Stochastic step flow model with growth in 1+1 dimensions

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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* and *all* times $t > 0$. 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.

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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 [1–4]. A related direction of active research in non-equilibrium statistical mechanics is the connection of particle schemes to macroscopic evolution laws [5, 6].

Material deposition (growth) on crystal surfaces is used to create building blocks of quantum wires and dots, and other nanoscale structures [3, 4]. 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.

In this work, a stochastic particle model for crystal terraces is studied in the limit of a large number of steps. A solvable case is treated, revealing an interplay of time and material parameters. *'Mean-field'* ideas are examined in the light of *kinetic hierarchies*, leading to a relatively simple criterion of particle (terrace) correlation.

The microscale constituents of crystal surfaces were introduced by Kossel [7], Stranski [8] and Burton, Cabrera and Frank (BCF) [9]. Surfaces evolve because steps move as adsorbed atoms (adatoms) hop on terraces, attach-detach at and move along step edges. A system of *deterministic* differential equations for step positions can thus be formulated. An alternative description invokes macroscopic evolution laws for the surface height [10–15]. These views have been connected to Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchies for *step position* correlation functions [16].

Distinctly different approaches have been followed for step *fluctuations* [2, 17]. Equilibrium properties such as the terrace width, or *step gap* [18], distribution (see footnote 1) for repulsively interacting steps have been studied extensively [2, 17, 19–21]. A key idea is to map steps onto worldlines of spinless fermions, because steps do not cross [19, 22]. The relaxation of the gap distribution is described by a *mean field*, via a Fokker-Planck equation (FPE), and by kinetic Monte Carlo simulations [23, 24]. 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 approach to BBGKY hierarchies for *gap* correlations has not been addressed previously.

In this paper, a BCF-type model in 1D under growth is explored by addition of Gaussian white noise for initially uniform step trains. One goal is to reconcile BBGKY hierarchies for joint gap densities with mean-field ideas for coupled SDEs [21, 23, 25]. 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 paper was inspired by the work of Hamouda, Pimpinelli and Einstein [25], 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 re-

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

sults with kinetic Monte Carlo simulations. Their density approaches a steady state at long times, captured both by the mean field and the kinetic Monte Carlo simulations. Here, the analysis complements [25] by focusing on the relation of the mean field with kinetic hierarchies, and the behavior of the one-gap density for *finite times.* In addition, finite-size effects for long times are discussed, exploring limitations of the linear model.

There is a long sequence of related works. Sources of surface fluctuations were laid out by Wolf [26] and aspects of noisy continuum theories were discussed by Krug [27,28] over a decade ago. A similar, minimal 1D model of growth is analyzed in [29] 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 captures *limiting forms* of effects such as finite step velocity [25, 30, 31], Ehrlich-Schwoebel barrier [32–35], electromigration [36], and variations in the number of atoms impinging on the surface [37]. This list is not exhaustive.

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

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

where $\mathcal{G}(t) = (\mathcal{G}_0(t), \mathcal{G}_1(t), \dots \mathcal{G}_{N-1}(t))$ is a vector-valued stochastic process with component $\mathcal{G}_i(t)$ representing the ith step gap; $\mathcal{B}(t) = (\mathcal{B}_0(t), \mathcal{B}_1(t), \dots \mathcal{B}_{N-1}(t))$ 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). The gaps are subject to screw periodic boundary conditions, i.e., each of the N particles corresponding to terraces lies on a ring.

The main contributions of this work are: (i) SDE (1) is 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 SDE 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). This f yields the mean field of [25] as a special case under an ansatz for two-gap independence.

The limits $N \to \infty$ and $t \to \infty$ are not allowed to 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.

The assumption is made that steps are entropically and energetically *non-interacting* [9]. The terrace widths in SDE (1) interact only through surface diffusion. This simplification retains elements of the essential physics and offers some advantages. (i) The coefficient $\check{A}$ in(1) is well-behaved; thus, for appropriate initial data, a unique strong solution exists [38] (see footnote 2). By contrast, repulsive step interactions would result in a singular $\check{A}$ [40, 41]. Although it is expected physically that step gaps

[2] For uniqueness, it suffices to have a Lipschitz continuous coefficient $\check{A}$ and initial data with finite mean and variance [38]. For an exposition to *strong* and *weak* solutions of SDEs, see, e.g., [39].

do not vanish (and thus $\breve{A}$ does not blow up), the modeling and analysis of step energies would require much more care in this case. (ii) SDE (1) have the appeal of a minimal model for gap correlations: as $F \to 0$ the gaps become *independent* random variables for all $t > 0$ [29]; hence, F *parameterizes* conveniently *deviations from decorrelation*.

A shortcoming of the present model, without step interactions, is its violation of the non-crossing condition for steps: gap densities acquire tails of nonzero probability for negative gaps. Hence, the analysis is deemed unphysical if the respective variance exceeds the mean terrace width (set by the initial condition) [25].

The BCF theory–which forms the core of this treatment–has an intrinsic near-equilibrium character. Hence, the model is expected to break down if the deposition flux, F, is too large [25]. 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 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. The precise relation of noise to geometry and the random hopping of adatoms, e.g., any plausible settings of kinetic Monte Carlo-type simulations, is not touched upon here. The steps are straight moving boundaries where the adatom flux satisfies certain kinetic conditions. Considering step fluctuations on a more fundamental basis calls for a revision of this *effective* description. The notion of noise should *emerge* as an appropriate limit and be intimately connected to dimensionality [42].

The present treatment is distinct from the renormalization group ideas by Haselwandter and Vvedensky [43], 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 may serve as a minimal model for exploring how discrete stochastic schemes are linked to large-scale fluctuations. The role of BBGKY hierarchies is exemplified with relative ease. The difference of an explicit formula for the gap variance from a mean-field counterpart is introduced as a *'measure' of terrace correlations*. The study of richer models could be guided by this treatment.

The analysis of this paper remains unconnected to the macroscopic limit of BBGKY hierarchies for step *position* correlations invoked in [16]. So, the relation to partial differential equations for the large-scale height profile is left for future work.

The paper is organized as follows. In section 2, the governing SDE system in 1D is formulated in the BCF framework [9]. 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 an extension and implications of these results: the variance is evaluated for large times t, $t > O(N)$; its approximation by the mean field [25] is compared to the explicit calculation for large N; and the modeling of noise is discussed. In section 7, the main results and pending issues are summarized. The appendices provide technical derivations needed in the main text.

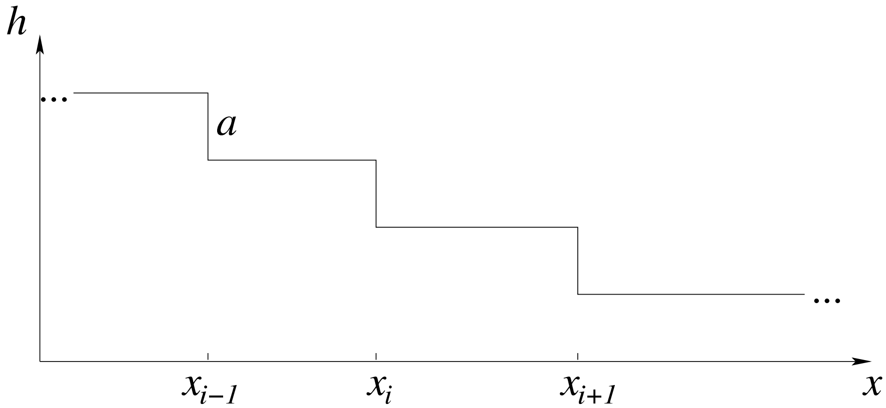

Figure 1. Schematic (cross section) of step configuration: $x = x_i(t)$ at the ith step edge, a is the step height, and h is the surface height; the ith step gap is $g_i = x_{i+1} - x_i$.

The notation is self-explanatory albeit non-standard. *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 $\vec{y}_l \equiv (y_0, \ldots, y_{l-1}) \in \mathbb{R}^l$, $1 \leq l \leq N-1$. 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 an extreme value.

2. Stochastic scheme: Formulation via BCF model

In this section, the SDE system for N step gaps under growth are formulated in the physical setting of Hamouda, Pimpinelli and Einstein [25]. First, the geometry and deterministic equations of motion for terrace widths are described via principles of the BCF model [9]. The physical effects include adatom terrace diffusion, atom attachment-detachment at steps, and material deposition from above. The diffusion of atoms along step edges is neglected. Second, the governing equations are non-dimensionalized. 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 the same 'sign'), steps have (nonrandom) positions $x_i(t)$ and height a, where $g_i = x_{i+1} - x_i > 0$ and $i = 0, \ldots, N-1$ (see footnote 3). Apply screw periodic boundary conditions, i.e., set $x_i(t) = x_{i+kN}(t)$ where k is any integer. (Steps as mapped onto particles on a ring).

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

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

[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).

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 $(x', t') = (x - vt, t)$ [31]; thus, (2) becomes [25, 31]

$$(D\partial_{x'}^2 + v\partial_{x'})C_i + F = \partial_{t'}C_i \approx 0 \ . \tag{3}$$

Now remove the primes for ease of notation: $x' \Rightarrow x$.

