Emergence of step flow from atomistic scheme of epitaxial growth in 1+1 dimensions

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The Burton-Cabrera-Frank (BCF) model for the flow of line defects (steps) on crystal surfaces has offered useful insights into nanostructure evolution. This model has rested on phenomenological grounds. Our goal is to show via scaling arguments the *emergence* of the BCF theory for non-interacting steps *from a stochastic atomistic scheme* of a simplified kinetic solid-on-solid model in one spatial dimension. Our main assumptions are: adsorbed atoms (adatoms) form a dilute system, and elastic effects of the crystal lattice are absent. The step edge is treated as a front that propagates via probabilistic rules for atom attachment and detachment at the step. We formally derive a quasistatic step flow description by averaging out the stochastic scheme when terrace diffusion, adatom desorption and deposition from above are present.

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I. INTRODUCTION

The design and fabrication of optoelectronic devices rely on understanding how crystalline features evolve across several length scales, from a few nanometers to hundreds of microns. At low enough temperatures, below the roughening transition, crystal surface structures evolve through the collective motion of line defects, steps [1, 2]. The motion of individual steps is a mesoscale phenomenon: On the one hand, it manifests defects of *atomic* size; on the other hand, steps appear to move in a *continuum* fashion by exchanging mass with nanoscale regions, terraces. For the description of crystal surface dynamics in a wide range of length and time scales, it is thus useful to explore the validity and applicability of mesoscale models for step flow. These models capture atomistic features in the direction vertical to the high-symmetry plane of the crystal, while retaining the advantages of continuum theories in the lateral directions.

Such a hybrid approach is the Burton-Cabrera-Frank (BCF) model [3]; for reviews, see, e.g., [1, 2]. In this model, step edges are represented by moving smooth curves, which are boundaries of terraces. The step motion is mediated by the continuous diffusion of adsorbed atoms (adatoms). A typical BCF-type description consists of the following [1, 2]: (i) a step velocity law; (ii) the diffusion equation for the adatom density on each terrace; and (iii) a linear kinetic relation, which is a Robin-type boundary condition involving the adatom flux normal to each step edge and forms an extension of the Dirichlet-type boundary condition for the adatom density in [3]. The motion laws for steps have been conceived primarily through a phenomenological framework by invoking the principles of mass conservation and local thermodynamic equilibrium. An issue is how this mesoscale picture can firmly be linked to fundamental atomistic processes.

In this paper, we present a stochastic scheme adopted from a simplified kinetic solid-on-solid (SOS) model [4] for the hopping of atoms on a stepped surface in 1+1 dimensions in the absence of elastic effects. We derive the entire BCF description for the flow of steps as a *scaling limit* of averaged equations from the atomistic model. First, we analyze an epitaxial system with a single step in the presence of external material deposition and desorption; and then extend our analysis to many steps. Our main assumption is that the adatoms are non-interacting and form a *dilute* system; on average, only a small number of adatoms occupy each lattice site at any given time. This diluteness has been observed experimentally [5], and simplifies the governing atomistic laws.

Our present approach is inspired by recent efforts to shed light on the nature of the BCF theory [6, 7]; see also [8–10]. It is tempting to explore whether the BCF model can be interpreted as the universal, in some appropriate sense, limit of fundamental atomistic processes at the mesoscale. Adopting a line of investigation that favors this view, we invoke basic mechanisms of atomistic motion in the presence of steps; these include generic local rules for the atom attachment/detachment at a step edge. Our hypotheses lead to a linear kinetic relation for the mesoscale adatom flux, which serves as a Robin-type boundary condition for the adatom diffusion on terraces [2]. The derivation of this relation from scaling arguments applied to an atomistic theory of crystal growth is one of our main achievements with this work.

This study is motivated by the broader question how to develop mesoscale models for far-from-equilibrium processes. A long-term objective is to construct by purely atomistic principles mesoscale theories for kinetic regimes far from thermodynamic equilibrium (for some related phenomenological models, see [11–14]). This task remains an open challenge.

A few comments on past works [6–10, 15] with a similar perspective are in order. In [6, 7], the starting point is a master equation for the probabilities of finding the system in atomistic configurations characterized by the total number, ℓ, of adatoms and their positions on a one-dimensional lattice; for every such configuration, the microscale step position at any given time is completely determined by this ℓ. The mesoscale motion of the step comes from the ensemble average of this microscale variable. In this setting, the entire BCF-type description for the one-step flow emerges as the low-density limit of the adatom system [6]. This formalism is not directly extensible to two spatial dimensions (2D). In [8], the authors connect atomistic rates to BCF-type parameters via balancing out discrete and continuum fluxes at the step edge in $1D$, without invoking a stochastic scheme or describing the effect of noise; their results are compatible with ours. On the other hand, the studies in [9, 10] concern geometries in 2D with focus on more particular aspects of step flow. For example, in [9] the step position is held fixed; and in [10] only numerical comparisons of kinetic Monte Carlo (KMC) simulations to the BCF model are pursued. Notably, in [15] the authors pursue the coarse-graining of a 2D master equation and reduce it to a Langevin-type description for continuous-in-time height columns by retaining discreteness in the lateral directions. We believe that a direct comparison of this last approach to the BCF theory is not compelling.

Our derivation of the BCF limit in this paper differs from the recent analysis of [6, 7] in several interrelated aspects. First, here we apply the hypothesis of a dilute adatom system, whereas in [6] the diluteness results as a special case, by neglect of multi-adatom states of the model. Second, we invoke a stochastic scheme, in contrast to the master-equation approach adopted in [6]. This, along with the diluteness hypothesis, presently enables us to include richer kinetic effects, namely, desorption and material deposition from above, and a larger number of steps with relative algebraic ease. Third, we introduce the step front position as an additional stochastic variable whose motion is *coupled* with the random number of adatoms per lattice site. We believe that this formalism is promising for 2D, where kinks play an important role [3]; this extension is the subject of work in progress. In the present work we resort to scaling arguments, thus offering a physically more transparent derivation of the step flow limit.

Our analysis here also reveals some details of the effect of stochastic noise on step motion as the lattice spacing approaches zero. In particular, we show that this noise tends to vanish; thus, the BCF-type description emerges in a regime where the law of large numbers is applicable.

