

Formulas for elastic interaction of surface line defects in 2 dimensions

John Quah¹, Li Peng Liang², and Dionisios Margetis^{3,4,5}

¹ 7201 Claymore Ave, Hyattsville MD 20782

² Department of Physics, Engineering and Geosciences, Montgomery College, Rockville MD 20850

³ Department of Mathematics, University of Maryland, College Park MD 20742

⁴ Institute for Physical Science and Technology, University of Maryland, College Park MD 20742

⁵ Center for Scientific Computation and Mathematical Modeling, University of Maryland, College Park MD 20742

Abstract. By use of asymptotics, we study the interplay of energetics and geometry on a crystal surface. We derive explicit, simplified formulas for integrals representing the *elastic-dipole interaction energy per unit length* between curved line defects (steps) of the same sign. Our starting point is linear elasticity whereby steps are represented as *force dipoles* lying in a high-symmetry plane, in accordance with the classic model by Marchenko and Parshin (1981 *Soviet Phys. JETP* **52** 129). We consider geometries that stem from *perturbations of concentric circular steps* (radial case). In the radial case, we define a small geometric parameter, δ^2 , expressing the smallness of interstep distance relative to the circle radii. We invoke the *Mellin transform* with respect to δ^2 and derive an approximation of the requisite integral; this technique offers an alternative to an exact evaluation in terms of elliptic integrals. We then demonstrate the use of the Mellin transform when calculating the elastic interaction energy between smoothly varying, non-circular steps, where a closed-form expression in terms of special functions is generally not available.

PACS numbers: 68.35.Md, 81.10.Aj, 62.20.D-, 02.30.Mv, 02.30.Uu, 68.35.-p

Keywords: Epitaxial growth, crystal surface, Burton-Cabrera-Frank (BCF) model, linear elasticity, step interactions, force dipoles, Mellin transform

Submitted to: *J. Phys. A: Math. Theor.*

1. Introduction

Modern small devices rely on the precise patterning of crystal surfaces to create nanostructures and thin films with desired properties. Below the roughening transition temperature, typical crystal surfaces are not atomically flat, but instead consist of nanoscale terraces separated by line defects, i.e., steps, of atomic height [1]. The interaction between steps plays a prominent role in surface morphological evolution.

Fundamental studies of step-step interactions include the model by Marchenko and Parshin (MP) [2], where each step is viewed as a distribution of force dipoles in the context of classical elasticity. The interaction energy of two such (infinitesimal) dipoles at distance r decays as r^{-3} . Effects such as atomic-scale roughness [3], elastic anisotropy [4], and surface elasticity under concentrated normal and shear loads [5] have enriched the MP model. Germane computations address mainly interactions between *straight* steps. In more complicated geometries, the requisite integrals in principle have an intricate, hardly transparent, dependence on the physical parameters.

In this paper, we focus on interactions between two-dimensional (2D) steps of the same sign in configurations that allow for simplifying (yet nontrivial) approximations. By considering smooth steps of *nonzero curvature* that form *perturbations of circles*, we illustrate analytically the calculation of elastic step interaction energies. Our resulting, explicit formulas aim to complement thermodynamic ingredients of step flow models describing crystal surface morphological evolution near equilibrium [1]. Such models are invoked extensively in the simulation and analysis of the motion of *many steps*; thus, it is expedient to have relatively simple formulas for the step interaction energies.

The basic ingredients of step flow were introduced by Burton, Cabrera and Frank (BCF) [6]. In their pioneering work, steps are non-interacting. Since then, modest progress has been made in illustrating analytically how to compute the interaction energies between steps of reasonably arbitrary shapes; for related reviews see, e.g., [1,7–9].

Our intention with the present work is to demonstrate the use of a computational technique for step interactions. This tool is the Mellin transform with respect to a suitable geometric parameter. Applications of this transform, although known in the context of, e.g., acoustics and electromagnetism [10, 11] and high-energy particle scattering [12], seem to have been previously unexplored in materials physics.

We choose to apply this asymptotic technique to perturbations of circular steps. The usual step flow equations are rotationally symmetric and, thus, allow for global rotational symmetry if the initial step configuration consists of concentric circles. Our setting is relevant to possible *deviations* from this symmetry, which can be caused by effects in the governing equations or the initial data. This issue is of practical importance in two space dimensions.

