Small fluctuations in epitaxial growth via flux-induced conservative noise

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Abstract. We study the joint effect of *growth* (material deposition from above) and nearest-neighbor *interactions* in a *stochastically perturbed* system of N line defects (steps) on a vicinal crystal in 1+1 dimensions. The noise stems from the deposition-flux-induced *asymmetric* attachment of atoms to step edges. The steps interact entropically and as force dipoles. Our main result is a simplified formula for the time dependent terrace width probability density as $N \to \infty$ for *small step fluctuations*. This work complements analyses by Margetis (2010 *J. Phys. A* **43** 065003) and Ben-Hamouda, Pimpinelli, and Einstein (2009 *Europhys. Lett.* **88** 26005) in which steps are non-interacting and the noise is deposition-independent.

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1. Introduction

A central question in nonequilibrium statistical mechanics is: how do *large-scale* evolution laws *emerge* from the deterministic or stochastic dynamics of *many-particle* systems [1]? Descriptions of linkages of particle models to full continuum theories lie at the heart of computational physics [2]. Related themes date back to classic works for the Boltzmann equation; see, e.g., [3–6].

Recently, one of us analyzed a stochastic model for the motion of many line defects (steps) on a vicinal crystal when material is deposited from above [7]. This setting is characterized by a constant average surface slope. The same system was studied in [8], where the increase of deposition rate was found to cause narrowing of the terrace width probability density (TWD), in qualitative agreement with kinetic Monte Carlo simulations. The starting point in [7, 8] is a large system of stochastic differential equations (SDEs) for the terrace widths. This is formulated by addition of ad hoc white noise to the Burton-Cabrera-Frank (BCF) model of step flow [9]. In [7] a self-consistent 'mean field', which reduces the SDEs to a single Langevin-type equation [8], is defined systematically via kinetic hierarchies for terrace correlation functions.

Three assumptions permeating [7] are: (i) steps are straight; (ii) steps are energetically non-interacting; and (iii) the white noise is non-conservative. These hypotheses have enabled simplifications in the analysis, yet are not entirely physical. For instance, enforcing (iii) yields a variance of the TWD that diverges at long times. Improvements of the stochastic model are offered in [10], where steps interact entropically and as force dipoles under conservative noise, albeit in the absence of growth. The step fluctuations are suppressed for sufficiently strong step interactions [10].

In this article, we relax assumptions (ii) and (iii) above, extending the analysis to straight steps that interact entropically and as force dipoles in the *presence of growth* and conservative white noise. For a given terrace, the noise is attributed to fluctuations in the number of atoms that attach to step edges. In the limit of *small fluctuations*, the corresponding (nonlinear) SDEs are *linearized* around the average terrace width. This approximation yields a prototypical linear model for *asymmetric* kinetic processes with conservative noise, which captures certain correlations (but leaves out nonlinearities). We solve this model exactly, and thereby quantify how the step interaction strength and deposition rate *combined* influence the TWD.

In accord with the BCF theory [9], the major kinetic processes incorporated in the model are: (a) diffusion of adsorbed atoms (adatoms) on terraces; (b) attachment and detachment of atoms at step edges; and (c) external deposition with (given) rate F. For the sake of simplicity, we impose diffusion-limited (DL) kinetics, in which the diffusion of adatoms on terraces is the slowest process. In this case, the adatom density at each step edge attains an equilibrium value [8, 11].

The kinetic process for the motion of terraces is *asymmetric* because of a drift (average lateral step velocity) proportional to F (see section 2.2). As a result, on every terrace the flux of deposited atoms toward an upstep is different from the flux at a downstep. A similar kinetic effect can arise by the Ehrlich-Schwoebel barrier [12–18], electromigration currents [19, 20], differences of atomistic origin in attachment rates [14, 21] and impurities [22, 23].

In our stochastic model, we account for a deposition-dependent noise that reflects the above kinetic asymmetry. In the spirit of Williams and Krishnamurthy [24], we include fluctuations in the number of deposited atoms that attach to step edges. For macroscopic times, such fluctuations are described by conservative white noise with a diffusion coefficient that expresses asymmetric attachment of atoms to step edges via a parameter, $p(F)$. The resulting SDEs are consistent with a fixed system size, i.e., the *total* length of the step system remains constant (and does not fluctuate).

Assuming small fluctuations of each terrace, induced by "small noise terms", we linearize the SDEs. The ensuing terrace width stochastic process is Gaussian. The average terrace width is fixed at its initial value (consistent with a vicinal crystal and set by the crystal miscut angle in experiments). We compute the variance analytically by allowing $N \to \infty$ while keeping the time t independent of N (see section 3).

In particular, we derive a relatively simple formula for the variance in the steady state. By comparing our result to the mean field approach introduced in [8] and further discussed in [7], we indicate the role of noise in terrace correlations at the steady state (see section 4.1). Plausible implications of our predictions are discussed in section 4.2. Because of our assumed dependence of the noise on the deposition rate (F), the effect of this rate on the TWD is found to be weaker than the respective effect found in [8] where the noise is flux-independent.

Our model, being amenable to basic analysis, is limited in its applicability. A limitation is due to the one-dimensional (1D) geometry. Because steps are straight, meandering is suppressed and the noise has a relatively simple form. This setting contrasts the two-dimensional (2D) geometry invoked e.g., in [15, 25, 26]. For instance, in [15, 25] Langevin forces are added to both the adatom diffusion equation and the boundary conditions for atom attachment-detachment at steps. For many steps, the resulting stochastic equations appear to have a complicated structure. In [26], the noise is white in both time and space (position along the step). Here, we resort to a tradeoff. On the one hand, we circumvent complications of 2D, aiming to capture effects (interaction and deposition growth) on *many* steps that cause narrowing of the TWD [8]. On the other hand, we exclude richer (more realistic) effects such as meandering.

Another limitation, which is a consequence of our approximation, is that steps can cross. This feature is unphysical. However, it has a negligibly small likelihood provided $(ga/T)(a/\varpi)(a\varrho_0) \gg 1$ (see section 4.3) where g is the step interaction strength in units of energy per length, T is the Boltzmann energy (or absolute temperature in units where $k_B = 1$), ϖ is the initial terrace width, ϱ_0 is a typical adatom density (in units of inverse length), and a is the atomic step height; $a\varrho_0 < 1$.

Throughout this paper, we assume familiarity with basic concepts of epitaxial systems. For reviews on the subject, the reader may consult, e.g., [11, 18, 27–30].