Mathematically, our starting scheme is akin to a random choice method ("Glimm scheme") invented for solving certain systems of conservation laws such as those arising in gas dynamics [16, 17]. The main idea is to construct the appropriate solution (say, a shock wave) through a sequence of operations; these include a sampling scheme by use of a random variable that is uniformly distributed over a fixed interval. Here, our approach has a similar flavor but bears particularities tailored to the physics of epitaxial growth. The time-dependent random variable that we employ takes discrete values corresponding to the distinct events of advancement, retreat or immobility of the step edge as adatoms attach to the step, detach from it or move otherwise, respectively. These events have prescribed probabilities involving known atomistic rates subject to the principle of detailed balance in the sense of [12] (see Sec. II for details).

Our work has several limitations. These are mainly due to restricting attention to: dilute systems, non-interacting steps, and 1D. In particular, the possible emergence of force-dipole step-step interaction [18] may require the alteration of the stochastic scheme to take into account an elastic lattice with spontaneous stress [19]. We expect that the extension of our formalism to 2D would have to possibly involve a space-time stochastic noise driving step fluctuations on the lattice. The scaling analysis of non-dilute adatom systems poses a challenge currently under investigation.

The remainder of the paper is organized as follows. In Sec. II, we formulate the discrete stochastic scheme for a single step. In Sec. III, we formally derive the scaling limit of this scheme. In Sec. IV, we discuss implications and extensions of our analysis, particularly the presence of more than one steps. Section V concludes our work with a summary of our results and an outline of open problems. Throughout the paper, the expression $Q = \mathcal{O}(h)$ means that the quantity Q/h is bounded by a constant as a parameter approaches an extreme value. The bar on top of a symbol for a stochastic variable implies the mean value (expectation) of that variable.

II. ATOMISTIC SCHEME WITH ONE STEP

The single-step geometry in 1D is shown in Fig. 1. The step lies on a lattice of uniform spacing a and length $L = Na$ where $N \gg 1$. Since L constitutes a natural length of the BCF setting, we set $L = 1$; thus, $a = 1/N \ll 1$. The step position at time t can be tracked by $q(t)$, an integer-valued Lagrangian coordinate expressing the number of the lattice site located immediately to the right of the step edge [$q(t) = 0, 1, \ldots, N-1$]; this q is distinct from j, the Eulerian coordinate for the lattice site. Hence, the step edge position is determined through the discrete stochastic variable $X(t) = q(t)a$.

It is useful to distinguish the edge atom, which has only one in-plane nearest neighbor (to its left), from the step atom, which has two in-plane nearest neighbors while all atoms to its left also have two in-plane nearest neighbors (see Fig. 1). In contrast, an adatom is a movable particle that is neither an edge atom nor a step atom.

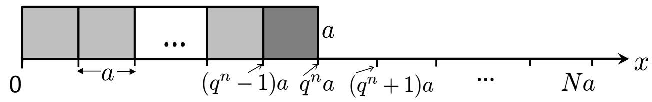

FIG. 1: Microscale view of a step edge at time $t = t_n$. The step has height a, an atomic length, and lies on a 1D lattice of spacing a and total length $L = Na$, where N is the total number of lattice sites ($N \gg 1$). The step position is determined by the lattice site $q^n = q(t_n)$ directly to the right of the edge ($q^n = 0, 1, \ldots N-1$). Notice that the step atoms (grey) of the upper terrace and the edge atom (dark grey) are represented by boxes; the atom position is indexed by the left side of each box, as indicated by arrows in the vicinity of the step. The Eulerian coordinate is $x = ja$ ($j = 0, \ldots N-1$).

A. Kinetic frame: Assumptions

To prescribe the adatom kinetics relative to the step edge, we apply the following main assumptions [7].

(i) An atom is only allowed to move horizontally, left or right, by one lattice site at any given time.

(ii) The adatoms are non-interacting and have low density, i.e., in the sense of some ensemble average, only a small average number of adatoms can occupy any lattice site at any given time. Therefore, it is unlikely that islands form and any height column may contain more than one adatom [see also (vi) below] [7].

(iii) An adatom can hop from a lattice site to an adjacent site of the same terrace with a probability proportional to the constant rate D. This rule gives rise to the usual, unbiased diffusion process as the result of a random walk [see Figs. 2(a), (b)].

(iv) An adatom from the upper ($-$) or lower ($+$) terrace attaches to the step edge and becomes an edge atom with probability proportional to the rate $D\phi_{\mp}$, where the nondimensional $\phi_{\pm}$ ($\phi_{\pm} \le 1$) is an Arrhenius factor accounting for the Ehrlich-Schwoebel barrier [1, 7, 20]; $\phi_{\pm} = e^{-E_{\pm}/T}$, $E_{\pm} > 0$, and T is the Boltzmann energy (absolute temperature). As a result, the step edge moves *forward* (to the right) by a distance equal to a [see Figs. 2(c), (d)].

(v) An edge atom can detach from a step, breaking a bond, become an adatom and hop to the upper ($-$) or lower ($+$) terrace with a probability proportional to $Dk\phi_{\mp}$, where $k = e^{-E_{\mathrm{b}}/T}$ and E_{b} is the edge-atom bond energy barrier, $E_{\mathrm{b}} > 0$. As a result, the step edge retreats (to the left) by distance a [see Figs. 2(e), (f)].

(vi) A step atom cannot become an adatom, or vice versa.

(vii) Only adatoms can evaporate from the surface.

(viii) Atoms deposited on the terrace from above instantly become adatoms.

Note that, within our atomistic model, steps can move only via rules (iv) and (v). By the above choice of kinetic rates at the step edge, detailed balance is satisfied in the sense of [12, 21, 22]. This principle implies that at equilibrium the microscale adatom fluxes toward the step edge must vanish [12]. In particular, by setting $D^-_{\mathrm{TE}} = D\phi_-$, $D^+_{\mathrm{TE}} = D\phi_+$, $D^-_{\mathrm{ET}} = Dk\phi_-$ and $D^+_{\mathrm{ET}} = Dk\phi_+$, we note the relation

$$D^-_{\mathrm{TE}} D^+_{\mathrm{ET}} = D^+_{\mathrm{TE}} D^-_{\mathrm{ET}}.$$

In the special case of a simple cubic SOS model [12, 23], it is expected that $D^{\pm}_{\mathrm{TE}} = D$ and $D^+_{\mathrm{ET}} = D^-_{\mathrm{ET}}$; thus, $\phi_+ = \phi_- = 1$. This case is known to lead to a Dirichlet-type boundary condition at the step edge [1], which is *not* the focus of the present treatment. For a discussion on the magnitudes of D, $\phi_{\pm}$ and k, see Sec. III A.