Elastic-dipole step interactions have taken on a prominent role in surface evolution, especially in the low-temperature regimes required for the fabrication of nanoscale features on crystal surfaces. At sufficiently low manufacturing temperatures, the thermal wandering of steps tends to be suppressed; hence, the influence of entropic

step repulsions [1] is considered relatively small and negligible here.

A detailed study of elastic interactions between steps in the context of essentially one-dimensional (1D) geometries is given by Pimpinelli and Villain [13]. They motivate and define the elastic interaction energy per unit length for straight steps via the MP model [2]. This energy decays as w^{-2} where w is the terrace width. The connection of step energetics to principles of linear elasticity is elucidated in [13].

In the present paper, we start with concentric circular steps, which form the basis of our treatment. A previously used formula for the step interaction energy in this case exhibits a simple geometric factor [14]. This formula has been adopted, but apparently not explained, in various works in crystal surface morphological evolution [15–19]. We derive this formula explicitly by invoking the MP model of interacting force dipoles and asymptotics following our definition of a small parameter. This parameter expresses the smallness of the interstep distance relative to the step radii. The example of concentric circles serves as a paradigm for understanding the related asymptotics in more complicated cases, e.g., non-concentric circular and other perturbed steps, which we examine here in due order.

To approximate the requisite integrals in the non-radial case, where steps are *not* concentric circles, we apply the Mellin transform with respect to an analogous geometric parameter. This technique leads to an asymptotic series for the interaction energy in the form of distinct contributions from residues associated with poles of the transformed function in the complex plane.

A goal is to answer the question: *how do the shapes of steps affect their elastic interaction energy?* We restrict attention to the interaction energy *per unit step length*. This quantity enters the step chemical potential of BCF-type models [1]. The dependence on geometry of an approximation for this interaction energy has been attributed to a smooth, multiplicative “geometric factor” Φ [20], by analogy with the case of concentric circular steps [14]. In [20], by use of local coordinates perpendicular and parallel to step edges, this Φ is assumed to depend locally only on the transverse coordinates of the interacting steps. For the perturbed geometries considered here, this hypothesis for the leading-order term is reasonable. The next higher-order term is logarithmic in the step distance, with a prefactor depending on the local slope of the step curve.

The results of this paper rest on several simplifying assumptions. First, the strain field due to a step edge is obtained as a *superposition* of the dipole strain fields arising from each point of the step edge. For this principle to be meaningful, the material must of course be in the *linear elastic* regime. Second, the dipole moment associated with each point of a step edge has a negligible (z -) component normal to the reference plane. In the same vein, we regard as constant the magnitude of the elastic dipole per unit step length. The geometries chosen are consistent with slowly varying step configurations [20], where the associated curvatures change appreciably over lengths comparable to or larger than the step radius of curvature, a macroscopic length.

The remainder of the paper is organized as follows. In section 2, we review some background for the motion of crystal steps; and discuss the role of elastic-dipole step

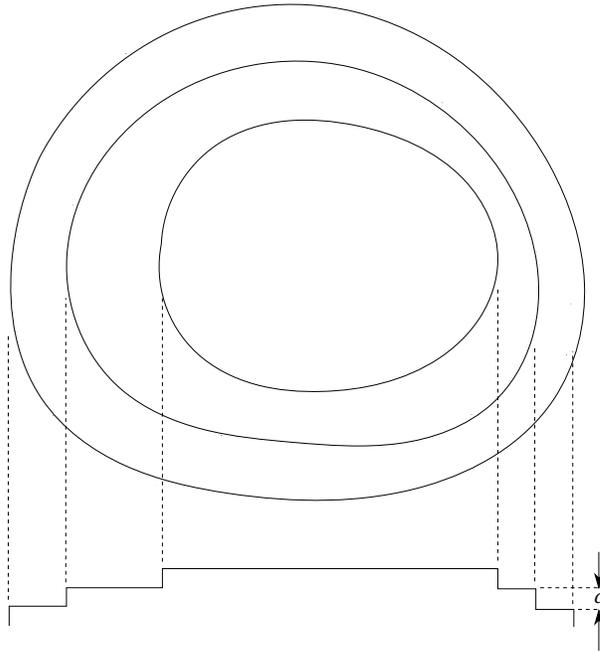


Figure 1. 2D steps. Top: projection on reference plane. Bottom: cross section.

interactions. In section 3, we demonstrate the application of the associated formula to the calculation of step interactions in one coordinate, including concentric circular steps (radial case). In section 4, we consider a geometry deviating from the radial case, namely, circular steps with different centers. In section 5, we allow the curvature of a step to vary slowly with the arc length. Finally, in section 6 we summarize our results.

