functions.

In general, in the smoothing process we change the original system for a p -times infinite family depending on p smoothing parameters $\vec{K} = K_0, K_1, K_2, \dots, K_{p-1}$. At the limit $\vec{K} \rightarrow \vec{\infty}$ the original model is recovered. The parameter K_0 , which appears directly in the evolution equation (17), will be called “principal smoothing parameter,” to distinguish it from the other smoothing parameters K_1, K_2, \dots, K_{p-1} that might appear in the smoothing of the transition probabilities.

Our expectation is that the statistical properties of the system will depend weakly on the smoothing introduced. This is, we expect that if \vec{K} is “sufficiently large,” the model will be a good approximation to the original one. It is expected that the loss of precision in the approximation will increase along with the decreasing of \vec{K} .

Not every statistical property is expected to have the same sensitivity to the smoothing parameters in the family of models. It is then possible to think that, even when the differences between the models are very important, some characteristics will be common or persist even for small values of \vec{K} .

Of particular relevance is the question of the characteristic exponents of the model: Is it possible for the scaling exponents to be the same for the full family of stochastic systems, even when the approximation to the original model substantially deteriorates? The answer to this question is not a simple one. Extensive numerical simulations over various well-known models appearing in the literature suggest that at least for the models so far considered, the answer is affirmative: the smoothing procedure is not expected to modify the universality class.

D. Evolution of the mean height in the smoothed system

A problem of fundamental importance in the modeling of real deposition processes is how to relate model parameters with experimentally measurable quantities. One of the most relevant quantities in deposition processes is the average deposition rate—i.e., the average height increase per time unit.

Considering Eq. (17), it is clear that the local rate is given by $\mathcal{F}(R_i, K_0) = \langle F_{K_0}(R_i - X_i) \rangle = \int_0^1 F_{K_0}(R_i - x) dx$ which represents the average over independent realizations of the height increase for a given (fixed) local deposition probability. In

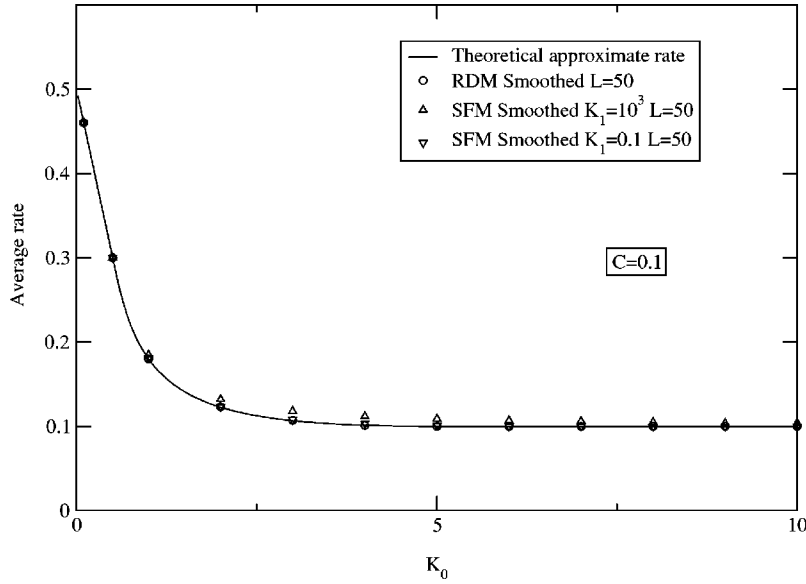


FIG. 2. Comparison of the approximate theoretical rate (21) with the rates obtained from Monte Carlo simulations averaged over ten independent runs. Results for the symmetric Family models (SFM), random deposition model (RDM), and a theoretical approximation described by Eqs. (21) and (18) are shown.

some cases, it is possible to obtain a closed form for this expression. For example, making the choice of smoothing functions proposed in Eq. (16) we obtain

$$\begin{aligned} \mathcal{F}(R_i, K_0) = & \frac{1}{2} + \frac{R_i}{\pi} \arctan(K_0 \pi R_i) \\ & - \frac{R_i - 1}{\pi} \arctan(K_0 \pi (R_i - 1)) \\ & + \frac{1}{2K_0 \pi^2} \ln \left(\frac{1 + K_0^2 \pi^2 (R_i - 1)^2}{1 + K_0^2 \pi^2 R_i^2} \right). \end{aligned} \quad (18)$$