Atoms are assumed to be deposited on the surface from above with constant flux f, which expresses number of atoms per unit time per lattice site, and can be evaporated with constant rate τ_{e}^{-1} where τ_{e} is a typical evaporation or desorption time. In addition, we introduce boundary conditions at $x = 0$ and $x = 1$ for definiteness. We consider a steady incoming flux, f_{in}, of adatoms from the left boundary, $x = 0$. Some of the incoming adatoms attach to the step so that the step moves forward; while some other adatoms leave the system from the right boundary, $x = 1$. Adatoms are not allowed to enter the prescribed spatial domain, $0 < x < 1$, from the right boundary or leave it from the left boundary. Note that our choice of conditions at the domain boundaries ($x = 0$, 1), is meant to form an example for definiteness; other choices are possible that do not distort the essential physics of step edge motion.

B. Stochastic scheme

Next, we formulate a discrete stochastic scheme for the (random) step front variable, $X(t)$, coupled with the (random) number, $\varrho_j(t)$, of adatoms at lattice site j ($j = 0, 1, \ldots, N-1$). By discretizing time, $t = t_n$, with a sufficiently small yet constant timestep, $\tau = t_{n+1} - t_n$, we describe how the step position, $X(t)$, varies with time. Now set $q^n = q(t_n)$, $\varrho^n_j = \varrho_j(t_n)$ and $X^n = X(t_n)$.

Consider the discrete random variable $\xi(t)$ that takes values in the set $\{-1, -2, 0, 1, 2\}$; $\xi^n = \xi(t_n)$. These integer values correspond to the possible atomistic events at $t = t_n$; see Fig. 2. In particular, regarding the motion of a step, $\xi^n = 1$ or 2 if an adatom attaches to the step from the upper or lower terrace, respectively; and $\xi^n = -1$ or -2 if the edge atom detaches toward the upper or lower terrace. Setting $\xi^n = 0$ amounts to processes that do not cause step motion for $t_n \le t < t_{n+1}$.

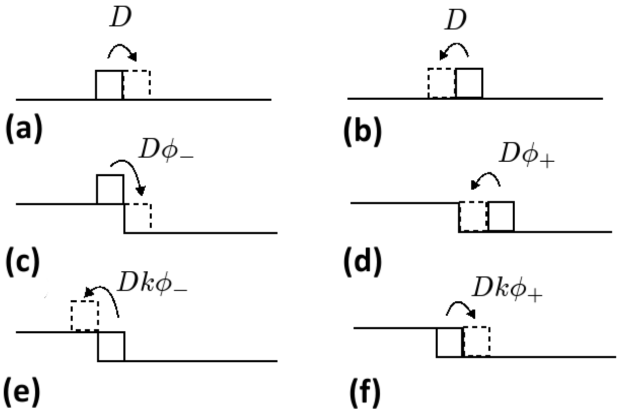

FIG. 2: Schematic of the basic atomistic processes of our model. *Upper panel* [(a), (b)]: Unbiased hopping of an adatom with constant rate D from a lattice site of a terrace to an adjacent site of the same terrace directly to the right [(a)] or left [(b)]. *Middle panel* [(c), (d)]: Attachment of an adatom to the step edge from the upper terrace with rate $D\phi_-$ [(c)], or the lower terrace with rate $D\phi_+$ [(d)]; the step edge moves to the right by one lattice spacing, a. *Lower panel* [(e), (f)]: Detachment of an edge atom from the step toward the upper terrace with rate $Dk\phi_-$ [(e)], or the lower terrace with rate $Dk\phi_+$ [(f)]; the step moves to the left by distance a.

Thus, the microscale step position is updated with time via the rule

$$X^{n+1} = \begin{cases} X^n & \text{if } \xi^n = 0, \\ X^n + a & \text{if } \xi^n = 1 \text{ or } 2, \\ X^n - a & \text{if } \xi^n = -1 \text{ or } -2. \end{cases} \tag{1}$$

We supplement this rule with the following probabilities:

$$\mathbb{P}(\xi^n = 1) = D\phi_- \tau \varrho^n_{q^n-1},\ \mathbb{P}(\xi^n = 2) = D\phi_+ \tau \varrho^n_{q^n+1},$$
$$\mathbb{P}(\xi^n = -1) = Dk\phi_- \tau,\ \mathbb{P}(\xi^n = -2) = Dk\phi_+ \tau, \tag{2}$$

which are mean-field expressions stemming from rules (iv) and (v) (Sec. II A). Note that the distribution of the random variable ξ^n in principle depends on the current position of the step edge and the local environment around it. Evidently,

$$\mathbb{P}(\xi^n = 0) = 1 - D\tau(\phi_- \varrho^n_{q^n-1} + \phi_+ \varrho^n_{q^n+1}) - D\tau k(\phi_- + \phi_+).$$

Given the above distribution of ξ^n, one can realize it from an independent, identically distributed random variable, uniformly distributed in some fixed interval (as is the common practice in KMC simulations).

It remains to prescribe the discrete scheme for ϱ^n_j. For lattice sites sufficiently away from the step edge, we have

$$\varrho^{n+1}_j = (1 - 2D\tau)\varrho^n_j + D\tau(\varrho^n_{j-1} + \varrho^n_{j+1}) - \frac{\tau}{\tau_{\mathrm{e}}}\varrho^n_j + \tau f,$$
$$j \neq 0,\ q^n - 2,\ q^n - 1,\ q^n,\ q^n + 1,\ N - 1, \tag{3}$$

which expresses the usual unbiased random walk on a lattice in the presence of desorption and external deposition. At the domain boundaries ($j = 0, N-1$), we additionally impose

$$\varrho^{n+1}_0 = (1 - D\tau)\varrho^n_0 + D\tau\varrho^n_1 + f_{\mathrm{in}}\tau - \frac{\tau}{\tau_{\mathrm{e}}}\varrho^n_0 + \tau f, \tag{4a}$$
$$\varrho^{n+1}_{N-1} = (1 - 2D\tau)\varrho^n_{N-1} + D\tau\varrho^n_{N-2} - \frac{\tau}{\tau_{\mathrm{e}}}\varrho^n_{N-1} + \tau f. \tag{4b}$$

