

Coarse-graining a restricted solid-on-solid model

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A procedure suggested by Vvedensky for obtaining continuum equations as the coarse-grained limit of discrete models is applied to the restricted solid-on-solid model with both adsorption and desorption. Using an expansion of the master equation, discrete Langevin equations are derived; these agree quantitatively with direct simulation of the model. From these, a continuum differential equation is derived, and the model is found to exhibit either Edwards-Wilkinson or Kardar-Parisi-Zhang exponents, as expected from symmetry arguments. The coefficients of the resulting continuum equation remain well-defined in the coarse-grained limit.

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I. INTRODUCTION

Driven, nonequilibrium interfaces have received much attention in recent years. Various models have been used to describe such systems. [1,2]. These models may usually be assigned to one of a small number of universality classes, each characterized by a set of scaling exponents. To each universality class corresponds a continuum Langevin equation; such an equation may therefore be identified for each lattice model if the exponents are known, for example, from kinetic Monte Carlo (KMC) simulations. This procedure, however, faces difficulties when crossover effects are important [3]. To overcome this, Vvedensky [4] has suggested using a combination of an expansion of the master equation [5–7] and the dynamic renormalization group (DRG) [8,9] to coarse-grain the resulting description, thereby obtaining a continuum Langevin equation in the large-scale, long-time limit. This program is a particular realization of a program suggested by Anderson [10].

In this paper we implement this procedure for a restricted solid-on-solid (RSOS) model with both adsorption and desorption. The master equation is expanded to obtain a set of discrete Langevin equations; these are then numerically integrated and compared to direct KMC simulations of the model, with which they are found to be in quantitative agreement. In the up and down symmetric case, an *ad hoc* procedure and the DRG both lead to the Edwards-Wilkinson (EW) equation,

$$\frac{\partial}{\partial t} \phi(x, t) = \nu_2 \frac{\partial^2}{\partial x^2} \phi(x, t) + \sqrt{D} \eta(x, t), \quad (1)$$

as the macroscopic description of the model; here, η is a zero-average Gaussian noise field with unit variance. For the asymmetric case, DRG arguments lead to the Kardar-Parisi-Zhang (KPZ) equation,

$$\frac{\partial}{\partial t} \phi(x, t) = \nu_2 \frac{\partial^2}{\partial x^2} \phi(x, t) + \lambda_2 \left(\frac{\partial}{\partial x} \phi(x, t) \right)^2 + \sqrt{D} \eta(x, t), \quad (2)$$

as the coarse-grained description. This is consistent with symmetry arguments and simulations [11]. The coefficients of the coarse-grained continuum equations remain well-defined in the macroscopic limit.

II. THE MODEL

The model is a simple generalization of the RSOS model introduced by Kim and Kosterlitz [11], and a special case of that introduced by Hinrichsen *et al.* [12]. It is described (in one dimension for simplicity) by a vector $\mathbf{h}(t)$ of L time-dependent, integer-valued heights $h_i(t)$, $i=1, 2, \dots, N$; time is also a discrete variable. The dynamical evolution is given by the following rules: At each time step, an integer $1 \leq i \leq L$ is randomly chosen; with probability p the height h_i is increased by 1, and with probability q attempt it is decreased by 1, provided that the resulting configuration does not violate $|h_i - h_{i\pm 1}| \leq 1$. Finally, periodic boundary conditions are imposed. The allowed transitions, together with the associated probabilities (equivalently, the rates) are shown in Fig. 1. The transition rate from configuration \mathbf{h} to $\mathbf{h} + \mathbf{r}$ is given by

$$W(\mathbf{h}; \mathbf{r}) = \sum_i [\{q \delta(r_i - 1) \theta(\Delta^+ h_i) \theta(-\Delta^- h_i) + p \delta(r_i + 1) \theta(-\Delta^+ h_i) \theta(\Delta^- h_i)\} \mathcal{F}_i], \quad (3)$$

with $\mathcal{F}_i = \prod_{j \neq i} \delta(r_j)$, the discrete derivatives

$$\Delta^\pm h_i = \pm (h_{i\pm 1} - h_i),$$

and

$$\theta(x) = \begin{cases} 1, & x \geq 0 \\ 0, & x < 0, \end{cases} \quad (4)$$

for integer (or zero) x . The temporal evolution of the probability density $P(\mathbf{h}, t)$ is given by the master equation