The organization of this paper is summarized as follows. In section 2, we formulate

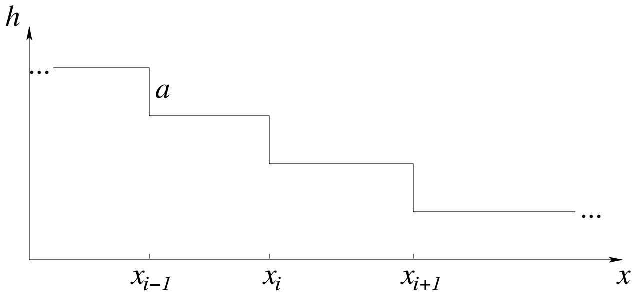

Figure 1. Schematic (cross section) of step geometry: $x = x_i(t)$ is the ith step position, a is the step height, and h is the surface height.

the governing SDE system for 1D step motion in the presence of growth and step interactions in the spirit of BCF [9]. In section 3, we solve the SDEs and compute the corresponding TWD. In section 4, we discuss implications of our results: we compare our prediction with a mean field approach, indicate conditions for the validity of our linearized model, and discuss comparisons to related past works and possible connections to experiment. The appendices contain technical derivations needed in the main text.

Notation and terminology. The symbol $\mathcal{B}(t)$ denotes Brownian motion, while $\eta(t) = \mathrm{d}\mathcal{B}/\mathrm{d}t$ is white noise (where the time derivative is interpreted in the sense of distributions) [31]. The probabilistic terms "average", "mean" and "expectation" are used interchangeably. Matrices and vectors are boldface. A matrix $\boldsymbol{C}$ is denoted by $[C_{k,l}]$ where $C_{k,l}$ is the entry at the kth row and lth column. The norm squared of the $N \times N$ circulant matrix $\boldsymbol{C}$ is $|\boldsymbol{C}|^2 = \sum_{l=0}^{N-1} |C_{0,l}|^2 = \sum_{k=0}^{N-1} |C_{k,0}|^2$. By $f = \mathcal{O}(g)$ we imply that f/g is bounded as a parameter or variable approaches an extreme value.

2. Formulation: Geometry, kinetics, energetics and noise

In this section we formulate SDEs for terrace widths in the spirit of the BCF theory [9]. The step flow model accounts for: (i) material deposition from above; (ii) nearest-neighbor force dipole and entropic step interactions; and (iii) deposition-related noise. The resulting SDEs are linearized via stochastic perturbations, i.e, when the noise term is sufficiently small (in some appropriate sense).

2.1. Deterministic model

We focus on deterministic motion. The geometry consists of straight steps at $x = x_i(t)$ (see figure 1). The ith terrace is the region $x_i < x < x_{i+1}$, where $w_i(t) = x_{i+1}(t) - x_i(t) > 0$ and $i = 0, \ldots, N-1$. Apply screw periodic boundary conditions so that steps are mapped onto point particles on a ring. We set $w_i(0) = \varpi$.

The formulation of equations for $x_i(t)$ is outlined in [7], and summarized here with a more precise description of step interactions. In the presence of material deposition from above, steps have a typical (drift) velocity $v = Fa\varpi$ where F is the deposition rate. By a Galilean transformation in the comoving frame [8, 32], the adatom concentration

$\varrho_i(x,t)$ on the ith terrace satisfies $(D\partial_{\tilde{x}}^2 + v\partial_{\tilde{x}})\varrho_i + F = \partial_{\tilde{t}}\varrho_i$, where D is the terrace diffusion constant and $(\tilde{x},\tilde{t}) = (x - vt, t)$. By the quasi-steady approximation we set $\partial_{\tilde{t}}\varrho_i \approx 0$, which holds if deviations of the actual step velocity from v are much smaller than the diffusive speed D/ϖ. Now remove the tildes for ease of notation ($\tilde{x} \Rightarrow x$).

By linear kinetics, the atom attachment-detachment at the steps bounding the ith terrace is expressed by [11] $-J_i(x_i) = k\,[\varrho_i(x_i) - \varrho_i^{\rm eq}]$ and $J_i(x_{i+1}) = k\,[\varrho_i(x_{i+1}) - \varrho_{i+1}^{\rm eq}]$, where $J_i(x) = -D\partial_x\varrho_i - v\varrho_i$ is adatom flux on the ith terrace, $\varrho_i^{\rm eq}$ is the equilibrium adatom concentration on the ith step edge, and k is a constant rate. The quantity $\varrho_i^{\rm eq}$ encapsulates energetics, e.g., force dipole step interactions [11, 33, 34]. Distinct rates $k_{\rm u}$, $k_{\rm d}$ for up- and down-step edges (Ehrlich-Schwoebel effect [12]) can also be included.

We enforce the conditions $v/k \ll 1$ and $D/k \ll \varpi$, which amount to DL kinetics[1]. This means that we let $k \to \infty$ in the attachment-detachment conditions at step edges so that $\varrho_i(x_i) \to \varrho_i^{\rm eq}$ since the flux is finite [8].

Each step advances or retreats in response to the total mass flux incident on it, by mass conservation. Thus, the step velocity reads $\dot{x}_i = {\rm d}x_i/{\rm d}t = (\Omega/a)[J_{i-1}(x_i) - J_i(x_i)]$ where Ω is the atomic area, $\Omega \approx a^2$. By solving the diffusion equation for ϱ_i (treating the positions x_i and densities $\varrho_i^{\rm eq}$ as fixed), and thus determining $J_i(x)$, we obtain a system of ordinary differential equations (ODEs) for $x_i(t)$, and in turn for $w_i(t)$ [7]:

$$
\begin{aligned}
\dot{w}_i = \frac{{\rm d}w_i}{{\rm d}t} = \frac{aF}{2}\Bigg\{ & \frac{w_{i+1}e^{\frac{vw_{i+1}}{2D}}}{\sinh(\frac{vw_{i+1}}{2D})} - \frac{2w_i\cosh(\frac{vw_i}{2D})}{\sinh(\frac{vw_i}{2D})} + \frac{w_{i-1}e^{\frac{vw_{i-1}}{2D}}}{\sinh(\frac{vw_{i-1}}{2D})} \\
& + a\varpi\Bigg[\varrho_{i+2}^{\rm eq}\frac{e^{\frac{vw_{i+1}}{2D}}}{\sinh(\frac{vw_{i+1}}{2D})} - \varrho_{i+1}^{\rm eq}\left(\frac{e^{-\frac{vw_{i+1}}{2D}}}{\sinh(\frac{vw_{i+1}}{2D})} + \frac{2e^{\frac{vw_i}{2D}}}{\sinh(\frac{vw_i}{2D})}\right) \\
& + \varrho_i^{\rm eq}\left(\frac{2e^{-\frac{vw_i}{2D}}}{\sinh(\frac{vw_i}{2D})} + \frac{e^{\frac{vw_{i-1}}{2D}}}{\sinh(\frac{vw_{i-1}}{2D})}\right) - \varrho_{i-1}^{\rm eq}\frac{e^{-\frac{vw_{i-1}}{2D}}}{\sinh(\frac{vw_{i-1}}{2D})}\Bigg]\Bigg\},
\end{aligned}
\tag{1}
$$

where $i = 0, 1, \ldots, N-1$. It remains to express each $\varrho_i^{\rm eq}$ in terms of positions x_i.