For the remaining sites, sufficiently close to the step edge, the scheme reads

$$\varrho^{n+1}_{q^n-2} = (1 - 2D\tau)\varrho^n_{q^n-2} + D\tau(\varrho^n_{q^n-3} + \varrho^n_{q^n-1}) - \frac{\tau}{\tau_{\mathrm{e}}}\varrho_{q^n-2} + f\tau + \mathbb{1}(\xi^n = -1), \tag{5a}$$
$$\varrho^{n+1}_{q^n-1} = (1 - D\tau)\varrho^n_{q^n-1} + D\tau\varrho^n_{q^n-2} - \frac{\tau}{\tau_{\mathrm{e}}}\varrho^n_{q^n-1} + f\tau - \mathbb{1}(\xi^n = 1), \tag{5b}$$
$$\varrho^{n+1}_{q^n} = (1 - D\tau)\varrho^n_{q^n} + D\tau\varrho^n_{q^n+1} - \frac{\tau}{\tau_{\mathrm{e}}}\varrho^n_{q^n} + f\tau + \mathbb{1}(\xi^n = -2), \tag{5c}$$
$$\varrho^{n+1}_{q^n+1} = (1 - 2D\tau)\varrho^n_{q^n+1} + D\tau(\varrho^n_{q^n} + \varrho^n_{q^n+2}) - \frac{\tau}{\tau_{\mathrm{e}}}\varrho^n_{q^n+1} + f\tau - \mathbb{1}(\xi^n = 2). \tag{5d}$$

In the above, $\mathbb{1}(\cdot)$ is the indicator function, viz., $\mathbb{1}(\mathrm{A}) = 1$ if the event A occurs, and $\mathbb{1}(\mathrm{A}) = 0$ otherwise. Thus, the presence of this indicator in Eqs. (5) signifies the addition or removal of an adatom to/from the corresponding lattice site when the step edge moves.

A few specific remarks on the meaning of Eqs. (5) are in order; see also Fig. 2. By Eqs. (5a) and (5d) pertaining to sites $q^n - 2$ and $q^n + 1$, an adatom at these sites can either hop to or from any of the two adjacent sites with rate D [Figs. 2(a), (b)]; or evaporate with rate τ_{e}^{-1}; or be deposited from the vapor to the surface with rate f; or come from an atom detaching from the step edge [Eq. (5a) and Fig. 2(e)]; or attach to the step [Eq. (5d) and Fig. 2(d)]. In the same vein, in regard to Eqs. (5b) and (5c) for sites $q^n - 1$ and q^n, an adatom at these sites can either hop to or from the adjacent site of the same terrace with rate D; or evaporate; or be deposited from above; or attach to the step edge [Eq. (5b) and Fig. 2(c)]; or come from the detachment of the edge atom [Eq. (5c) and Fig. 2(f)].

C. Averaging of stochastic scheme

We now average out the governing stochastic laws of Sec. II B in the limit $\tau \to 0$ by keeping the spacing a fixed. To simplify the analysis, we henceforth apply the condition that $a \ll 1$ and take into account that, as argued in Sec. III B, the stochastic noise for the step position, $X(t)$, is negligible for small enough a. Therefore, we carry out the averaging procedure for the stochastic scheme involving the step position and adatom number in the regime where the law of large numbers holds, allowing the mean of $\varrho_q(t)$, where q is a stochastic variable, to be set approximately equal to $\bar{\varrho}_{\bar{q}}(t)$ [24].

By Eqs. (1) and (2), we obtain the expectation

$$\begin{aligned}\mathbb{E}[X^{n+1}-X^n] &= a\{\mathbb{P}(\xi^n = 1 \text{ or } 2) - \mathbb{P}(\xi^n = -1 \text{ or } -2)\}\\ &\approx Da\{(\phi_-\bar{\varrho}^n_{\bar{q}^n-1} + \phi_+\bar{\varrho}^n_{\bar{q}^n+1})\\ &\quad - k(\phi_- + \phi_+)\}\tau, \end{aligned}\tag{6}$$

where $\mathbb{E}[X] \equiv \bar{X}$. In the same vein, we compute the variance of $X^{n+1} - X^n$:

$$\begin{aligned}\mathbb{V}[X^{n+1}-X^n] &= Da^2\{(\phi_-\bar{\rho}_{\bar{q}-1} + \phi_+\bar{\rho}_{\bar{q}+1})\\ &\quad + k(\phi_- + \phi_+)\}\tau + \mathcal{O}(\tau^2).\end{aligned}\tag{7}$$

In the limit $\tau \to 0$, we thus derive a mean step velocity law at $t = t_n$ in terms of $\bar{\varrho}^n_j$ where j belongs to adjacent sites of the step edge:

$$\begin{aligned}\frac{dx_\mathrm{s}}{dt} &\equiv \lim_{\tau\to 0}\mathbb{E}\left[\frac{X^{n+1}-X^n}{\tau}\right]\\ &\approx a\{D(\phi_-\bar{\varrho}_{\bar{q}-1} + \phi_+\bar{\varrho}_{\bar{q}+1}) - Dk(\phi_- + \phi_+)\};\end{aligned}\tag{8}$$

here, $\bar{q} = \bar{q}(t)$ and $x_\mathrm{s}(t) = \bar{X}(t) = \bar{q}(t)a$.

