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2010 J. Phys. A: Math. Theor. 43 065003

(http://iopscience.iop.org/1751-8121/43/6/065003)

IOP PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL

J. Phys. A: Math. Theor. **43** (2010) 065003 (22pp) doi:10.1088/1751-8113/43/6/065003

A stochastic step flow model with growth in 1+1 dimensions

Dionisios Margetis

Department of Mathematics, and Institute for Physical Science and Technology, and Center for Scientific Computation and Mathematical Modeling, University of Maryland, College Park, MD 20742-4111, USA

E-mail: dio@math.umd.edu

Received 16 August 2009, in final form 21 December 2009
Published 22 January 2010
Online at stacks.iop.org/JPhysA/43/065003

Abstract

Mathematical implications of adding *Gaussian white noise* to the Burton–Cabrera–Frank model for N terraces ('gaps') on a crystal surface are studied under external material deposition for *large* N. The terraces separate *straight, non-interacting* line defects (steps) with uniform spacing initially ($t = 0$). As the growth tends to vanish, the gaps become uncorrelated. First, simple closed-form expressions for the gap variance are obtained directly for *small fluctuations*. The leading-order, linear stochastic differential equations are *prototypical* for discrete *asymmetric* processes. Second, the Bogoliubov–Born–Green–Kirkwood–Yvon (BBGKY) *hierarchy* for joint gap densities is formulated. Third, a self-consistent *'mean field'* is defined via the BBGKY hierarchy. This field is then determined approximately through a terrace decorrelation hypothesis. Fourth, comparisons are made of directly obtained and mean-field results. Limitations and issues in the modeling of noise are outlined.

PACS numbers: 81.15.Aa, 05.10.Gg, 68.35.−p, 05.40.−a, 02.10.Yn

1. Introduction

The drive toward ever smaller and faster devices has fueled interest in crystal surface dynamics and fluctuations across scales. For broad reviews, the reader may consult [1–3]. A related direction of active research in non-equilibrium statistical mechanics is the connection of particle schemes to macroscopic evolution laws [4, 5].

Material deposition (growth) on crystal surfaces is used to create building blocks of quantum wires and dots, and other nanoscale structures [3]. On *vicinal* crystals, nanoscale terraces are oriented in the high-symmetry direction and separated by line defects (steps) typically one atomic layer high. At temperatures of interest, the steps are monotonic (of the same 'sign') with their number *fixed* by the miscut angle set by the experiment [2].

Understanding how microscale processes for steps are linked to the fluctuation of surface features at larger scales paves the way to controlling epitaxy.

Here, we study a stochastic particle model for crystal terraces. A solvable case is treated by methods of kinetic theory, revealing an interplay of time and material parameters. *'Mean-field'* ideas are examined in the light of *kinetic hierarchies* and compared to an exact result for the terrace variance. This leads to a simple correlation criterion.

The microscale constituents of crystal surfaces were introduced by Kossel [6], Stranski [7] and Burton, Cabrera and Frank (BCF) [8]. Surfaces evolve because steps move as adsorbed atoms (adatoms) hop on terraces, attach–detach at and move along step edges. This picture leads to a system of differential equations for step positions. An alternative description invokes macroscopic evolution laws for the surface height, e.g., in [9, 10]. Both of these descriptions have been connected to Bogoliubov–Born–Green–Kirkwood–Yvon (BBGKY) hierarchies for *step position* correlation functions [11].

Distinctly different approaches have been followed for step *fluctuations* [2, 12]. Equilibrium properties such as the terrace width, or *step gap* [13], distribution[1] for repulsively interacting steps have been studied extensively [2, 12, 14–16]. A key idea is to map steps onto worldlines of spinless fermions, because steps do not cross [14, 17]. The relaxation of the gap distribution is described by a *mean field*, via a Fokker–Planck equation (FPE), and by kinetic Monte Carlo simulations [18, 19]. In the former approach, stochastic differential equations (SDEs) for gaps approximately decouple, yielding a one-dimensional (1D) FPE for the one-gap density. The relation of this simplified mean-field approach to BBGKY hierarchies, which form the basis of any statistical–mechanical system with particle correlations, is not well understood and needs to be explored. This issue lies at the core of computational physics and motivates our work.

In this paper, a BCF-type model in 1D under growth is explored by the addition of Gaussian white noise for initially uniform step trains. One goal is to reconcile BBGKY hierarchies for joint gap probability densities with mean-field ideas for coupled SDEs [18, 16, 20]. Another goal is to treat the SDEs for N step gaps under a *small-fluctuation* expansion. The zeroth-order equations are linear and solved explicitly for all times and large N.

This problem was inspired by the recent work of Hamouda *et al* [20], who addressed non-equilibrium properties of terrace width fluctuations during growth. These authors apply a mean field for the one-gap density, and compare analytical results for long times with kinetic Monte Carlo simulations. Their density approaches a steady state captured both by the mean field and the kinetic Monte Carlo simulations. Here, the analysis complements [20] by focusing on (i) the relation of their mean field to the exact formalism of kinetic hierarchies, and (ii) the behavior of the one-gap density for *finite times*. This study aims to clarify the precise nature of previous, simple mean-field approximations, especially their limitations due to terrace correlations.

Sources of surface fluctuations were laid out by Wolf [21], and aspects of noisy continuum theories were discussed by Krug [22, 23] over a decade ago. A similar, minimal 1D model of growth is analyzed in [24] with emphasis on continuum equations for the surface height. The small-fluctuation model solved here (sections 5 and 6.1) is *prototypical* for a class of *asymmetric* discrete processes: a parameter (p) captures *limiting forms* of effects such as finite step velocity [20, 25, 26], Ehrlich–Schwoebel barrier [27–30], electromigration [31] and fluctuations in the number of atoms impinging on the surface [32]. This list is not exhaustive. Our approach, especially the modeling of noise, is compared to a few previous works, e.g. [30, 33, 34], in section 6.4.

[1] Throughout this paper, the terms *terrace width* and *step gap* are used interchangeably.

The SDE system for N terrace widths has the general (nondimensional) form

$$\mathrm{d}\mathcal{G}(t) = \check{A}(\mathcal{G}; F)\,\mathrm{d}t + \mathrm{d}\mathcal{B}(t) \qquad (t : \text{time},\ t \geqslant 0), \tag{1}$$

where $\mathcal{G}(t) = (\mathcal{G}_0(t), \mathcal{G}_1(t), \ldots, \mathcal{G}_{N-1}(t))$ is a vector-valued stochastic process with component $\mathcal{G}_i(t)$ representing the ith step gap; $\mathcal{B}(t) = (\mathcal{B}_0(t), \mathcal{B}_1(t), \ldots, \mathcal{B}_{N-1}(t))$ is vector Brownian motion (with independent and identically distributed components $\mathcal{B}_i(t)$); the vector-valued $\check{A}$ is smooth and has components $\check{A}_i = A(\mathcal{G}_{i-1}, \mathcal{G}_i, \mathcal{G}_{i+1})$ and F is the material deposition flux (see section 2 for a formulation). The gaps are subject to screw periodic boundary conditions, i.e. the N particles corresponding to terraces lie on a ring.

The main contributions of our work are: (i) SDEs (1) are converted to a BBGKY hierarchy for joint gap densities; (ii) by expansion of $\check{A}$ for sufficiently small fluctuations of $\mathcal{G}(t)$, an explicit solution of the leading-order SDEs and the corresponding gap variance are obtained; (iii) a self-consistent mean field f is introduced systematically via the BBGKY hierarchies, where $\mathcal{G}_{i-1}(t) \equiv f(t, \mathcal{G}_i) \equiv \mathcal{G}_{i+1}(t)$ in (1) and (iv) the mean-field gap variance is compared to an exact result for the linear model. The mean field f of [20] follows as a special case under the ansatz of two-gap independence.

The limits $N \to \infty$ and $t \to \infty$ do not commute in the main computation of section 5.2. The time t is taken to be fixed, which is physically meaningful (and better illustrates the relation of white noise to gap variance). Specifically, if t is physical time, $(Fa\varpi)^2 t/D < O(N)$ where ϖ is the initial step gap, a is the step size and D is the terrace diffusivity. This time restriction is, nonetheless, *relaxed* in section 6.1, revealing *finite-size* effects within a linear stochastic model.

For the main derivations, the assumption is made that steps are entropically and energetically *non-interacting* [8]. The terrace widths in SDEs (1) interact only through surface diffusion. This simplification, which retains the essential physics of growth and offers some advantages, can be motivated as follows. (i) The terrace fluctuations, partly controlled by the deposition flux F and initial step gap ϖ, can be kept sufficiently small so that leaving out step interactions has a negligible effect. This is further discussed in section 6.3. (ii) Without interactions, the coefficient $\check{A}$ in (1) is well behaved. Thus, for reasonable initial data, a unique strong solution exists[2]. By contrast, repulsive step interactions would result in a singular $\check{A}$ [36, 37]. Although it is expected physically that step gaps do not vanish (and thus $\check{A}$ does not blow up), the analysis of step energies would require much more care. (iii) SDEs (1) have the appeal of a minimal model for gap correlations with noise. As $F \to 0$, the gaps become *independent* for all $t > 0$ [24]. Hence, F *parameterizes* in a simple nontrivial setting *terrace correlation*.

A shortcoming of our model, without step interactions, appears to be its violation of the non-crossing condition for steps: gap densities acquire tails of nonzero probability for negative gaps. However, if the gap variance is much smaller than the mean terrace width squared, as can happen, e.g., by controlling the initial terrace width ϖ and flux F, negative gaps are unlikely and their probability is small. Hence, the results are deemed physical provided ϖ, F and t suitably conspire to keep fluctuations small enough [20]. This possibility is quantified in section 5 as an outcome of our analysis.

The BCF theory—which forms the core of this treatment—has an intrinsically near-equilibrium character. Hence, the model is expected to break down if the deposition flux, F, is too large [20]. In the other extreme limit, $F \to 0$, the inclusion of step interactions is compelling since fluctuations tend to grow. The view is adopted that step interactions are

[2] For uniqueness, it suffices to have a Lipschitz continuous coefficient $\check{A}$ and initial data with finite mean and variance. For an exposition to strong and weak solutions of SDEs, see, e.g., [35].

negligible for $F > F_{\rm th}$ where $0 < F_{\rm th}a\varpi^2/D \ll 1$. The idealized limit $Fa\varpi^2/D \to 0$ is invoked in the analysis as a reference case, to show how terraces tend to decorrelate.

A bothersome feature of (1) is that the form of the noise term is *assumed* ad hoc rather than derived. This approach relies on widely appealing features of the (Brownian motion-based) white noise. The relation of this noise to geometry and the random hopping of adatoms, e.g., any plausible settings of kinetic Monte Carlo-type simulations, is not touched upon. In the same vein, aspects of step meandering [30, 34] are beyond our present scope. The steps are straight moving boundaries. Considering step meandering leads to a more elaborate setting and formulation (see section 6.4 for a discussion).

The present treatment is distinct from the renormalization group ideas by Haselwandter and Vvedensky [38], who derive stochastic *partial* differential equations for the surface height from an atomistic model. The connection of their approach to fluctuating steps and terraces is not addressed.

Despite its idealizations, the present setting is viewed as a minimal model for linking discrete stochastic schemes to large-scale fluctuations. The role of BBGKY hierarchies is exemplified with relative ease. In this analytically tractable context, an explicit result for the gap variance is compared to a previous mean-field formula. This indicates a *'measure' of terrace correlations* which, although quantified here in the absence of step interactions, is believed to capture universal features of fluctuations such as the narrowing of the terrace width distribution with increasing flux F. The study of richer models can be guided by this treatment.

