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Crossover and universality in the Wolf-Villain model

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The transition rules of the Wolf-Villain model for the deposition and instantaneous relaxation of particles on a lattice are expressed as a Langevin equation for the height fluctuations at each site. A coarse-graining transformation of this equation shows directly that this model belongs to the Edwards-Wilkinson universality class, in agreement with kinetic Monte Carlo simulations. The crossover from the Mullins-Herring equation is explained by the transformation under coarse graining of the coefficients in the equation of motion.

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The widespread application of lattice models to epitaxial kinetics [1–3] has fostered a huge literature on the statistical mechanics of growth fronts [4–6]. A central concern in this work is the identification of scaling regimes at long length and time scales and their assignment to universality classes [4]. Such studies are typically based either on kinetic Monte Carlo (KMC) simulations of lattice rules or on a renormalization-group analysis of a Langevin equation deemed to capture the coarse-grained evolution of the front. However, simulation requirements can be considerable if crossover effects are to be eliminated, and the renormalization-group method suffers from there being no systematic way of obtaining a Langevin equation from the rules of a lattice model.

In this paper, we examine the coarse graining of the Wolf-Villain model [7] for the deposition and instantaneous relaxation of particles on a lattice. First introduced for the low-temperature growth of group-IV materials [8], this model has been the subject of many studies [9–19]. KMC simulations show a slow crossover to the Edwards-Wilkinson universality class [9–11,15,16], a conclusion supported by arguments based on surface diffusion currents [12]. Attempts at a direct demonstration of this result by coarse graining the lattice Langevin equation [17–20] have relied on *ad hoc* regularizations of the step functions in the transition rules. The resulting analysis is thereby purely formal, which preempts any meaningful discussion about crossover and universality. In contrast, the method presented here produces a regular continuum limit, so we are able to show explicitly that the Wolf-Villain model belongs to the Edwards-Wilkinson universality class. Moreover, the transformation under coarse graining of the coefficients in the equation of motion explains the crossover from the Mullins-Herring equation observed in simulations.

We consider a one-dimensional lattice onto which particles are deposited randomly. The deposition rate is taken as the unit of time. In the Wolf-Villain model [7,8], an arriving particle remains on the original (randomly chosen) site only if its coordination (the number of nearest neighbors) cannot be increased by moving to a nearest neighbor site. If only one nearest neighbor site offers greater coordination than the original site, deposition is onto that site. However, if both nearest neighbor sites offer greater coordination than the original site, the deposition site is chosen randomly between the two. The equation of motion for the height h_i at site i is [20]

$$\frac{dh_i}{d\tau} = [w_i^{(1)} + w_{i+1}^{(2)} + w_{i-1}^{(3)}] + \eta_i , \tag{1}$$

in which the $w_i^{(j)}$ are transition probabilities for a particle incident on site i to remain there ($j=1$), to relax to site $i-1$ ($j=2$), or to relax to site $i+1$ ($j=3$), with

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

and the η_i are Gaussian noises that have mean zero and covariance

$$\langle \eta_i(\tau)\, \eta_j(\tau') \rangle = [w_i^{(1)} + w_{i+1}^{(2)} + w_{i-1}^{(3)}]\, \delta_{ij}\, \delta(\tau - \tau'). \tag{3}$$

The $w_i^{(j)}$ are obtained by applying the relaxation rules to local height configurations. Since these rules are based on coordination, we must include sites out to the second-nearest neighbors of the original site. The required configurations can be tabulated by using the step function

$$\theta(x) = \begin{cases} 1 & \text{if } x \geqslant 0 \\ 0 & \text{if } x < 0 \end{cases} \tag{4}$$

to express the pertinent relative heights between nearest neighbors as an identity:

$$\begin{aligned} &[\theta(h_{i-1} - h_{i-2}) + \Theta(h_{i-1} - h_{i-2})][\delta(h_i, h_{i-1}) \\ &\quad + \Theta(h_{i-1} - h_i) + \Theta(h_i - h_{i-1})][\delta(h_i, h_{i+1}) \\ &\quad + \Theta(h_i - h_{i+1}) + \Theta(h_{i+1} - h_i)][\theta(h_{i+1} - h_{i+2}) \\ &\quad + \Theta(h_{i+1} - h_{i+2})] = 1, \end{aligned} \tag{5}$$