Accordingly, as $\tau \to 0$ the heuristic limit of the mean of Eqs. (3) and (4), for $j \neq q-2, q-1, q, q+1$, reads

$$\frac{d\bar{\varrho}_j}{dt} = D(\bar{\varrho}_{j-1} - 2\bar{\varrho}_j + \bar{\varrho}_{j+1}) - \frac{1}{\tau_\mathrm{e}}\bar{\varrho}_j + f;\tag{9}$$

$$\frac{d\bar{\varrho}_0}{dt} = D(\bar{\varrho}_1 - \bar{\varrho}_0) + f_\mathrm{in} - \frac{1}{\tau_\mathrm{e}}\bar{\varrho}_0 + f,\tag{10a}$$

$$\frac{d\bar{\varrho}_{N-1}}{dt} = -2D\bar{\varrho}_{N-1} + D\bar{\varrho}_{N-2} - \frac{1}{\tau_\mathrm{e}}\bar{\varrho}_{N-1} + f.\tag{10b}$$

On the other hand, for lattice sites near the step edge, the scheme reads

$$\begin{aligned}\frac{\partial\bar{\varrho}_{\bar{q}-2}}{\partial t} &= D(\bar{\varrho}_{\bar{q}-3} - 2\bar{\varrho}_{\bar{q}-2} + \bar{\varrho}_{\bar{q}-1}) - \frac{1}{\tau_\mathrm{e}}\bar{\varrho}_{\bar{q}-2}\\ &\quad + f + Dk\phi_-,\end{aligned}\tag{11a}$$

$$\begin{aligned}\frac{\partial\bar{\varrho}_{\bar{q}-1}}{\partial t} &= D(\bar{\varrho}_{\bar{q}-2} - \bar{\varrho}_{\bar{q}-1}) - \frac{1}{\tau_\mathrm{e}}\bar{\varrho}_{\bar{q}-1} + f\\ &\quad - D\phi_-\bar{\varrho}_{\bar{q}-1},\end{aligned}\tag{11b}$$

$$\frac{\partial\bar{\varrho}_{\bar{q}}}{\partial t} = D(\bar{\varrho}_{\bar{q}+1} - \bar{\varrho}_{\bar{q}}) - \frac{1}{\tau_\mathrm{e}}\bar{\varrho}_{\bar{q}} + f + Dk\phi_+,\tag{11c}$$

$$\begin{aligned}\frac{\partial\bar{\varrho}_{\bar{q}+1}}{\partial t} &= D(\bar{\varrho}_{\bar{q}+2} - 2\bar{\varrho}_{\bar{q}+1} + \bar{\varrho}_{\bar{q}}) - \frac{1}{\tau_\mathrm{e}}\bar{\varrho}_{\bar{q}+1} + f\\ &\quad - D\phi_+\bar{\varrho}_{\bar{q}+1}.\end{aligned}\tag{11d}$$

Equations (9) and (11) are recast into the compact form

$$\begin{aligned}\frac{\partial\bar{\varrho}_j}{\partial t} &= D(\bar{\varrho}_{j-1} - 2\bar{\varrho}_j + \bar{\varrho}_{j+1}) - \frac{1}{\tau_\mathrm{e}}\bar{\varrho}_j + f\\ &\quad + Dk\phi_-\delta_{j,\bar{q}-2} + [D(\bar{\varrho}_{\bar{q}-1} - \bar{\varrho}_{\bar{q}}) - D\phi_-\bar{\varrho}_{\bar{q}-1}]\delta_{j,\bar{q}-1}\\ &\quad + [D(\bar{\varrho}_{\bar{q}} - \bar{\varrho}_{\bar{q}-1}) + Dk\phi_+]\delta_{j,\bar{q}} - D\phi_+\bar{\varrho}_{\bar{q}+1}\delta_{j,\bar{q}+1},\end{aligned}\tag{12}$$

in which $j \neq 0$, $N-1$ and $\delta_{i,j}$ denotes Kronecker's delta.

A few remarks on the mean motion laws are in order. Equation (8) couples the discrete mean step velocity law with the average adatom numbers on each side of the step. In the limit $a \to 0$, this coupling will give rise to a mass conservation statement involving the values of the adatom flux directly to the left and right of the edge (Sec. III). This flux can be determined via Eqs. (9)–(11), which pertain to the adatom diffusion and kinetic conditions at all the associated boundaries. To reduce the discrete equations to BCF-type laws, we need to appropriately scale variables and parameters of the problem with the system size, $N = a^{-1}$; and then take the limit $a \to 0$ by assuming that the adatom number per lattice site, ϱ_j, becomes a smooth function of coordinate $x = ja$ on the terrace, away from the step edge.

III. SCALING LIMIT AS $a \to 0$

In this section, we carry out the scaling limit of Eqs. (8)–(11) as $a \to 0$ by use of Eq. (12). For this purpose, we restrict attention to macroscopic times by defining

$$\tilde{t} = at, \quad \tilde{\tau}_\mathrm{e} = a\tau_\mathrm{e},\tag{13}$$

and the variable

$$\tilde{\rho}_j(\tilde{t}) = \bar{\varrho}_j(t)/a,\tag{14}$$

which plays the role of the adatom number density as $a \to 0$. In this vein, we consider $\tilde{t}, \tilde{\tau}_\mathrm{e} = \mathcal{O}(1)$ and $\tilde{\rho}_j = \mathcal{O}(1)$. For notational economy, we will drop the tildes and replace $\bar{q}$ by q from now on.

By Eq. (8), the mean step velocity law reads

$$\frac{dx_\mathrm{s}}{dt} = (r^-_\mathrm{a}\rho_{q-1} - r^-_\mathrm{d}) + (r^+_\mathrm{a}\rho_{q+1} - r^+_\mathrm{d}),\tag{15}$$

where both sides should be considered as $\mathcal{O}(1)$ quantities. In Eq. (15), the kinetic coefficients are defined by

$$r^\pm_\mathrm{d} = Dk\phi_\pm, \quad r^\pm_\mathrm{a} = D\phi_\pm a,\tag{16}$$

which serve the roles of mesoscopic detachment (d) and attachment (a) rates to the left ($-$) or right ($+$) of the step edge. Hence, it is reasonable to assume that, as $a \to 0$, the rates of Eqs. (16) are finite and independent of a (see Sec. III A). This assumption will enable us to recover the entire Robin-type boundary conditions at the step edge.

Thus, Eq. (12) for the adatom number density becomes

$$\begin{aligned}a\frac{\partial\rho_j}{\partial t} &= D(\rho_{j-1} - 2\rho_j + \rho_{j+1}) - \frac{1}{\tau_\mathrm{e}}\rho_j + fa^{-1}\\ &\quad + \{Da(\rho_q - \rho_{q-1})(\delta_{j,q} - \delta_{j,q-1})\\ &\quad + (r^+_\mathrm{d}\delta_{j,q} - r^+_\mathrm{a}\rho_{q+1}\delta_{j,q+1})\\ &\quad + (r^-_\mathrm{d}\delta_{j,q-2} - r^-_\mathrm{a}\rho_{q-1}\delta_{j,q+1})\}a^{-1},\end{aligned}\tag{17}$$

where $j = 1, \ldots, N-2$. A task is to express the right-hand side of Eq. (15) as a sum of adatom fluxes defined through the limit of Eq. (17). Note that Eqs. (10), suitably scaled, should additionally be imposed at the domain boundaries, $x = 0, 1$.