The paper is organized as follows. In section 2, the governing SDE system in 1D is formulated in the BCF framework [8]. In section 3, an equivalent formulation is provided in terms of BBGKY hierarchies for joint probability *step gap* densities. In section 4, a self-consistent mean field is introduced via the two-gap density. In section 5, the one-gap variance is computed explicitly for fixed time. Section 6 addresses extensions and implications of these results. In section 7, the main results and pending issues are summarized. The appendices provide technical derivations needed in the main text.

Note on notation. Calligraphic capital letters denote scalar or vector *stochastic processes*. Matrices are boldface; a vector $y \in \mathbb{R}^N$ (N-dimensional space) is not boldface and has components y_k, $k = 0, \ldots, N-1$, whereas $\vec{y}_l \equiv (y_0, \ldots, y_{l-1}) \in \mathbb{R}^l$, $1 \leqslant l \leqslant N-1$. Joint gap densities are ρ_n with $n = 1, \ldots, N$. The symbol $f = O(g)$ implies that f/g is bounded by a constant as a parameter or variable approaches a certain limit.

2. Stochastic scheme: formulation via the BCF model

In this section, the SDE system for N step gaps under growth is formulated in the physical setting of Hamouda *et al* [20]. First, the geometry and deterministic equations of motion for terrace widths are described via BCF principles [8]. The effects include adatom terrace diffusion, atom attachment-detachment at steps and material deposition from above. Second, the governing equations are nondimensionalized. Third, Gaussian white noise is added to the equations of motion.

2.1. Deterministic equation of motion

Consider noiseless dynamics. The step geometry is shown in figure 1. The step train is monotonic, steps have (nonrandom) positions $x_i(t)$ and height a, where $g_i = x_{i+1} - x_i > 0$

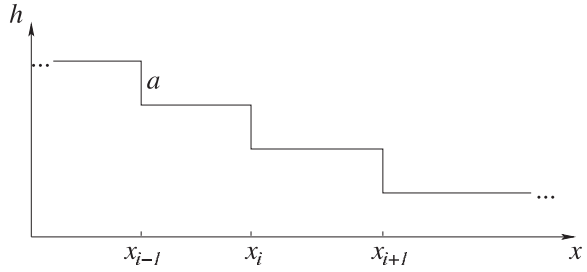

Figure 1. Schematic (cross section) of step configuration: $x = x_i(t)$ at the ith step edge, a is the step height and h is the surface height; the ith step gap is $g_i = x_{i+1} - x_i$.

and $i = 0, \ldots, N-1$.[3] Apply screw periodic boundary conditions, i.e. set $x_i(t) = x_{i+kN}(t)$ where k is any integer.

The adatom concentration $C_i(t, x)$ on the ith terrace satisfies the diffusion equation

$$\partial_t C_i = D\partial_x^2 C_i + F, \qquad x_i < x < x_{i+1} \qquad (\partial_t \equiv \partial/\partial t), \tag{2}$$

where D is the terrace diffusion constant and F is the external deposition rate.

A usual approach to solving (2) for $F = 0$ is the *quasi-steady approximation*, $\partial_t C_i \approx 0$. In growth ($F \neq 0$), a nonzero relative step velocity, $v \propto F$, is included via the Galilean transformation $(x', t') = (x - vt, t)$ [26]. Thus, (2) becomes [20, 26]

$$\left(D\partial_{x'}^2 + v\partial_{x'}\right)C_i + F = \partial_{t'} C_i. \tag{3}$$

It is reasonable to set $v = Fa\varpi$, the mean step velocity, where ϖ is the initial or mean gap (see section 5). So, the diffusion equation is transformed to the comoving frame [20]. Apply the quasi-steady approximation $\partial_{t'} C \approx 0$ in the kinetic regime where deviations of the actual step velocity from this v are small compared to the speed $D/(x_{i+1} - x_i)$. Now, remove the primes for ease of notation (i.e. $x' \Rightarrow x$).

Next, linear kinetics are enforced at steps bounding the ith terrace [2]:

$$-j_i(x_i) = k\left[C_i(x_i) - C_i^{\mathrm{eq}}\right], \quad j_i(x_{i+1}) = k\left[C_i(x_{i+1}) - C_{i+1}^{\mathrm{eq}}\right], \tag{4}$$

where $j_i(x) = -D\partial C_i/\partial x - vC_i$ is the ith-terrace adatom flux, C_i^{eq} is the ith-edge equilibrium adatom concentration and k is the rate for atom attachment–detachment. The time dependence of C_i and j_i is suppressed. Each C_i^{eq} accounts for step energetics, i.e. elastic-dipole step interactions [2, 36, 37] (see section 6). Kinetic rates different for up- and down-step edges (i.e. the Ehrlich–Schwoebel barrier [27]) can be included.

By mass conservation, the velocity of the ith step edge is

$$\dot{x}_i = \mathrm{d}x_i/\mathrm{d}t = (\Omega/a)[j_{i-1}(x_i) - j_i(x_i)], \tag{5}$$

where Ω is the atomic volume, $\Omega \approx a^2$. Once each C_i is obtained for fixed positions $\{x_i\}$, (5) leads to a system of ordinary differential equations for $x_i(t)$.

Equations (3) and (4) are solved explicitly, but the details are omitted; $j_i(x)$ reads

$$j_i(x) = FDv^{-1} + F(x - x_i) - \Lambda_i, \tag{6}$$

where $\Lambda_i = \Lambda\left(g_i; C_i^{\mathrm{eq}}, C_{i+1}^{\mathrm{eq}}\right)$, $g_i = x_{i+1} - x_i$, and

$$\Lambda(g; \alpha, \beta) = \frac{F[(1 + \mathrm{e}^{-vg/D})D/k + (1 + v/k)g] + v(\beta - \alpha\,\mathrm{e}^{-vg/D})}{1 + v/k - (1 - v/k)\,\mathrm{e}^{-vg/D}}. \tag{7}$$

[3] Figure 1 and the discussion of this section imply that steps have a fixed ordering. Consistent with this picture, the starting formulation in this subsection incorporates step repulsions via the C_i^{eq} in (4).

By virtue of (5), the differential equations for the step gaps, g_i, read

$$\dot{g}_i = (\Omega/a)[F(g_i - g_{i-1}) + \Lambda_{i+1} - 2\Lambda_i + \Lambda_{i-1}]. \tag{8}$$

A distinguished limit of (8) follows by taking

$$vg_i/D \leqslant O(1), \qquad v/k \ll 1, \qquad D/k \ll g_i, \qquad vC_i^{\mathrm{eq}} \ll Fg_i.$$

Consequently, $\Lambda_i \sim Fg_i(1 - \mathrm{e}^{-vg_i/D})^{-1}$ and (8) reduces to [20]

$$\dot{g}_i = \frac{\Omega F}{2a}\left[\frac{g_{i+1}\,\mathrm{e}^{vg_{i+1}/(2D)}}{\sinh\left(\frac{vg_{i+1}}{2D}\right)} - \frac{2g_i\cosh\left(\frac{vg_i}{2D}\right)}{\sinh\left(\frac{vg_i}{2D}\right)} + \frac{g_{i-1}\,\mathrm{e}^{-vg_{i-1}/(2D)}}{\sinh\left(\frac{vg_{i-1}}{2D}\right)}\right]. \tag{9}$$

If $g_i(0) = \varpi = \text{const.}$, then $g_i(t) \equiv \varpi$ solves (9) for all $t > 0$.

2.2. Nondimensional equations

Consider $Na/L \geqslant O(1)$ where L is the size of the sample. Each gap g_i, and thus ϖ, is comparable to or larger than the step height, a. The positive surface slope $m_0 = a/\varpi$ $(0 < m_0 < 1)$ is independent of N. In many physically appealing situations $v\varpi/D \leqslant 1$.

A few related observations are in order.

Deposition rate. The continuum analog of the step velocity law (5) is $\partial_t h + \Omega\partial_x j = \Omega F$ where $\Omega = O(a^2)$, $h(t, x)$ is the surface height and $j(t, x)$ is the large-scale flux [9]. Thus, it is reasonable to think of $F\Omega$ as an $O(1)$, macroscopically measurable parameter.

Length scales. Two obvious length scales are (i) the, usually microscopic, length $\ell_1 = \varpi$, set by the initial condition for a vicinal crystal and (ii) $\ell_2 = O(D/v)$. For a fixed surface slope, ℓ_2 is considered as N-independent.

Time scales. By the inspection of (9), two possible time scales are (i) $\tau_1 = O[(Fa)^{-1}]$ and (ii) $\tau_2 = O[D/(Fa^2)^2]$, which is considered as N-independent. To unravel τ_2 when $v\varpi/D \ll 1$, think of (9) as a second-order difference scheme for a step-continuous equation. By the Taylor expansion in i, the right-hand side manifestly becomes $O\left(\tau_2^{-1}\varpi\right)$.

Equation (9) can be recast to a nondimensional form for later algebraic convenience. Emphasis is placed on manifestly N-independent scales. Define[4]

$$\tilde{g}_i = g_i/\ell_2, \qquad \tilde{t} = t/\tau_2; \qquad \ell_2 = \frac{2D}{v}, \qquad \tau_2 = \frac{2D}{F\Omega}\frac{1}{Fa^2} \qquad (\Omega \approx a^2). \tag{10}$$

Next, we drop the tildes ($\tilde{g}_i \Rightarrow g_i$ and $\tilde{t} \Rightarrow t$). The units are chosen so that $vm_0a/(2D) \equiv 1$ $(m_0 = a/\varpi)$ and the factor of $1/2$ is included for later algebraic convenience; see also section 5. Equation (9) is written accordingly (see (11)).

2.3. Gaussian white noise

Consider the N-dimensional Brownian motion $\mathcal{B}(t) = (\mathcal{B}_0(t), \ldots, \mathcal{B}_{N-1}(t)) \in \mathbb{R}^N$ ($\mathbb{R}$: set of real numbers). The white noise, $\mathcal{N}(t)$, is the generalized stochastic process $\mathcal{N}(t) = \mathrm{d}\mathcal{B}(t)/\mathrm{d}t$. Such an $\mathcal{N}(t)$, if interpreted as the usual derivative of $\mathcal{B}(t)$, suffers from pathologies, e.g. lack of continuous paths. The relation $\mathrm{d}\mathcal{B}(t) = \mathcal{N}(t)\mathrm{d}t$ amounts to $\int_{t_0}^{t}\mathcal{N}(\tau)\,\mathrm{d}\tau = \mathcal{B}(t) - \mathcal{B}(t_0)$ for any t_0, t. Hence, this $\mathcal{N}(t)$ has units of (time)$^{-1/2}$.