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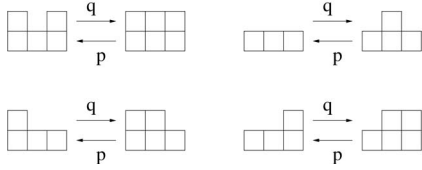


FIG. 1. Allowed transitions and associated transition rates.

$$\frac{\partial}{\partial t} P(\mathbf{h}, t) = \int d^L r [W(\mathbf{h} - \mathbf{r}; \mathbf{r}) P(\mathbf{h} - \mathbf{r}, t) - W(\mathbf{h}; \mathbf{r}) P(\mathbf{h}, t)]. \quad (5)$$

In Ref. [13], the special case $q=1, p=0$ is studied, and the KPZ equation derived as the coarse-grained description. However, the treatment of Ref. [13] leads to ill-defined coefficients precisely in the coarse-grained limit. In particular, the authors find the coarse-grained description to be Eq. (2) with ν_2, λ_2 , and D proportional to different powers of a parameter, a , which controls the degree of coarse-graining; indeed, their results are valid as $a \rightarrow 0$. Such a problem does not arise in our approach.

III. A VARIANT OF THE VAN KAMPEN EXPANSION

An often-used method for deriving Fokker-Planck equations for stochastic processes is the van Kampen expansion [5–7]. The method as described in [6,7] is not directly applicable to systems such as the RSOS model because it requires a small parameter, $1/\Omega$, in which to expand. In effect, it *assumes* the existence of a macroscopic law along with stochastic corrections to it, the relative size of which is controlled by the expansion parameter [6]. In stochastic growth models, this is not the case; it is impossible to separate the time evolution into deterministic and stochastic parts: the stochastic evolution is all there is. A more extended discussion of this point may be found in Refs. [14,15], where it is shown that Eq. (5) may nevertheless be approximated by a Fokker-Planck equation, which corresponds to the Itô Langevin equation

$$\frac{d}{dt} h_i = K_i^{(1)}(\mathbf{h}) + \sqrt{K_{ij}^{(2)}(\mathbf{h})} \eta_j(t), \quad (6)$$

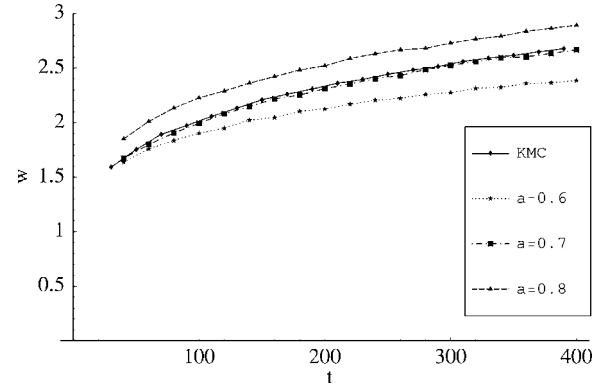
where summation over repeated indices is implied and the jump moments are defined by

$$K_{i_1, \dots, i_n}^{(n)}(\mathbf{h}) = \int d\mathbf{r} r_{i_1} \cdots r_{i_n} W(\mathbf{h}; \mathbf{r}).$$

Equation (6) is essentially a set of simultaneous coupled Langevin equations. Obtaining a continuum version is conceptually similar to the (inverse of the) method of lines used to solve partial differential equations. However, in the case of discrete interface models, the jump moments $K^{(n)}$ contain nonanalytic step functions which necessitate a regularization procedure. This is done in the next section.