The step interactions are introduced explicitly in the ith-step chemical potential, μ_i, through the relation $\varrho_i^{\rm eq} = \varrho_0(1 + \mu_i/T)$ [11]. If $E_N(\{x_i\})$ is the total energy per unit length of the step system, we have $\mu_i = \Omega(\delta E_N/\delta x_i)$. For entropic and force dipole interactions, this E_N reads [11, 33, 34]

$$
E_N = g\sum_i \left(\frac{a}{w_i}\right)^2 \Rightarrow \mu_i = ga\left[\left(\frac{a}{w_i}\right)^3 - \left(\frac{a}{w_{i-1}}\right)^3\right] \quad (g > 0). \tag{2}
$$

Equation (1) is rewritten accordingly. We leave this task to the interested reader. Evidently, $w_i(t) \equiv \varpi$ is a solution for all $t > 0$ if $w_i(0) = \varpi$.

2.2. Stochastic perturbation

Next, we add noise to ODEs (1) in view of (2). Features of this extension are suggested via perturbations of these ODEs around a constant, c (e.g., $c = \varpi$).

[1]For $v = \mathcal{O}(1) > 0$, a more precise condition on v reads $v/k \ll \tanh[v\varpi/(2D)]$.

Set $w_i(t) = c[1+\xi_i(t)]$, $|\xi_i| \ll 1$. By (1) and (2), the linearized equations are

$$\dot{\xi}_i = aF\{(1-p)(\xi_{i+1}-\xi_i) + p(\xi_i - \xi_{i-1}) + \breve{g}[-(1+\text{ß})(\xi_{i+2} - 3\xi_{i+1} + 3\xi_i - \xi_{i-1}) + \text{ß}(\xi_{i+1} - 3\xi_i + 3\xi_{i-1} - \xi_{i-2})]\}, \tag{3}$$

where (abusing notation) we use the same symbol (ξ_i) for the approximation of ξ_i, i.e., the solution of the linearized equations. The parameters p, ß and $\breve{g}$ are defined by

$$p = \frac{1}{2}\left(\frac{\nu}{\sinh^2\nu} - \frac{e^{-\nu}}{\sinh\nu}\right), \quad \text{ß} = \frac{1}{2}\frac{e^{-\nu}}{\sinh\nu}, \quad \breve{g} = 3\frac{ga}{T}m_0^3(a\varrho_0), \tag{4}$$

with $\nu = v\varpi/(2D)$, $m_0 = a/\varpi$ (slope) and $0 < p < 1/2$; cf. (34) in [7] where $g = 0$.

Let us pause for a moment and take a closer look at (3). For $\breve{g} = 0$ (no step interaction), this equation reduces to $\dot{w}_i \approx Fa[(1-p)(w_{i+1} - w_i) + p(w_i - w_{i-1})]$. We can consider p as the fraction of deposited atoms from above that attach to the downstep of terrace i, in the setting of figure 1. So, $1-p$ is the fraction of atoms that move to an upstep. Hence, the number of atoms per unit time that cause increase of the ith terrace size is $pF(w_i - w_{i-1})$ by competition with the upper terrace, and $(1-p)F(w_{i+1} - w_i)$ from the lower terrace. For a similar model see the early work by Gossmann, Sinden and Feldman for step motion in a diffusion bias [35] (see also [36] for an effect of impurities).

To add noise, we inspect the linearized deterministic equations for $\breve{g} = 0$ [24]. The idea is to consider the number of atoms arriving at each step edge as fluctuating in accord with the p-induced *asymmetry*, i.e., allow lateral fluxes that cause noise to distinguish downsteps from upsteps. Let $\mathcal{N}_i^{\pm}(t)$ be the (random) number of atoms attaching to an upstep (+) or a downstep (−) of the ith terrace. For macroscopic times and each i, we posit that the increments $\mathcal{N}_i^{\pm}(t_{n+1}) - \mathcal{N}_i^{\pm}(t_n)$ are independent, normally distributed and stationary random variables, with mean zero and variance proportional to $1-p$ (+) or p (−) times $(t_{n+1} - t_n)Fw_i$, where $0 < t_n < t_{n+1}$.

Accordingly, we perturb (3), or (1), for the ith terrace motion by: (i) the noise $\sqrt{(1-p)Fw_{i+1}\Omega}\,\eta_{i+1}$ (which has the dimension of speed where $\Omega \approx a^2$) for fluctuations in the number of atoms attaching to the upstep bounding the $(i+1)$th terrace; (ii) $\sqrt{pFw_{i-1}\Omega}\,\eta_{i-1}$ regarding the downstep of the $(i-1)$th terrace; and (iii) $[\sqrt{pFw_i\Omega} - \sqrt{(1-p)Fw_i\Omega}]\,\eta_i$ for mass conservation purposes. Here, $(\eta_0, \ldots, \eta_{N-1})$ is a vector white noise–having independent, identically distributed components $\eta_i = \mathrm{d}\mathcal{B}_i/\mathrm{d}t$ with dimension of $(\mathrm{time})^{-1/2}$. We propose the SDEs ($i = 0, \ldots, N-1$)

$$\dot{\xi}_i = aF\{(1-p)(\xi_{i+1}-\xi_i) + p(\xi_i - \xi_{i-1}) + \breve{g}[-(1+\text{ß})(\xi_{i+2} - 3\xi_{i+1} + 3\xi_i - \xi_{i-1}) + \text{ß}(\xi_{i+1} - 3\xi_i + 3\xi_{i-1} - \xi_{i-2})]\} + \frac{a}{\varpi}\sqrt{F\varpi}\left[\sqrt{1-p}\,(\eta_{i+1} - \eta_i) + \sqrt{p}\,(\eta_i - \eta_{i-1})\right], \tag{5}$$

where $\xi_i = (w_i - \varpi)/\varpi$ is now a *stochastic* process. We assume that fluctuations are small in probability, $1 - \Pr[\sup_{t>0}|\xi_i(t)| \ll 1] \ll 1$ for all i (Pr denotes the probability)[2].

[2]In (5), notice the replacement of w_i and $w_{i\pm1}$ by the initial terrace width, ϖ, in the noise diffusion coefficients. A formal argument for this approximation can be made by adding to ODEs (1) the "small noises" $\epsilon\eta_i\sqrt{Fw_ia^2}(\sqrt{p} - \sqrt{1-p})$, $\epsilon\eta_{i+1}\sqrt{Fw_{i+1}a^2}$ and $-\epsilon\eta_{i-1}\sqrt{Fw_{i-1}a^2}$ where $0 < \epsilon \ll 1$. Then, use the expansion $w_i(t) = \varpi[1 + \epsilon\xi_i(t) + \ldots]$. Equations (5) are viewed as the lowest-order equations in ϵ.