Next, the vector-valued *function* $g(t) = (g_0(t), \ldots, g_{N-1}(t))$ is replaced by the *stochastic process* $\mathcal{G}(t) = (\mathcal{G}_0(t), \ldots, \mathcal{G}_{N-1}(t))$. The components $\mathcal{G}_i(t)$ satisfy the SDEs

$$\mathrm{d}\mathcal{G}_i(t) = \frac{1}{2}\left(\frac{\mathcal{G}_{i+1}\mathrm{e}^{\mathcal{G}_{i+1}}}{\sinh\mathcal{G}_{i+1}} - 2\mathcal{G}_i\coth\mathcal{G}_i + \frac{\mathcal{G}_{i-1}\mathrm{e}^{-\mathcal{G}_{i-1}}}{\sinh\mathcal{G}_{i-1}}\right)\mathrm{d}t + \mathrm{d}\mathcal{B}_i(t), \tag{11}$$

[4] Alternatively, one may define $\tau_2 = (F\varpi^2)^{-1}(2D/(F\Omega))$, replacing a by ϖ.

where $0 \leqslant i \leqslant N-1$. Apply (nonrandom) initial data $\mathcal{G}_i(0) = \nu \equiv \nu\varpi/(2D) = \aleph_i$ where $\aleph \equiv (\nu, \ldots, \nu) \in \mathbb{R}^N$.

Definition 1. *By* $1 - \mathrm{Prob}[\sup_{t\in[0,T)}|\mathcal{G}_i(t)| \ll 1] \ll 1$, *SDEs (11) become*

$$\mathrm{d}\mathcal{G}_i = \tfrac{1}{2}(\mathcal{G}_{i+1} - \mathcal{G}_{i-1})\mathrm{d}t + \mathrm{d}\mathcal{B}_i, \quad \mathcal{G}_i(0) = \nu. \tag{12}$$

This model will be referred to as the 'reference case'.

Equation (11) relies on an ad hoc introduction of noise. The coefficient of $\mathrm{d}\mathcal{B}_i(t)$ is a constant. Thus, the solution to (11) admits a unique interpretation. By contrast, the inclusion of a $\mathcal{G}$-dependent noise coefficient, not precluded by any physical principle [32], poses a question as to what stochastic calculus (e.g. of Itô or Stratonovich) would be more appropriate [35]. An advantage of the Itô calculus is the relative ease by which connections can be made to BBGKY hierarchies. Issues of noise are discussed in section 6.

Note in passing that, upon returning to *dimensional* variables, the $\mathrm{d}\mathcal{B}_i(t)$ acquires the dimensional coefficient $\ell_2/\sqrt{\tau_2} = m_0\sqrt{2D}$, independent of N (with $\Omega = a^2$).

3. BBGKY hierarchy

In this section, the SDE system for step gaps (Lagrangian coordinates) is recast to coupled partial differential equations for joint probability densities (Eulerian variables). The starting point is a generalization of SDEs (11), namely,

$$\mathrm{d}\mathcal{G}_i(t) = A(\mathcal{G}_{i-1}(t), \mathcal{G}_i(t), \mathcal{G}_{i+1}(t))\,\mathrm{d}t + \mathrm{d}\mathcal{B}_i(t). \tag{13}$$

3.1. Formulation

First, appropriate probability densities are introduced. The N-gap density is

$$\rho_N(t, y)\,\mathrm{d}y = \mathrm{Prob}\big[\cap_{k=0}^{N-1}\{y_k < \mathcal{G}_k(t) < y_k + \mathrm{d}y_k\}\big], \qquad \mathrm{d}y = \prod_{k=0}^{N-1}\mathrm{d}y_k, \tag{14}$$

where y_k is the value of the kth gap, and $y = (y_0, \ldots, y_{N-1}) \in \mathbb{T}^N$, the N-dimensional torus. In view of (13), the joint density of *any* n consecutive gaps is defined by

$$\rho_n(t, \vec{s}_n) := \frac{1}{N}\sum_{k=0}^{N-1}\int_{\mathbb{T}^{N-n}} \rho_N(t, (\vec{y}'_{N-n}, \vec{s}_n)^c_k)\,\mathrm{d}\vec{y}'_{N-n}, \qquad 1 \leqslant n < N, \tag{15}$$

where $\vec{y}'_l$, $\vec{s}_l$ are l-dimensional vectors ($\vec{s}_l \in \mathbb{R}^l$, $0 \leqslant l \leqslant N-1$) with $\vec{s}_l = (s_0, \ldots, s_{l-1})$. The vector $\zeta_k \equiv (\vec{y}'_{N-n}, \vec{s}_n)^c_k \in \mathbb{R}^N$ is formed by the *cyclic* permutation of coordinates in $(\vec{y}'_{N-n}, \vec{s}_n)$, i.e. $\zeta_k = (y'_k, \ldots, y'_{N-n-1}, \vec{s}_n, y'_0, \ldots, y'_{k-1})$ if $0 \leqslant k \leqslant N-n-1$ while $\zeta_k = (s_{k-N+n}, \ldots, s_{n-1}, \vec{y}'_{N-n}, s_0, \ldots, s_{k-N+n-1})$ if $N-n \leqslant k \leqslant N-1$. Note that, for $N \gg 1$ and $n = O(1)$, this latter possibility has a small, $O(n/N)$, likelihood. The factor of $1/N$ in (15) accounts for each terrace in the step train with equal probability. Of particular interest is the density of any single gap, given explicitly by

$$\rho_1(t, s \in \mathbb{T}) = N^{-1}\sum_{k=0}^{N-1}\int_{\mathbb{T}^{N-1}} \rho_N(t, y'_0, \ldots, y'_{k-1}, s, y'_k, \ldots, y'_{N-2})\,\mathrm{d}\vec{y}'_{N-1}. \tag{16}$$

Second, equations of motion for ρ_n are derived under $N \gg 1$ and $n = O(1)$. Define the N-dimensional vector field $\check{A}(y)$ that has the kth component $\check{A}_k = A(y_{k-1}, y_k, y_{k+1})$, $0 \leqslant k \leqslant N-1$; cf (13). The FPE (or, the forward Kolmogorov equation) for $\rho_N(t, y)$ reads

$$\partial_t \rho_N(t, y) + \mathrm{div}_N[\check{A}(y)\rho_N] = \frac{1}{2}\Delta_N \rho_N(t, y); \quad \mathrm{div}_N F \equiv \sum_{k=0}^{N-1} \partial_{y_k} F_k, \tag{17}$$

and Δ_n is the n-dimensional Laplacian (with $n = N$ above). For a vicinal crystal, the initial condition is $\rho_N(0, y) = \delta_{\aleph}(y)$, where $\aleph = (\nu, \ldots, \nu) \in \mathbb{R}^N$, $\nu \equiv \aleph_i = \upsilon\varpi/(2D)$ and $\delta_{\aleph}(y)$ is the Dirac measure ('delta function') on $\mathbb{R}^N$ centered at the point $\aleph$.

The BBGKY hierarchy stems (formally) from differentiation of (15) with respect to t. For $n = 1$, the equation for $\rho_1(s)$ (by suppression of the t dependence) is

$$\begin{aligned}\partial_t \rho_1(s) = -\partial_s \Bigg[N^{-1} \sum_{k=0}^{N-1} \int_{\mathbb{T}^2} \mathrm{d}y'_{k-1}\, \mathrm{d}y'_k\, A(y'_{k-1}, s, y'_k) \\ \times \int_{\mathbb{T}^{N-3}} \mathrm{d}\vec{y}'_{N-3}\, \rho_N((\vec{y}'_{N-1}, s)^c_k) \Bigg] + \frac{1}{2}\partial_s^2 \rho_1, \qquad s \in \mathbb{T};\end{aligned}$$

$$\Rightarrow \partial_t \rho_1(s) + \partial_s \left[\int \mathrm{d}s'_0\, \mathrm{d}s'_1\, A(s'_0, s, s'_1)\, \rho_3(s'_0, s, s'_1) \right] = \frac{1}{2}\partial_s^2 \rho_1. \tag{18}$$

Terms pertaining to the permutations (s, s'_0, s'_1) and (s'_0, s'_1, s) are $O(1/N)$ and neglected. The integration range is implied by the variables and omitted.

The hierarchy for ρ_n is generalized for $n \geqslant 2$:

$$\begin{aligned}\partial_t \rho_n(\vec{s}_n) + \partial_{s_0} \left[\int \mathrm{d}s'\, A(s', s_0, s_1)\, \rho_{n+1}(s', \vec{s}_n) \right] + \sum_{k=1}^{n-2} \partial_{s_k}[A(s_{k-1}, s_k, s_{k+1})\, \rho_n(\vec{s}_n)] \\ + \partial_{s_{n-1}} \left[\int \mathrm{d}s'\, A(s_{n-2}, s_{n-1}, s')\, \rho_{n+1}(\vec{s}_n, s') \right] = \frac{1}{2}\Delta_n \rho_n(\vec{s}_n).\end{aligned} \tag{19}$$

As an initial condition for a vicinal crystal, set $\rho_n|_{t=0} = \prod_{k=0}^{n-1} \delta_v(s_k)$.

The analysis here is distinct from [11], where noise is absent, the hierarchies involve correlation functions for step *positions* (not terrace widths), and delta functions are invoked explicitly in the derivation; cf equations (3.17)– (3.19) in [11].

3.2. Example: Growth model

In correspondence to (11), equations (18) and (19) are now written for the coefficient

$$A(y_1, y_2, y_3) \equiv K_a(y_1) - K_{ab}(y_2) + K_b(y_3), \qquad K_{ab} \equiv K_a + K_b, \tag{20}$$

where, e.g., $K_a(s) = s\,\mathrm{e}^s/(2\sinh s)$ and $K_b(s) = s\,\mathrm{e}^{-s}/(2\sinh s) = K_a(-s)$:

$$\partial_t \rho_1(s) + \partial_s \left\{ \int \mathrm{d}s' \,[K_a(s')\rho_2(s', s) + K_b(s')\rho_2(s, s')] - K_{ab}(s)\rho_1(s) \right\} = \frac{1}{2}\partial_s^2 \rho_1, \tag{21}$$

$$\begin{aligned}\partial_t \rho_n(\vec{s}_n) + \partial_{s_0} \left\{ \int \mathrm{d}s'\, K_a(s')\rho_{n+1}(s', \vec{s}_n) + [K_b(s_1) - K_{ab}(s_0)]\rho_n(\vec{s}_n) \right\} \\ + \sum_{k=1}^{n-2} \partial_{s_k}\{[K_a(s_{k-1}) - K_{ab}(s_k) + K_b(s_{k+1})]\rho_n(\vec{s}_n)\}\end{aligned}$$

$$+\partial_{s_{n-1}}\left\{\int \mathrm{d}s'\, K_b(s')\,\rho_{n+1}(\vec{s}_n, s') + [K_a(s_{n-2}) - K_{ab}(s_{n-1})]\rho_n(\vec{s}_n)\right\}$$
$$= \frac{1}{2}\Delta_n \rho_n, \qquad n \geqslant 2. \tag{22}$$

3.3. Linear model and decorrelation

Consider scheme (12) in definition 1 (section 2.3), which amounts to the *small-fluctuation, linear model* $A(y_1, y_2, y_3) = (1-p)y_1 - (1-2p)y_2 - py_3$ of section 5.2 for $p = 1/2$; see also [20, 24] as well as (34) and (35). First, it is shown that the step gaps are *uncorrelated* for any N and $t > 0$. An underlying assumption is that the evolution equation (FPE) for the density ρ_N and the ensuing BBGKY hierarchy for ρ_n—supplemented with the initial data for a vicinal surface—have at most one solution.

The step gap independence amounts to the product form

$$\rho_N(t, y) = \prod_{k=0}^{N-1} \rho_1(t, y_k), \qquad \rho_1(0, s) = \delta_v(s). \tag{23}$$

Then, $\rho_n(\vec{s}_n) = \prod_{k=0}^{n-1} \rho_1(s_k)$, suppressing time dependence unless indicated otherwise.