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

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

where $j_i(x) = -D\partial C_i/\partial x - vC_i$ is the i-th terrace adatom flux, C_i^{eq} is the equilibrium adatom concentration at the ith edge, and k is the kinetic rate for atom attachment-detachment; the time dependence of C_i and j_i is suppressed. The quantity C_i^{eq} accounts for step energetics, say elastic-dipole step interactions [2, 40, 41]. Kinetic rates different for up- and down-step edges (i.e., the Ehrlich-Schwoebel effect [32]) 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 $\{x_i\}$, (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 $\Lambda_i = \Lambda(g_i; C_i^{\mathrm{eq}}, C_{i+1}^{\mathrm{eq}})$, $g_i = x_{i+1} - x_i$, and

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

By virtue of (5), the differential equations for the step gaps (terrace widths), 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

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

Consequently, $\Lambda_i \sim Fg_i(1 - e^{-vg_i/D})^{-1}$ and (8) reduces to [25]

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

By (9), an initially uniform step geometry is preserved by the flow: if $g_i(0) = \varpi = $ const., then $g_i(t) \equiv \varpi$ for all $t > 0$. So, to have (nontrivial deterministic) evolution, the vicinal crystal needs to be perturbed off uniformity.

A particular limit of (9) is

$$\dot{g}_i \sim \frac{\Omega F}{2a}(g_{i+1} - g_{i-1}) \qquad \text{as } \ vg_i/D \to 0 \ . \tag{10}$$

2.2. Nondimensional equations

Consider $Na/L \geq O(1)$ 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 $v\varpi/D \ll 1$.

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 [15]. 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 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 Taylor expansion in i, the right hand side manifestly becomes $O(\tau_2^{-1}\varpi)$.

Equation (9) is now recast to a nondimensional form for later algebraic convenience. Emphasis is placed on manifestly N-independent scales. Define (see footnote 4)

$$\tilde{g}_i = g_i/\ell_2 \ , \qquad \tilde{t} = t/\tau_2 \ ; \quad \ell_2 = \frac{2D}{v} \ , \ \tau_2 = \frac{2D}{F\Omega}\frac{1}{Fa^2} \qquad (\Omega \approx a^2) \ . \quad (11)$$

Next, drop the tildes ($\tilde{g}_i \Rightarrow g_i$ and $\tilde{t} \Rightarrow t$). Equation (9) reads

$$\dot{g}_i = \frac{1}{2}\left(\frac{g_{i+1}e^{g_{i+1}}}{\sinh g_{i+1}} - \frac{2g_i \cosh g_i}{\sinh g_i} + \frac{g_{i-1}e^{-g_{i-1}}}{\sinh g_{i-1}} \right) , \qquad (12)$$

where units are chosen so that $v m_0 a/(2D) \equiv 1$ $(m_0 = a/\varpi)$ and the factor of $1/2$ is included for later algebraic convenience; see also section 5.

2.3. Gaussian white noise

Preliminaries: For the sake of clarity, a brief review of the underlying stochastic vocabulary is given first. 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). By construction, $\mathcal{B}(t)$ is assumed to have the following interrelated properties [38].

(i) The 1D processes $\mathcal{B}_i(t)$ are independent 1D Brownian motions $(0 \leq i \leq N-1)$. Hence, each $\mathcal{B}_i(t)$ has the mean $\mathbb{E}[\mathcal{B}_i(t)] = 0$ and variance $\mathbb{E}[\mathcal{B}_i(t)^2] = t$, where $\mathcal{B}_i(0) = 0$. Apply the periodic extension $\mathcal{B}_{i+lN}(t) = \mathcal{B}_i(t)$ for all integers l and $0 \leq i \leq N-1$.

(ii) The vector $\mathcal{B}(t)$ is a Gaussian process, i.e., the random variable $(\mathcal{B}(t_1), \ldots, \mathcal{B}(t_k)) \in \mathbb{R}^{kN}$ has a multinormal distribution for all $0 \leq t_1 \leq \ldots \leq t_k$.

(iii) $\mathcal{B}(t)$ has independent increments, i.e., $\mathcal{B}(t_1), \mathcal{B}(t_2) - \mathcal{B}(t_1), \ldots, \mathcal{B}(t_k) - \mathcal{B}(t_{k-1})$ are independent random variables for all $0 \leq t_1 < t_2 < \ldots < t_k$.

[4] Alternatively, one may define $\tau_2 = (F\varpi^2)^{-1}\big(2D/(F\Omega)\big)$, replacing a by ϖ. This only affects the chosen units by a factor involving the initial slope, $m_0 = a/\varpi = O(1)$.

(iv) $\mathcal{B}(t)$ has continuous paths (with $\mathcal{B}(0) = 0$).

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 severe pathologies, e.g., lack of continuous paths. By standard notation, $\mathrm{d}\mathcal{B}(t) = \mathcal{N}(t)\mathrm{d}t$ 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 $(\mathrm{time})^{-1/2}$.

Equations of motion: Next, the vector-valued *function* $g(t) = (g_0(t), \ldots, g_{N-1}(t))$ is replaced by the N-dimensional *stochastic process* $\mathcal{G}(t) = (\mathcal{G}_0(t), \ldots, \mathcal{G}_{N-1}(t))$. The components $\mathcal{G}_i(t)$ are required to satisfy the SDEs $(0 \le i \le N-1)$

$$\mathrm{d}\mathcal{G}_i(t) = \frac{1}{2}\left(\frac{\mathcal{G}_{i+1}e^{\mathcal{G}_{i+1}}}{\sinh \mathcal{G}_{i+1}} - 2\mathcal{G}_i \coth \mathcal{G}_i + \frac{\mathcal{G}_{i-1}e^{-\mathcal{G}_{i-1}}}{\sinh \mathcal{G}_{i-1}}\right)\mathrm{d}t + \mathrm{d}\mathcal{B}_i(t)\ , \qquad (13)$$

which stem from (12) by addition of white noise, $\mathcal{N}(t)$; apply *nonrandom* initial data $\mathcal{G}_i(0) = \upsilon\varpi/(2D)$. Hence, it is understood that, for any $t > 0$,

$$\mathcal{G}_i(t) = \nu + \frac{1}{2}\int_0^t \left[\frac{\mathcal{G}_{i+1}(\tau)e^{\mathcal{G}_{i+1}}}{\sinh \mathcal{G}_{i+1}} - \frac{2\mathcal{G}_i(\tau)\cosh \mathcal{G}_i}{\sinh \mathcal{G}_i} + \frac{\mathcal{G}_{i-1}(\tau)e^{-\mathcal{G}_{i-1}}}{\sinh \mathcal{G}_{i-1}}\right]\mathrm{d}\tau$$
$$+ \mathcal{B}_i(t)\ ; \qquad \nu \equiv \frac{\upsilon\varpi}{2D} \equiv \aleph_i\ ,\ \aleph \equiv (\nu, \ldots, \nu) \in \mathbb{R}^N\ . \qquad (14)$$

Definition 1. *Consider (13) for small* $\mathcal{G}_i$*, i.e., if* $\mathrm{Prob}[\sup_{t\in[0,T)}|\mathcal{G}_i(t)| \ll 1] = 1$*:*

$$\mathrm{d}\mathcal{G}_i = \tfrac{1}{2}(\mathcal{G}_{i+1} - \mathcal{G}_{i-1})\mathrm{d}t + \mathrm{d}\mathcal{B}_i\ , \quad \mathcal{G}_i(0) = \nu\ . \qquad (15)$$

This model will be referred to as the 'reference case'; cf (10) for the deterministic analog.

A few comments on modeling are in order. Equation (13) relies on an ad hoc introduction of noise. Notably, the coefficient of $\mathrm{d}\mathcal{B}_i(t)$ is a constant. The solution to (13) admits a unique interpretation, dictated by (14). By contrast, the inclusion of a $\mathcal{G}$-dependent noise coefficient, which is not precluded by any physical principle [37], poses a question as to what stochastic calculus (e.g., in the sense of Itô or Stratonovich) would be more appropriate to use [38]. Issues of modeling noise are further discussed in section 6.3.

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). This BBGKY hierarchy serves the introduction of the mean field in section 4. The starting point is a generalization of SDEs (13), viz.,

$$\mathrm{d}\mathcal{G}_i(t) = A(\mathcal{G}_{i-1}(t), \mathcal{G}_i(t), \mathcal{G}_{i+1}(t))\,\mathrm{d}t + \mathrm{d}\mathcal{B}_i(t)\ . \qquad (16)$$

3.1. Formulation

First, appropriate probability densities are introduced. Consider the N-gap density $\rho_N(t,y)$, where

$$\rho_N(t,y)\,\mathrm{d}y=\mathrm{Prob}[\cap_{k=0}^{N-1}\{y_k<\mathcal{G}_k(t)<y_k+\mathrm{d}y_k\}]\ ,\quad \mathrm{d}y=\prod_{k=0}^{N-1}\mathrm{d}y_k\ ,\quad (17)$$

y_k is the value of the kth gap, and $y=(y_0,\,\dots\,,y_{N-1})\in\mathbb{T}^N$, the N-dimensional torus. In view of (16), the joint density of *any* n consecutive gaps is strictly defined by

$$\rho_n(t,\vec{s}_n):=\frac{1}{N}\sum_{k=0}^{N-1}\int_{\mathbb{T}^{N-n}}\rho_N(t,(\vec{y}\,'_{N-n},\vec{s}_n)^c_k)\,\mathrm{d}\vec{y}\,'_{N-n}\ ,\quad 1\le n<N\ ,\qquad (18)$$

where $\vec{y}\,'_l$, $\vec{s}_l$ are l-dimensional vectors ($\vec{s}_l\in\mathbb{R}^l$, $0\le l\le N-1$) with $\vec{s}_l=(s_0,\,\dots\,,s_{l-1})$. 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., $\zeta_k=(y'_k,\dots,y'_{N-n-1},\vec{s}_n,y'_0,\dots,y'_{k-1})$ if $0\le k\le N-n-1$ while $\zeta_k=(s_{k-N+n},\dots,s_{n-1},\vec{y}\,'_{N-n},s_0,\dots,s_{k-N+n-1})$ if $N-n\le k\le N-1$; note that, for $N\gg1$ and $n=O(1)$, this latter possibility has a small, $O(n/N)$, likelihood. The factor of $1/N$ in (18) accounts for each terrace in the step train with equal probability. Of particular interest is the density of any single gap, given explicitly by

$$\rho_1(t,s\in\mathbb{T})=N^{-1}\sum_{k=0}^{N-1}\int_{\mathbb{T}^{N-1}}\rho_N(t,y'_0,\dots,y'_{k-1},s,y'_k,\dots,y'_{N-2})\,\mathrm{d}\vec{y}\,'_{N-1}\ .(19)$$