Equation (5) is fully non-dimensionalized via $t \mapsto \tilde{t} = tFa$ and $\eta_i \mapsto \tilde{\eta}_i = \eta_i(Fa)^{-1/2}$. Hence, we formulate the SDEs

$$\begin{aligned}\frac{\mathrm{d}\xi_i}{\mathrm{d}\tilde{t}} &= (1-p)(\xi_{i+1}-\xi_i) + p(\xi_i - \xi_{i-1}) + \breve{g}[-(1+ß)(\xi_{i+2}-3\xi_{i+1} \\ &\quad + 3\xi_i - \xi_{i-1}) + ß(\xi_{i+1} - 3\xi_i + 3\xi_{i-1} - \xi_{i-2})] \\ &\quad + \sqrt{m_0}\Big[\sqrt{1-p}\,\tilde{\eta}_{i+1} - \sqrt{p}\,\tilde{\eta}_{i-1}) + (\sqrt{p} - \sqrt{1-p})\tilde{\eta}_i\Big],\ \xi_i(0) = 0,\end{aligned} \quad (6)$$

where each ξ_i has zero expectation, $\mathbb{E}\xi_i = 0$.

Remark 1. The choice of signs of the noise terms is not unique, but guarantees $\sum_i \dot{w}_i(t) = 0$, i.e., a constant, non-fluctuating, system size. Further, the overall noise is *first-order conservative.* Indeed, let $\tilde{\eta}_i(\tilde{t}) = \aleph(\chi, \tilde{t})$ for $\chi = i\delta$ with δ appropriately small, e.g., $\delta = \mathcal{O}(\frac{a}{N\varpi})$, and (space-)continuous $\aleph(\cdot, \tilde{t})$. The Taylor expansion in δ for the overall noise yields $\delta\partial_\chi \aleph + \mathcal{O}(\delta^2)$. Similar terms come from the ξ_i's via $\xi_i(t) = \Xi(\chi, t)$. In the limit $N \to \infty$ with fixed m_0, SDEs (6) reduce to a continuum conservation law, $\partial_t \Xi + \partial_\chi \Phi[\Xi, \aleph] = 0$ where Φ is an appropriate "flux" (depending linearly on Ξ and $\aleph$).

3. Solution of linearized stochastic system

In this section we solve SDEs (6) with particular emphasis on the single-terrace width variance, $\sigma(t; N)^2 = \mathbb{E}\xi_i(t)^2$. The SDEs are recast to the matrix form

$$\frac{\mathrm{d}\boldsymbol{\xi}}{\mathrm{d}\tilde{t}} = -\boldsymbol{A}\cdot\boldsymbol{\xi} + \boldsymbol{Q}\cdot\widetilde{\boldsymbol{\eta}}\ , \quad (7)$$

where $\boldsymbol{\xi} = (\xi_0, \dots, \xi_{N-1})$, $\widetilde{\boldsymbol{\eta}} = (\tilde{\eta}_0, \dots, \tilde{\eta}_{N-1})$, and $\boldsymbol{A}$ and $\boldsymbol{Q}$ are sparse *circulant* matrices with first-row entries $[1-2p+3\breve{g}(1+2ß), -1+p-\breve{g}(3+4ß), \breve{g}(1+ß), 0, \dots, 0, \breve{g}ß, p-\breve{g}(1+4ß)]$ and $\sqrt{m_0}[\sqrt{p}-\sqrt{1-p}, \sqrt{1-p}, 0, \dots, 0, -\sqrt{p}]$, respectively.

By integrating (7), we obtain

$$\boldsymbol{\xi}(t) = \int_0^{\tilde{t}} e^{-\boldsymbol{A}(\tilde{t}-\tau)}\boldsymbol{Q}\cdot\widetilde{\boldsymbol{\eta}}(\tau)\,\mathrm{d}\tau, \qquad \tilde{t} = tFa. \quad (8)$$

Evidently, for every $t > 0$, (8) describes a vector Gaussian variable with zero expectation. The variance of each component, ξ_i, is

$$\sigma(t; N)^2 = \int_0^{tFa} \left|e^{-\boldsymbol{A}\tau}\boldsymbol{Q}\right|^2 \mathrm{d}\tau\ . \quad (9)$$

The probability density for each ξ_i is[3]

$$P(\xi, t) = \frac{1}{\sqrt{2\pi\,\sigma(t; N)^2}} \exp\left[-\frac{\xi^2}{2\sigma(t; N)^2}\right], \quad -\infty < \xi < \infty,\ t > 0, \quad (10)$$

by which the TWD for the dimensional terrace width is obtained via $\xi = (w - \varpi)/\varpi$, $-\infty < w < \infty$. *Within this approximation* $\Pr[w_i < 0] > 0$: there exists a nonzero probability of step crossing. This can be controlled by the step interaction strength, deposition rate and initial terrace width (see section 4.3). We consider $\Pr[w_i < 0]$ as negligibly small.

[3]By abusing notation, we use the same symbol, ξ, to denote both the independent real variable of the TWD and the stochastic process associated with each terrace width.

3.1. Terrace width variance

Next, we compute $\sigma(t;N)^2$ by (9). First, we derive an equivalent expression valid for finite N and t. Second, we take the limit as $N\to\infty$ and thereby extract a single-integral formula for $\sigma(t;\infty)^2$. By this formula, we find a simple expression for $\sigma(t;\infty)^2$ at long times, $1\ll tFa<\mathcal{O}(N)$. In our study, tFa is treated as large yet independent of N.

By a property of circulant matrices (see appendix A) [10], we write (9) as

$$\sigma(t;N)^2=\int_0^{tFa}N^{-1}\sum_{k=0}^{N-1}\vartheta_k\,e^{-\lambda_k\tau}\,\mathrm{d}\tau=N^{-1}\sum_{k=0}^{N-1}\vartheta_k\lambda_k^{-1}(1-e^{-\lambda_k Fat}),\quad(11)$$

where λ_k and ϑ_k are the eigenvalues of $\boldsymbol{A}+\boldsymbol{A}^T$ and $\boldsymbol{Q}\boldsymbol{Q}^T$, respectively ($\boldsymbol{C}^T$ is the transpose of $\boldsymbol{C}$). The eigenvalues of (square) circulant matrices can be evaluated directly via the discrete Fourier transform [37]. A simple calculation yields the eigenvalues

$$\lambda_k=2\Big[1-2p+2\breve{g}(1+2\text{ß})\Big(1-\cos\frac{2\pi k}{N}\Big)\Big]\Big(1-\cos\frac{2\pi k}{N}\Big),$$

$$\vartheta_k=2m_0\left[1+2\sqrt{p(1-p)}\cos\frac{2\pi k}{N}\right]\left(1-\cos\frac{2\pi k}{N}\right).$$

Consequently, we obtain the formula

$$\sigma(t;N)^2=m_0\frac{1}{N}\sum_{k=0}^{N-1}\left[1+2\sqrt{p(1-p)}\cos\frac{2\pi k}{N}\right]\times\frac{1-e^{-2[1-2p+2\breve{g}(1+2\text{ß})(1-\cos\frac{2\pi k}{N})](1-\cos\frac{2\pi k}{N})tFa}}{1-2p+2\breve{g}(1+2\text{ß})\left(1-\cos\frac{2\pi k}{N}\right)}.\quad(12)$$