By (17), the N-dimensional FPE for the reference case is

$$\partial_t \rho_N(y) + \frac{1}{2}\sum_{k=0}^{N-1} \partial_{y_k}[(y_{k+1} - y_{k-1})\rho_N] = \frac{1}{2}\sum_k \partial_{y_k}^2 \rho_N, \qquad y \in \mathbb{R}^N. \tag{24}$$

The first equation of the hierarchy stems from (21) with $K_a(s) = \frac{1}{2}(1+s) = K_b(-s)$.

Start with (24). The substitution of (23) into (24) yields

$$\sum_{l=0}^{N-1}\left\{\left(\partial_t - \frac{1}{2}\partial_{y_l}^2\right)\rho_1(y_l) + \partial_{y_l}\left[\frac{1}{2}(y_{l+1} - y_{l-1})\rho_1(y_l)\right]\right\}\prod_{k\neq l}\rho_1(y_k) = 0.$$

This is satisfied if ρ_1 solves the heat equation, $\partial_t \rho_1 = \frac{1}{2}\partial_s^2 \rho_1$. The solution is $\rho_1(t, s) = (2\pi t)^{-1/2}\,\mathrm{e}^{-\frac{(s-v)^2}{2t}}$, i.e. a Gaussian of mean $\mu = v$ and variance $\sigma^2 = t$. (For the derivation, note that $\partial_s \rho_1 = -(s-\mu)\rho_1(s)/\sigma^2$ while y lies on a torus: $\sum_l (y_{l+1} - y_{l-1})\partial_{y_l}\rho_1(y_l) = 0$.) This result is consistent with (21) under $\rho_2(s_0, s_1) = \rho_1(s_0)\rho_1(s_1)$.

One can show (as a trivial exercise) that for $p = 1/2$ the remaining equations of the BBGKY hierarchy collapse to the same equation for ρ_1 under $\rho_n(\vec{s}_n) = \prod_{k=0}^{n-1}\rho_1(s_k)$.

By contrast, this product form does *not* satisfy the BBGKY hierarchy in the physical range $0 < p < 1/2$ (see section 5.2). The equation for $\rho_1(s)$ collapses to $\partial_t \rho_1 + (1-2p)\partial_s[(v-s)\rho_1] = \frac{1}{2}\partial_s^2\rho_1$, solved by a Gaussian of mean v and variance $[2(1-2p)]^{-1}(1 - \mathrm{e}^{-2(1-2p)t})$ (see also [20] and section 4.2). However, equation (22) for the pair density ρ_2 (if $n = 2$), under $\rho_2(s_0, s_1) \sim \rho_1(s_0)\rho_1(s_1)$ and $\rho_3(\vec{s}_3) \sim \rho_2(s_0, s_1)\rho_1(s_2)$, yields $(1-p)(s_1 - v)\partial_{s_0}\rho_1(s_0)/\rho_1(s_0) = p(s_0 - v)\partial_{s_1}\rho_1(s_1)/\rho_1(s_1)$, which is false if $p \neq 1/2$.

Remark 1. By the model $A(y_1, y_2, y_3) = (1-p)y_1 - (1-2p)y_2 - py_3$, gap correlations are induced if $0 < p < 1/2$. By contrast, the step gaps are uncorrelated if $p = 1/2$.

4. Mean-field formalism

In this section, a self-consistent mean field is defined via exploiting the BBGKY hierarchy of (18) and (19) at the level of the one-gap density. This formulation will facilitate comparisons of a previous approach based on step gap independence [20] to results obtained in section 5.2 from an explicit large-N computation (see section 6.2).

4.1. Formal generalities

Consider the stochastic scheme (13). A goal is to reduce these *coupled* SDEs to a single SDE by slaving G_{i-1} and G_{i+1} to G_i through an (*a priori* unknown) function f [20]. A starting point is to introduce the stochastic processes $\widehat{\mathcal{G}}_i(t)$ satisfying

$$\mathrm{d}\widehat{\mathcal{G}}_i(t) = A(f(t,\widehat{\mathcal{G}}_i),\widehat{\mathcal{G}}_i,f(t,\widehat{\mathcal{G}}_i))\,\mathrm{d}t + \mathrm{d}\mathcal{B}_i(t), \qquad 0\leqslant i\leqslant N-1, \tag{25}$$

under the initial data $\widehat{\mathcal{G}}_i(0) = \mathcal{G}_i(0)$. The function $f(t,\,s)$ is to be determined (see definition 2). Assume that A and f are such that (25) is solvable. Note that (25) comes from (13) with replacement of the variables $\mathcal{G}_{i-1}$ and $\mathcal{G}_{i+1}$ by $f(t,\widehat{\mathcal{G}}_i)$.

Definition 2. *Suppose that $f = f^{\mathrm{mf}}$ exists such that this f^{mf} generates a probability density, $\widehat{\rho}_1(t,s;[f])$, for $\widehat{\mathcal{G}}_i(t)$ equal to the density $\rho_1(t,s)$ for $\mathcal{G}_i(t)$ in a weak sense (wk),*

$$\int \mathrm{d}s\;\rho_1(t,s)\,\vartheta(s) = \int \mathrm{d}s\;\widehat{\rho}_1(t,s;[f^{\mathrm{mf}}])\,\vartheta(s) \tag{26}$$

for every reasonably arbitrary (smooth) test function $\vartheta(s)$ and fixed time $t>0$. Then, f^{mf} is called the mean field for SDEs (13).

A way to introduce f^{mf} is this. By (25), for fixed initial data and reasonably arbitrary f, think of $\widehat{\rho}_1$ as a functional of f: $\widehat{\rho}_1 = \widehat{\rho}_1[f]$. By variations of f, it is presumed that there exists some $f = f^{\mathrm{mf}}$ for which $\widehat{\rho}_1[f^{\mathrm{mf}}] = \rho_1$. No guarantee is given here that this f^{mf} exists. Equation (26) has been invoked for *static* variables in other physical contexts, e.g., non-uniform liquids where f amounts to an external potential [39]. The BBGKY formalism here will allow us to place this idea in a dynamical context.

It is of interest to derive an (implicit) formula for f^{mf} via the BBGKY hierarchy of (18) and (19). One only needs to use evolution law (18) for ρ_1.

Proposition 1. *Suppose that a mean field f^{mf} exists. Then, f^{mf} is given by the formula*

$$A(f^{\mathrm{mf}}(s),s,f^{\mathrm{mf}}(s))\rho_1(s) = \int \mathrm{d}s_1'\,\mathrm{d}s_2'\,A(s_1',s,s_2')\,\rho_3(s_1',s,s_2') \quad (wk). \tag{27}$$

Proof. This follows directly from (18), (25) and (26). Note that $\widehat{\rho}_1(t,s;[f])$ obeys

$$\partial_t\widehat{\rho}_1 + \partial_s[A(f(t,s),s,f(t,s))\widehat{\rho}_1] = \tfrac{1}{2}\partial_s^2\widehat{\rho}_1. \tag{28}$$

The multiplication of (28) by a test function, $\phi(s)$, and integration result in

$$\partial_t\int \mathrm{d}s\;\widehat{\rho}_1\,\phi(s) - \frac{1}{2}\int \mathrm{d}s\;\widehat{\rho}_1\,\partial_s^2\phi = \int \mathrm{d}s\;\widehat{\rho}_1\,A\,\partial_s\phi \quad \forall\,\phi. \tag{29}$$

In view of (26), now replace f by f^{mf} and thus $\widehat{\rho}_1$ by ρ_1 in (29). A similar result involving ρ_3 is obtained via multiplication of (18) by $\phi(s)$ and subsequent integration. Equation (27) follows by comparison of (29) and its counterpart involving ρ_3 for $\widehat{\rho}_1 = \rho_1$. □

4.2. Growth model

If A is given by (20), then (27) is simplified to

$$\begin{aligned} K_{ab}(f^{\mathrm{mf}}(s)) &= \int \mathrm{d}s'\,[K_a(s')\rho_{1/2}(s',s) + K_b(s')\rho_{2/1}(s',s)] \\ &= \mathbb{E}[K_a(\mathcal{G}_a)\big|\mathcal{G}_b = s] + \mathbb{E}[K_b(\mathcal{G}_b)\big|\mathcal{G}_a = s] \qquad (s\in\mathbb{T}). \end{aligned} \tag{30}$$

Here, $\rho_{1/2}(s', s) \equiv \rho_2(s', s)/\rho_1(s)$ and $\rho_{2/1}(s', s) \equiv \rho_2(s, s')/\rho_1(s)$ are conditional probability densities for *any pair* of consecutive step gaps $(\mathcal{G}_a, \mathcal{G}_b)$, given that one of these gaps equals s. $\mathbb{E}[K_c(\mathcal{G}_c)\big|s]$ $(c = a,\ b)$ denotes the respective mean.

In the special case with the *linear* model $A(y_1, y_2, y_3) = (1-p)y_1 - (1-2p)y_2 - py_3$, $0 < p < 1/2$ (see section 5.2), (30) reduces to the more explicit formula

$$f^{\mathrm{mf}}(s) = (1-2p)^{-1}\{(1-p)\,\mathbb{E}[\mathcal{G}_a|\mathcal{G}_b = s] - p\mathbb{E}[\mathcal{G}_b|\mathcal{G}_a = s]\}. \tag{31}$$

4.2.1. Pair decorrelation approximation. By $\rho_2(s_0, s_1) \sim \rho_1(s_0)\,\rho_1(s_1)$, (31) entails $f^{\mathrm{mf}} \sim E[\mathcal{G}_a]$, where the gaps are taken identically distributed. This relation is consistent with the approach in [20]. Thus, the processes $\widehat{\mathcal{G}}_i$ satisfy [20]

$$\mathrm{d}\widehat{\mathcal{G}}_i = (1-2p)(\nu - \widehat{\mathcal{G}}_i)\,\mathrm{d}t + \mathrm{d}\mathcal{B}_i, \qquad \nu = \mathbb{E}[\mathcal{G}_i] = \mathcal{G}_i(0).$$

For fixed t, the solution is the Gaussian random variable with variance

$$\widehat{\sigma}_{\mathrm{pc}}(t)^2 = \int_0^t \mathrm{e}^{-2(1-2p)\tau}\,\mathrm{d}\tau = [2(1-2p)]^{-1}\{1 - \mathrm{e}^{-2(1-2p)t}\}, \tag{32}$$

in agreement with [20]. This approximation is further discussed in section 6.2.

5. Small fluctuations and large-N limit

SDEs (11) are now expanded for small fluctuations. The leading-order equations are treated explicitly as $N \to \infty$ for fixed $t > 0$ (see section 6.1 for an extension). Deviations of $\mathcal{G}_i(t)$ from their initial value $\nu \equiv \aleph_i = v\varpi/(2D)$ are small in the sense $1 - \mathrm{Prob}[\sup_{t\in[0,T)} |\mathcal{G}(t) - \aleph| \ll |\aleph|] \ll 1$.[5] Set $\aleph = (\aleph_0, \ldots, \aleph_{N-1})$.

In the following, it is assumed that material parameter groups—which depend on F and enter through ν coefficients of related SDEs—are fixed, i.e. independent of the deviation of $\mathcal{G}_i$ from $\mathbb{E}[\mathcal{G}_i]$. So, the fluctuation of $\mathcal{G}_i$, which depends on F, is considered as controllable mainly by the time t, where $t \in [0, T)$ for some suitable T, while $\nu = O(1)$.