IV. DISCRETE LANGEVIN EQUATIONS

To apply Eq. (6), the first two jump moments are needed. These can be calculated from W given by Eq. (3) and are


 FIG. 2. Variation of the evolution of the interfacial width with time for three values of a , as well as KMC simulation; $q=1$ and $p=0, L=100$. Both KMC and stochastic integration results averaged over 2000 runs.

$$K_i^{(1)}(\mathbf{h}) = q\theta(\Delta^+ h_i)\theta(-\Delta^- h_i) - p\theta(-\Delta^+ h_i)\theta(\Delta^- h_i) \quad (7a)$$

and

$$K_{ij}^{(2)}(\mathbf{h}) = [q\theta(\Delta^+ h_i)\theta(-\Delta^- h_i) + p\theta(-\Delta^+ h_i)\theta(\Delta^- h_i)]\delta_{ij}, \quad (7b)$$

where δ_{ij} is a Kronecker delta.

Equations (7a) and (7b) are not completely specified by the lattice transition rules of Sec. II, but must be extended to noninteger values of the h_i . Furthermore, in deriving Eq. (6), the implicit assumption that $W(\mathbf{h}; \mathbf{r})$ is analytic in \mathbf{h} was made, which in turn implies that the extension of $\theta(x)$ to nonintegers must be differentiable. This continuation of the $K^{(n)}$ to noninteger arguments is known as regularization [4,5,16,17]. We choose the representation of θ given by

$$\theta(x) = \lim_{\Delta \rightarrow 0^+} \theta_\Delta(x), \quad (8)$$

where, following [4,16,17],

$$\theta_\Delta(x) = \frac{\Delta}{a} \ln \left[\frac{\exp[(x+a)/\Delta] + 1}{\exp(x/\Delta) + 1} \right]. \quad (9)$$

The parameter a is the value of x below which $\theta(x)=0$ and must therefore satisfy $0 < a < 1$ in order to agree with the lattice rules; it is otherwise free at this stage. Δ is effectively a “smoothing” parameter, and θ_Δ is an analytic function of x at the origin for all $\Delta > 0$. More details may be found in [4].

In some cases, such as the Wolf-Villain model analyzed in [15], the lattice rules can be used to infer the value of a . Here, simple arguments [14] show that $a=0$ leads to a discontinuous (nonanalytic) dependence of $K^{(1)}(\mathbf{h})$ on \mathbf{h} ; this is against the spirit of the model, so $a \neq 0$. Unfortunately, the argument cannot fix the exact value; this must be determined by comparing the results of numerical integration of Eq. (6) to simulations of the lattice model. Accordingly, Fig. 2 shows a plot of w against t for $L=100$ with $q=1$ and $p=0$; results from a KMC simulation and numerical integration of the Langevin equations for each of $a=0.6, a=0.7$ and $a=0.8$ are presented. It is evident that $a \approx 0.7$ gives a result that agrees closely with the KMC simulation. To test this agreement in

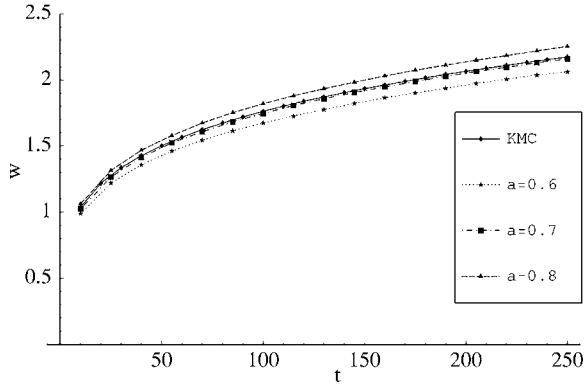


FIG. 3. Early-time behavior of the width for $L=1000$ and $q=p=0.5$. Both KMC and stochastic integration results averaged over 1000 runs.

the case $q=p=0.5$, we simulate a system of size $L=1000$; Fig. 3 shows the early-time behavior. It again shows that $a \approx 0.7$ gives the best agreement between KMC simulations and the stochastic formulation.

In conclusion, the system of discrete Langevin equations with the choice $a \approx 0.7$ gives quantitatively the same results as the original model.