As $N\to\infty$, let $\phi=\frac{2\pi k}{N}$ and $N^{-1}\sum_{k=0}^{N-1}(\cdot)\to\frac{1}{2\pi}\int_0^{2\pi}(\cdot)\,\mathrm{d}\phi$. By periodicity we have

$$\sigma(t;\infty)^2=\frac{m_0}{2\pi}\int_{-\pi}^{\pi}[1+2\sqrt{p(1-p)}\cos\phi]\times\frac{1-e^{-2[1-2p+2\breve{g}(1+2\text{ß})(1-\cos\phi)](1-\cos\phi)tFa}}{1-2p+2\breve{g}(1+2\text{ß})(1-\cos\phi)}\,\mathrm{d}\phi.\quad(13)$$

We have not been able to evaluate this integral in simple closed form in terms of elementary functions if $0<p<1/2$ and $\breve{g}>0$. In the *special (idealized) case* with $\breve{g}\downarrow 0$ (vanishing step interaction), we obtain [38]

$$\frac{\sigma(t,\infty)^2|_{\breve{g}\downarrow 0}}{m_0}=\frac{1}{1-2p}\Big\{1-e^{-\breve{t}}[I_0(\breve{t})+2\sqrt{p(1-p)}\,I_1(\breve{t})]\Big\},\quad(14)$$

where $\breve{t}=2(1-2p)tFa$. In the limit $\breve{t}\to\infty$, $\sigma(t,\infty)^2|_{\breve{g}\downarrow 0}\to m_0(1-2p)^{-1}$.

For $tFa\to\infty$ with $\breve{g},\nu=\mathcal{O}(1)>0$, (13) becomes (see appendix B)

$$\frac{\sigma(t,\infty)^2}{m_0}\to\frac{\sigma_{\rm st}(p,\breve{g})^2}{m_0}=\frac{1}{\sqrt{1-2p+4\breve{g}(1+2\text{ß})}}\,\frac{1}{\sqrt{1-2p}}\times\left\{1+\frac{8\breve{g}(1+2\text{ß})\sqrt{p(1-p)}}{[\sqrt{1-2p}+\sqrt{1-2p+4\breve{g}(1+2\text{ß})}]^2}\right\}.\quad(15)$$

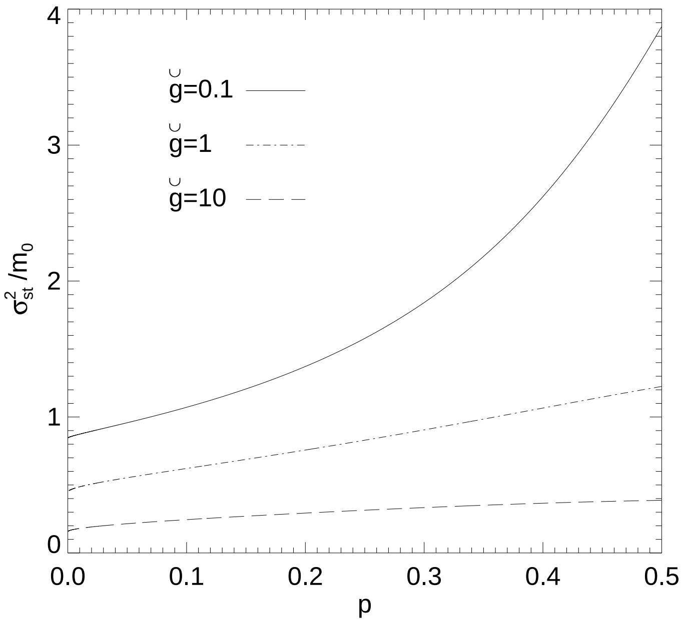

Figure 2. Steady state variance $\sigma_{\rm st}^2/m_0$ as function of p for different values of interaction parameter $\breve{g}$ ($\breve{g} = 0.1, 1, 10$). The narrowing of the TWD with F (decreasing p) is evident but is suppressed for large values of $\breve{g}$.

Recall that, by (4), $ß = ß(p)$ through ν. Figure 2 shows plots for $\sigma_{\rm st}(p, \breve{g})^2/m_0$ as function of p for different values of $\breve{g}$. Notably, (15) differs from the corresponding value obtained within the mean field approximation of [7, 8], as discussed in section 4.1.

Remark 2. If $\nu = Fa\varpi^2/(2D) \downarrow 0$ $(p \uparrow 1/2)$ and $\breve{g} = \mathcal{O}(1) > 0$, by (13) the variance approaches *zero* for any time t. This behavior is derived by use of $ß = \mathcal{O}(\nu^{-1})$ as $\nu \downarrow 0$, and is consistent with SDEs (5) since these become (deterministic) ODEs as $F \downarrow 0$. Details for the precise role of time t in this limiting case are provided in appendix C.

Remark 3. The limits $\nu \downarrow 0$ and $t \to \infty$ of (13) do *not* commute: the steady state result (15) approaches the finite value $(2\breve{g}/3)^{-1/2}$ as $\nu \downarrow 0$ (see section 4.2) whereas $\sigma(t)^2 \to 0$ as $p \uparrow 1/2$ for fixed t and $\breve{g}$ (remark II). To resolve this apparent paradox, we point out a transition in the asymptotics for $\sigma(t)^2$ if $tFa = \mathcal{O}(\breve{g}\nu^{-3})$. If ν is small, (15) is recovered from (13) if aFt is large enough to suppress the singularity in the time-independent term of the integrand in (13). For $\nu aFt \gg 1$ the major contribution to integration comes from the vicinity of $\phi = 0$. Thus, to extract the finite limit of (15) we require $1 - 2p > \mathcal{O}[\breve{g}(1 + 2ß)\phi^2]$ and $(1 - 2p)\phi^2 aFt = \mathcal{O}(1)$, by which $tFa \gg \breve{g}\nu^{-3}$. By contrast, if $aFt \ll \breve{g}\nu^{-3}$ the variance can be arbitrarily small (see appendix C for further technical details).

Remark 4. Consider the steady state variance $\sigma_{\rm st}(p, \breve{g})^2$ by (15) for $1 - 2p > 0$ (see figure 2). For fixed p, $\sigma_{\rm st}^2$ decreases with $\breve{g}$. For finite and fixed $\breve{g}$, $\sigma_{\rm st}^2$ increases with p, thus decreasing with F. Recall that ß decreases with F and becomes exponentially small (compared to unity) if $\nu = v\varpi/(2D) \gg 1$. Therefore, (15) predicts a narrowing of the TWD with increasing step interaction or deposition rate (see section 4.2).

4. Discussion

In this section we discuss implications of (15). In particular, we compare this result to a mean field approach [7, 8]; outline a plausible connection to experiments; and state conditions on the validity of our linearized model.