5.1. Small-fluctuation expansion

Apply the substitution

$$\mathcal{G}(t) = \aleph + \bar{\mathcal{G}}(t); \qquad \aleph = \mathcal{G}(0), \qquad \bar{\mathcal{G}}(0) = 0.$$

Equation (11) leads to

$$\begin{aligned}\mathrm{d}\bar{\mathcal{G}}_i = \big\{&(1-p)(\bar{\mathcal{G}}_{i+1} - \bar{\mathcal{G}}_i) + p(\bar{\mathcal{G}}_i - \bar{\mathcal{G}}_{i-1}) + q_1\big(\bar{\mathcal{G}}_{i+1}^2 + \bar{\mathcal{G}}_{i-1}^2 - 2\bar{\mathcal{G}}_i^2\big)\\ &- q_2\big(\bar{\mathcal{G}}_{i+1}^3 + \bar{\mathcal{G}}_{i-1}^3 - 2\bar{\mathcal{G}}_i^3\big) + O\big(\bar{\mathcal{G}}_{i-1}^4, \bar{\mathcal{G}}_i^4, \bar{\mathcal{G}}_{i+1}^4\big)\big\}\,\mathrm{d}t + \mathrm{d}\mathcal{B}_i(t).\end{aligned} \tag{33}$$

The parameter $p = O(1)$ is defined by

$$p = \frac{1}{2}\left(\frac{\nu}{\sinh^2\nu} - \frac{e^{-\nu}}{\sinh\nu}\right), \tag{34}$$

in accord with [20], whereas q_1 and q_2 are not needed for our purposes. Expansion (33) can be extended to higher orders, but the algebra becomes increasingly cumbersome.

[5] The term *small fluctuations* refers to deviations of $\mathcal{G}(t)$ from $\mathcal{G}(0)$, rather than from the mean $\mathbb{E}[\mathcal{G}(t)]$ as is, strictly speaking, more appropriate. This distinction is practically unimportant here [20].

Equation (33) is now simplified via the formal expansion $\bar{\mathcal{G}}(t) \sim \sum_{j=0}^{k-1} \bar{\mathcal{G}}^{(j)}(t)$ where $k = 3$ and $1 - \text{Prob}[\sup|\bar{\mathcal{G}}^{(j+1)}(t)| \ll \sup|\bar{\mathcal{G}}^{(j)}(t)|] \ll 1$.[6] The $\bar{\mathcal{G}}_i^{(0)}$ satisfy

$$\mathrm{d}\bar{\mathcal{G}}_i^{(0)} = \left[(1-p)\left(\bar{\mathcal{G}}_{i+1}^{(0)} - \bar{\mathcal{G}}_i^{(0)}\right) + p\left(\bar{\mathcal{G}}_i^{(0)} - \bar{\mathcal{G}}_{i-1}^{(0)}\right)\right]\mathrm{d}t + \mathrm{d}\mathcal{B}_i(t), \tag{35}$$

with the initial condition $\bar{\mathcal{G}}_i^{(0)}(0) = 0$. Higher order equations of the $\bar{\mathcal{G}}^{(j)}$-cascade are linear but not considered here. Equation (35) forms the basis of the perturbation scheme.

5.2. *One-gap variance to zeroth order: derivation for $t = O(1)$, $N \to \infty$*

Next, (35) is solved as $N \to \infty$ (see proposition 2). Note that, by (34), $p(\nu) \uparrow 1/2$ as $\nu \downarrow 0$; $p \downarrow 0$ as $\nu \to \infty$ and $\mathrm{d}p(\nu)/\mathrm{d}\nu < 0$ for $\nu > 0$. Hence, we have $0 < p < 1/2$ for $\nu > 0$. By Taylor expansion, we obtain $p = 1/2 - \nu/3 + O(\nu^2)$ as $\nu \downarrow 0$.[7]

So, consider $0 < p < 1/2$. Equation (35) is recast to the vector form

$$\mathrm{d}\bar{\mathcal{G}}^{(0)}(t) = -\mathbf{A}(p)\cdot\bar{\mathcal{G}}^{(0)}(t)\,\mathrm{d}t + \mathrm{d}\mathcal{B}(t), \qquad \bar{\mathcal{G}}^{(0)}(0) = 0 \qquad (\bar{\mathcal{G}}^{(0)} \in \mathbb{T}^N), \tag{36}$$

where $\mathbf{A} = [A_{i,k}]_{0\leqslant i,k\leqslant N-1}$ is a sparse *circulant* matrix. The first row ($i = 0$) of $\mathbf{A}$ has zero entries *except* $A_{0,k} = 1 - 2p$ if $k = 0$; $-(1-p)$ if $k = 1$ and p if $k = N-1$. The remaining rows ($1 \leqslant i \leqslant N-1$) form *cyclic permutations* of the first row. Set

$$\mathbf{A}(p) \equiv \mathbf{A}_0(p) + (1-2p)\mathbf{1},$$

where $\mathbf{1}$ denotes the $N \times N$ unit matrix. So, the first row ($i = 0$) of the circulant matrix $\mathbf{A}_0 = [(A_0)_{i,k}]$ has entries $(A_0)_{0,k} = -(1-p)$ if $k = 1$; p if $k = N-1$ and 0 otherwise.

Evidently, the solution to (36) is written as

$$\bar{\mathcal{G}}^{(0)}(t) = \int_0^t \mathrm{e}^{-\mathbf{A}(t-\tau)}\,\mathrm{d}\mathcal{B}(\tau) = \int_0^t \mathrm{e}^{-(1-2p)(t-\tau)}\,\mathrm{e}^{-\mathbf{A}_0(t-\tau)}\,\mathrm{d}\mathcal{B}(\tau). \tag{37}$$

Thus, the mean is $\mathbb{E}[\bar{\mathcal{G}}^{(0)}(t)] = 0$, by the known property $\mathbb{E}[\mathrm{d}\mathcal{B}(\tau)] = 0$.

Remark 2. By (37), each component $\bar{\mathcal{G}}_i^{(0)}$ of $\bar{\mathcal{G}}^{(0)}(t)$ is a sum of increments of linear superpositions of 1D independent Brownian motions. Thus, for fixed t and p, $\bar{\mathcal{G}}_i^{(0)}(t)$ are, in principle correlated, Gaussian variables with zero mean.

Therefore, it suffices to compute the variance, ${\sigma_i^{(0)}}^2$, of each $\bar{\mathcal{G}}_i^{(0)}(t)$. By (37), this variance is i-independent and given by

$$\sigma^{(0)}(t)^2 = \mathbb{E}\left[\bar{\mathcal{G}}_i{}^{(0)}(t)^2\right] = \int_0^t \mathrm{e}^{-2(1-2p)\tau}|\mathrm{e}^{-\mathbf{A}_0\tau}|^2\,\mathrm{d}\tau, \tag{38}$$

where $|C|^2$ denotes the magnitude squared of any row-vector of the circulant matrix C. Given $\sigma^{(0)}$, and in view of remark 2, the density of any step gap is

$$\rho_1(t,s) \approx \rho_1^{(0)}(t,s) = \frac{1}{\sqrt{2\pi\sigma^{(0)}(t)^2}}\exp\left\{-\frac{(s-\nu)^2}{2\sigma^{(0)}(t)^2}\right\}, \tag{39}$$

where $\approx$ is used loosely to imply that the difference of the two sides approaches 0 in the limit of small fluctuations.

[6] It appears perhaps paradoxical that no small parameter is involved in this expansion. To remedy this, consider $\mathrm{d}\mathcal{B}_i(t)$ as small. For instance, multiply $\mathrm{d}\mathcal{B}_i$ by a (presumably temperature-dependent) parameter $\bar{\epsilon}$, $\bar{\epsilon} \ll 1$. Expand $\bar{\mathcal{G}}(t) \sim \bar{\epsilon}\sum_{j=0}^{k-1}\bar{\epsilon}^j\,\bar{\mathcal{G}}^{(j)}(t)$. The interpretation of the perturbation scheme is the subject of work in progress. Related rigorous theory can be found in Freidlin and Wentzell [40].

[7] The symbol $x \downarrow a$ ($x \uparrow a$) implies that x approaches a from the right (left).

To explicitly compute $\sigma^{(0)}$, consider $t = O(1)$ and set

$$\mathrm{e}^{-\mathbf{A}_0 t} = \sum_{n=0}^{\infty} (-1)^n \frac{\mathbf{A}_0^n t^n}{n!} \sim \sum_{n=0}^{N-1} (-1)^n \frac{\mathbf{A}_0^n t^n}{n!}, \qquad N \gg 1. \tag{40}$$

This replacement is justified provided $\mathbf{A}_0$ has a finite norm and the series converges accordingly as $N \to \infty$ [8] [41]. Note that the n in the summand of *finite* sum (40) does not exceed the dimension of $\mathbf{A}_0$.

The large-N computation of $\mathrm{e}^{-\mathbf{A}_0 t}$ on the basis of (40) is outlined in two lemmas (lemmas 1 and 2), proved in appendix A.

Lemma 1. *The circulant matrix $\mathbf{A}_0^n$ has the first-row entries*

$$\left(\mathbf{A}_0^n\right)_{0,k} = \sum_{j=0}^{n} (-1)^{n-j} p^j (1-p)^{n-j} \binom{n}{j} \delta^n_{k+2j}; \qquad \binom{n}{j} = \frac{n!}{j!(n-j)!},$$

δ^n_k is Kronecker's delta, modulo N ($\delta^n_{k+lN} = \delta^n_k$ for any integer l), and $0 \leqslant j, n \leqslant N-1$.

Lemma 2. *For large N, the matrix $\mathrm{e}^{-\mathbf{A}_0 t}$ has the first-row entries*

$$(\mathrm{e}^{-\mathbf{A}_0 t})_{0,k} \sim \left(\frac{1-p}{p}\right)^{k/2} J_k(\check{t}) + (-1)^{N-k} \left(\frac{p}{1-p}\right)^{\frac{N-k}{2}} J_{N-k}(\check{t}),$$

where $\check{t} = 2[p(1-p)]^{1/2} t$ and J_k is the kth-order Bessel function [42]. This approximation is interpreted in the sense of an appropriate matrix norm [41].

Some requisite formulas involving Bessel functions are derived in appendix B. A few observations on properties of the matrix $\mathrm{e}^{-\mathbf{A}_0 t}$ are outlined in appendix C. In particular, it is shown that lemma 2 is consistent with $\det(\mathrm{e}^{-\mathbf{A}_0 t}) = 1$, valid for *all* N and t.

It remains to compute the one-gap variance via (38) and lemma 2. Note that

$$|\mathrm{e}^{-\mathbf{A}_0 \tau}|^2 \sim \sum_{k=-N}^{N-1} \left(\frac{1-p}{p}\right)^k J_k(\check{\tau})^2 + 2 \sum_{k=0}^{N-1} (-1)^{N-k} \left(\frac{1-p}{p}\right)^{\frac{2k-N}{2}} J_k J_{N-k}(\check{\tau})$$

$$\sim \sum_{k=-\infty}^{\infty} \left(\frac{1-p}{p}\right)^k J_k(\check{\tau})^2 = I_0[2(1-2p)\tau], \qquad \check{\tau} = 2\sqrt{p(1-p)}\tau,$$

with recourse to appendix B, where I_k is the kth-order modified Bessel function of the first kind [42]. The following result is obtained directly by use of an integral of I_0 [42].