A. Scaling of atomistic rates

We now discuss the scaling of the kinetic parameters with a, by inspection of Eqs. (15)–(17). First, it is reasonable to set

$$\mathfrak{D} \equiv Da^2 = \mathcal{O}(1), \tag{18}$$

i.e., require that the rate D scale with the system size ($N = a^{-1}$) as $1/a^2 = N^2$. This $\mathfrak{D}$ expresses the usual macroscopic diffusivity resulting from a random walk on a lattice [25]. By Eqs. (10), (16) and (17), we also assume that

$$\phi_\pm = \mathcal{O}(a),\ k = \mathcal{O}(a),\ f = \mathcal{O}(a),\ f_{\rm in} = \mathcal{O}(1), \tag{19}$$

and define

$$F \equiv fa^{-1} = \mathcal{O}(1). \tag{20}$$

Equations (18) and (19) provide a set of conditions sufficient for deriving a kinetic relation for the adatom flux as a linear function of the adatom density at the step edge. Note that the parameters $\mathfrak{D}^{-1}f_{\rm in}$ and $\mathfrak{D}^{-1}F$ should be sufficiently small, consistent with our diluteness hypothesis.

We alert the reader that Eqs. (18) and (19) preclude $\phi_+ \approx 1$ or $\phi_- \approx 1$, a choice known to imply a Dirichlet boundary condition at the step edge [1]. This special case, which signifies the absence of an Ehrlich-Schwoebel barrier, is not strictly treated by our present asymptotics.

B. On limit of stochastic noise

It is worthwhile addressing the stochastic noise that underlies mean step velocity law (15). The stochastic differential equation for the step position variable, $X(t)$, can be written as

$$dX_t \approx c_{\rm s}\, dt + \sqrt{a} c_{\rm n}\, dW_t, \tag{21}$$

where $dt = t^{n+1} - t^n$, $dX_t = X^{n+1} - X^n$ and W_t is the Wiener process [25] so that $dW_t = W^{n+1} - W^n$ represents discrete "white noise". The $\mathcal{O}(1)$-quantities $c_{\rm s}$ and $c_{\rm n}$ come from the expectation $\mathbb{E}[dX_t]$ [Eq. (6)] and standard deviation $\sqrt{\mathbb{V}[dX_t]}$ [Eq. (7)] of $X^{n+1} - X^n$ as $dt \to 0$, under the definitions of Eqs. (13), (14), (18) and (19):

$$c_{\rm s} = r_{\rm a}^- \rho_{q-1} - r_{\rm d}^- + r_{\rm a}^+ \rho_{q+1} - r_{\rm d}^+,$$

$$c_{\rm n} = (r_{\rm a}^- \rho_{q-1} + r_{\rm d}^- + r_{\rm a}^+ \rho_{q+1} + r_{\rm d}^+)^{1/2}; \tag{22}$$

cf. Eq. (15).

Evidently, in the limit $a \to 0$ the term pertaining to white noise vanishes in Eq. (21), provided ρ_{q-1} and ρ_{q+1} approach finite values on each side of the step edge. This observation is not surprising, originating from the assumption that the step front can only move by $\pm a$ each time, which in turn causes a negligibly small variance of its random motion. Hence, in this regime, step motion can be viewed as a phenomenon in the context of the law of large numbers. It should be noted, however, that a stochastic mesoscale description, in which the noise is preserved as $a \to 0$, may result under different kinetics or scaling scenarios. This issue deserves to be the subject of future work.

C. Step flow limit

Next, we complement Eq. (15) by a description of the adatom number density, $\rho_j(t)$, as $a \to 0$. Suppose the step position is still denoted $x_{\rm s}(t)$ in this limit. By slightly abusing notation, we formally replace $\rho_j(t)$ by the $\mathcal{O}(1)$-function $\rho(t, x)$, assuming that this limit exists in some appropriate sense for $x = ja$ and $t > 0$, where $0 < x < 1$ with $x \neq x_{\rm s}(t)$; also, $\mathfrak{D}$, $r_{\rm d}^\pm$, $r_{\rm a}^\pm$, $\tau_{\rm e}$, and F should take their finite limiting values. In the following, we suppress the time dependence of $\rho(t, x)$ for algebraic convenience.

Consider Eq. (17). First, $a(\partial\rho_j/\partial t) \approx a[\partial\rho(t, x)/\partial t] \to 0$ for fixed time t, since $\partial\rho_j/\partial t$ is bounded. Second, it is tempting to replace the second-order difference term, $a^{-2}(\rho_{j+1} - 2\rho_j + \rho_{j-1})$, by the Laplacian of $\rho(x)$, $\Delta_x \rho$, for $x < x_{\rm st}$ and $x > x_{\rm st}$. A word of caution is in order. If $j = q-1$ or $j = q$, the above discrete term involves values of ρ_j on both sides of the step edge; however, $\rho(x)$ can be discontinuous across the step. In an effort to describe the limit of Eq. (17) transparently, we introduce reference densities $\rho_{\rm s}^\pm$ such that the scheme for the adatom number density at sites adjacent to the step edge reads [1, 6]

$$\begin{aligned} j = q-1:\ \ 0 &= \mathfrak{D}[a^{-2}(\rho_{j-1} - 2\rho_j + \rho_{\rm s}^-)] - \frac{1}{\tau_{\rm e}}\rho_j + F \\ &\quad - \{r_{\rm a}^- \rho_j + \mathfrak{D}[a^{-1}(\rho_{\rm s}^- - \rho_j)]\}a^{-1}, \end{aligned} \tag{23a}$$

$$\begin{aligned} j = q:\ \ 0 &= \mathfrak{D}[a^{-2}[(\rho_{j+1} - 2\rho_j + \rho_{\rm s}^+)] - \frac{1}{\tau_{\rm e}}\rho_j + F \\ &\quad + \{r_{\rm d}^+ + \mathfrak{D}[a^{-1}(\rho_j - \rho_{\rm s}^+)]\}a^{-1}. \end{aligned} \tag{23b}$$

The densities $\rho_{\rm s}^\pm$ can be thought of as representing the continuum limits of ρ_j at either side of the step edge, and can be determined so that they produce the appropriate adatom fluxes to the right (+) or left (−) of the step. Specifically, $\pm a^{-1}(\rho_j - \rho_{\rm st}^\pm)$ is let to approach $(\partial\rho/\partial x)^\pm$, the respective value of the derivative of $\rho(x)$, for $j = q$ (+) or $j = q-1$ (−). These terms contribute to the desired Robin boundary conditions as shown below.