where

$$\Theta(h_i - h_j) = 1 - \theta(h_i - h_j) \tag{6}$$

and

$$\delta(h_i, h_j) = \theta(h_i - h_j) + \theta(h_j - h_i) - 1 \tag{7}$$

is the Kronecker delta. The functions in Eq. (5) test whether $h_i = h_j$, by $\delta(h_i, h_j)$, $h_i \geqslant h_j$, by $\theta(h_i - h_j)$, or $h_i < h_j$, by $\Theta(h_i - h_j)$. The expansion of Eq. (5) produces 36 configurations, each of which is assigned to one of the $w_i^{(j)}$ by the relaxation rules, so Eq. (2) is satisfied by construction. The configurations for $w_i^{(1)}$ are shown in Fig. 1, those for $w_i^{(2)}$ in

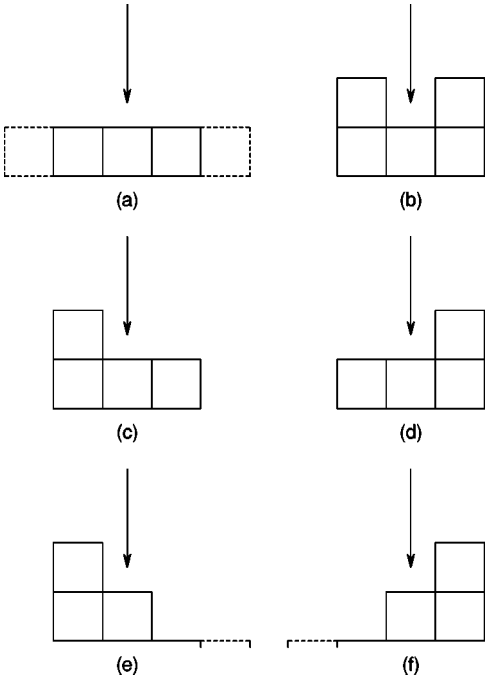

FIG. 1. The local configurations that contribute to $w_i^{(1)}$. The arrow indicates an atom incident on the ith site. Column heights strictly greater than and strictly equal to h_i are as indicated, while those less than or equal to h_i are indicated by broken lines.

Fig. 2, and those for $w_i^{(3)}$ are mirror images about the central (ith) site of the configurations in Fig. 2.

The step functions in Eqs. (5) present a major obstacle for coarse graining the equations of motion (1). We have addressed this issue [21] by using the following representation of $\theta(x)$:

$$\theta(x) = \lim_{\Delta \to 0^+} \left\{ \frac{\Delta}{a} \ln \left[\frac{e^{(x+a)/\Delta}+1}{e^{x/\Delta}+1} \right] \right\}, \tag{8}$$

where $0 < a \leqslant 1$. The Taylor series of the regularized form of θ is

$$\theta(x) = A + \frac{Bx}{2a} - \frac{B^2x^2}{8a\Delta} - \frac{Cx^3}{6a\Delta^2} + \cdots, \tag{9}$$