Proposition 2. *For $N \to \infty$ and fixed t, the leading-order variance of each gap is*

$$\sigma^{(0)}(t)^2 \sim t\, \mathrm{e}^{-2(1-2p)t} [I_0(2(1-2p)t) + I_1(2(1-2p)t)]. \tag{41}$$

For an extension of this result to arbitrarily large values of t, see section 6.1.

For fixed t, the density ρ_1 of any step gap is given by (39). Formula (41) diverges as $O(\sqrt{t/(1-2p)})$ if $(1-2p)t \gg 1$. Hence, the system does not settle to a steady state.

The procedure leading to (41) is questionable if t is of the order of N or larger. Most importantly, the stochastic model needs to be revised if $\sigma^{(0)} > \nu$. Then, the step-crossing probability is appreciable and step interactions must be included. If $\sigma^{(0)} \ll \nu$ (say, for sufficiently small times or large ν), the present model provides a reasonable description for fixed t. Compare (41) to the mean-field result (32) (see section 6.2).

[8] Consider the weak (Hilbert-Schmidt) norm, $|\cdot|_2$: for an $N \times N$ matrix A, $|A|_2 \equiv (N^{-1} \sum_{i,k} |(A)_{i,k}|^2)^{1/2}$. For a circulant matrix C, $|C|_2 = |C|$ where $|\cdot|$ is introduced in (38). Note that $|\mathbf{A}_0| = [p^2 + (1-p)^2]^{1/2} < \infty$. In this metric, the remainder in (40) approaches 0 as $N \to \infty$.

6. Extension and discussion

In this section, the terrace width variance is computed for arbitrary $t > 0$ within the linear model (36). In addition, the exact result is compared to mean-field formula (32), also derived in [20]. The neglect of step interactions, and possible connections of the present approach to experiments and other models are also discussed.

6.1. Extension: exact variance for arbitrary N and t > 0

To explore the limitations of model (36), we study how the gap variance behaves if t and N are unrestricted. The methodology leading to proposition 2 (section 5.2) must be modified since in that approach the limits $N \to \infty$ and $t \to \infty$ do not commute. In particular, (40) is inapplicable if t is larger than $O(N)$.

Consider formula (38) for the variance. The key idea here is to use the relation [41]

$$|\mathrm{e}^{-\mathbf{A}_0 t}|^2 = N^{-1}\,\mathrm{tr}[(\mathrm{e}^{-\mathbf{A}_0 t})^T\,\mathrm{e}^{-\mathbf{A}_0 t}] = N^{-1}\,\mathrm{tr}[\mathrm{e}^{-(\mathbf{A}_0^T+\mathbf{A}_0)t}] = N^{-1}\sum_{k=0}^{N-1}\mathrm{e}^{-\widetilde{\lambda}_k t},$$

since $\mathbf{A}_0$ and its transpose, $\mathbf{A}_0^T$, commute. The set $\{\widetilde{\lambda}_k\}$ consists of all eigenvalues of the circulant $\mathbf{A}_0 + \mathbf{A}_0^T$, and is the discrete Fourier transform of its first row. We compute $\widetilde{\lambda}_k = -2(1-2p)\cos(2\pi k/N)$. By substitution in (38), we obtain

$$\sigma^{(0)}(t)^2 = N^{-1}\sum_{k=0}^{N-1}\frac{1-\mathrm{e}^{-2(1-2p)[1-\cos(2\pi k/N)]t}}{2(1-2p)[1-\cos(2\pi k/N)]}. \tag{42}$$

The task is to evaluate (42) when *t and N* are large. Distinguish the following cases.

Case $0 \leqslant (1-2p)t \leqslant O(1)$: sum (42) is converted to an integral by use of the continuous variable $\psi = 2\pi k/N$, where $2\pi/N \to \mathrm{d}\psi$ and $0 \leqslant \psi < 2\pi$ as $N \to \infty$:

$$\sigma^{(0)}(t)^2 \sim \int_0^{2\pi}\frac{\mathrm{d}\psi}{2\pi}\frac{1-\mathrm{e}^{-2(1-2p)(1-\cos\psi)t}}{2(1-2p)(1-\cos\psi)} = \int_0^t \mathrm{d}\tau\int_0^{2\pi}\frac{\mathrm{d}\psi}{2\pi}\,\mathrm{e}^{-2(1-2p)(1-\cos\psi)\tau},$$

which reduces to (41) by integration. Hence, this alternate procedure confirms proposition 2. Further, it can be inferred that the correction term for $\sigma^{(0)}(t)^2$ is $O(1/N)$.

Case $(1-2p)t \gg 1$: the major contribution to sum (42) comes from the vicinity of $n = 0,\ N-1$. Then, by $1-\cos(2\pi n/N) \sim 2\pi^2 n^2/N^2$ the sum reduces to

$$\sigma^{(0)}(t)^2 \sim \frac{2t}{N}\left[1+\sum_{n=1}^{\infty}\frac{1-\mathrm{e}^{-\zeta(t)n^2}}{\zeta(t)n^2}\right], \qquad \zeta(t) \equiv \frac{4\pi^2(1-2p)t}{N^2}. \tag{43}$$

It has been impossible to simplify this formula if $\zeta(t) = O(1)$, i.e. $(1-2p)t = O(N^2)$ or $\sigma^{(0)}(t)^2 = O(N)$. The underlying stochastic model is not reliable if $\sigma^{(0)}(t) > \nu$, since negative terrace widths are predicted with appreciable probability. On the other hand, having $\sigma^{(0)} < \nu$ in this regime would imply that ν may be too large for the BCF theory to be meaningful. Note that the size(N)-dependent result (43) has been influenced by the assumed boundary conditions.

As a check, take $\zeta(t) \ll 1$ in (43). Then, $\sigma^{(0)}(t)^2 \sim \sqrt{t/(\pi(1-2p))}$, which matches the limit of proposition 2. Thus, (43) connects smoothly to the fixed-t behavior of ${\sigma^{(0)}}^2$.

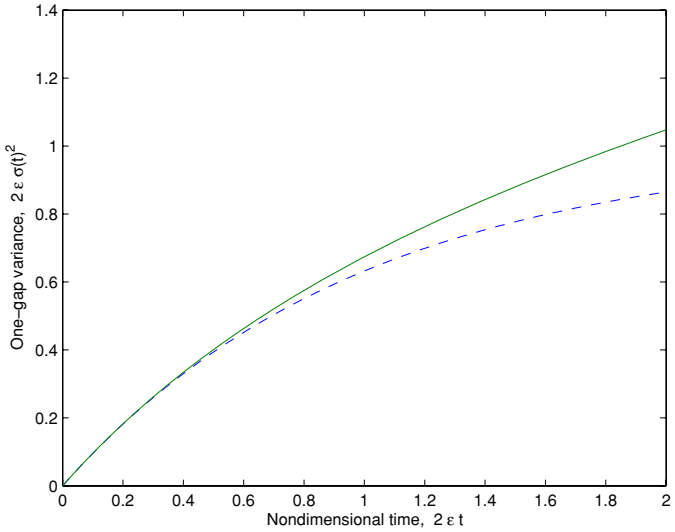

Figure 2. Two (scaled) variances, as functions of $2\epsilon t$ ($\epsilon = 1 - 2p$), for model (11) under small fluctuations: (i) $2\epsilon\sigma^{(0)}(t)^2$ (solid line), by (41) from explicit large-N limit; and (ii) $2\epsilon\widehat{\sigma}_{\rm pc}(t)^2$ (dashed line), by (32) via mean field under two-gap independence.

6.2. *Comparison to mean-field variance*

The mean field is defined rigorously via the pair density ρ_2 (see (27)). The independence ansatz $\rho_2(s_0, s_1) \sim \rho_1(s_0)\rho(s_1)$, which underlies the approximation in [20], provides an appealing alternative to fully computing ρ_2 for $N \gg 1$. We next show *how* terrace correlations cause deviations of the one-gap variance from its mean-field approximation.

Figure 2 depicts the two (scaled) variances as functions of $2(1-2p)t$. The discrepancy between them implies that two consecutive step gaps are *correlated* for $t > 0$, regardless of how large N is. The analysis indicates that a plausible 'measure' of gap correlation is $\left[\sigma^{(0)^2} - \widehat{\sigma}_{\rm pc}^2\right]/t$. For $2(1-2p)t \ll 1$, we find [42]

$$\begin{aligned}
&\widehat{\sigma}_{\rm pc}(t)^2 = \frac{1}{2\epsilon}(1 - {\rm e}^{-2\epsilon t}) = t\left[1 - \epsilon t + \frac{2}{3}\epsilon^2 t^2 + O(\epsilon^3 t^3)\right],\\
&\sigma^{(0)}(t)^2 = t\left[1 - \epsilon t + \epsilon^2 t^2 + O(\epsilon^3 t^3)\right], \qquad \epsilon \equiv 1 - 2p,\\
&\qquad \Rightarrow \ \frac{\sigma^{(0)}(t)^2 - \widehat{\sigma}_{\rm pc}(t)^2}{t} = \frac{1}{3}\epsilon^2 t^2 + O(\epsilon^3 t^3). \qquad (44)
\end{aligned}$$

Note the influence of p: as p gets closer to the value $1/2$ ($\epsilon \downarrow 0$) of the reference case (definition 1), i.e. as the deposition flux decreases, correlations tend to disappear.

6.3. *Step interactions under small fluctuations*

Thus far, we have neglected step interactions. If repulsive elastic-dipole and entropic interactions are included in the deterministic equations, $C_i^{\rm eq}$ in (4) is expressed as [2]

$$C_i^{\rm eq} = C_s {\rm e}^{\mu_i/T}, \qquad \mu_i = \xi a^3\left(g_i^{-3} - g_{i-1}^{-3}\right),$$

where μ_i is the step chemical potential, and ξ and C_s are positive constants.

For small fluctuations, μ_i can be expanded around $g_i(0) = \varpi$. If $\mu_i \ll T$, which is typical in semiconductor vicinal surfaces [2], the ith step equilibrium density is

$$C_i^{\rm eq} \sim C_s \left[1 + \frac{3\xi a^3}{\varpi^4 T}(g_{i-1} + g_i)\right]. \tag{45}$$

By inspection of (7), (8) and (45), the SDEs for gaps acquire terms proportional to $(a/\varpi)^3(aC_s)(\xi/T)\mathcal{G}_{i\pm 2}\mathrm{e}^{\pm v\mathcal{G}_{i\pm 1}/(2D)}$; cf (11). By $aC_s \leqslant 1$, these terms are deemed negligible if $(\xi/T)\,(a/\varpi)^3 \ll 1$. The last condition is met in typical situations. For example, for Si(1 1 1), by table I in [43] we obtain $\xi/T \sim 1$ at $T \sim 1000\,\mathrm{K}$ while $a/\varpi \lesssim 0.1$. This estimate indicates that the neglect of step interactions, which simplifies the analysis, can be made compatible with the small-fluctuation limit.

The effect of the *singularity* in the step interactions remains unexplored. It can be conjectured that the gap density $\rho_1(s,t)$ and all its derivatives approach zero rapidly as $s \downarrow 0$ while $\rho_1 \equiv 0$ for $s < 0$. This result can be derived by a heuristic mean-field approximation but has not been proved rigorously. Our discussion implies that if the standard deviation of each terrace is much smaller than the mean gap, the actual behavior of ρ_1 at $s = 0$ should not affect the predictions of the linear model practically.

6.4. Models of noise and connection to experiments

Next, we comment on a few other models of noise and plausible connections of the present approach to laboratory experiments.