Consequently, in the limit $a \to 0$ Eq. (17) becomes

$$\begin{aligned} 0 = {} & \{\mathfrak{D}\Delta_x\rho - \tau_{\mathrm{e}}^{-1}\rho(x) + F\}[\theta(x - x_{\mathrm{s}}) + \theta(x_{\mathrm{s}} - x)] \\ & + \delta^{+}_{x_{\mathrm{s}}}(-\mathcal{J}^{+} + r^{+}_{\mathrm{d}} - r^{+}_{\mathrm{a}}\rho^{+}) \\ & + \delta^{-}_{x_{\mathrm{s}}}(\mathcal{J}^{-} + r^{-}_{\mathrm{d}} - r^{-}_{\mathrm{a}}\rho^{-}), \qquad 0 < x < 1. \end{aligned} \tag{24}$$

Note the elimination of the time derivative of the adatom number density in this scaling regime. In the above, $\theta(x)$ is the Heaviside function [$\theta(x) = 0$ if $x < 0$ and $\theta(x) = 1$ if $x > 0$]; $\delta^{\pm}_{x_{\mathrm{s}}} = \lim_{a\to 0}(a^{-1}\delta_{j,l})$ is the Dirac mass, delta function, centered at x_{s} to the left ($-$) or right ($+$) of the step edge, for $l = q-2, q-1$ and $l = q, q+1$, respectively; and $\mathcal{J}^{\pm}$ is the corresponding x-directed adatom flux restricted at the step edge, viz.,

$$\begin{aligned} \mathcal{J}^{+} &= -\mathfrak{D}\left(\frac{\partial\rho}{\partial x}\right)^{+} = -\mathfrak{D}\lim_{a\to 0}\left(\frac{\rho_q - \rho^{+}_{\mathrm{s}}}{a}\right), \\ \mathcal{J}^{-} &= -\mathfrak{D}\left(\frac{\partial\rho}{\partial x}\right)^{-} = -\mathfrak{D}\lim_{a\to 0}\left(\frac{\rho^{-}_{\mathrm{s}} - \rho_{q-1}}{a}\right). \end{aligned} \tag{25}$$

Evidently, there is no convective term present in $\mathcal{J}^{\pm}$, which is consistent with the elimination of $\partial\rho/\partial t$. This feature signifies the quasistatic regime.

Equation (24) is equivalent to a diffusion equation on each terrace along with kinetic Robin-type boundary conditions at the step edge:

$$\mathfrak{D}\Delta_x\rho - \tau_{\mathrm{e}}^{-1}\rho(x) + F = 0,\ 0 < x < x_{\mathrm{s}} \text{ or } x_{\mathrm{s}} < x < 1, \tag{26}$$

$$\begin{aligned} \mathcal{J}^{+} &= -r^{+}_{\mathrm{a}}(\rho^{+} - r^{+}_{\mathrm{d}}/r^{+}_{\mathrm{a}}), & x &= x^{+}_{\mathrm{s}}, \\ \mathcal{J}^{-} &= r^{-}_{\mathrm{a}}(\rho^{-} - r^{-}_{\mathrm{d}}/r^{-}_{\mathrm{a}}), & x &= x^{-}_{\mathrm{s}}, \end{aligned} \tag{27}$$

where

$$\frac{r^{+}_{\mathrm{d}}}{r^{+}_{\mathrm{a}}} = \frac{r^{-}_{\mathrm{d}}}{r^{-}_{\mathrm{a}}} \equiv \rho_{\mathrm{eq}} = \lim_{a\to 0}\left(\frac{k}{a}\right), \tag{28}$$

which is finite by Eq. (19). This ρ_{eq} represents the equilibrium number density of adatoms at the step edge; cf. [1, 6, 8]. Thus, step velocity law (15) reads

$$\frac{dx_{\mathrm{s}}}{dt} = r^{-}_{\mathrm{a}}(\rho^{-} - \rho_{\mathrm{eq}}) + r^{+}_{\mathrm{a}}(\rho^{+} - \rho_{\mathrm{eq}}) = \mathcal{J}^{-} - \mathcal{J}^{+}. \tag{29}$$

Equations (26), (27) and (29) provide the BCF-type step motion laws.

For the sake of completeness, we need to include conditions at the boundaries, $x = 0$ and 1, of the domain. These come from Eqs. (10) as $a \to 0$; specifically, using the scaling of Sec. III A, we obtain the following relations:

$$\begin{aligned} 0 &= \lim_{a\to 0}\{\mathfrak{D}[a^{-1}(\rho_1 - \rho_0)] + f_{\mathrm{in}} - a\tau_{\mathrm{e}}^{-1}\rho_0 + aF\} \\ &\Rightarrow \mathcal{J}(0) = -\mathfrak{D}\left(\frac{\partial\rho}{\partial x}\right)\bigg|_{x=0} = f_{\mathrm{in}}, \end{aligned} \tag{30}$$

$$\begin{aligned} 0 &= \lim_{a\to 0}\{-\mathfrak{D}\rho_{N-1} - \mathfrak{D}(\rho_{N-1} - \rho_{N-2})\} \\ &\Rightarrow \rho(1) = 0. \end{aligned} \tag{31}$$

At the risk of redundancy, we note that this set of boundary conditions at $x = 0$ and 1 is not meant to be special; other choices of conditions are possible without distorting the essential physics of the BCF model.

IV. DISCUSSION

In this section, we discuss issues that underlie the exposition and formal analysis of Secs. II and III. In particular, we (i) provide remarks on the convergence of our atomistic scheme, and (ii) extend the formulation to multiple non-interacting steps.