V. THE CONTINUUM LIMIT

The continuum (coarse-grained) limit of the symmetric case $q=p$ may be taken using a simple *ad hoc* method, which is direct but physically opaque and cannot be extended to the asymmetric case. The DRG is necessary to analyze the full model; it is considerably more general and conceptually clear, but correspondingly more complicated to carry out. The analysis presented in this section confirms the results of symmetry arguments and constitutes the final step in the identification of the stochastic differential equation (SDE) corresponding to the RSOS model.

A. Ad hoc approach

Using the regularization of Sec. IV, the step functions may be expanded about $x=0$ as

$$\theta_{\Delta}(x) = \sum_{n=0}^{\infty} b_n(\Delta)x^n. \quad (10)$$

Replacing the set $h_i(t)$ by a function of a continuous argument x , $\phi(x,t)$ [which coincides with $h_i(t)$ for $x=i$], and expanding the discrete derivatives transforms the discrete set of SDEs of Eq. (6) into a (partial) stochastic differential equation for $\phi(x,t)$.

By using power counting arguments (see [14] for details), we find that the relevant terms in this equation are, at most,

$$\begin{aligned} \frac{\partial \phi}{\partial t} = & \nu_2 \frac{\partial^2 \phi}{\partial x^2} + \nu_4 \frac{\partial^4 \phi}{\partial x^4} + \nu_6 \frac{\partial^6 \phi}{\partial x^6} + \kappa_{13} \frac{\partial \phi}{\partial x} \frac{\partial^3 \phi}{\partial x^3} + \lambda_2 \left(\frac{\partial \phi}{\partial x} \right)^2 \\ & + \lambda_{13} \frac{\partial}{\partial x} \left(\frac{\partial \phi}{\partial x} \right)^3 + \kappa_{22} \left(\frac{\partial^2 \phi}{\partial x^2} \right)^2 + \sqrt{D} \eta, \end{aligned} \quad (11)$$

where η is Gaussian noise with unit variance and the coeffi-

icients may be found explicitly as functions of the b_n . The coefficients $\nu_2, \nu_4, \nu_6, \lambda_{13}$, and D are proportional to $q+p$, while the rest are proportional to $q-p$; this is consistent with arguments based on up and down reflection symmetry.

In the symmetric case $q=p$, the only surviving terms are given by $\nu_2=12\nu_4=360\nu_6=b_0b_1$, $\lambda_{13}=(3b_0b_3+b_1b_2)/3$, and $D=1$. The coefficients b_n may be found explicitly from Eq. (9). These satisfy the following inequality [19]:

$$b_n(\Delta) \leq \frac{A_n(\Delta)}{\Delta^{n-1}}, \quad (12)$$

where $A_n \rightarrow \text{const}$ as $\Delta \rightarrow 0^+$.

A simple scaling approach would involve rescaling space, time, and the field as $x \rightarrow \epsilon x$, $t \rightarrow \epsilon^z t$, and $\phi \rightarrow \epsilon^\alpha \phi$, respectively, followed by taking the limit $\epsilon \rightarrow 0^+$. Instead, following [4,16], we will take the two limits $\epsilon \rightarrow 0$ and $\Delta \rightarrow 0$ together. Setting $\Delta = \epsilon^\delta$, with $\delta > 0$ to be determined, the limit $\epsilon \rightarrow 0^+$ is well-defined only if $z=2$, $\alpha=1/2$, and $\delta=1/2$. The space-time scaling is diffusive (EW), while the value of δ has no direct physical significance. At the limit, the only surviving terms are the ν_2 term and the noise; all the others vanish. We therefore conclude that the coarse-grained limit of the symmetric RSOS model is the EW equation [20].

Unfortunately, this direct coarse-graining procedure cannot be applied to the asymmetric case. In the next section, both the symmetric and asymmetric version of the model are studied using DRG arguments.

B. Dynamic renormalization group

An equation corresponding to the limit of Eq. (11) for $q=p$ has previously been analyzed by das Sarma and Kotlyar [18]; however, the DRG flow equation for λ_{13} is not derived in Ref. [18].