where

$$A \equiv \frac{\Delta}{a} \ln[\tfrac{1}{2}(1+e^{a/\Delta})], \tag{10}$$

$$B \equiv \frac{e^{a/\Delta}-1}{e^{a/\Delta}+1}, \tag{11}$$

$$C \equiv \frac{e^{a/\Delta}(e^{a/\Delta}-1)}{(e^{a/\Delta}+1)^3}. \tag{12}$$

As $\Delta \to 0^+$, $A \to 1$, $B \to 1$, and $C \to 0$, with

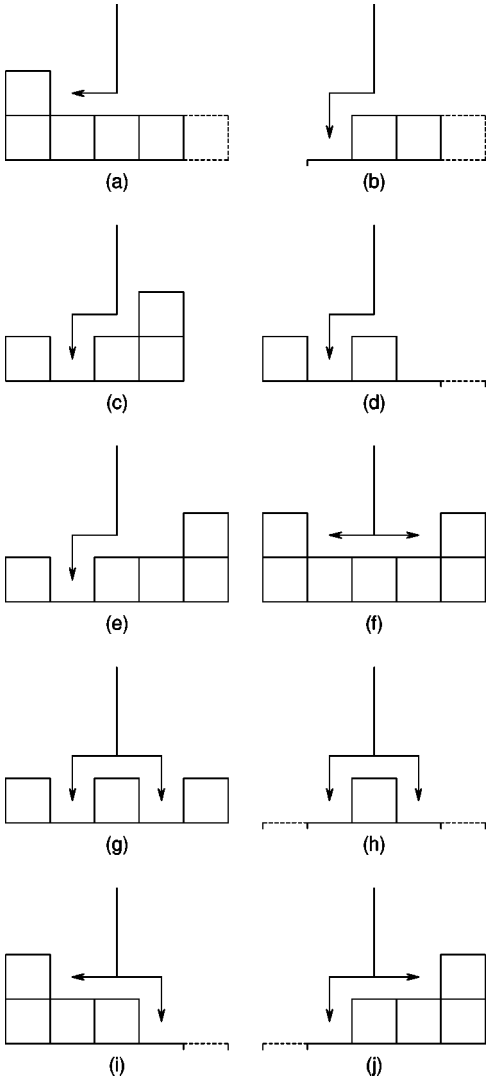

FIG. 2. The local configurations that contribute to $w_i^{(2)}$. The arrow indicates the deposition site for an atom incident on the ith site. Where more than one such site is indicated, both choices are equally likely. Column heights strictly greater than and strictly equal to h_i are as indicated, while those less than or equal to h_i are indicated by broken lines.

$$A = 1 - \frac{\Delta}{a} \ln 2 + \cdots. \tag{13}$$

Note that the first two terms in the expansion of θ are *finite* as $\Delta \to 0$, with $A = \theta(0)$, and

$$\frac{1}{2a} \lim_{\Delta \to 0^+} B = \tfrac{1}{2} \left[\lim_{x \to 0^-} \left(\frac{d\theta}{dx} \right) + \lim_{x \to 0^+} \left(\frac{d\theta}{dx} \right) \right] \tag{14}$$

is the average of the left-hand and right-hand derivatives of θ at $x = 0$. The regularization in Eq. (8) exploits the fact that θ is required only at the discrete values $h_{i\pm1} - h_i$, so we have chosen an interpolation between these points that yields a *continuous* function.

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

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

where z is to be determined and ϵ is the coarse-graining parameter: $\epsilon = 1$ corresponds to the smoothed lattice model and $\epsilon \to 0$ to the continuum limit. The coarse-grained height function u is

$$u(x,t) = \epsilon^\alpha (h_i - \tau), \tag{16}$$

where τ is the average growth rate and α is to be determined. Upon applying these transformations and the expansion in Eq. (9) to Eqs. (1) and (3), we obtain the following leading terms in the equation of motion:

$$\epsilon^{z-\alpha}\frac{\partial u}{\partial t} = \nu\epsilon^{2-\alpha}\frac{\partial^2 u}{\partial x^2} + \lambda_1\epsilon^{4-2\alpha}\frac{\partial^2}{\partial x^2}\left(\frac{\partial u}{\partial x}\right)^2 + \lambda_2\epsilon^{4-3\alpha}\frac{\partial}{\partial x}\left(\frac{\partial h}{\partial x}\right)^3 + K\epsilon^{4-\alpha}\frac{\partial^4 u}{\partial x^4} + \epsilon^{(1+z)/2}\xi, \tag{17}$$

where

$$\nu = \frac{B}{a^4}(2A-a)(A-a)^2, \tag{18}$$

$$\lambda_1 = \frac{B^2}{4a^4}(a^2+2aA-4A^2) + \frac{B^2}{4a^4\Delta} \times (4A^3-8aA^2+5a^2A-2a^3), \tag{19}$$