Second, equations of motion for ρ_n are derived under $N\gg1$ and $n=O(1)$. Define the N-dimensional vector field $\check{A}(y)$ that has kth component $\check{A}_k=A(y_{k-1},y_k,y_{k+1})$, $0\le k\le N-1$; cf (16). The FPE (or, forward Kolmogorov equation) for $\rho_N(t,y)$ reads (see appendix A)

$$\partial_t\rho_N(t,y)+\mathrm{div}_N[\check{A}(y)\rho_N]=\frac{1}{2}\Delta_N\rho_N(t,y)\ ;\quad \mathrm{div}_N F\equiv\sum_{k=0}^{N-1}\partial_{y_k}F_k\ ,\quad (20)$$

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 $\aleph=(\nu,\dots,\nu)\in\mathbb{R}^N$, $\nu\equiv\aleph_i=v\varpi/(2D)$, and $\delta_0(y)$ is the Dirac measure ('delta function') on $\mathbb{R}^N$ (giving unit mass to point 0).

The BBGKY hierarchy stems (formally) from differentiation of (18) with respect to t. For $n=1$, the equation for $\rho_1(s)$ (by suppression of the t dependence) is

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

$$\Rightarrow\qquad \partial_t\rho_1(s)+\partial_s\left[\int\mathrm{d}s'_0\mathrm{d}s'_1\ A(s'_0,s,s'_1)\,\rho_3(s'_0,s,s'_1)\right]=\frac{1}{2}\partial_s^2\rho_1\ ,\quad (21)$$

where $s \in \mathbb{T}$. 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.

Evolution equations for ρ_n, $n \geq 2$, are extracted similarly. If $n = 2$, ρ_n satisfies

$$\partial_t \rho_2(s_0, s_1) + \partial_{s_0}\left[\int \mathrm{d}s'\, A(s', s_0, s_1)\, \rho_3(s', s_0, s_1)\right] + \partial_{s_1}\left[\int \mathrm{d}s'\, A(s_0, s_1, s')\, \rho_3(s_0, s_1, s')\right] = \frac{1}{2}\Delta_2 \rho_2 \ . \qquad (22)$$

The hierarchy for ρ_n is generalized for $n \geq 3$:

$$\partial_t \rho_n(\vec{s}_n) + \partial_{s_0}\left[\int \mathrm{d}s'\, A(s', s_0, s_1)\, \rho_{n+1}(s', \vec{s}_n)\right] + \sum_{k=1}^{n-2} \partial_{s_k}[A(s_{k-1}, s_k, s_{k+1})\, \rho_n(\vec{s}_n)] + \partial_{s_{n-1}}\left[\int \mathrm{d}s'\, A(s_{n-2}, s_{n-1}, s')\, \rho_{n+1}(\vec{s}_n, s')\right] = \frac{1}{2}\Delta_n \rho_n(\vec{s}_n) \ ; \qquad (23)$$

$\rho_n|_{t=0} = \prod_{k=0}^{n-1} \delta_\nu(s_k)$ where $\delta_0(s)$ is the delta function on $\mathbb{R}$ centered at 0.

Evidently, the above hierarchies consist of conservation laws, and are interpreted in the weak sense, i.e., after multiplication by appropriate test functions and application of integration by parts [5]. The analysis here is distinct from [16], 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 [16].

3.2. Example: Growth model

In correspondence to (13), hierarchy (21)–(23) is now written for the coefficient

$$A(y_1, y_2, y_3) \equiv K_a(y_1) - K_{ab}(y_2) + K_b(y_3) \ , \qquad K_{ab} \equiv K_a + K_b \ , \qquad (24)$$

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

$$\partial_t \rho_1(s) + \partial_s\left\{\int \mathrm{d}s'\, [K_a(s')\rho_2(s', s) + K_b(s')\rho_2(s, s')] - K_{ab}(s)\rho_1(s)\right\} = \frac{1}{2}\partial_s^2 \rho_1 \ , \qquad (25)$$

$$\partial_t \rho_n(\vec{s}_n) + \partial_{s_0}\left\{\int \mathrm{d}s'\, K_a(s')\rho_{n+1}(s', \vec{s}_n) + [K_b(s_1) - K_{ab}(s_0)]\rho_n(\vec{s}_n)\right\} + \sum_{k=1}^{n-2} \partial_{s_k}\{[K_a(s_{k-1}) - K_{ab}(s_k) + K_b(s_{k+1})]\rho_n(\vec{s}_n)\} + \partial_{s_{n-1}}\left\{\int \mathrm{d}s'\, K_b(s')\, \rho_{n+1}(\vec{s}_n, s') + [K_a(s_{n-2}) - K_{ab}(s_{n-1})]\rho_n(\vec{s}_n)\right\} = \frac{1}{2}\Delta_n \rho_n \ , \qquad n \geq 2 \ . \qquad (26)$$

3.3. Linear model and decorrelations

Consider scheme (15) in definition I (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 [25, 29], as well as (41) and (44). First, it is shown that in this case the step gaps of a vicinal surface 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 in some appropriate sense.

The step gap independence amounts to the product form

$$\rho_N(t, y) = \prod_{k=0}^{N-1} \rho_1(t, y_k) \ , \qquad \rho_1(0, s) = \delta_\nu(s) \ . \tag{27}$$

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

By (20), the N-dimensional FPE for the reference case is

$$\partial_t \rho_N(y) + \frac{1}{2} \sum_{k=0}^{N-1} \partial_{y_k} [(y_{k+1} - y_{k-1})\rho_N] = \frac{1}{2} \sum_k \partial_{y_k}^2 \rho_N \ , \quad y \in \mathbb{R}^N \ . \tag{28}$$

The 1st equation of the hierarchy stems from (25) with $K_a(s) = \frac{1}{2}(1+s) = K_b(-s)$:

$$\partial_t \rho_1(s) + \frac{1}{2} \partial_s \int \mathrm{d}y_1 \, y_1 [\rho_2(s, y_1) - \rho_2(y_1, s)] = \frac{1}{2} \partial_s^2 \rho_1 \ . \tag{29}$$

Start with (28). The substitution of (27) into (28) yields

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

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 $\rho_1(t, s) = (2\pi t)^{-1/2} \, e^{-\frac{(s-\nu)^2}{2t}}$, i.e., a Gaussian of mean $\mu = \nu$ 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; so, $\sum_l (y_{l+1} - y_{l-1})\partial_{y_l}\rho_1(y_l) = 0$.) This result is consistent with (29) 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 if in the linear model $A(y_1, y_2, y_3) = (1-p)y_1 - (1-2p)y_2 - py_3$ one has $0 < p < 1/2$ (this range is explained in section 5). The equation for $\rho_1(s)$ collapses to the FPE $\partial_t \rho_1 + (1-2p)\partial_s[(\nu - s)\rho_1] = \frac{1}{2}\partial_s^2 \rho_1$, which is solved by a Gaussian of mean ν and variance $[2(1-2p)]^{-1}(1 - e^{-2(1-2p)t})$; see [25] and section 4.2. However, (26) 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 $(1-p)(s_1 - \nu)\partial_{s_0}\rho_1(s_0)/\rho_1(s_0) = p(s_0 - \nu)\partial_{s_1}\rho_1(s_1)/\rho_1(s_1)$, 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 BBGKY hierarchy (21)–(23) at the level of the one-gap density. This formulation will facilitate comparisons of a previous approach based on step gap independence [25] 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 (16). The 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. A starting point is to introduce the stochastic processes $\widehat{\mathcal{G}}_i(t)$ satisfying

$$\mathrm{d}\widehat{\mathcal{G}}_i(t) = A(f(t,\widehat{\mathcal{G}}_i), \widehat{\mathcal{G}}_i, f(t,\widehat{\mathcal{G}}_i))\,\mathrm{d}t + \mathrm{d}\mathcal{B}_i(t)\ , \qquad 0 \le i \le N-1\ , \tag{30}$$

under the initial data $\widehat{\mathcal{G}}_i(0) = \mathcal{G}_i(0)$, i.e., same as for the original process $\mathcal{G}_i(t)$. The function $f(t,s)$ is to be determined (see definition II). Assume that A and f are such that (30) is solvable in an appropriate sense. Notice that (30) comes from (16) with replacement of the variables $\mathcal{G}_{i-1}$ and $\mathcal{G}_{i+1}$ by $f(t,\widehat{\mathcal{G}}_i)$.

The following heuristic definition can now be stated.

Definition 2. *The function $f(t,s)$, $f:(0,\infty)\times\mathbb{T}\to\mathbb{R}$, is called the mean field, $f=f^{\mathrm{mf}}$, for SDEs (16) if this f^{mf} generates a probability density, $\widehat{\rho}_1(t,s;[f])$, for $\widehat{\mathcal{G}}_i(t)$ that equals the density $\rho_1(t,s)$ for $\mathcal{G}_i(t)$ in the weak sense (wk), i.e.,*

$$\int \mathrm{d}s\,\rho_1(t,s)\,\vartheta(s) = \int \mathrm{d}s\,\widehat{\rho}_1(t,s;[f^{\mathrm{mf}}])\,\vartheta(s) \tag{31}$$

for every reasonably arbitrary test function $\vartheta(s)$ and fixed time $t>0$.