For this section, Eq. (11) will be generalized to d dimensions in the obvious way. Defining $K_d = S_d / (2\pi)^d$, $S_d = 2\pi^{d/2} / \Gamma(d/2)$, and $g = \lambda_{13} D / \nu_2^2$, we find, to first order in g (which plays the role of an effective coupling constant),

$$\frac{d\nu_2}{dl} = \nu_2 \left(z - 2 + \frac{1}{2} g K_d \frac{d+2}{d} \right), \quad (13a)$$

$$\frac{d\lambda_{13}}{dl} = \lambda_{13} \left(2\alpha + z - 4 - \frac{1}{2} g K_d \frac{d^2 + 6d + 20}{d(d+2)} \right), \quad (13b)$$

$$\frac{dD}{dl} = D(z - d - 2\alpha) \quad (13c)$$

(the nonrenormalization of D is a well-known consequence of the fact that the deterministic part of the equation is conservative). The flow equation for g is given by

$$\frac{dg}{dl} = -g \left(d + g \frac{K_d}{2d(d+2)} (3d^2 + 14d + 28) \right). \quad (14)$$

For any positive $g(l=0)$ (which is the case here [14]), $g=0$ is an attractive fixed point [21]. This fixed point

corresponds to $z=2$ and $\alpha=(2-d)/2$, with $\lambda_{13}=0$, that is, it is the fixed point of the EW universality class, in agreement with the *ad hoc* approach of the previous section (as well as symmetry arguments and computer simulations).

Application of the full machinery of the DRG to Eq. (11)

is unnecessary because definite conclusions may be reached by inspection of the equation. In terms of the Fourier transform of $\phi(x,t)$, which we denote by the same symbol $\phi(\mathbf{k},\omega)$, Eq. (11) (generalized to d dimensions) becomes

$$G_0(\mathbf{k},\omega)\phi(\mathbf{k}) = \eta(\mathbf{k},\omega) + \int_{\mathbf{q},\Omega} M_2(\mathbf{q},\mathbf{k}-\mathbf{q})\phi(\mathbf{q})\phi(\mathbf{k}-\mathbf{q}) + \int_{\mathbf{q},\mathbf{q}',\Omega'} [M_3(\mathbf{k},\mathbf{k}-\mathbf{q}-\mathbf{q}',\mathbf{q},\mathbf{q}')\phi(\mathbf{q})\phi(\mathbf{q}')\phi(\mathbf{k}-\mathbf{q}-\mathbf{q}')], \quad (15)$$

where the argument ω has been suppressed for ϕ , the bare response function is

$$G_0(\mathbf{k},\omega) = \nu_2 k^2 - \nu_4 k^4 + \nu_6 k^6 - i\omega,$$

and the two vertices are

$$M_3(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4) = \lambda_{13}[\mathbf{k}_1 \cdot \mathbf{k}_4][\mathbf{k}_2 \cdot \mathbf{k}_3] \quad (16)$$

and

$$M_2(\mathbf{k}_1,\mathbf{k}_2) = -\lambda_2(\mathbf{k}_1 \cdot \mathbf{k}_2) + \kappa_{22}(\mathbf{k}_1)^2(\mathbf{k}_2)^2 + \frac{1}{2}\kappa_{13}(\mathbf{k}_1 \cdot \mathbf{k}_2) \times [(\mathbf{k}_1)^2 + (\mathbf{k}_2)^2]. \quad (17)$$

In the long-wavelength limit $k \rightarrow 0$ the 2-vertex of Eq. (17) will be dominated by the λ_2 (KPZ) term, with the κ_{ij} terms playing the role of higher-order corrections. Similarly, the 3-vertex is of higher order than the KPZ term; in addition, it has been shown to be irrelevant previously. Therefore, the KPZ term λ_2 determines the universality class of the model.

Since $\lambda_2, \kappa_{ij} \propto (q-p)$, if $q=p$ then $M_2=0$ initially. If only vertices with an odd number of legs are present in the bare (unrenormalized) equation, then vertices with an even number of vertices cannot be produced under renormalization. Therefore, if $q=p$ the KPZ term is not present and the coarse-grained dynamics of the system is described by the EW equation. If $q \neq p$, the dynamics is described by the KPZ equation. This result is consistent with symmetry arguments and simulation results [14].