From the experimentalist point of view, who generally watches as a single system evolves, more relevant than an statistical ensemble average is the lattice average

$$\mathcal{F}_A(K_0) = \{F_{K_0}(R_i - X_i)\}_L \equiv \frac{1}{L} \sum_i F_{K_0}(R_i - X_i). \quad (19)$$

In general it is not possible to obtain a closed expression for $\mathcal{F}_A(K_0)$, since R_i is a stochastic variable whose statistical properties are *a priori* unknown. Nevertheless, an attempt to achieve a suitable approximation to this quantity comes from the “reasonable” (but nonrigorous) supposition that the spatial average of $F_{K_0}(R_i - X_i)$ is close to the statistical average:

$$\{F_{K_0}(R_i - X_i)\}_L \sim \langle F_{K_0}(\{R_i\}_L - X_i) \rangle. \quad (20)$$

From the general expression (5) for the local amplitudes, we obtain $\{J_{ij}\}_L = 1/L$, so $\{R_i\}_L = C$. Combining this relationship with Eqs. (19) and (20) we produce an estimation for the average rate:

$$\mathcal{F}_A(K_0) \sim \mathcal{F}(C, K_0). \quad (21)$$

The average deposition rate emerging from this expression is compared in Fig. 2 with numerical simulations, showing excellent agreement. The figure shows that the average depends weakly on the value of the probability smoothing parameter K_1 , being determined mostly by the main smoothing parameter K_0 , in agreement with the approximated result

(21). Notice that this means that in terms of the average growth rate, all the models behave as the corresponding smoothed random deposition model for the same value of K_0 .

E. Connection with spatially continuous models

Stochastic partial differential equations and discrete models are normally portrayed as two alternatives approaches to study interface dynamics.

Most of the support for this conjecture comes from numerical studies that have related pairs of models within the same universality class: for example, the Edwards-Wilkinson and the Family models.

The Edwards-Wilkinson (EW) model reads [11]

$$\dot{h}(x, t) = F + \nu \nabla^2 h(x, t) + \eta(x, t), \quad (22)$$

where F represents an average constant flow and ν is the diffusion constant (sometimes called evaporation-condensation coefficient), while the noise term $\eta(x, t)$ is assumed to be a Gaussian white noise, with zero mean and correlation given by

$$\langle \eta(x, t) \eta(x', t') \rangle = \Gamma \delta(x - x') \delta(t - t'). \quad (23)$$

Although considerable theoretical effort has been devoted to relate continuous equations with discrete models, using a variety of techniques such as Master equation formulations followed by a Kramers-Moyal expansions [9,19,20], Van Kampen’s Ω expansions [21], and others [10,22,23], at present not one of this attempts can be considered fully satisfactory, and the problem continues to be open [24].

We will follow the proposed smoothing procedure with the symmetric Family model defined in Sec. II A. We simply have to replace the step functions in the expression of the local amplitude given in Eq. (9) for a function F_{K_1} and the step function in Eq. (2) for a F_{K_0} function. Thus, from the symmetric Family model we obtain a three-parameter family of smoothed models; i.e., we have a model for each (C, K_0, K_1) point in parameter space.