$$\lambda_2 = -\frac{B^3}{4a^4}(2A-a) - \frac{B^3}{4a^4\Delta}(3A-2a)(A-a) - \frac{C}{3a^4\Delta^2}(2A-a)(A-a)^2, \tag{20}$$

$$K = \frac{B}{12a^4}(44A^3-95aA^2+64a^2A-19a^3), \tag{21}$$

and ξ is a Gaussian noise with mean zero and covariance

$$\langle \xi(x,t)\xi(x',t')\rangle = \delta(x-x')\delta(t-t'). \tag{22}$$

There are two key considerations for taking the continuum limit of Eq. (17). The first is that, to obtain bounded coefficients, we take the limit $\Delta \to 0^+$ in Eq. (8) *together* with the continuum limit $\epsilon \to 0^+$ [21,22]. Accordingly, we set $\Delta = \epsilon^\delta$, where $\delta > 0$ can be chosen at our convenience. The second concerns the magnitudes of the coefficients as $\epsilon \to 0^+$. There are two cases: $a \neq 1$ and $a = 1$. If $a \in (0,1)$, then as $\epsilon \to 0^+$, the leading terms in the coefficients in Eqs. (18)–(21) are

$$\nu = \frac{1}{a^4}(2-a)(1-a)^2 + O(\Delta), \tag{23}$$

$$\lambda_1 = \frac{1}{4a^4\Delta}(4-8a+5a^2-2a^3) + O(1), \tag{24}$$

$$\lambda_2 = -\frac{1}{4a^4\Delta}(3-2a)(1-a) + O(1), \tag{25}$$

$$K = \frac{1}{12a^4}(44-95a+64a^2-19a^3) + O(\Delta). \tag{26}$$

If $a = 1$, Eqs. (24) and (26) remain valid, but Eqs. (23) and (25) are replaced by

$$\nu = (\Delta \ln 2)^2, \tag{27}$$

$$\lambda_2 = -\frac{1}{4}(1-\ln 2) + O(\Delta). \tag{28}$$

The most direct approach to the continuum limit is obtained for $0 < a < 1$, and by requiring (i) that u_t, u_{xx}, and ξ have the same scaling dimensions and (ii) that these are the dominant terms as $\epsilon \to 0$. Condition (i) necessitates setting $z = 2$ and $\alpha = \frac{1}{2}$, while (ii) requires that $0 < \delta < 1$, so that the term $(u_x^3)_x$ does not become more relevant than these other terms solely as a result of coarse graining. Then, in the limit $\epsilon \to 0^+$, we obtain the Edwards-Wilkinson [23] equation:

$$\frac{\partial u}{\partial t} = \nu_0\frac{\partial^2 u}{\partial x^2} + \xi, \tag{29}$$

with

$$\nu_0 = \frac{1}{a^4}(2-a)(1-a)^2. \tag{30}$$

Since the values of z and α are also those of the Edwards-Wilkinson model [4], our procedure demonstrates that the Wolf-Villain model belongs to this universality class.

The Edwards-Wilkinson can also be obtained for $a = 1$, in which case $\nu_0 = (\ln 2)^2$. We must now choose δ in the range $(0, \frac{1}{4})$ to ensure that the dominant terms remain u_t, u_{xx}, and ξ. The corresponding values of α and z, $z = 2 + 2\delta$ and $\alpha = \frac{1}{2} + \delta$, have an explicit dependence on δ. Therefore, we regard this as an anomalous special case that we exclude from further discussions.

The transformation of the coefficients under coarse graining can be used to examine the crossover to the Edwards-Wilkinson universality class. We first observe that for $0 < a < 1$, $\nu > 0$, and $\lambda_2 < 0$, while $K < 0$ only for $1 > a \geq a_K \equiv 0.774\,03\ldots$ and $\lambda_1 < 0$ only for $1 > a \geq 0.741\,94\ldots$; for other values of a, K and λ_2 may be positive, negative, or change sign as a function of ϵ. Thus, to avoid introducing unstable behavior purely as a result of an inappropriate choice of coarse-graining parameters, we will restrict a to the interval $(a_K, 1)$.