VI. SUMMARY

We have implemented a procedure suggested by Vvedensky (and in more general terms by Anderson [10]) to obtain macroscopic equations from microscopic models.

Discrete Langevin equations are first derived and numerically integrated; they are found to be in quantitative agreement with KMC simulations of the underlying model. Next, these equations are expanded, leading to a continuum Langevin equation, from which it is shown that the coarse-grained description of the model is the KPZ equation with the coefficient of the nonlinear term λ_2 vanishing in the symmetric case, so that the EW equation is obtained. The coefficients appearing in the equation are well-defined in the coarse-grained limit.

The advantage of this procedure over the identification of the universality class by direct determination of the exponents from simulations is that slow convergence to the asymptotic regime is not a problem. In addition, the DRG approach allows, in principle, investigation of crossover effects (although this has not been pursued here). Application of this procedure to other models would be a fruitful area for the future.

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- [1] T. Halpin-Healey and Y.-C. Zhang, *Phys. Rep.* **254**, 215 (1995).
- [2] A.-L. Barabási and H. E. Stanley *Fractal Concepts in Surface Growth* (Cambridge University Press, Cambridge, 1995).
- [3] M. Kotrla and P. Smilauer, *Phys. Rev. B* **53**, 13777 (1996).
- [4] D. D. Vvedensky, *Phys. Rev. E* **67**, 025102(R) (2003).
- [5] D. D. Vvedensky, A. Zangwill, C. N. Luse, and M. R. Wilby, *Phys. Rev. E* **48**, 852 (1993).

- [6] N. G. van Kampen, *Stochastic Processes in Physics and Chemistry* (North Holland, Amsterdam, 1992).
- [7] R. F. Fox and J. Keizer, *Phys. Rev. A* **43**, 1709 (1991).
- [8] D. Forster, D. R. Nelson, and M. J. Stephen, *Phys. Rev. A* **16**, 732 (1977).
- [9] M. Kardar, G. Parisi, and Y.-C. Zhang, *Phys. Rev. Lett.* **56**, 889 (1986).
- [10] P. W. Anderson, *Basic Notions of Condensed Matter Physics*

- (Benjamin, Cummings, CA, 1984), p. 212.
- [11] J. M. Kim and J. M. Kosterlitz, *Phys. Rev. Lett.* **62**, 2289 (1989).
- [12] H. Hinrichsen, R. Livi, D. Mukamel, and A. Politi, *Phys. Rev. Lett.* **79**, 2710 (1997).
- [13] K. Park and B. N. Kahng, *Phys. Rev. E* **51**, 796 (1995).
- [14] A. Lazarides, Ph.D. thesis, Department of Mathematics, Imperial College London, 2005 (unpublished).
- [15] Alvin L.-S. Chua, C. A. Haselwandter, C. Baggio, and D. D. Vvedensky, *Phys. Rev. E* **72**, 051103 (2005).
- [16] D. D. Vvedensky, *Phys. Rev. E* **68**, 010601(R) (2003).
- [17] T. Nagatani, *Phys. Rev. E* **58**, 700 (1998).
- [18] S. Das Sarma and R. Kotlyar, *Phys. Rev. E* **50**, R4275 (1994).
- [19] This may be verified by direct inspection of the first few coefficients; unfortunately, we have not found a convenient closed-form expression for b_n allowing a direct verification. However, the conjecture is supported to at least $n=18$ by explicit calculation of the b_n [14].
- [20] It is important that the value of δ is uniquely fixed, and that the resulting coarse-grained equation does not depend on this value. Another crucial point is that the terms neglected in Eq. (11) may also be shown to vanish in the limit. For a detailed discussion of these points, see [14].
- [21] There exists also a repulsive fixed point for $g < 0$; however, this is irrelevant for the model in question because initially $g > 0$. Furthermore, as pointed out to the author by Bray, had the initial λ_{13} been negative, the model would not have been well-defined.