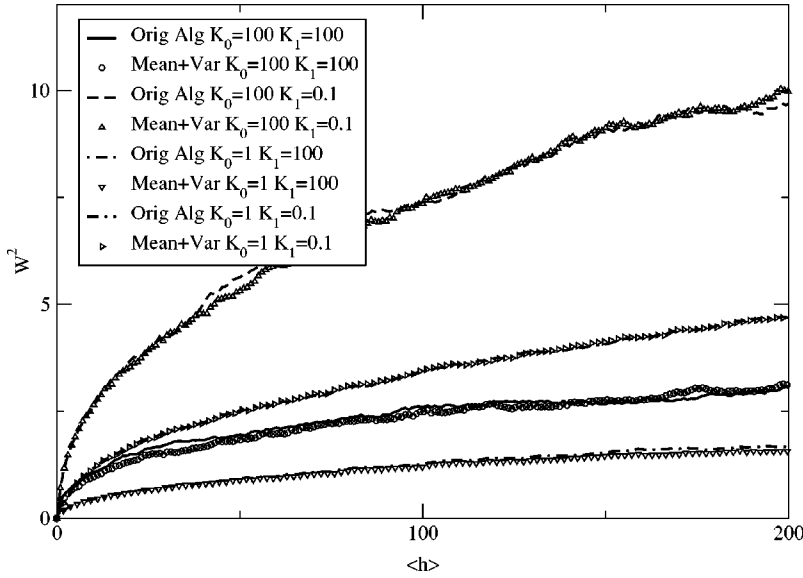


FIG. 3. Curves obtained, for different parameter values on the smoothed symmetric Family model using the evolution dictated by Eq. (29) (Orig Alg) and the approximation in terms of mean and variance (28) (Mean +Var). In all cases $L=100$ and $C=0.1$ and an average over 100 independent runs was performed.

Numerical simulations show (as we shall see in Sec. IV) that the family shares the same set of scaling exponents. This means that despite the fact that we change the parameters the model remain in the same universality class than the symmetric Family model.

In particular, this is true for the models with a value of \bar{K} sufficiently small such that linear approximations are possible (*how* small should \bar{K} be will depend on the argument of $F_{\bar{K}}$).

Expanding both in K_0 and K_1 up to the first nontrivial contribution, we get

$$h_i(n+1) - h_i(n) = \frac{1}{2} + K_0 C - \frac{K_0}{2} + CK_0 K_1 \left(h_{i+1} + h_{i-1} - 2h_i + \frac{h_{i+2} + h_{i-2} - 2h_i}{4} \right) + K_0 \eta_i, \quad (24)$$

where η_i are uncorrelated random variables distributed uniformly in $[-\frac{1}{2}, \frac{1}{2}]$. The expressions $h_{i+1} + h_{i-1} - 2h_i$ and $(h_{i+2} + h_{i-2} - 2h_i)/4$ are two discrete realizations of the one-dimensional Laplace's operator.

Equation (24) can be considered a discrete form of the EW equation (22). In fact, Eq. (24) is equivalent to a numerical integration (in an Euler forward scheme) of the EW equation with parameters:

$$F = \frac{1}{2} + K_0 C - \frac{K_0}{2}, \quad (25)$$

$$\nu = 2CK_0 K_1, \quad (26)$$

$$\Gamma = \frac{K_0^2}{12}. \quad (27)$$

Γ was introduced in Eq. (23) and the integration steps are $\Delta t = \Delta x = 1$.

Therefore, an interpolation has been produced linking the Family model and the Edwards-Wilkinson equation. Note, however, that the link is established smoothing rather than differentiating; smoothing is associated with the deposition of blobs rather than particles and is expected to be relevant at a mesoscopic scale in consonance with the ideas in [11].

F. Simplified models

We will further explore the smoothed systems in terms of the flux and variance model introduced in Sec. III A for the system (2).

For every stochastic system in the smoothing family, a flux and variance counterpart can be produced along the lines of Eq. (17) using state-dependent noise:

$$\Delta h_i = E[CLJ_i, K_0] + \sqrt{12 \text{Var}(CLJ_i, K_0)} \eta_i. \quad (28)$$

here E and “Var” denote mean and variance of $F_{K_0}(CLJ_i - X_i)$, respectively, while the η_i are independent random variables uniformly distributed in $[-1/2, 1/2]$.

We present in Fig. 3 the W^2 vs $\langle h \rangle$ curves obtained for the smoothed symmetric Family models as dictated by Eqs. (29) and (30) and those obtained from the approximated equation (28) for different parameters values. The figure shows excellent agreement between both approaches, since it is almost impossible to distinguish between corresponding pairs of curves.

IV. NUMERICAL RESULTS

In this section we present an extensive numerical study using Monte Carlo simulations. We focus on the properties of the models obtained by applying the smoothing procedure as explained above to the symmetric Family model.

We aim at getting an understanding of the main properties of the models in the different regions of the parameter space (C, K_0, K_1) , avoiding as much as possible the details that will eventually emerge as characteristics of the particular smoothing used.