A way to think about f^{mf} is this. By (30), fixed initial data and reasonably arbitrary f, describe $\widehat{\rho}_1$ as a functional of f: $\widehat{\rho}_1 = \widehat{\rho}_1[f]$. By variations of f in an appropriate space, it is presumed that some $f = f^{\mathrm{mf}}$ exists for which $\widehat{\rho}_1[f^{\mathrm{mf}}] = \rho_1$ (wk). No guarantee is given here that this f^{mf} exists; proving existence lies beyond the present scope. Equation (31) has essentially been invoked for static variables in other physical contexts, e.g., non-uniform liquids [44].

It is of interest to derive an (implicit) formula for f^{mf} via the BBGKY hierarchy (21)–(23). In fact, one only needs to use evolution law (21) for ρ_1.

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

$$A(f^{\mathrm{mf}}(s), s, f^{\mathrm{mf}}(s))\rho_1(s) = \int \mathrm{d}s_1'\mathrm{d}s_2'\,A(s_1', s, s_2')\,\rho_3(s_1', s, s_2') \quad (wk)\ . \tag{32}$$

Equation (32) has the flavor of a *self-consistency condition.*

Proof. This follows directly from (21), (30) and (31). First, note that $\widehat{\rho}_1(t,s;[f])$ obeys (see appendix A)

$$\partial_t\widehat{\rho}_1 + \partial_s[A(f(t,s), s, f(t,s))\widehat{\rho}_1] = \frac{1}{2}\partial_s^2\widehat{\rho}_1\ . \tag{33}$$

The multiplication of (33) by a test function, $\phi(s)$, and integration result in

$$\partial_t \int \mathrm{d}s\, \widehat{\rho}_1\, \phi(s) - \frac{1}{2} \int \mathrm{d}s\, \widehat{\rho}_1\, \partial_s^2 \phi = \int \mathrm{d}s\, \widehat{\rho}_1\, A\, \partial_s \phi \qquad \forall\, \phi\ . \tag{34}$$

In view of (31), now replace f by f^{mf} and thus $\widehat{\rho}_1$ by ρ_1 in (34). Similarly, the multiplication of (21) by $\phi(s)$ and integration result in

$$\begin{aligned} &\partial_t \int \mathrm{d}s\, \rho_1\, \phi(s) - \frac{1}{2} \int \mathrm{d}s\, \rho_1\, \partial_s^2 \phi \\ &= \int \mathrm{d}s \int \mathrm{d}s_1' \mathrm{d}s_2'\ A(s_1', s, s_2')\, \rho_3(s_1', s, s_2')\, \partial_s \phi(s)\ . \end{aligned} \tag{35}$$

The comparison of (35) and (34), for $\widehat{\rho}_1 = \rho_1$, leads to (32). □

4.2. Growth model

If A is given by (24), then (32) is simplified to

$$\begin{aligned} K_{ab}(f^{\mathrm{mf}}(s)) &= \int \mathrm{d}s'\, [K_a(s')\rho_{1/2}(s', s) + K_b(s')\rho_{2/1}(s', s)] \\ &= \mathbb{E}[K_a(\mathcal{G}_a)|\mathcal{G}_b = s] + \mathbb{E}[K_b(\mathcal{G}_b)|\mathcal{G}_a = s] \qquad (s \in \mathbb{T})\ . \end{aligned} \tag{36}$$

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. $\mathbb{E}[K_c(\mathcal{G}_c)|s]$ ($c = a,\, b$) denotes the respective mean of K_c.

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), (36) reduces to the more explicit formula

$$\begin{aligned} f^{\mathrm{mf}}(s) &= (1-2p)^{-1} \int \mathrm{d}s'\, s'[(1-p)\, \rho_{1/2}(s', s) - p\, \rho_{2/1}(s', s)] \\ &\equiv (1-2p)^{-1}\{(1-p)\, \mathbb{E}[\mathcal{G}_a|\mathcal{G}_b = s] - p\mathbb{E}[\mathcal{G}_b|\mathcal{G}_a = s]\}\ . \end{aligned} \tag{37}$$

Pair *decorrelation* approximation: By $\rho_2(s_0, s_1) \sim \rho_1(s_0)\, \rho_1(s_1)$, (37) entails

$$f^{\mathrm{mf}} \sim E[\mathcal{G}_a]\ , \tag{38}$$

where the gaps are taken identically distributed. Equation (38) is consistent with the approach in [25]. Thus, the processes $\widehat{\mathcal{G}}_i$ satisfy the Langevin equations [25]

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

For fixed t, the solution is the Gaussian random variable given by $\widehat{\mathcal{G}}_i(t) = \nu + \int_0^t e^{-(1-2p)(t-\tau)} \mathrm{d}\mathcal{B}_i(\tau)$, which has the variance [45]

$$\widehat{\sigma}_{\mathrm{pc}}(t)^2 = \int_0^t e^{-2(1-2p)\tau} \mathrm{d}\tau = [2(1-2p)]^{-1}\{1 - e^{-2(1-2p)t}\}, \tag{39}$$

in agreement with [25]. This approximation is further discussed in section 6.2.

5. Small fluctuations and large-N limit

In this section, SDEs (13) are expanded for small fluctuations. The leading-order equations are treated explicitly as $N \to \infty$. The asymptotic limit of the variance is illustrated for fixed t (see section 6.1 for an extension). Deviations of $\mathcal{G}(t)$ from its initial value $\aleph$, where $\nu \equiv \aleph_i = v\varpi/(2D)$, are taken small in the sense $\mathrm{Prob}[\sup_{t\in[0,T)} |\mathcal{G}(t) - \aleph| \ll |\aleph|] \sim 1$ (see footnote 5); this is in the spirit of [25].

A word of caution: in the following, it is implicitly assumed that material parameter groups–which depend on F and enter, through ν, coefficients of related SDEs–are fixed, i.e., independent of the (relatively small) deviation of $\mathcal{G}_i$ from ν and $\mathbb{E}[\mathcal{G}_i]$. 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 $\nu = O(1)$. This hypothesis is convenient for bookkeeping purposes in the perturbation scheme.

5.1. Small-fluctuation expansion

Apply the substitution

$$\mathcal{G}(t) = \aleph + \bar{\mathcal{G}}(t)\ , \qquad \aleph = \mathcal{G}(0) \quad (\bar{\mathcal{G}} \in \mathbb{R}^N)\ ,$$

where $\mathrm{Prob}[\sup_{[0,T)} |\bar{\mathcal{G}}(t)| \ll |\aleph|] \sim 1$. Equation (13) then leads to

$$\begin{aligned} \mathrm{d}\bar{\mathcal{G}}_i = \{&(1-p)(\bar{\mathcal{G}}_{i+1} - \bar{\mathcal{G}}_i) + p(\bar{\mathcal{G}}_i - \bar{\mathcal{G}}_{i-1}) + q_1(\bar{\mathcal{G}}_{i+1}^2 + \bar{\mathcal{G}}_{i-1}^2 - 2\bar{\mathcal{G}}_i^2) \\ &- q_2(\bar{\mathcal{G}}_{i+1}^3 + \bar{\mathcal{G}}_{i-1}^3 - 2\bar{\mathcal{G}}_i^3) + O(\bar{\mathcal{G}}_{i-1}^4, \bar{\mathcal{G}}_i^4, \bar{\mathcal{G}}_{i+1}^4)\}\mathrm{d}t + \mathrm{d}\mathcal{B}_i(t)\ . \end{aligned} \tag{40}$$

Notice the linear terms in the right hand side; p and q_j $(j = 1, 2)$ are defined by

$$p = \frac{1}{2}\left(\frac{\nu}{\sinh^2\nu} - \frac{e^{-\nu}}{\sinh\nu}\right)\ , \tag{41}$$

in accord with [25]; and

$$\begin{aligned} q_1 &= \frac{1}{2}\left(-\frac{1}{\sinh^2\nu} + \nu\,\frac{\cosh\nu}{\sinh^3\nu}\right)\ , \\ q_2 &= \frac{1}{2}\frac{1}{\sinh^2\nu}\left[-\frac{\cosh\nu}{\sinh\nu} + \nu\left(-\frac{1}{3} + \frac{\cosh^2\nu}{\sinh^2\nu}\right)\right]\ ; \quad p,\, q_j = O(1)\ . \end{aligned} \tag{42}$$

The expansion in the right hand side of (40) can be extended directly to higher orders, but the evaluation of the respective coefficients, $q_{j\geq 3}$, becomes increasingly cumbersome.

Equation (40) is now simplified via the formal expansion

$$\bar{\mathcal{G}}(t) \sim \sum_{j=0}^{k-1} \bar{\mathcal{G}}^{(j)}(t)\ ; \quad k = 3\ ,\ \mathrm{Prob}[\sup|\bar{\mathcal{G}}^{(j+1)}(t)| \ll \sup|\bar{\mathcal{G}}^{(j)}(t)|] = 1\ . \tag{43}$$

[5] The term *small fluctuations* here 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 for vicinal surfaces. In fact, evidently, $\mathcal{G}(0) = \mathbb{E}[\mathcal{G}(t)]$ to the leading order; see section 5.2.