4.1. Mean field approach and decorrelation hypothesis

Heuristically speaking, the main goal with a mean field is to reduce the SDE system to a single Langevin-type equation that produces the *same* TWD as the starting, coupled system [7, 10]. For SDEs of the form

$$\dot{\xi}_i = G(\xi_{i-2}, \xi_{i-1}, \xi_i, \xi_{i+1}, \xi_{i+2}) + \sum_{k=0}^{N-1} Q_{i,k}\eta_k \tag{16}$$

(where η_k: independent white noises and $\boldsymbol{Q} = [Q_{i,k}]$: circulant), this task is pursued via the replacements $\xi_i \Rightarrow \xi^{\mathrm{mf}}$ and $\xi_{i\pm1}, \xi_{i\pm2} \Rightarrow f(\xi^{\mathrm{mf}}, t)$ where f is a (deterministic) field to be determined [7, 10]. In principle, this f depends on the joint probability density, p_5, of five terraces. This p_5 satisfies a Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy (involving the joint probability densities, p_n, of n terraces) [10].

Since the η_k are independent, it can be argued that the term $\sum_{k=0}^{N-1} Q_{i,k}\eta_k$ should be replaced by $q\,\eta$ where $q^2 = \sum_{k=0}^{N-1} Q_{i,k}^2 = |\boldsymbol{Q}|^2$. A formal justification comes from considering the first equation of the BBGKY hierarchy, which is an evolution equation for $p_1 = P(\xi, t)$, where the coefficient of $\partial_{\xi\xi}P(\xi, t)$ is $\frac{1}{2}|\boldsymbol{Q}|^2$. Thus, (16) is reduced to

$$\dot{\xi}^{\mathrm{mf}} = G(f(\xi^{\mathrm{mf}}, t), f(\xi^{\mathrm{mf}}, t), \xi^{\mathrm{mf}}, f(\xi^{\mathrm{mf}}, t), f(\xi^{\mathrm{mf}}, t)) + q\,\eta. \tag{17}$$

By comparison of the Fokker-Planck equation for (17) with the first equation of the BBGKY hierarchy for (16), one obtains a (self-consistent) formula for f [10]. For *linear* G, such a self-consistent f requires knowing the pair correlation. Specifically, one needs to know the conditional expectation for a terrace width, i.e., the average width of a terrace in a pair of terraces *given* the value of the width of the other terrace [7].

To avoid complications of solving the BBGKY hierarchy, it is tempting to apply the decorrelation ansatz $p_n(\vec{w}_n, t) = \prod_{j=1}^{n} P(w_j, t)$ where $\vec{w}_n = (w_0, \ldots, w_n)$ [7, 10]. For a *linear* SDE system, i.e., when G is linear, the ensuing f is the expectation $\mathbb{E}\xi_i = 0$ [7,10]. In [10], where the first-row entries for $\boldsymbol{Q}$ are set to $[2, -1, 0 \ldots, 0, -1]$ (second-order conservative noise scheme), it was verified for the linearized SDEs that the long-time limit of the mean field variance *coincides* with that of the exact solution.

Motivated by these previous studies, we compute the mean field variance for SDEs (6). By taking $f = \mathbb{E}\xi_i = 0$, these equations are reduced to the Langevin equation

$$\frac{\mathrm{d}\hat{\xi}}{\mathrm{d}\tilde{t}} = -[1 - 2p + 3\breve{g}(1 + 2ß)]\xi + q\,\tilde{\eta}(\tilde{t}), \quad q^2 = 2m_0[1 - \sqrt{p(1-p)}], \tag{18}$$

where $\hat{\xi}$ is the mean field stochastic process for a terrace width under the decorrelation ansatz. Thus, $\hat{\xi}$ is a Gaussian random variable with zero mean and variance

$$\hat{\sigma}(t)^2 = m_0 \frac{1-\sqrt{p(1-p)}}{1-2p+3\breve{g}(1+2ß)} \{1 - e^{-2Fa[1-2p+3\breve{g}(1+2ß)]t}\} \ , \tag{19}$$

which approaches $\hat{\sigma}(\infty)^2 = m_0[1-\sqrt{p(1-p)}][1-2p+3\breve{g}(1+2ß)]^{-1}$ as $t \to \infty$.

Since the long time limit of (19) differs from (15), terrace correlations persist at large times. For strong enough step interactions, i.e., $\breve{g}(1+2ß) \gg 1-2p$, we have $\hat{\sigma}(\infty)^2 = \mathcal{O}(\breve{g}^{-1})$ while by (15) $\sigma_{\rm st}^2 = \mathcal{O}(\breve{g}^{-1/2})$. The decorrelation hypothesis exaggerates the narrowing of the TWD, and correlations favor broadening of the TWD.

4.2. Related past works and possible connection to experiments

Next, we point out features of our prediction for the variance $\sigma_{\rm st}^2$ that may be experimentally testable, and compare these to results of [8, 24].

(i) *Narrowing of TWD* [8]. By (15) for large $\nu = aF\varpi^2/(2D)$, $\sigma_{\rm st}$ becomes

$$\sigma_{\rm st} \to \sqrt{m_0}\,(1+4\breve{g})^{-1/4} \quad \text{as } \nu \to \infty, \tag{20}$$

under the assumption that the quasi-steady approximation is meaningful. This prediction should be contrasted to the one in [8] where $\sigma = \mathcal{O}(F^{-1/2})$ for large F. For small deposition rate F ($p \uparrow 1/2$), (15) yields (see appendix C)

$$\sigma_{\rm st} \to \sqrt{m_0}\,(2\breve{g}/3)^{-1/4} \qquad \text{as } \nu \downarrow 0, \tag{21}$$

in contrast to the behavior $\sigma = \mathcal{O}(F^{-1})$ predicted in [8]. Hence, the deposition-dependent noise of our model significantly tones down the narrowing of the TWD reported in [8] where deposition is the only source of TWD narrowing and the noise is F-independent. Other models of noise in SDEs for terrace widths can be built by "mixing" elements of the diffusion matrix $\boldsymbol{Q}$ used here with F-independent elements while retaining the overall conservative character of the noise.

(ii) *Comparison to* [24]. In the model of [24] the deterministic equations account for the same kinetic (flux-induced) asymmetry in step motion but steps are *non-interacting*. The noise used in [24] for every terrace, w_i, appears to have the form $\sqrt{Fpw_{i-1}}\,\eta_{i,1} + \sqrt{Fpw_i}\eta_{i,2} + \sqrt{F(1-p)w_i}\eta_{i,3} + \sqrt{F(1-p)w_{i+1}}\eta_{i,4}$ where $\eta_{i,k}$ ($k = 1, \ldots, 4$) are independent white noises and units with $a = 1$ are apparently used. In the mean field approximation (under the decorrelation ansatz for terrace widths), this model yields the (scaled by ϖ^2) steady state variance $\hat{\sigma}(t \to \infty)^2 = (1-2p)^{-1}$ [24]. In [24] this prediction is found to appreciably overestimate the variance produced by kinetic Monte Carlo simulations for small rate F (see figure 4 in [24]). Since the simulations do *not* allow for step crossing, it is expected that these simulations include *entropic repulsions* between steps. On the other hand, our analytical model does contain the effect of step repulsion explicitly (via $\breve{g}$) and predicts a lower value of the variance for small F.