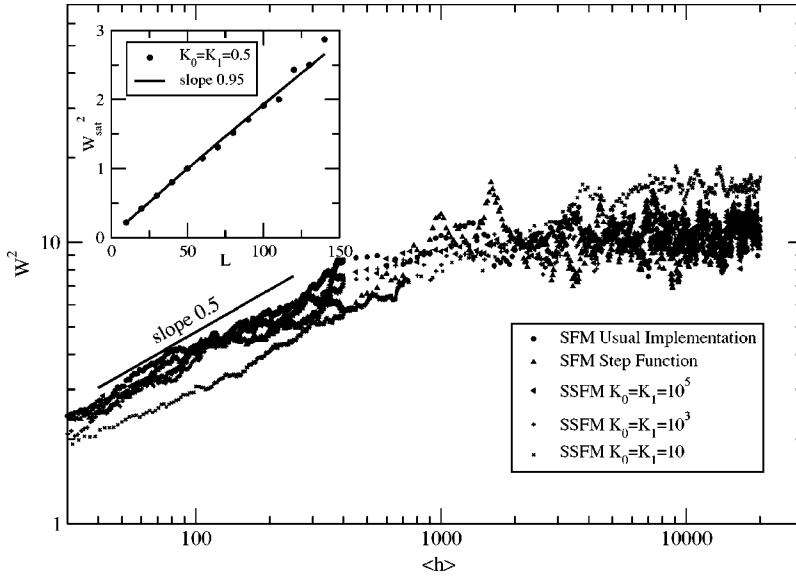


FIG. 4. Comparison of the squared roughness vs mean height evolution for the original symmetric Family model (SFM) and the smoothed symmetric Family model (SSFM) for various values of smoothing parameters for $L=200$, $C=0.01$ and averaging over 25 independent runs. Inset: saturation squared roughness as a function of system size, showing, approximately, a roughness exponent $2\alpha \sim 0.95$.

The smoothed symmetric Family model (SSFM) with parameters (C, K_0, K_1) is defined by the following equations:

$$h_i(n+1) - h_i(n) = F_{K_0}(CLJ_i(n) - X_i(n)) \quad (29)$$

$$\begin{aligned} J_i^{SSFM} = & \{1 + F_{K_1}(h_{i+1} - h_i) + F_{K_1}(h_{i-1} - h_i) - F_{K_1}(h_i - h_{i+1}) \\ & - F_{K_1}(h_i - h_{i-1}) + 0.5[2F_{K_1}(h_i - h_{i+1})F_{K_1}(h_i - h_{i-1}) \\ & - F_{K_1}(h_{i+1} - h_i)F_{K_1}(h_{i+1} - h_{i+2}) - F_{K_1}(h_{i-1} - h_i) \\ & \times F_{K_1}(h_{i-1} - h_{i-2})]\}/L. \end{aligned} \quad (30)$$

In terms of scaling laws we find that, for the SSFM, the roughness scales with the average height and system size in agreement with the Family-Vicsek [2] picture since the scaling exponents obtained are close to those corresponding to the EW universality class (see Fig. 4)—i.e., in one dimension $\alpha=0.5$ and $\beta=0.25$.

Although the number of lattice sites is relatively small due to computational restrictions, we find that the numerical evidence sustains the claim that the full family of stochastic systems belong to the same universality class.

A qualitative understanding of the properties of the smoothed symmetric Family model in parameter space comes from considering the generic shape assumed for the F functions. In fact, roughly speaking, the F functions have an almost linear part and an almost constant part (this would be exactly the case for a smoothing performed with the linear piecewise functions proposed above). Then, we can make a partition of the parameter space in regions in which the linear approximation in Eqs. (29) and (30) is valid or not valid—i.e., when the differences $|h_i - h_{i+1}|K_1 \ll 1$ or $|h_i - h_{i+1}|K_1 \gg 1$ (leaving a transition region for $|h_i - h_{i+1}|K_1 \approx 1$).

Certainly, these regions depend on the proper choice of the smoothing functions F and have not, generally, well-defined boundaries; instead, there are crossover regions with intermediate behavior that make it harder to obtain a full characterization of the parameter space. Nevertheless, we

have found that our more relevant numerical findings can be qualitatively understood by means of this characterization.