The meaning of expansion (43) is not analyzed (see footnote 6). The term $\bar{\mathcal{G}}^{(0)}$ satisfies

$$\mathrm{d}\bar{\mathcal{G}}_i^{(0)} = [(1-p)(\bar{\mathcal{G}}_{i+1}^{(0)} - \bar{\mathcal{G}}_i^{(0)}) + p(\bar{\mathcal{G}}_i^{(0)} - \bar{\mathcal{G}}_{i-1}^{(0)})]\mathrm{d}t + \mathrm{d}\mathcal{B}_i(t) \tag{44}$$

with the initial condition $\bar{\mathcal{G}}_i^{(0)}(0) = 0$. By dominant balance, the next 2 higher-order terms $\bar{\mathcal{G}}^{(j)}$ ($j = 1, 2$) obey

$$\begin{aligned}\mathrm{d}\bar{\mathcal{G}}^{(1)} = \{&(1-p)\,(\bar{\mathcal{G}}_{i+1}^{(1)} - \bar{\mathcal{G}}_i^{(1)}) + p\,(\bar{\mathcal{G}}_i^{(1)} - \bar{\mathcal{G}}_{i-1}^{(1)}) \\ &+ q_1[\bar{\mathcal{G}}_{i+1}^{(0)}(t)^2 + \bar{\mathcal{G}}_{i-1}^{(0)}(t)^2 - 2\bar{\mathcal{G}}_i^{(0)}(t)^2]\}\mathrm{d}t\ , \quad \bar{\mathcal{G}}^{(1)}(0) = 0\ ,\end{aligned} \tag{45}$$

$$\begin{aligned}\mathrm{d}\bar{\mathcal{G}}^{(2)} = \{&(1-p)\,(\bar{\mathcal{G}}_{i+1}^{(2)} - \bar{\mathcal{G}}_i^{(2)}) + p(\bar{\mathcal{G}}_i^{(2)} - \bar{\mathcal{G}}_{i-1}^{(2)}) \\ &+ 2q_1(\bar{\mathcal{G}}_{i+1}^{(0)}\bar{\mathcal{G}}_{i+1}^{(1)} + \bar{\mathcal{G}}_{i-1}^{(0)}\bar{\mathcal{G}}_{i-1}^{(1)} - 2\bar{\mathcal{G}}_i^{(0)}\bar{\mathcal{G}}_i^{(1)}) \\ &- q_2[\bar{\mathcal{G}}_{i+1}^{(0)}(t)^3 + \bar{\mathcal{G}}_{i-1}^{(0)}(t)^3 - 2\bar{\mathcal{G}}_i^{(0)}(t)^3]\}\mathrm{d}t\ , \quad \bar{\mathcal{G}}^{(2)}(0) = 0\ .\end{aligned} \tag{46}$$

Every equation of the $\bar{\mathcal{G}}^{(j)}$-cascade is linear. Equation (44), which has a white noise, forms the basis of the perturbation scheme. Equations (45) and (46) (for $j \geq 1$) contain lower orders, e.g., $\bar{\mathcal{G}}^{(0)}$, as sources and are thus in principle solvable by superposition; see section 5.3.

5.2. *Zeroth order and one-gap variance,* $0 < p \leq 1/2$

Next, (44) is solved in the limit $N \to \infty$. Note that, by (41), $p(\nu) \uparrow 1/2$ as $\nu \downarrow 0$, $p \downarrow 0$ as $\nu \to \infty$, and $\mathrm{d}p(\nu)/\mathrm{d}\nu < 0$ for $\nu > 0$; hence, $0 < p < 1/2$ for $\nu > 0$. By Taylor expansion [25], $p = 1/2 - \nu/3 + O(\nu^2)$ as $\nu \downarrow 0$ (see footnote 7).

I. Nonzero deposition, $0 < p < 1/2$ **:** Equation (44) is recast to the vector form

$$\mathrm{d}\bar{\mathcal{G}}^{(0)}(t) = -\mathbf{A}(p)\cdot\bar{\mathcal{G}}^{(0)}(t)\,\mathrm{d}t + \mathrm{d}\mathcal{B}(t)\ , \quad \bar{\mathcal{G}}^{(0)}(0) = 0 \quad (\bar{\mathcal{G}}^{(0)} \in \mathbb{T}^N)\ , \tag{47}$$

where $\mathbf{A} = [A_{i,k}]_{0\leq i,k\leq N-1}$ is a sparse *circulant* matrix [46]. The 1st 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 ($1 \leq i \leq N - 1$) form *cyclic permutations* of the 1st 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 1st 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 (47) is written as

$$\bar{\mathcal{G}}^{(0)}(t) = \int_0^t e^{-\mathbf{A}(t-\tau)}\,\mathrm{d}\mathcal{B}(\tau) = \int_0^t e^{-(1-2p)(t-\tau)}e^{-\mathbf{A}_0(t-\tau)}\,\mathrm{d}\mathcal{B}(\tau)\ . \tag{48}$$

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

[6] It appears perhaps paradoxical that no small parameter is manifestly involved in this expansion. A plausible way, amenable to analysis, to think about (43) is this. Consider $\mathrm{d}\mathcal{B}_i(t)$ as small in some sense; for instance, one may multiply $\mathrm{d}\mathcal{B}_i$ by a small (p-dependent) parameter, say $\bar{\epsilon}(p) \ll 1$. Then (43) is written formally as $\bar{\mathcal{G}}(t) \sim \bar{\epsilon}\sum_{j=0}^{k-1}\bar{\epsilon}^j\,\bar{\mathcal{G}}^{(j)}(t)$. The precise definition of this $\bar{\epsilon}$ and study of conditions for an appropriate interpretation (e.g., convergence) of (43) are the subject of work in progress.

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

Remark 2. *By (48), each component $\bar{\mathcal{G}}_i^{(0)}$ of $\bar{\mathcal{G}}^{(0)}(t)$ is a (Riemann) 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 inspection of (48), this variance is i-independent and given by [45]

$$\sigma^{(0)}(t)^2 = \mathbb{E}[\bar{\mathcal{G}}_i^{(0)}(t)^2] = \int_0^t e^{-2(1-2p)\tau}\,|e^{-\mathbf{A}_0\tau}|^2\,\mathrm{d}\tau\ , \tag{49}$$

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

$$\rho_1(t,s) \approx \rho_1^{(0)}(t,s) = \frac{1}{\sqrt{2\pi\sigma^{(0)}(t)^2}}\ \exp\left\{-\frac{(s-\nu)^2}{2\sigma^{(0)}(t)^2}\right\}\ , \tag{50}$$

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

To explicitly compute $\sigma^{(0)}$ via (48), it is desirable to find a formula for $e^{-\mathbf{A}_0 t}$ in the limit $N\to\infty$ (see section 6.1 for an alternate route). Consider $t = O(1)$ and set

$$e^{-\mathbf{A}_0 t} = \sum_{n=0}^{\infty}(-1)^n\,\frac{\mathbf{A}_0^n t^n}{n!} \sim \sum_{n=0}^{N-1}(-1)^n\,\frac{\mathbf{A}_0^n t^n}{n!} \qquad (N\gg 1)\ , \tag{51}$$

bearing in mind that the dimension of $\mathbf{A}_0$ is N. This replacement should be interpreted appropriately, provided $\mathbf{A}_0$ has a finite norm and the series converges accordingly as $N\to\infty$ (see footnote 8) [47]. Note that the n in the summand of *finite* sum (51) does not exceed the dimension of $\mathbf{A}_0$; this facilitates the computation below.

The large-N computation of $e^{-\mathbf{A}_0 t}$ on the basis of (51) is outlined in two lemmas (lemmas I and II), proved in appendix B. First, $\mathbf{A}_0^n$ is provided by the following.

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

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

δ_k^n is Kronecker's delta, modulo N ($\delta_{k+lN}^n = \delta_k^n$ for any integer l), and $0\le j,\ n\le N-1$.

Lemma I enables the explicit computation of $e^{-\mathbf{A}_0 t}$ through (51). The relevant result is stated as follows.

Lemma 2. *For large N, the matrix $e^{-\mathbf{A}_0 t}$ has the 1st-row entries*

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

where $\breve{t} = 2[p(1-p)]^{1/2}\,t$ and J_k is the kth-order Bessel function [48]. This approximation is interpreted in the sense of an appropriate matrix norm (see footnote 9).

[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 (49). Note that $|\mathbf{A}_0| = [p^2 + (1-p)^2]^{1/2} < \infty$. In this metric, the remainder in (51) approaches 0 as $N\to\infty$.

[9] As in (51), the symbol $\sim$ for $e^{-\mathbf{A}_0 t}$ in lemma II implies that the difference of the two matrices (exact and approximate one) approaches 0 as $N\to\infty$ in the Hilbert-Schmidt metric [47].

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

It remains to compute the one-gap variance via (49) and lemma II. Note that

$$\begin{aligned}|e^{-\mathbf{A}_0\tau}|^2 &= \sum_{k=0}^{N-1}[(e^{-\mathbf{A}_0\tau})_{0,k}]^2\\ &\sim \sum_{k=-N}^{N-1}\left(\frac{1-p}{p}\right)^k J_k(\breve{\tau})^2 + 2\sum_{k=0}^{N-1}(-1)^{N-k}\left(\frac{1-p}{p}\right)^{\frac{2k-N}{2}} J_k J_{N-k}(\breve{\tau})\\ &\sim \sum_{k=-\infty}^{\infty}\left(\frac{1-p}{p}\right)^k J_k(\breve{\tau})^2 = I_0[2(1-2p)\tau]\ , \quad \breve{\tau} = 2\sqrt{p(1-p)}\,\tau\ ,\end{aligned}$$

with recourse to appendix C, where I_k is the kth-order modified Bessel function of the first kind [48]. The following result is obtained directly by use of an integral of I_0 derived in appendix C.

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

$$\sigma^{(0)}(t)^2 \sim te^{-2(1-2p)t}[I_0(2(1-2p)t) + I_1(2(1-2p)t)]\ . \tag{52}$$

For an alternate derivation and extension of the above computation to arbitrarily large values of t, see section 6.1.

For fixed t, the density ρ_1 of any step gap is given by (50). It is worthy of notice that (52) diverges as $O(\sqrt{t/(1-2p)})$ if $(1-2p)t \gg 1$. Hence, no steady state is indicated.