(iii) *Experiment on Si(111)* [39]. As mentioned in [8], experimental techniques that enable observation of equilibrium TWD can in principle probe narrowing due to the combined influence of growth *and* step interactions. An example is the reflection electron microscopy applied in [39]. In this experiment [39], TWD narrowing is observed on vicinal Si(111) at 1100°C and attributed solely to electromigration (which also causes a drift in the adatom flux) although a deposition flux from above and step interactions are present.

4.3. On validity of linearized model

We repeat that a limitation of our model is connected to its 1D character. Another limitation is related to the perturbation expansion for "small" noise, which underlies our linearization. Within this approximation, an indication that the linearization may not be valid arises if $\sigma_{\rm st}^2 > 1$: then, the negative tail of the (approximate) TWD $P(\xi, t)$ of (10) may have an appreciable effect on moments. This possible pathology is more pronounced for zero step interaction, and is worsened as the rate F approaches small values. Indeed, for $\breve{g}(1+2ß) \ll 1-2p$, (15) yields $\sigma_{\rm st}^2 \approx m_0(1-2p)^{-1}$ which may be significantly greater than unity if p is close enough to 1/2 (cf [24] and section 4.2).

To provide a condition necessary for the validity of our model, we require that $\sigma_{\rm st}^2 < 1$. In view of (21), this condition is satisfied if $\breve{g} > (3/2)m_0^2$ or, by (4),

$$\frac{ga}{T}\, m_0(a\rho_0) > \frac{1}{2},$$

which is a condition for small fluctuations on the basis of strong step interactions so that the linearization makes sense. A systematic study of the underlying perturbation scheme lies beyond our present purposes.

5. Conclusion

In this paper, we studied a model for *small stochastic fluctuations* of line defects on a crystal surface when material is deposited from above in 1+1 dimensions. This work has been inspired by [24], and aims to complement recent studies in the steady state distribution of terrace widths on vicinal crystals [7,8]. Noteworthy features of the model are the conservative character of noise, a deposition-flux-induced kinetic asymmetry in the noise coefficients, and the inclusion of step repulsion effects.

Our perturbation analysis led to a Gaussian TWD and a simple closed form for the associated variance. This TWD, which is symmetric about the expectation of the terrace width, is plausibly valid for values of terrace widths near the peak of the actual TWD. On the basis of this result, we inferred that growth combined with the noise kinetic asymmetry and step interaction sustain a reduced narrowing of the TWD with the deposition rate, F, in juxtaposition to the corresponding (more exaggerated) F-dependence of [8]. Furthermore, we applied a previous mean field approach [7, 8], and thereby indicated (but not analyzed) the role of terrace correlations at long times.

Our analysis points to several open questions. For example, terrace correlations, although evident, have not been described explicitly. The nonlinearities left out from our stochastic scheme should cause the TWD to be non-symmetric about the mean [10]. The derivation of such a modified TWD remains unresolved. The model with multiplicative noise (where the noise coefficients depend on terrace widths) is left for future work. Another open question concerns 2D geometries, which were not considered here. In real systems, edge atoms also diffuse along steps (besides diffusing on terraces and attaching/detaching at step edges). In addition, kinks on steps influence the form of noise. Many-step interacting systems in 2D are the subject of work in progress.

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Appendix A. On norm of circulant matrices

In this appendix, we derive (11) from (9). So, we prove the following statement [10].

Proposition 1. *For $N \times N$ circulant matrices $\boldsymbol{X}$ and $\boldsymbol{Y}$, the norm squared of $\boldsymbol{X}e^{\boldsymbol{Y}}$ is*

$$|\boldsymbol{X}e^{\boldsymbol{Y}}|^2 = |e^{\boldsymbol{Y}}\boldsymbol{X}|^2 = N^{-1}\sum_{k=0}^{N-1} \vartheta_k e^{\psi_k}, \tag{A.1}$$

where $\{\vartheta_k\}_{k=0}^{N-1}$ and $\{\psi_k\}_{k=0}^{N-1}$ are sets of eigenvalues of $\boldsymbol{X}\boldsymbol{X}^T$ and $\boldsymbol{Y}+\boldsymbol{Y}^T$, respectively.
Proof. Note that any two (square) circulant matrices commute. Consider the relations [37] $|\boldsymbol{X}e^{\boldsymbol{Y}}|^2 = N^{-1}\mathrm{tr}[\boldsymbol{X}\boldsymbol{X}^T e^{\boldsymbol{Y}^T+\boldsymbol{Y}}]$ and $\boldsymbol{F}^{-1}\exp(\boldsymbol{C})\boldsymbol{F} = \exp(\boldsymbol{F}^{-1}\boldsymbol{C}\boldsymbol{F})$. Here, $\boldsymbol{F} = [F_{k,l}]$ is the $N \times N$ discrete Fourier transform matrix, with entries $F_{k,l} = e^{-i2\pi(kl)/N}$ ($i^2 = -1$), and $\boldsymbol{C}$ is a square circulant matrix, e.g., $\boldsymbol{C} = \boldsymbol{Y}+\boldsymbol{Y}^T$. Since $\boldsymbol{F}^{-1}(\boldsymbol{X}\boldsymbol{X}^T)\boldsymbol{F} = \mathrm{diag}(\vartheta_k)$ and $\boldsymbol{F}^{-1}(\boldsymbol{Y}+\boldsymbol{Y}^T)\boldsymbol{F} = \mathrm{diag}(\psi_k)$, we assert that

$$\begin{aligned} |\boldsymbol{X}e^{\boldsymbol{Y}}|^2 &= N^{-1}\mathrm{tr}[(\boldsymbol{F}^{-1}\boldsymbol{X}\boldsymbol{X}^T\boldsymbol{F})(\boldsymbol{F}^{-1}e^{\boldsymbol{Y}+\boldsymbol{Y}^T}\boldsymbol{F})] \\ &= N^{-1}\mathrm{tr}[\mathrm{diag}(\vartheta_k e^{\psi_k})]. \end{aligned} \tag{A.2}$$

The last identity concludes our proof, cf (11). □

Appendix B. Steady-state variance

In this appendix, we derive steady-state formula (15) from exact expression (13) for the variance. We assume that $\breve{g} > 0$ and $0 < p < 1/2$.

First, we split integral (13) into two terms. For the integral containing the time-dependent exponential, change the variable of integration to $z = \sin(\phi/2)$ for

$\phi \in (-\pi, \pi]$, and apply the even symmetry of the integrand. By a steepest-descent argument [40], we assert that

$$\lim_{t\to\infty}\int_0^1 [1+2\sqrt{p(1-p)}(1-2z^2)]\frac{e^{-4[1-2p+4\breve{g}(1+2ß)z^2]tFa\,z^2}}{1-2p+4\breve{g}(1+2ß)z^2}\,\frac{\mathrm{d}z}{\sqrt{1-z^2}}=0,$$

if $1-2p, \breve{g}(1+2ß)=\mathcal{O}(1)>0$. Note in passing that the major contribution to integration comes from a vicinity of $z=0$. Thus, the integral behaves as $\mathcal{O}(t^{-1/2})$ as $t\to\infty$.