A. Convergence of atomistic scheme

Thus far, we have provided a derivation of the BCF-type model from an atomistic scheme based on heuristic asymptotics. To make the derivation mathematically rigorous, it is useful to make the analogy of the atomistic dynamics to a finite-difference scheme approximating the continuous description from the BCF-type model, where the parameter a is identified as the mesh size of the discretization. Indeed, as already mentioned above, the first term on the right-hand side of Eq. (17) can be viewed as a central difference of the Laplacian operator acting on ρ, except near the step edge which in turn results in suitable boundary conditions there. Moreover, the evolution of the step edge in the atomistic scheme, given by Eq. (1), can be viewed as a stochastic scheme for the step velocity law (29). This is very similar to the Glimm scheme used for front propagation [16, 17]. Therefore, to establish the limiting behavior of the atomistic scheme as $a \to 0$, it is desirable to prove the convergence of the particular numerical scheme to the BCF-type step flow model.

Let us briefly sketch the main ideas of the convergence proof; the details lie beyond the scope of the present paper. As usual, the convergence of the scheme involves both consistency and stability analysis. The consistency for the scheme essentially follows the heuristic asymptotic arguments provided above in the derivation. The stability is more subtle. A difficulty comes from the quasistatic time scaling on the left-hand side of Eq. (17): The small parameter a multiplying the time derivative of ρ requires stability for effectively long time evolution. Hence, an energy estimate is needed to show that the discrete system is dissipative. This amounts to establishing a gradient flow structure for the atomistic scheme, which is expected to be similar to that on the continuous scale for the BCF-type system with detailed balance [21].

B. Multiple steps

Our analysis can be extended to more than one non-interacting ordered steps without difficulty. The main observation is that the above derivation of step motion laws is local, based on local atomistic laws. Specifically, the Robin boundary conditions (27) for adatom diffusion and step velocity law (29) both result from the mass exchange between the edge atom and adatoms in the neighboring lattice sites. Hence, the derivation of mesoscale laws for systems with a monotone step train should not present any difficulty, provided the steps do not interact elastically and are sufficiently far apart, so that the local atomistic laws at the step edges are not distorted. In particular, if the system consists of M non-interacting steps with the same kinetic rates everywhere, the atomistic scheme near the kth step edge, which is at site q_k ($k = 1,\, 2,\, \ldots M$), is assumed to be

$$\begin{aligned}
\varrho^{n+1}_{q^n_k-2} &= (1-2D\tau)\varrho^n_{q^n_k-2} + D\tau(\varrho^n_{q^n_k-3} + \varrho^n_{q^n_k-1}) \\
&\quad - \frac{\tau}{\tau_{\mathrm{e}}}\varrho_{q^n_k-2} + f\tau + \mathbb{1}(\xi^n_k = -1), \\
\varrho^{n+1}_{q^n_k-1} &= (1-D\tau)\varrho^n_{q^n_k-1} + D\tau\varrho^n_{q^n_k-2} - \frac{\tau}{\tau_{\mathrm{e}}}\varrho^n_{q^n_k-1} + f\tau \\
&\quad - \mathbb{1}(\xi^n_k = 1), \\
\varrho^{n+1}_{q^n_k} &= (1-D\tau)\varrho^n_{q^n_k} + D\tau\varrho^n_{q^n_k+1} - \frac{\tau}{\tau_{\mathrm{e}}}\varrho^n_{q^n_k} + f\tau \\
&\quad + \mathbb{1}(\xi^n_k = -2), \\
\varrho^{n+1}_{q^n_k+1} &= (1-2D\tau)\varrho^n_{q^n_k+1} + D\tau(\varrho^n_{q^n_k} + \varrho^n_{q^n_k+2}) \\
&\quad - \frac{\tau}{\tau_{\mathrm{e}}}\varrho^n_{q^n_k+1} + f\tau - \mathbb{1}(\xi^n_k = 2), \qquad (32)
\end{aligned}$$

where the random variable $\xi_k(t)$ indicates the atomistic events relevant to the kth step; cf. Eqs. (5). The local probabilistic rules for ξ_k follow directly from Eqs. (2).

In this case, in the scaling limit each step moves according to velocity law (29) with the adatom density determined by quasistatic diffusion on each terrace with the same Robin-type boundary conditions at each step edge. However, as our atomistic model does not include elastic response of the lattice, the system of multiple steps is deemed as physically incomplete. It is an interesting and challenging research direction to understand the elastic interaction between multiple steps starting from atomistic models.

V. CONCLUSION

In this paper, starting from a stochastic scheme for the hopping of atoms on a crystal lattice we formally derived a set of quasistatic motion laws for a system of non-interacting steps in 1+1 dimensions. These laws form the core of mesoscale BCF-type theories. Our scheme was adopted on the basis of a simplified SOS model for a dilute system of adatoms. Within our discrete model, the step edge is treated as a front that propagates via the attachment/detachment of atoms. This process is described by a random variable that takes values under mean-field probabilistic rules associated with the kinetics at the step. Our approach here differs from the more traditional master-equation viewpoint of previous treatments, e.g., [6, 7, 15]. We believe that our present formalism is promising for extensions to 2D, including more realistic effects in step motion.

Our formal analysis reveals some key features of the passage from atomistic rules to mesoscale laws for line defects. In our treatment, the emergence of BCF-type laws, including the full Robin boundary conditions for the adatom density at the step edge, is intimately connected to certain scalings of the time variable and the atomistic rates with the system size, $N = a^{-1}$. This entails a particular dominant balance for the adatom density and flux in the stochastic scheme as the lattice spacing, a, approaches zero. Our analysis also reveals that the stochastic noise vanishes in this limit, thus suggesting the interpretation of BCF theory as a consequence of the law of large numbers.

The present work points to several pending issues, not addressed in this paper. An issue is the possible emergence from atomistic rules of a *stochastic* mesoscale model, in which the noise plays a significant role as $a \to 0$. This requires a careful examination of the underlying kinetics. Furthermore, in experimental situations, steps interact as force dipoles in homoepitaxy and force monopoles or otherwise in hereroepitaxy. Hence, our current treatment needs to include elastic effects by taking into account the strain dependence of kinetic rates. Lastly, the derivation of a BCF-type description in 2D, where steps are curved in the presence of step-edge diffusion and kinks, and islands form, is a viable direction of future research.

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