6.4.1. Modeling noise. Within our zeroth-order model, the fluctuation of the total length of the step train grows with time. Specifically, $N^{-1}\sum_{i=0}^{N-1}\bar{\mathcal{G}}_i = \bar{\mathcal{G}}_{\rm av} \sim \bar{\mathcal{G}}_{\rm av}^{(0)}$ satisfies the SDE $\mathrm{d}\bar{\mathcal{G}}_{\rm av}^{(0)}(t) = N^{-1}\sum_i \mathrm{d}\mathcal{B}_i(t)$, which has solution $\bar{\mathcal{G}}_{\rm av}^{(0)}(t) = N^{-1}\sum_i \mathcal{B}_i(t)$, with variance t/N. This feature is consistent with the divergence of the one-gap variance found in section 6.1. By contrast, if white noise is added to the equations of motion for step *positions*, noise terms mutually cancel in adding all equations for the time derivatives of terrace widths. Hence, $\sum_{i=0}^{N-1}\mathrm{d}\bar{\mathcal{G}}_i^{(0)}(t) = 0$ which yields $\mathcal{G}_{\rm av}^{(0)}(t) = v$. In this case, it can be shown that the one-gap variance approaches a finite limit for large t [44].

Williams and Krishnamurty [32] proposed related SDEs encapsulating fluctuations in the number of atoms adsorbed on terraces. Slightly modified, their SDEs read

$$\begin{aligned}\mathrm{d}\mathcal{G}_i(t) = {} & [(1-p)(\mathcal{G}_{i+1} - \mathcal{G}_i) + p(\mathcal{G}_i - \mathcal{G}_{i-1})]\,\mathrm{d}t + \sqrt{(1-p)\mathcal{G}_{i+1}}\,\mathrm{d}\mathcal{B}_{i+1}(t) \\ & + (\sqrt{p} - \sqrt{1-p})\sqrt{\mathcal{G}_i}\,\mathrm{d}\mathcal{B}_i(t) - \sqrt{p\,\mathcal{G}_{i-1}}\,\mathrm{d}\mathcal{B}_{i-1}(t).\end{aligned} \tag{46}$$

Hence, $\sum_i \mathcal{G}_i(t) = \text{const.}$ via cancelation of the noise terms. It is expected that the gap variance from this model approaches a finite limit for long times.

The consideration of $\mathcal{G}_i$-dependent (multiplicative) noise, e.g. equation (46), brings forth the issue of what is the proper interpretation of the stochastic integrals. An appealing feature of the Itô (versus, say, Stratonovich) calculus is, e.g. the property that each gap $\mathcal{G}_i(t)$ satisfies $\mathbb{E}[\mathcal{G}_i(t)\mathrm{d}\mathcal{B}_i(t)] = 0$, $\mathbb{E}\big[\big(\int_0^t \mathcal{G}_i(t')\,\mathrm{d}\mathcal{B}_i(t')\big)^2\big] = \mathbb{E}\big[\int_0^t \mathcal{G}_i(t')^2\,\mathrm{d}t'\big]$.

It is tempting to compare our choice of white noise, $\mathcal{N}_i(t) = \mathrm{d}B_i(t)/dt$, to the random force for step meandering in two space dimensions (2D), used, e.g., in [34]. Here, we suppress any dependence on the position along a step (eliminating meandering). Thus, the noise autocorrelation function involves only the time variable, and thus differs from the model in [34], where the noise is white in both time and position along the step. In the same vein, we have not tried to fix the noise coefficient via any fluctuation-dissipation theorem [34].

Our formulation, where noise is added to the equations of motion for terrace widths, is distinct from the work by Pierre-Louis and Misbah [30, 33]. These authors add explicitly Langevin forces to the adatom diffusion equation and to the boundary conditions for atom attachment–detachment at steps. Their approach offers a thermodynamically self-consistent model for step meandering in 2D [30]. The addition of noise at the level of adatom diffusion apparently leads to SDEs different from (1). An appealing feature of our approach, as in [20], lies in the ease of defining a mean field for the *coupled motion* of many steps. The incorporation of richer Langevin terms in the spirit of [30] for small fluctuations is more elaborate and left for future work.

6.4.2. Possible connection to experiments. Our analysis complements [20] where narrowing of the terrace width distribution with increasing flux F is pointed out via mean-field theory and kinetic Monte Carlo simulations. In [20] the focus is the steady state of the distribution. Here, we describe the *transient behavior* of the gap density. This result may be relevant to the distribution narrowing observed by reflection electron microscopy on Si(1 1 1) at $T \approx 1370$ K [45] (as is also mentioned in [20]).

7. Conclusion

An N-dimensional SDE system for terraces on vicinal crystals was studied analytically with emphasis on the terrace width variance for large N. In the small-fluctuation limit, the SDE system was linearized. The resulting equations involve a parameter, p, that expresses asymmetry in the adatom kinetics. For $p = 1/2$, the process is symmetric. The present paper complements the recent work by Hamouda *et al* [20] who applied kinetic Monte Carlo simulations and mean-field ideas to predict narrowing of the one-gap density with increasing deposition flux.

The stochastic model was analyzed from two perspectives. First, a BBGKY hierarchy was formulated for joint probability gap densities. The hierarchy forms a basis for defining a self-consistent mean field in terms of the two-gap density (ρ_2). By an ansatz of gap decorrelation, this mean field reduces to a simple form invoked previously, e.g., in [20, 32]. In the symmetric case, $p = 1/2$, the mean-field density becomes exact.

Second, the one-gap variance was computed for all times $t > 0$ when N is large. The analysis shows how *nonzero* values of $1 - 2p$ induce correlations, and thus cause the variance to deviate from its mean-field limit. If $p \neq 1/2$ and (the nondimensional) t is large yet $t < O(N)$, the exact variance of the linear model diverges as $O(\sqrt{t})$. In contrast, the mean-field variance approaches a finite value, in qualitative agreement with kinetic Monte Carlo simulations [20]. The variance was also computed for $t \geqslant O(N)$.

The BBGKY hierarchy may offer a systematic procedure for predicting features of several-terrace-width distributions. The mean field provides an approximation at the level of the two-gap correlation. Finer approximations may be introduced at the level of higher correlations. This direction should be further explored.

This work admits extensions, has limitations and points to pending issues. The large-t limit of the gap variance depends on the assumptions for the noise term. By adding properly periodic white noise, so that the total length of the step train is constant, the variance can approach a finite value. An open problem is to justify rigorously the small-fluctuation expansion. The expansion is questionable when the standard deviation becomes comparable to the terrace width mean. This calls for including energetic and entropic step repulsions to enforce a non-crossing condition for steps.

Actual steps and terraces are of course two dimensional, giving rise to much richer phenomena [46]. The (1+1)-dimensional model fails to capture important features such as step meandering. The linkage of the kinetic formalism adopted herein with settings in 2D is left for future work. This aspect is truly crucial for making predictions for lab experiments and kinetic Monte Carlo simulations.

Acknowledgments

I am indebted to T L Einstein for bringing [20] to my attention and making valuable remarks on the manuscript. I wish to thank A Pimpinelli, A E Tzavaras and J D Weeks for useful conversations. Special thanks are due to P Patrone, K Spiliopoulos and R Wang. This research was supported by NSF under grant DMS-0847587.

Appendix A. Proofs of lemmas 1 and 2

(Proof of lemma 1). Since $\mathbf{A}_0$ is a circulant matrix, so is $\mathbf{A}_0^n$ for every $n \geqslant 0$. From the definition of $\mathbf{A}_0$, the first-row elements of $\mathbf{A}_0^n$ ($n \geqslant 1$) satisfy the difference scheme

$$\left(A_0^n\right)_{0,k} = -(1-p)\left(A_0^{n-1}\right)_{0,k-1} + p\left(A_0^{n-1}\right)_{0,k+1}; \qquad \left(A_0^0\right)_{0,k} = \delta_k^0. \quad \text{(A.1)}$$

The main statement of lemma 1 then follows by induction in n.

For $n = 0$, lemma 1 holds trivially. So, assume that, for some $n \geqslant 0$,

$$\left(A_0^n\right)_{0,k} = \sum_{j=0}^{n} (-1)^{n-j} p^j (1-p)^{n-j} \binom{n}{j} \delta_{k+2j}^n, \qquad 0 \leqslant k \leqslant N-1,$$

and proceed to show that this is also true for $n \Rightarrow n+1$. By (A.1), $\left(A_0^{n+1}\right)_{0,k}$ is (by omission of the index $i = 0$ indicating first row)

$$\begin{aligned}
\left(A_0^{n+1}\right)_k &= -(1-p)\left(A_0^n\right)_{k-1} + p\left(A_0^n\right)_{k+1} \\
&= \sum_{j=0}^{n} (-1)^{n-j+1} p^j (1-p)^{n-j+1} \binom{n}{j} \delta_{k+2j}^{n+1} \\
&\quad + \sum_{j=1}^{n+1} (-1)^{n+1-j} p^j (1-p)^{n-j+1} \binom{n}{j-1} \delta_{k+2j}^{n+1} \\
&= \sum_{j=1}^{n} (-1)^{n+1-j} p^j (1-p)^{n+1-j} \left[\binom{n}{j} + \binom{n}{j-1} \right] \delta_{k+2j}^{n+1} \\
&\quad + (-1)^{n+1} (1-p)^{n+1} \delta_k^{n+1} + p^{n+1} \delta_{k+2n+2}^{n+1} \\
&= \sum_{j=0}^{n+1} (-1)^{n+1-j} p^j (1-p)^{n+1-j} \binom{n+1}{j} \delta_{k+2j}^{n+1}.
\end{aligned}$$

The last equation ensures that lemma 1 holds for all $n \geqslant 0$ and concludes the proof. □

(Proof of lemma 2). For definiteness, set $N = 2M + 1$: odd. The proof is very similar for even N and hence is omitted. The plan is to use formula (40) for large N in conjunction with lemma 1, noting that

$$\left(A_0^n\right)_k = \sum_{\substack{j \\ k+2j = n \bmod N}} (-1)^{n-j} p^j (1-p)^{n-j} \binom{n}{j}.$$

Thus, having $0 \leqslant n \leqslant N-1$ simplifies the evaluation of this sum, since there are at most two contributing values of j. These values are: (i) $j = (n-k)/2$ provided $n \geqslant k$ and $n-k$: even; (ii) $j = (N+n-k)/2$ if $n+k \geqslant N$ and $n-k$: odd. Hence,

$$\left(A_0^n\right)_k = \begin{cases} p^{\frac{n-k}{2}}[-(1-p)]^{\frac{n+k}{2}}\binom{n}{\frac{n-k}{2}}, & n-k: \text{even}, \qquad n \geqslant k, \\ p^{\frac{n+N-k}{2}}[-(1-p)]^{\frac{n-N+k}{2}}\binom{n}{\frac{n+N-k}{2}}, & n-k: \text{odd}, \qquad n+k \geqslant N, \\ 0, & \text{otherwise}. \end{cases}$$

By (40), the kth first-row element of the circulant matrix $\mathrm{e}^{-\mathbf{A}_0 t}$ is given by

$$(\mathrm{e}^{-\mathbf{A}_0 t})_k \sim \sum_{\substack{n \leqslant N-1 \\ n:\text{even}}} \frac{t^n}{n!}\left(A_0^n\right)_k - \sum_{\substack{n \leqslant N-1 \\ n:\text{odd}}} \frac{t^n}{n!}\left(A_0^n\right)_k.$$