So, we are left with the integral

$$\frac{\sigma_{\mathrm{st}}^2}{m_0}=\frac{1}{2\pi}\int_{-\pi}^{\pi}\frac{1+2\sqrt{p(1-p)}\,\cos\phi}{1-2p+2\breve{g}(1+2ß)(1-\cos\phi)}\,\mathrm{d}\phi. \tag{B.1}$$

We proceed to compute σ_{st}^2 by contour integration. By the change of variable $\zeta=e^{i\phi}$ ($i^2=-1$) and analytic continuation in the ζ complex plane, integral (B.1) becomes

$$\frac{\sigma_{\mathrm{st}}^2}{m_0}=\frac{1}{2\pi i}\oint_{|\zeta|=1}\frac{1+\sqrt{p(1-p)}(\zeta+\zeta^{-1})}{1-2p+2\breve{g}(1+2ß)[1-\frac{1}{2}(\zeta+\zeta^{-1})]}\,\frac{\mathrm{d}\zeta}{\zeta}, \tag{B.2}$$

where ζ is viewed as a variable in the complex plane, $\mathbb{C}$. By the residue theorem, we can evaluate (B.2) from contributions of simple poles of the integrand in the interior of the unit disk, $\{\zeta\in\mathbb{C}:\,|\zeta|<1\}$. The poles are located at the points $\zeta=0$ and

$$\zeta_{\pm}=\frac{1-2p+2\breve{g}(1+2ß)\pm\sqrt{(1-2p)[1-2p+4\breve{g}(1+2ß)]}}{2\breve{g}(1+2ß)},$$

where $0<\zeta_-<1$ and $\zeta_+>1$. Thus, only ζ_- lies inside the unit disk. By computing the residues at $\zeta=0,\zeta_-$ we find

$$\frac{\sigma_{\mathrm{st}}^2}{m_0}=\frac{1}{\breve{g}(1+2ß)}\left[\frac{\zeta_-+\sqrt{p(1-p)}(1+\zeta_-^2)}{(\zeta_+-\zeta_-)\zeta_-}-\sqrt{p(1-p)}\right], \tag{B.3}$$

which yields (15) after some algebra.

Appendix C. Limit of time dependent variance as $\nu\to 0$

In this appendix, we evaluate integral (13) for small $\nu=Fa\varpi^2/(2D)$ and $\breve{g}=\mathcal{O}(1)$. For algebraic convenience, we set $m_0=1$ (only in this appendix).

By the change of the integration variable to $z=\sin(\phi/2)$, the integral becomes

$$\sigma(t)^2=\frac{1}{2\pi}\frac{1}{\breve{g}(1+2ß)}\int_0^1\frac{\mathrm{d}z}{\sqrt{1-z^2}}\,[1+2\sqrt{p(1-p)}(1-2z^2)]\times\frac{1-e^{-(\alpha_1^2+z^2)\alpha_2^2z^2}}{z^2+\alpha_1^2}, \tag{C.1}$$

where $\alpha_1^2=(1-2p)[4\breve{g}(1+2ß)]^{-1}$ and $\alpha_2^2=16tFa\breve{g}(1+2ß)$. For $\nu\downarrow 0$ with fixed $\breve{g}$ and $tFa\geq\mathcal{O}(1)$, we have $\alpha_1^2=\mathcal{O}(\nu^2)$ while $\alpha_2^2\geq\mathcal{O}(\nu^{-1})$. Thus, the task is to evaluate $\sigma(t)^2$ by (C.1) for *small* α_1 and *large* α_2 (where $\alpha_1,\alpha_2>0$).

By inspection of the integrand in (C.1), we distinguish the following cases.

(i) $\alpha_2^{-1} \gg \alpha_1^2$, i.e., $tFa \ll \breve{g}(1+2\text{ß})(1-2p)^{-2}$: The major contribution to integration comes from a neighborhood of width $\mathcal{O}(\alpha_2^{-1/2})$ around $z=0$, and α_1^2 is neglected compared to z^2. Specifically, we have

$$\begin{aligned}\sigma(t)^2 &\approx \frac{1}{\pi}\frac{1}{\breve{g}(1+2\text{ß})}\int_0^1 \sqrt{1-z^2}\,\frac{1-e^{-\alpha_2^2 z^4}}{z^2}\,\mathrm{d}z \\ &= \frac{1}{\pi}\frac{1}{\breve{g}(1+2\text{ß})}\left(\int_0^A + \int_A^{\alpha_2^2}\right)\int_0^1 \sqrt{1-z^2}\,z^2\,e^{-yz^4}\,\mathrm{d}z\,\mathrm{d}y \qquad \text{(C.2)}\end{aligned}$$

where A is any fixed yet large positive number. Thus, the y in $\int_A^{\alpha_2^2}$ is large and the respective integral in z is evaluated by expanding the integrand near $z=0$. Finally, we obtain

$$\sigma(t)^2 \approx \frac{2}{\pi}\,\Gamma(\tfrac{3}{4})\,[\breve{g}(1+2\text{ß})]^{-3/4}\,(tFa)^{1/4}, \qquad \text{(C.3)}$$

where $\Gamma(\zeta)$ is the Gamma function [41]. So, if tFa is fixed as $\nu \downarrow 0$, then $\sigma(t)^2$ vanishes as $\mathcal{O}(\nu^{3/4})$. However, if instead $2Dt/\varpi^2$ is kept fixed as $\nu \downarrow 0$, then $\sigma(t)^2 = \mathcal{O}(\nu) = \mathcal{O}(F)$.

(ii) $\alpha_2^{-1} \ll \alpha_1^2$, i.e., $tFa \gg \breve{g}(1+2\text{ß})(1-2p)^{-2}$: The major contribution to integration in the time dependent term of (C.1) arises from a vicinity of width $\mathcal{O}((\alpha_1\alpha_2)^{-1}) = \mathcal{O}((\nu tFa)^{-1/2})$ around $z=0$. Thus, we obtain

$$\sigma(t)^2 \approx \frac{1}{2\pi}\frac{1}{\breve{g}(1+2\text{ß})}\int_{-1}^1 \frac{\sqrt{1-z^2}}{z^2+\alpha_1^2}\,\mathrm{d}z. \qquad \text{(C.4)}$$

To evaluate this integral to leading order in ν, we apply analytic continuation of the integrand to complex z. So, deform the path of integration to the upper complex z-plane so as to pick up the residue from the simple pole at $z = i\alpha_1$ ($i^2=-1$). Thus, compute

$$\sigma(t)^2 = (2\breve{g}/3)^{-1/2} + \mathcal{O}(\nu) = \sigma_{\mathrm{st}}(p \uparrow 1/2, \breve{g}), \qquad \text{(C.5)}$$

which is the limit of (15) for small $\nu = Fa\varpi^2/(2D)$, cf (21).

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