We shall speak of four main regions in parameter space, noted as $\{(L, L); (L, N); (N, L); (N, N)\}$, where, for example, the (L, N) region is the one where the linear approximation is valid in Eq. (29) while the F_{K_1} functions in Eq. (30) behave practically as step functions. It is obvious that, setting a fixed C value, at the limit $(K_0, K_1) \rightarrow (0, 0)$ we are in the (L, L) region, while for $(K_0, K_1) \rightarrow (\infty, \infty)$ we are in the region (N, N) .

In accordance with this classification scheme, we can understand many facts that emerge from numerical simulations, such as the following:

(i) The simulations show that little variation is observed by varying the K_0 and K_1 parameters between 10 and ∞ , while C is kept fixed at a constant value, $C=0.1$. This means that, in this region of parameter, the smoothing procedure has not an appreciable effect. A fact that can be understood by noting that, for these (C, K_0, K_1) values, we are in the region (N, N) , and the arguments inside of the F functions in Eqs. (29) and (30) evaluate the F functions as almost constant. No substantial change takes place moving the parameters inside this region.

(ii) Points in parameter space with $C=0.1$ and $K_0, K_1 \leq \frac{1}{2}$ lie in the (L, L) region in which the evolution equation reduces to the “EW-like” form discussed in Sec. III E. In Fig. 5, we use this connection with the EW equation to obtain data collapse between different simulations in which the parameters are included in the rescaling of the axis in the form given by the exact solution of the EW equation [25].

The collapse of data in Fig. 5 should not be expected to be complete since the data correspond to different stochastic systems and the scaling is adjusted just for the limit case corresponding to the EW equations rather than for each one individually.

Finally, we give an example of a transition between the (N, N) to the (N, L) region. This transition can be observed in Fig. 6, where fixed values $C=0.1$, $K_0=1000$ were taken, while the K_1 value was varied in the range $0.1, 10^6$. This

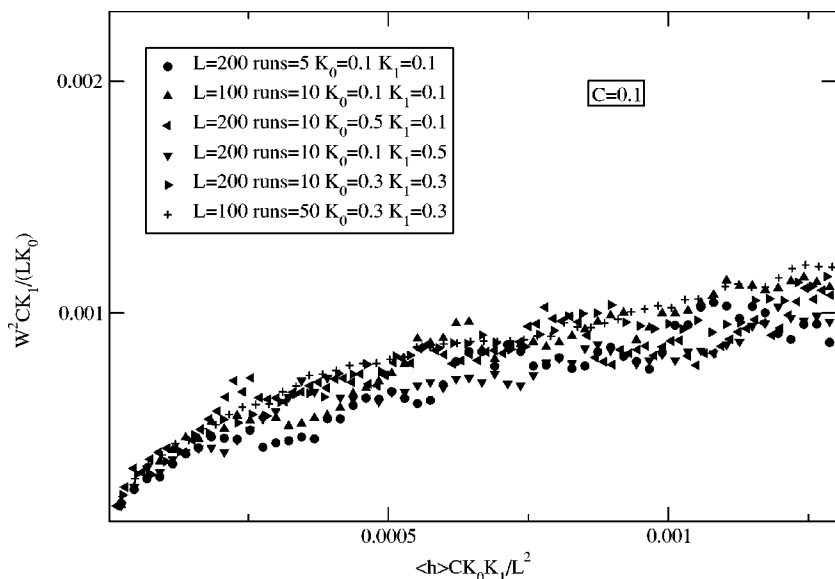


FIG. 5. Data collapse, obtained by rescaling the axis in agreement with the exact solution of the EW equation. The word “runs” in the box indicates the number of independent realizations in which the data has been averaged.

figure shows that varying K_1 between approximately 0.4 and 10^6 [which corresponds to the (N, N) region], a nearly constant value of the saturation squared roughness is obtained, while for $K_1 < \sim 0.4$ (corresponding to the (N, L) region) the saturation squared roughness grows as K_1^{-1} .

The influence of the parameter C depends on the region being considered. In the (N, N) region the influence is negligible (provided C is sufficiently small) as it only results in changing the time between observations. In the (L, L) region it controls the amount of diffusion without changing the fluctuations. Finally, the location of the transition regions in the (K_0, K_1) plane depends on C since the conditions for linearizing the probability rates depends both on C and K_1 .