In Fig. 3, we show $\nu\epsilon^{2-\alpha}$, $\lambda_1\epsilon^{4-2\alpha}$, $K\epsilon^{4-\alpha}$, and $\lambda_2\epsilon^{4-3\alpha}$, with $\alpha = \frac{1}{2}$ and $\delta = \frac{1}{2}$, as a function of ϵ for $a \in (a_K, 1)$. For $\epsilon = 1$, the magnitude of K is greater than those of ν and λ_2 by more than an order of magnitude, and greater than that of λ_1 by at least a factor of 6. Thus, the equation of motion for $\epsilon = 1$, which corresponds to a smoothed lattice

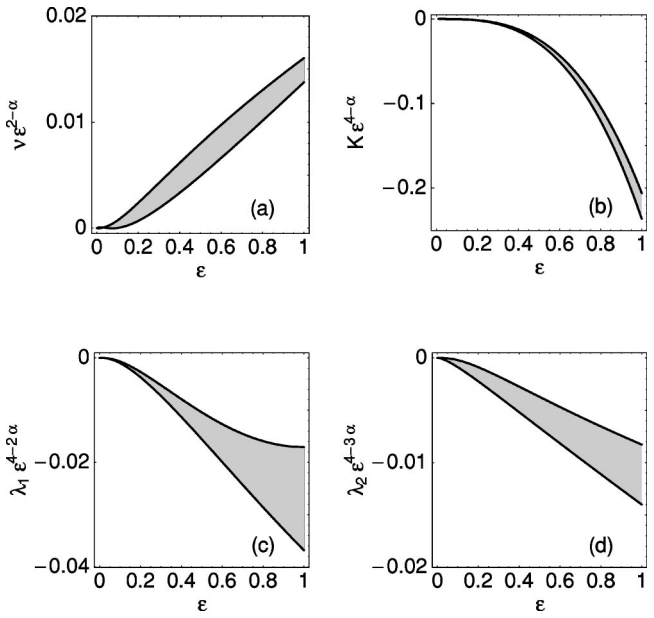

FIG. 3. The transformation of the coefficients in Eq. (17) under coarse graining. The shaded region indicates the values of these coefficients for $a \in (a_K,1)$, which guarantees that $K<0$ and $\lambda_1 <0$. In each panel, the upper curve corresponds to $a=1$ and the lower curve to $a=a_K$.

model, but with no coarse graining, is given approximately by the stochastic Mullins-Herring equation [24,25]:

$$\frac{\partial h}{\partial t} = K_0 \frac{\partial^4 h}{\partial x^4} + \xi, \tag{31}$$

where $K_0 \approx -0.2$. This result has been known for some time from simulations [7], but our analytic discussion provides additional confidence that our method captures the essential features of this model at the two extremes of coarse graining.

Simulations [9] also observe an intermediate crossover to the Villain-Lai-Das Sarma [26,27] equation prior to the final crossover to the Edwards-Wilkinson universality class. Within the framework of our analysis, this situation can arise from the compensating effects of negative λ_2 and positive ν. In fact, if we are in a regime where the propagator of the model is determined by u_{xxxx}, rather than u_{xx}, dynamical renormalization-group calculations [28] support this scenario. However, a more detailed analysis is required to establish a firm conclusion.

In summary, we have used a coarse-graining method to show that, at short length and time scales, the Wolf-Villain model is approximately described by the Mullins-Herring equation, and that, at long length and time scales, the universality class is that of the Edwards-Wilkinson model. Our method is quite general and can be applied in higher spatial dimensions. Indeed, the rich variety of phenomena seen in simulations of the Wolf-Villain model on higher-dimensional substrates [9,11] presents an inviting challenge to our method. Taking a broader perspective, if a direct coarse-graining transformation is not suitable, our method can be used to generate an equation of motion as the initial condition for a subsequent renormalization group analysis. This will provide the basis for an understanding of conservative nonlinear growth models as the natural expression of particular atomistic processes.

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