The procedure leading to (52) is questionable if t is too large, of the order of N or larger; also, *the starting stochastic model must be modified if $\sigma^{(0)} > \nu$*. Compare (52) to the mean-field result (39) of section 6.2. The two results are discussed in section 6.2.

II. Geometric picture for reference case, $p = 1/2$**:** As is pointed in section 3.3 on the basis of joint *distributions*, step gaps *decorrelate* if $p = 1/2$, for any N and $t \geq 0$. A geometric interpretation of this behavior is now provided in light of (48).

For any N, the matrix $\mathbf{A}_0(p = 1/2)$ is skew symmetric, i.e., $\mathbf{A}_0 = -\mathbf{A}_0^T$ ($\mathbf{A}_0^T$: transpose). Hence, $e^{-\mathbf{A}_0 t}$ is orthogonal, i.e., $e^{-\mathbf{A}_0 t}(e^{-\mathbf{A}_0 t})^T = \mathbf{1} = (e^{-\mathbf{A}_0 t})^T e^{-\mathbf{A}_0 t}$. In addition, for any p, $\det(e^{-\mathbf{A}_0 t}) = 1$ (see appendix D). Thus, $e^{-\mathbf{A}_0(p=1/2)\,t}$ represents rotations in $\mathbb{R}^N$. (So, $\mathbf{A}_0$ via $t \in \mathbb{R}$ generates a 1D subgroup of the special orthogonal group, SO(N).) Hence, in (48), $e^{-\mathbf{A}_0\,(t-\tau)}\,\mathrm{d}\mathcal{B}(\tau)$ describes a rotation of the N-dimensional Brownian motion increment $\mathrm{d}\mathcal{B}(\tau)$; the independence of the components $\mathrm{d}\mathcal{B}_i$ and the variance, $\mathrm{d}\tau$, of $\mathrm{d}\mathcal{B}(\tau)$ are preserved by each rotation. After successive rotations in $[0, t)$, the components $\mathcal{G}_i(t) = \nu + \bar{\mathcal{G}}_i^{(0)}(t)$ emerge as independent Gaussian variables with mean ν and variance t. (Note: $|e^{-\mathbf{A}_0\tau}|^2 = [e^{-\mathbf{A}_0 t}(e^{-\mathbf{A}_0 t})^T]_{0,0} = 1$, which by (49) yields a variance equal to t.)

This result is in agreement with proposition II: in the limit $\nu \downarrow 0$, variance (52) approaches t, since $I_0(0) = 1$ and $I_1(0) = 0$; see also [29].

5.3. On higher-order terms

Corrections to the zeroth-order variance, ${\sigma^{(0)}}^2$, can in principle be obtained via expansion (43) but explicit computations lie beyond the scope of this paper. Next, the higher-order solutions $\bar{\mathcal{G}}^{(1)}(t)$ and $\bar{\mathcal{G}}^{(2)}(t)$ are described formally.

For ease of notation, define the N-dimensional vectors

$$\bar{\mathcal{G}}^{(l)\gamma}(t) \equiv (\bar{\mathcal{G}}_0^{(l)}(t)^\gamma, \ldots, \bar{\mathcal{G}}_{N-1}^{(l)}(t)^\gamma) \ , \quad \gamma = 2,\, 3 \ ,$$
$$\bar{\mathcal{G}}^{(01)}(t) \equiv (\bar{\mathcal{G}}_0^{(0)}\bar{\mathcal{G}}_0^{(1)}(t), \ldots, \bar{\mathcal{G}}_{N-1}^{(0)}\bar{\mathcal{G}}_{N-1}^{(1)}(t)) \ .$$

Accordingly, (45) and (46) have the solutions (in vector form)

$$\bar{\mathcal{G}}^{(1)}(t) = q_1 \int_0^t e^{-(1-2p)(t-\tau)} e^{-\mathbf{A}_0(t-\tau)} A_1 \bar{\mathcal{G}}^{(0)2}(\tau)\, \mathrm{d}\tau \ ,$$
$$\bar{\mathcal{G}}^{(2)}(t) = \int_0^t e^{-(1-2p)(t-\tau)} e^{-\mathbf{A}_0(t-\tau)} A_1 \Big\{ 2q_1 \bar{\mathcal{G}}^{(01)}(\tau) - q_2 \bar{\mathcal{G}}^{(0)3}(\tau) \Big\}\, \mathrm{d}\tau \ , \quad (53)$$

where A_1 is the $N \times N$ circulant matrix with *zero* 1st-row elements *except* $(A_1)_{0,0} = -2$ and $(A_1)_{0,k} = 1$ if $k = 1,\, N-1$; $\bar{\mathcal{G}}^{(0)}(t)$ is given by (48).

6. Extension and discussion

In this section, the terrace width variance is computed for large t within the linear model (47). So, the time restriction of section 5.2 is removed. It is shown how the variance grows with time, indicating that the small-fluctuation hypothesis may break down. In addition, implications and open questions regarding results of sections 3, 4 and 5 are discussed. Of particular interest are: (i) the comparison of variance (39), which stems from the mean-field formalism and gap independence ansatz [25], to explicit formula (52) of proposition II; and (ii) issues of modeling noise in epitaxy.

6.1. Long-t variance and finite-size effects

To explore the limitations of linear model (47), it is advisable to study how the gap variance behaves if t is *arbitrarily* large. The methodology leading to proposition II in section 5.2 must be modified. Formula (52) gives a variance that *diverges* as $\sigma^{(0)}(t)^2 \sim \sqrt{2t/(\pi(1-2p))}$. The starting model becomes *questionable* if $\sigma^{(0)} > \nu$.

The limits $N \to \infty$ and $t \to \infty$ do not commute within the technique of section 5.2. Equation (51), and the subsequent proofs, call for constraining t: for example, asymptotic formula (51) is inapplicable if t is larger than $O(N)$. In this regime, $\sigma^{(0)}(t)$ is sensitive to the choice of boundary conditions for steps.

Consider formula (49) for the variance. The key idea here is to use the relation [47]

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

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 1st row [46]; by a simple computation, $\widetilde{\lambda}_k=-2(1-2p)\cos(2\pi k/N)$. By substitution in (49) and integration,

$$\sigma^{(0)}(t)^2=N^{-1}\sum_{k=0}^{N-1}\frac{1-e^{-2(1-2p)[1-\cos(2\pi k/N)]t}}{2(1-2p)[1-\cos(2\pi k/N)]}\ . \tag{54}$$

The task is to evaluate (54) when t *and* N are large. Distinguish the following cases.

Case $0\le(1-2p)t\le O(1)$**:** Sum (54) 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 $0\le\psi<2\pi$ as $N\to\infty$:

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

which reduces to (52) by integration. Hence, this alternate procedure confirms proposition II. 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 (54) comes from the vicinity of $n=0,\ N-1$. Then, by $1-\cos(2\pi n/N)\sim 2\pi^2n^2/N^2$ the sum reduces to

$$\sigma^{(0)}(t)^2\sim\frac{2t}{N}\left[1+\sum_{n=1}^{\infty}\frac{1-e^{-\zeta(t)n^2}}{\zeta(t)n^2}\right]\ ,\qquad \zeta(t)\equiv\frac{4\pi^2(1-2p)t}{N^2}\ . \tag{55}$$

It has been impossible to simplify this formula if $\zeta(t)=O(1)$, i.e., $(1-2p)t=O(N^2)$; then, $\sigma^{(0)}(t)^2=O(N)$. 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 $\sigma^{(0)}<\nu$ would imply that ν might be too large for the BCF theory to be meaningful. Note that the size(N)-dependent result (55) has been influenced by the assumed boundary conditions.

As a check, take $\zeta(t)\ll 1$ in (55). Then, $\sigma^{(0)}(t)^2\sim\sqrt{t/(\pi(1-2p))}$, which matches the limit of proposition II. Thus, (55) connects smoothly to the fixed-t behavior of ${\sigma^{(0)}}^2$.

Notably, the stochastic process for the *average* terrace width, $\mathcal{G}_{\rm av}(t)=N^{-1}\sum_{i=0}^{N-1}\mathcal{G}_i(t)$ ($\mathcal{G}_{\rm av}\in\mathbb{R}$), can be described simply. To the leading order (for small fluctuations), $\mathcal{G}_{\rm av}-\nu\sim\mathcal{G}_{\rm av}^{(0)}$ satisfies the SDE $\mathrm{d}\mathcal{G}_{\rm av}^{(0)}(t)=N^{-1}\sum_i \mathrm{d}\mathcal{B}_i(t)$, which has solution $\mathcal{G}_{\rm av}^{(0)}(t)=N^{-1}\sum_i\mathcal{B}_i(t)$; its variance is t/N for $t\ge 0$ (see footnote 10).