V. SUMMARY AND DISCUSSION

The study of a three-parameter family of stochastic systems related to the symmetric Family model by smoothing of the probabilities and the surfaces allows us to interpolate

between the solid-on-solid deposition and an Edwards-Wilkinson equation, being all the models within the same universality class.

We have shown that there is a Langevin-like equation that cannot be distinguished from the symmetric Family model in terms of roughness evolution. The Langevin-like stochastic model (12) presents a mean value contribution (flux) plus a state-dependent (denso-dependent or multiplicative) noise.

The smoothing procedure introduced in this work could actually be applied to a large class of solid-on-solid deposition models, but the final linearization requires the saturation of the roughness; hence, in those situations where, for example, instabilities in the form of fingers appear (unstable growing), the linearization is not possible and the relation with differential equations is lost.

It is worth mentioning that in the present work smoothing is understood as a continuous process in terms of the smoothing parameters; hence, the degree of smoothness introduced can be regulated. This idea is in sharp contrast with

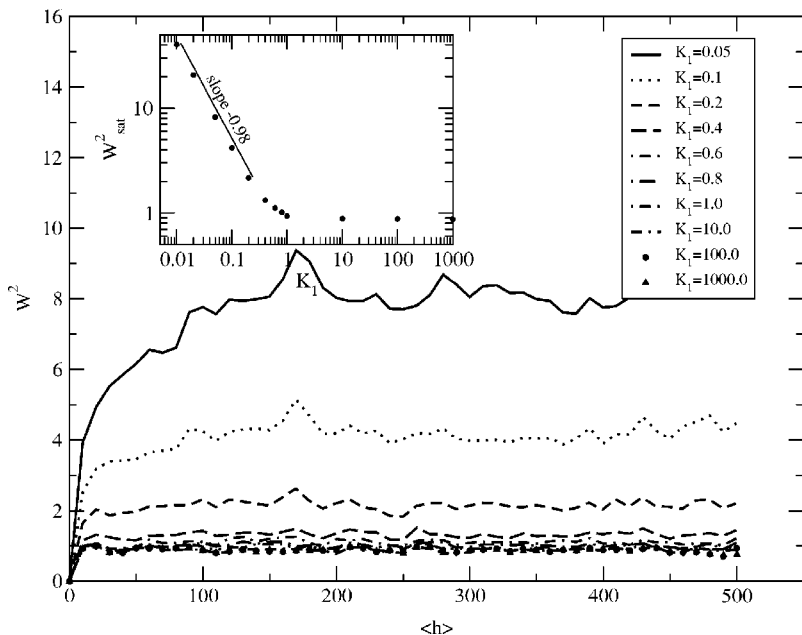


FIG. 6. Curves of W^2 vs $\langle h \rangle$ for different values of the parameter K_1 . Inset: saturation values of W^2 as a function of K_1 , showing a transition between different behaviors close to $K_1=0.4$. The remaining parameters are $K_0=1000$ and $C=0.1$.

previous works [9,10,19,20] where the step function is replaced by a polynomial moving from the (N,N) region to the (L,L) region discontinuously.

We have further shown that the evolution of the roughness with time is insensitive to most features of the stochastic process if exception is made for the conditional flux and variance of the model; hence, we can conjecture that just the conditional flux and variance are reflected in universality classes.

Conversely, notice that model validation beyond conditional mean and variance requires one to go beyond the standard statistical analysis of roughness.

Not every interesting property is shared by all members of a universality class. Of particular relevance is the fact that the maximum roughness achieved with different models is model dependent, being sensitive to the transition probabilities $Y_{i,j}$ and, hence, to the microscopic laws describing particle interactions.

Intuitively, the higher the value of the probability smoothing parameter K_1 is, the higher the sensitivity to the height differences $h_i - h_{i+1}$, hence, the system is expected to respond more effectively to height differences for large K_1 values, achieving smoother surfaces. Our results show that this intuitive thinking is relevant only for moderate values of the probability smoothing parameter K_1 and insensitivity to this feature becomes the rule for larger values of K_1 .

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