Distinguish the cases $k = 2l$ and $k = 2l+1$, where $0 \leqslant k \leqslant N-1$. For $k = 2l$,

$$\begin{aligned}(\mathrm{e}^{-\mathbf{A}_0 t})_{k=2l} \sim & \sum_{\substack{m=l \\ (n=2m)}}^{M} (-1)^{m+l} t^{2m} \frac{p^{m-l}(1-p)^{m+l}}{(m-l)!(m+l)!} \\ & - \sum_{\substack{m=M-l \\ (n=2m+1)}}^{M-1} (-1)^{m-M+l} \frac{t^{2m+1} p^{M+m-l+1}(1-p)^{m-M+l}}{(M+1+m-l)!(m-M+l)!} \\ = & [(1-p)t]^{2l} \sum_{m=0}^{M-l} \frac{[-p(1-p)t^2]^m}{m!\Gamma(m+2l+1)} \\ & - (pt)^{2(M-l)+1} \sum_{m=0}^{l-1} \frac{[-p(1-p)t^2]^m}{m!\Gamma(m+2(M-l)+2)} \qquad \text{as } M \to \infty,\end{aligned}$$

where $\Gamma(z)$ is the Gamma function. The first sum of the last equation is negligible if $l = O(M)$ and is evaluated for $l = O(1)$. In the same vein, the second sum above is negligible if $l = O(1)$ and is now evaluated for $M - l = O(1)$. In these considerations, $p(1-p)t^2$ is kept fixed (finite). Hence, for reasonably all l $(0 \leqslant l \leqslant M)$,

$$\begin{aligned}(\mathrm{e}^{-\mathbf{A}_0 t})_{k=2l} \sim & [(1-p)t]^{2l} \sum_{m=0}^{\infty} (-1)^m \frac{[p(1-p)t^2]^m}{m!\Gamma(m+2l+1)} \\ & - (pt)^{2(M-l)+1} \sum_{m=0}^{\infty} (-1)^m \frac{[p(1-p)t^2]^m}{m!\Gamma(m+2(M-l)+2)} \\ = & \left(\frac{1-p}{p}\right)^{k/2} J_k(\check{t}) - \left(\frac{p}{1-p}\right)^{\frac{N-k}{2}} J_{N-k}(\check{t}), \qquad k: \text{even},\end{aligned}$$

where $\check{t} = 2\sqrt{p(1-p)}\,t$ and J_k is the kth-order Bessel function [42].

For $k = 2l+1$, the analogous computation for $0 \leqslant l \leqslant M-1$ reads

$$\begin{aligned}(\mathrm{e}^{-\mathbf{A}_0 t})_{k=2l+1} \sim & \sum_{m=M-l}^{M} (-1)^{m+l-M} t^{2m} \frac{p^{M+m-l}(1-p)^{m-M+l}}{(M+m-l)!(m+l-M)!} \\ & + \sum_{m=l}^{M-1} (-1)^{l+m} \frac{t^{2m+1} p^{m-l}(1-p)^{m+l+1}}{(m-l)!(m+1+l)!} \\ \sim & \left(\frac{p}{1-p}\right)^{\frac{N-k}{2}} J_{N-k}(\check{t}) + \left(\frac{1-p}{p}\right)^{k/2} J_k(\check{t}), \qquad k: \text{odd}.\end{aligned}$$

This concludes the proof of lemma 1 for odd N. The case with even N is treated similarly. □

Appendix B. On series of Bessel functions

This appendix addresses the computation of two power series and an integral involving Bessel functions, which are needed in section 5 and in appendix C.

First, consider the known Fourier series [42]

$$S_1(z = \mathrm{e}^{\mathrm{i}\theta};\, \eta) = \sum_{k=-\infty}^{\infty} \mathrm{e}^{\mathrm{i}k\theta}\, J_k(\eta) = \mathrm{e}^{\mathrm{i}\eta \sin\theta}, \qquad \theta \in [0, 2\pi), \qquad \eta \in \mathbb{R}, \tag{B.1}$$

where $J_k(\eta)$ denotes the kth-order Bessel function. The replacements $\mathrm{e}^{\mathrm{i}\theta} = z(\chi) = [(1 + \mathrm{i}\chi)/(1 - \mathrm{i}\chi)]^{1/2}\, \mathrm{e}^{-\mathrm{i}2\pi n/N}$, where $\chi \in \mathbb{R}$ and n: integer, and $2\mathrm{i}\sin\theta = z - z^{-1}$ in (B.1) produce the formula

$$\begin{aligned} S_1(z(\chi);\, \eta) &= \sum_{k=-\infty}^{\infty} \left(\frac{1 + \mathrm{i}\chi}{1 - \mathrm{i}\chi}\right)^{k/2} \mathrm{e}^{-\mathrm{i}2\pi kn/N}\, J_k(\eta) \\ &= \exp\left[\frac{1}{2}\eta\left(\sqrt{\frac{1 + \mathrm{i}\chi}{1 - \mathrm{i}\chi}}\, \mathrm{e}^{-\mathrm{i}2\pi n/N} - \sqrt{\frac{1 - \mathrm{i}\chi}{1 + \mathrm{i}\chi}}\, \mathrm{e}^{\mathrm{i}2\pi n/N}\right)\right]. \end{aligned} \tag{B.2}$$

Now let χ be *complex*: both sides of (B.2) represent analytic functions in the complex χ-plane *except* at the points $\chi = \pm\mathrm{i}$. So, by analytic continuation, it is legitimate to set $\chi = -\mathrm{i}\epsilon$ in (B.2) where $\epsilon \in (-1,\, 1)$. (Appropriate branch cuts are defined for $z(\chi)$.)

As another application of analytic continuation, compute

$$\widetilde{S}_2(\epsilon) = \sum_{k=-\infty}^{\infty} z(\epsilon)^k\, J_k(\eta)^2, \qquad z(\epsilon) = \frac{1 + \epsilon}{1 - \epsilon}, \qquad -1 < \epsilon < 1, \qquad \eta \in \mathbb{R}. \tag{B.3}$$

For complex z and fixed real η, this series $\widetilde{S}_2$ converges everywhere in $\{z :\ 0 < |z| < \infty\}$.

To find $\widetilde{S}_2(\epsilon)$ apply a version of Graf's addition formula [42], namely the Fourier series

$$S_2(z = \mathrm{e}^{\mathrm{i}\theta};\, \eta) = \sum_{k=-\infty}^{\infty} \mathrm{e}^{\mathrm{i}k\theta}\, J_k(\eta)^2 = J_0(\eta\sqrt{2}\sqrt{1 - \cos\theta}), \qquad \theta \in [0, 2\pi). \tag{B.4}$$

Next, set $2\cos\theta = z + z^{-1}$ with $z = (1 + \mathrm{i}\chi)/(1 - \mathrm{i}\chi)$, $\chi \in \mathbb{R}$. Hence, (B.4) becomes

$$S_2(z = (1 + \mathrm{i}\chi)/(1 - \mathrm{i}\chi);\, \eta) = J_0\left(\frac{2\eta\chi}{\sqrt{1 + \chi^2}}\right); \qquad \chi,\ \eta \in \mathbb{R}. \tag{B.5}$$

The variable χ is now continued to the complex plane. Both sides of (B.5) represent functions of χ analytic everywhere except at $\chi = \pm\mathrm{i}$ (for fixed $\eta \in \mathbb{R}$). By analytic continuation, (B.5) is continued to the imaginary axis, $\chi = -\mathrm{i}\epsilon$ and $\epsilon \in (-1, 1)$:

$$\widetilde{S}_2(\epsilon) \equiv S_2(z = (1 + \epsilon)/(1 - \epsilon);\, \eta) = J_0\left(\frac{-2\mathrm{i}\eta\epsilon}{\sqrt{1 - \epsilon^2}}\right) = I_0\left(\frac{2\eta\epsilon}{\sqrt{1 - \epsilon^2}}\right), \tag{B.6}$$

where I_0 is the zeroth-order modified Bessel function of the first kind [42].

Appendix C. On spectral properties of matrix $\mathrm{e}^{-\mathbf{A}_0 t}$

In this appendix, the eigenvalues and determinant of the $N \times N$ matrix $\mathrm{e}^{-\mathbf{A}_0(p)t}$ are computed. Note that, since $\mathrm{e}^{-\mathbf{A}_0 t}$ is circulant, its (normalized to unity) eigenvectors are $\Psi_l = N^{-1/2}(1, \mathrm{e}^{\mathrm{i}2\pi l/N}, \ldots, \mathrm{e}^{\mathrm{i}2\pi lj/N}, \ldots, \mathrm{e}^{\mathrm{i}2\pi l(N-1)/N})$, $0 \leqslant l,\ j \leqslant N - 1$.

Result 1. *For any N and t, the determinant of* $\mathrm{e}^{-\mathbf{A}_0 t}$ *equals unity:* $\det\left(\mathrm{e}^{-\mathbf{A}_0 t}\right) = 1$.

Proof. By inspection, $\mathrm{tr}(\mathbf{A}_0) = 0$. Thus, $\det(\mathrm{e}^{-\mathbf{A}_0 t}) = \mathrm{e}^{-\mathrm{tr}(\mathbf{A}_0)\, t} = 1$. □

Result 2. *For fixed time t and large N, the eigenvalues of* $\mathrm{e}^{-\mathbf{A}_0 t}$ *are*

$$\lambda_l(t) \sim \exp\left[\frac{1}{2}\breve{t}\left(\sqrt{\frac{1-p}{p}}\,\mathrm{e}^{-\mathrm{i}2\pi l/N} - \sqrt{\frac{p}{1-p}}\mathrm{e}^{\mathrm{i}2\pi l/N}\right)\right], \tag{C.1}$$

where $\breve{t} = 2\sqrt{p(1-p)}\,t$ *and* $0 \leqslant l \leqslant N-1$.

Proof. The desired eigenvalues are the discrete Fourier transform of the first row of $\mathrm{e}^{-\mathbf{A}_0 t}$. By lemma 2 (section 5.2) in the limit $N \to \infty$,

$$\begin{aligned}\lambda_l &\sim \sum_{k=0}^{N-1}\left[\left(\frac{1-p}{p}\right)^{k/2} J_k(\breve{t}) + (-1)^{N-k}\left(\frac{p}{1-p}\right)^{\frac{N-k}{2}} J_{N-k}(\breve{t})\right]\mathrm{e}^{-\mathrm{i}2\pi kl/N} \\ &= \sum_{k=-N}^{N-1}\left(\frac{1-p}{p}\right)^{k/2}\mathrm{e}^{-\mathrm{i}2\pi kl/N} J_k(\breve{t}) \sim \sum_{k=-\infty}^{\infty}\left(\frac{1-p}{p}\right)^{k/2}\mathrm{e}^{-\mathrm{i}2\pi kl/N} J_k(\breve{t}),\end{aligned}$$

which furnishes (C.1) through (B.2) of appendix B with $\epsilon \equiv 1-2p$, $\epsilon \in [0, 1)$. □

It is of interest to show that (C.1), although obtained in the large-N limit, is consistent with result 1. Indeed, by the well-known formula $\det(\mathrm{e}^{-\mathbf{A}_0 t}) = \prod_{l=0}^{N-1}\lambda_l(t)$, result 1 follows from result 2 via the trivial identities $\sum_{l=0}^{N-1}\mathrm{e}^{\pm\,\mathrm{i}2\pi l/N} = 0$.

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