6.2. Comparison to mean-field variance

The small-fluctuation system described by SDEs (44) was studied from two perspectives: (i) a mean-field formalism leading to the variance $\widehat{\sigma}^2_{\rm pc}$, equation (39), under two-gap independence, in accord with [25]; and (ii) an explicit solution for large N and fixed t, yielding variance (52) of proposition II. The mean field is strictly defined via BBGKY hierarchies, especially the (a priori unknown) pair density ρ_2; see (32) of proposition I. In this context, the independence ansatz $\rho_2(s_0,s_1)\sim\rho_1(s_0)\rho(s_1)$ provides an attractive

[10] This assertion and the derivations of this paper rely on the independence of $\mathrm{d}\mathcal{B}_i(t)$, $i=0,\ \ldots,\ N-1$. By contrast, if periodic white noise is added to the equations of motion for step *positions*, then the resulting noise components for gaps satisfy $\sum_{i=0}^{N-1}\mathrm{d}\mathcal{B}_i(t)=0$ yielding $\mathcal{G}_{\rm av}(t)=\text{const.}$ [49]

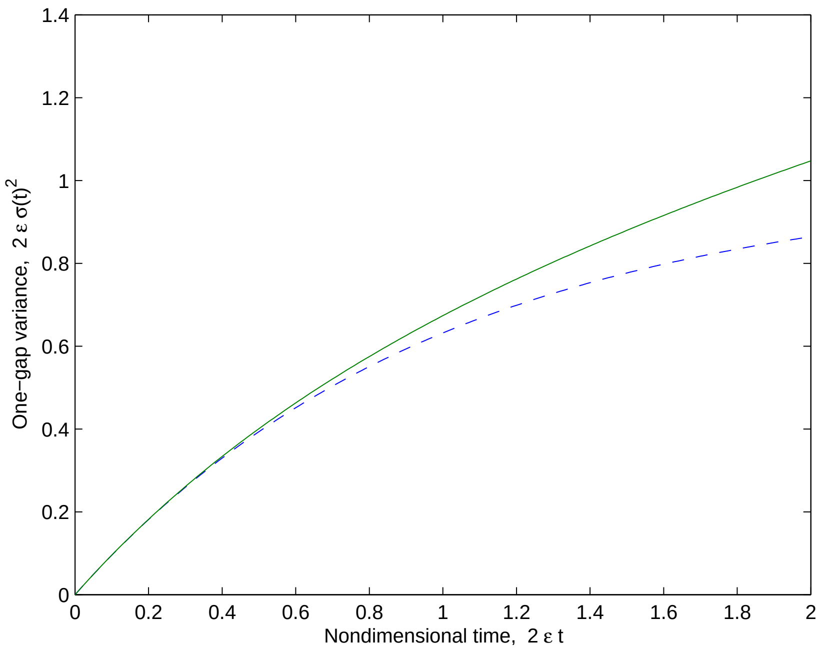

Figure 2. Two (scaled) variances, as functions of $2\epsilon t$ ($\epsilon = 1 - 2p$), for model (13) under small fluctuations: (i) $2\epsilon\sigma^{(0)}(t)^2$ (solid line), by (52) from explicit large-N limit; and (ii) $2\epsilon\widehat{\sigma}_{\rm pc}(t)^2$ (dashed line), by (39) via mean field under two-gap independence.

alternative to complications of fully computing ρ_2 for $N \gg 1$. The ensuing SDEs are decoupled and the one-gap variance is thus determined directly, as in [25]; see (39).

Figure 2 shows the two (scaled) variances as functions of $2(1-2p)t$. The discrepancy between them simply implies that two consecutive step gaps are *correlated* for $t > 0$, regardless of how large N is. The analysis further indicates that a plausible 'measure' of gap correlation is $[{\sigma^{(0)}}^2 - \widehat{\sigma}_{\rm pc}^2]/t$. For $2(1-2p)t \ll 1$, the use of expansions for modified Bessel functions yields [48]

$$\begin{aligned}
\widehat{\sigma}_{\rm pc}(t)^2 &= \frac{1}{2\epsilon}(1 - e^{-2\epsilon t}) = t[1 - \epsilon t + \tfrac{2}{3}\epsilon^2 t^2 + O(\epsilon^3 t^3)] \ , \\
\sigma^{(0)}(t)^2 &= t[1 - \epsilon t + \epsilon^2 t^2 + O(\epsilon^3 t^3)] \ , \qquad \epsilon \equiv 1 - 2p \ , \\
\Rightarrow \ \frac{\sigma^{(0)}(t)^2 - \widehat{\sigma}_{\rm pc}(t)^2}{t} &= \frac{1}{3}\epsilon^2 t^2 + O(\epsilon^3 t^3) \ . \qquad (56)
\end{aligned}$$

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

Remark 3. *For fixed t, (56) may quantify how the deposition flux controls the two-gap correlation, or how 'far' terraces are from decorrelation.*

6.3. Notions of noise

At the risk of redundancy, it is emphasized that the noise has been introduced on an *ad hoc* basis in the equations of motion for terrace widths. Although sources of surface fluctuations have been documented (e.g., [26]), it is of interest to mention possible improvements of the present model that are amenable to analysis by kinetic theory. These include (i) *step-gap dependence* of the white noise coefficient by phenomenology, and (ii) derivation of the noise from perhaps more basic concepts. This discussion concerns the noise at the level of steps; for an exposition on aspects of continuum theory, see [27]. Two tractable possibilities are outlined as follows.

Terrace-width-dependent noise: A plausible *nonlinear* extension of the present linear growth model stems from the work of Williams and Krishnamurty [37]:

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

Here, the $\mathcal{G}$-dependent coefficients of the white noise express stochastic variations in the number of atoms being deposited on neighboring terraces [37]. One subtlety of the analysis is the choice of the stochastic calculus, e.g., Itô or Stratonovich calculus [38]. It is expected that the retainment of linear, $\mathcal{G}$-dependent coefficients of $\mathrm{d}\mathcal{B}$ in this model yields a finite variance for sufficiently long times under $N \to \infty$. A germane complication concerns the definition of a mean field in terms of correlation functions. The analysis of this model is the subject of work in progress.

Random initial data and memory effects; Zwanzig-Mori formalism: So far, the initial data for terrace widths is *nonrandom*. An obvious alternative is to apply deterministic equations of motion with random initial data. This is the approach by Gossmann et al [50], and is incorporated in the formulation of [16]. For the linear model (47), it has been found that the variance behaves as $t^{-1/2}$ for large t [50].

A natural extension is to allow that the noise be induced by randomness in the initial data for terraces that *cannot be measured*, i.e., are 'unresolved'. This approach originates from works by Zwanzig [51] and Mori [52] for non-equilibrium interacting Hamiltonian systems, and permeates current computational approaches (see, e.g., [45] and references therein). The key principle is to separate the step gap variables into *resolved* and *unresolved* ones, and eliminate the latter from the equations of motion. The ensuing SDEs for the resolved variables contain: (i) memory terms (deterministic integrals over $[0,t)$) with a kernel depending on features of the unresolved motion; and (ii) *non-white* noise terms, which come from random initial data for unresolved terraces. Complications arise from the analysis of the nontrivial noise term and the analytical description of the memory kernel. This direction is left for future work.

7. Conclusion

A N-dimensional SDE system for widths of terraces on vicinal crystals was studied analytically with emphasis on the terrace variance for large N. This description originated from a BCF-type model with non-interacting steps, diffusion-limited kinetics and constant material deposition from above [25]. In the small-fluctuation limit, the SDEs were linearized. The resulting matrix Langevin equation involves a parameter, p, that expresses asymmetry in the adatom kinetics; for $p = 1/2$ the process becomes symmetric. The present paper aimed to offer a systematic treatment via elements of kinetic theory, thus complementing analytically recent work by Hamouda, Pimpinelli and Einstein [25] based on kinetic Monte Carlo simulations and mean-field ideas.

The model was analyzed from two perspectives. First, a BBGKY hierarchy was formulated generally for joint probability densities. The BBGKY hierarchy sets the basis for a rigorous definition of a self-consistent mean field in terms of the two-gap density. By an ansatz for gap independence (decorrelation), this mean field reduces to a simple form, adopted in previous works, e.g., [25,37]. In the symmetric case, $p = 1/2$, the joint gap densities have product forms, consistent with a corresponding limit in [29]. Then, the mean field gives the exact one-gap density.

Second, the one-gap variance was computed for all positive times when N is large. For fixed t and $N \to \infty$ ('thermodynamic limit'), the results are expected to be independent of the boundary conditions. The analysis shows how *nonzero* values of $1 - 2p$ induce correlations and thus cause the variance to deviate from its mean-field counterpart. However, if $p \neq 1/2$ and t increases, the exact variance of the linear model diverges as $O(\sqrt{t})$ while the mean-field variance attains a finite value, in qualitative agreement with kinetic Monte Carlo simulations [25]. Finite-size effects were also described by allowing the (nondimensional) t to be larger than N. The physical relevance of this regime is unclear at the moment.

This work has limitations and points to several pending issues. An open problem is to justify rigorously the small-fluctuation expansion and the ensuing zeroth-order SDE. The expansion is questionable when the standard deviation becomes comparable to the terrace width mean. A related issue is that the methods here apply to linear equations. The higher-order equations are linear but, since it is conceivable that the expansion can break down, fully nonlinear terms may have to be considered. This calls for studying the nonlinear SDEs (13), possibly with energetic and entropic step repulsions to enforce a non-crossing condition. Since explicit formulas for the variance are not readily available for this case, one may resort to *a priori estimates*, or a mean-field approach as a guide.

An avenue to understanding the notion of the mean field is to study discrepancies of joint gap densities from their product (decorrelation) forms via weak solutions of BBGKY hierarchies. This plausible direction of research has not been explored.

Extensions of the present model were outlined; for instance, stochastic models with terrace-size dependent noise or incorporation of a Zwanzig-Mori-type formalism. Connections with noisy continuum theories, including renormalization group approaches, were not pursued.

Finally, actual steps and terraces are of course two dimensional (2D), producing much richer phenomena [53]. The (1+1)-dimensional model fails to capture important features such as step meandering, which would alter the predictions. The linkage of the kinetic formalism adopted herein with 2D settings is left for future work. This is crucial for making predictions for experiments and kinetic Monte Carlo simulations.

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Appendix A. Review of Itô formula and Fokker-Planck equation

This appendix provides a brief review of the derivation of the FPE (or, forward Kolmogorov equation) for the N-dimensional SDE

$$\mathrm{d}\mathcal{X}(t) = \check{A}(\mathcal{X}(t))\,\mathrm{d}t + \mathrm{d}\mathcal{B}(t)\ ; \quad \mathcal{X} \in \mathbb{T}^N\ , \tag{A.1}$$

$\mathcal{B}(t)$ is N-dimensional Brownian motion, and $\mathcal{X}(0) = \mathcal{Z}$ where $\mathcal{Z}$ is a random variable with known density $\rho_N^{\mathcal{Z}}(x)$ $(x \in \mathbb{T}^N)$; for precise conditions on $\check{A}$, see [54]. Although the coefficient of $\mathrm{d}\mathcal{B}(t)$ is set to unity here, the derivation can be extended to the case with an $\mathcal{X}$-dependent coefficient via Itô calculus.

The starting point is the Itô formula, i.e., a rule for differentiating with respect to t functions of stochastic processes [38, 54]. If $\phi(x)$, $\phi : \mathbb{T}^N \to \mathbb{R}$, is twice continuously differentiable and $\mathcal{X}(t)$ satisfies (A.1), then the Itô formula reads

$$\mathrm{d}\phi(\mathcal{X}(t)) = [\nabla_N \phi(\mathcal{X}(t))] \cdot \mathrm{d}\mathcal{X}(t) + \frac{1}{2}[\Delta_N \phi(X(t))]\,\mathrm{d}t\ , \tag{A.2}$$

which by direct integration yields

$$\phi(\mathcal{X}(t)) - \phi(\mathcal{Z}) = \int_0^t \{[\nabla_N \phi(\mathcal{X}(\tau))] \cdot \mathrm{d}\mathcal{X}(\tau) + \frac{1}{2}[\Delta_N \phi(X(\tau))]\,\mathrm{d}\tau\}\ .$$

Taking the mean of both sides, with recourse to the density $\rho_N^{\mathcal{X}}(t, x)$ for $\mathcal{X}(t)$, and applying integration by parts yields

$$\int_{\mathbb{T}^N} \phi(x)\rho_N^{\mathcal{X}}(t, x)\,\mathrm{d}x - \int_{\mathbb{T}^N} \phi(x)\rho_N^{\mathcal{Z}}(x)\,\mathrm{d}x$$
$$= \int_{\mathbb{T}^N}\int_0^t \mathrm{d}\tau\mathrm{d}x\,\phi(x)\,\{-\mathrm{div}_N[\check{A}(x)\,\rho_N^{\mathcal{X}}(\tau, x)] + \tfrac{1}{2}\Delta_N \rho_N^{\mathcal{X}}(\tau, x)\} \qquad \forall\,\phi\ .$$

In the above, use was made of the Itô isometry $\mathbb{E}[\nabla_N\phi(\mathcal{X}(\tau))\cdot \mathrm{d}\mathcal{B}(\tau)] = 0$ [54]. It follows that $\rho_N^{\mathcal{X}}(t,x)$ satisfies

$$\int_{\mathbb{T}^N}\int_0^t \mathrm{d}\tau\mathrm{d}x\, \phi(x)\, \{\partial_\tau + \mathrm{div}_N[\check{A}(x)\,\cdot\,] - \tfrac{1}{2}\nabla_N\}\rho_N^{\mathcal{X}}(\tau,x) = 0 \quad \forall\,\phi\ , \tag{A.3}$$

with the initial condition $\rho_N^{\mathcal{X}}(0,x) = \rho_N^{\mathcal{Z}}(x)$. Equation (A.3) leads to the FPE for (A.1) in an appropriate weak sense:

$$\partial_t\rho_N^{\mathcal{X}}(t,x) + \mathrm{div}_N[\check{A}(x)\rho_N^{\mathcal{X}}(t,x)] = \frac{1}{2}\nabla_N\rho_N^{\mathcal{X}}(t,x)\ . \tag{A.4}$$

Note that using the Itô formula is not necessary here because the coefficient of $\mathrm{d}\mathcal{B}(t)$ is a constant, and thus the choice of stochastic calculus becomes immaterial.

Appendix B. Proofs of lemmas I and II

This appendix presents proofs of the elementary lemmas I and II of section 5.2.

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

$$(A_0^n)_{0,k} = -(1-p)\,(A_0^{n-1})_{0,k-1} + p\,(A_0^{n-1})_{0,k+1}\ ; \quad (A_0^0)_{0,k} = \delta_k^0\ . \tag{B.1}$$

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

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

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

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

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

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

Proof of lemma II: 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 (51) for large N in conjunction with lemma I, noting that

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

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

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

By (51), the kth 1st-row element of the circulant matrix $e^{-\mathbf{A}_0 t}$ is given by

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

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

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

where $\Gamma(z)$ is the Gamma function [55]. 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 $(0 \le l \le M)$,

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

where $\breve{t} = 2\sqrt{p(1-p)}\,t$ and J_k is the kth-order Bessel function [48].

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

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

This concludes the proof of lemma I for odd N. The case with even N is similar, left as an exercise to the interested reader. □

Appendix C. On series and an integral 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 D.

Power series: First, consider the known Fourier series [48]

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

where $J_k(\eta)$ denotes the kth-order Bessel function. The replacements $e^{i\theta} = z(\chi) = [(1+i\chi)/(1-i\chi)]^{1/2} e^{-i2\pi n/N}$, where $\chi \in \mathbb{R}$ and n: integer, and $2i \sin\theta = z - z^{-1}$ in (C.1) produce the formula

$$
\begin{aligned}
S_1(z(\chi); \eta) &= \sum_{k=-\infty}^{\infty} \left(\frac{1+i\chi}{1-i\chi}\right)^{k/2} e^{-i2\pi kn/N} J_k(\eta) \\
&= \exp\left[\frac{1}{2}\eta \left(\sqrt{\frac{1+i\chi}{1-i\chi}} e^{-i2\pi n/N} - \sqrt{\frac{1-i\chi}{1+i\chi}} e^{i2\pi n/N} \right)\right] \ . \qquad \text{(C.2)}
\end{aligned}
$$

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

As another application of analytic continuation, compute

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

which is needed for determining the one-gap variance in section 5.2. For complex z ($z \in \mathbb{C}$), or ϵ, and fixed real η, this series $\widetilde{S}_2$ converges everywhere in $\mathbb{C}_0 = \{z : \ 0 < |z| < \infty\}$ and represents an analytic function in the punctured plane $\mathbb{C}_0$.

To find $\widetilde{S}_2(\epsilon)$ apply a version of Graf's addition formula [48], viz., the Fourier series

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

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

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

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

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

where I_0 is the 0th-order modified Bessel function of the first kind [48].

Integral of a modified Bessel function: The next task is to show that

$$\int_0^t e^{-\tau}\, I_0(\tau)\, \mathrm{d}\tau = te^{-t}[I_0(t) + I_1(t)] \ . \tag{C.7}$$

Indeed, the integrand is written as

$$e^{-t}I_0(t) = e^{-t}[t(I_0' + I_1' - I_0 - I_1) + I_0 + I_1] = \frac{\mathrm{d}}{\mathrm{d}t}[e^{-t}t(I_0 + I_1)] \ , \tag{C.8}$$

where $I_0' = I_1$ and $t(I_1' - I_0) + I_1 = 0$ [48]; the prime here denotes differentiation in t.

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

In this appendix, the eigenvalues and determinant of the $N \times N$ matrix $e^{-\mathbf{A}_0(p)t}$ are computed. Note that, since $e^{-\mathbf{A}_0 t}$ is circulant, its (normalized to unity) eigenvectors are $\Psi_l = N^{-1/2}(1, e^{i2\pi l/N}, \ldots, e^{i2\pi lj/N}, \ldots, e^{i2\pi l(N-1)/N})$, $0 \le l,\, j \le N-1$ [46].

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

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

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

$$\lambda_l(t) \sim \exp\left[\frac{1}{2}\breve{t}\left(\sqrt{\frac{1-p}{p}}\, e^{-i2\pi l/N} - \sqrt{\frac{p}{1-p}} e^{i2\pi l/N}\right)\right] \ , \tag{D.1}$$

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

Proof. The desired eigenvalues are the discrete Fourier transform of the 1st row of $e^{-\mathbf{A}_0 t}$ [46]. By lemma II (section 5.2) in the limit $N \to \infty$,

$$\begin{aligned}\lambda_l &\sim \sum_{k=0}^{N-1}\left[\left(\frac{1-p}{p}\right)^{k/2} J_k(\breve{t}) + (-1)^{N-k}\left(\frac{p}{1-p}\right)^{\frac{N-k}{2}} J_{N-k}(\breve{t})\right] e^{-i2\pi kl/N} \\ &= \sum_{k=-N}^{N-1}\left(\frac{1-p}{p}\right)^{k/2} e^{-i2\pi kl/N}\, J_k(\breve{t}) \sim \sum_{k=-\infty}^{\infty}\left(\frac{1-p}{p}\right)^{k/2} e^{-i2\pi kl/N}\, J_k(\breve{t}) \ ,\end{aligned}$$

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

It is of interest to show that (D.1), although obtained in the large-N limit, is consistent with result I. Indeed, by the well-known formula $\det(e^{-\mathbf{A}_0 t}) = \prod_{l=0}^{N-1} \lambda_l(t)$, result I follows from result II via the trivial identities $\sum_{l=0}^{N-1} e^{\pm i2\pi l/N} = 0$.

Application of result II to the *reference case*, $p = 1/2$, yields the following corollary.

Corollary 1. For $p = 1/2$, fixed t and large N, the eigenvalues of $e^{-\mathbf{A}_0 t}$ are

$$\lambda_l(t; p = 1/2) \sim \exp\left[-it \sin\left(\frac{2\pi l}{N}\right)\right] . \tag{D.2}$$

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