2. Background

In this section we review the underlying geometry and basics of step interactions. The geometry of crystal steps is depicted from two perspectives in figure 1. The cross-sectional view illustrates steps of atomic height, a , that descend from a surface peak. The steps are projected onto non-crossing, non-self-intersecting, smooth curves on the reference ('basal') plane (see footnote 1), shown in the upper part of figure 1. In the radial case studied, e.g., in [15, 17], these curves are concentric circles.

¹The usual requirement of continuously differentiable curves would suffice for normal and tangent vectors to be well defined at each point of the step curve. Here, we impose the stronger condition of *infinitely* differentiable (smooth) curves since this in principle allows for asymptotics (by our method) to *arbitrary* order in the small geometric parameter (to be defined below).

To place step interactions in the broader context of crystal surface motion, we briefly discuss major elements of BCF-type models (see footnote 2). Then, we review the main ideas underlying the modeling of interacting steps by force dipoles.

2.1. Evolution of crystal surfaces: role of step interactions

In surface diffusion, the motion of steps is mediated by diffusion of adsorbed atoms (adatoms) on terraces between steps, and by attachment and detachment of adatoms at step edges. The adatom density, C_j , on terrace j satisfies

$$\text{div}(D\nabla C_j) = \partial_t C_j, \quad (1)$$

where D is the diffusivity, assumed to be constant. Each step moves by mass conservation, as the step velocity balances out atom fluxes. Specifically, in the absence of edge atom diffusion [1, 21], the normal velocity of step j is given by

$$v_j = \frac{\Omega}{a}(\varphi_{j-1,\perp} - \varphi_{j,\perp}) \quad \text{at step } j,$$

where φ_j is the (vector-valued) flux from terrace j and Ω is the atomic volume; the subscript \perp denotes the component normal to the step. In the quasisteady approximation, where $\partial_t C_j \approx 0$, we set $\varphi_j = -D\nabla C_j$; for more details, see, e.g., [20, 22].

The atom attachment-detachment at step edges is expressed through appropriate boundary conditions for (1). By linear kinetics [1], the normal flux $\varphi_{j,\perp}$ at the bounding steps $j, j+1$ is proportional to concentration differences according to

$$\begin{aligned} -\varphi_{j,\perp} &= k_u(C_j - C_j^{\text{eq}}) \quad \text{at step } j, \\ \varphi_{j,\perp} &= k_d(C_j - C_{j+1}^{\text{eq}}) \quad \text{at step } j+1. \end{aligned} \quad (2)$$

In the above, C_j^{eq} is an equilibrium adatom density and k_u, k_d are kinetic rates. This C_j^{eq} quantifies the propensity of a step edge to incorporate or release atoms. By recourse to notions of thermodynamic equilibrium, this propensity is expressed by the law [1]

$$C_j^{\text{eq}} = C^0 \exp\left(\frac{\mu_j}{\vartheta}\right), \quad (3)$$

where μ_j is the step chemical potential, a thermodynamic force, $\vartheta = k_B T$ is the Boltzmann energy, and C^0 is a constant.

The μ_j above is the *change of the j th-step energy per atom captured or released by the step edge* and links step motion to energetics [20]. It can be shown that μ_j in principle involves the step curvature (line tension), entropic step repulsions, and elastic interactions between steps [1, 23]. The latter two energies decay as the inverse square of step separation in the special case of straight steps [13, 23].

In the radial case, the step chemical potential is [14, 17, 18] (see footnote 3)

$$\mu_j = \frac{\Omega g_1}{r_j} + \frac{\Omega}{ar_j} \frac{\partial}{\partial r_j} \{r_j[V(r_j, r_{j+1}) + V(r_{j-1}, r_j)]\}, \quad (4)$$

²As mentioned in section 1, in the original BCF theory [6] steps are non-interacting.

³Our definition of V in (4) and (5) is slightly different from that in [18].

where r_j are radii of concentric circles representing steps, and $V(r_j, r_{j+1})$ is the elastic interaction energy between steps $j, j + 1$ per unit length of step j . By [14], this V is

$$V(r_j, r_{j+1}) = g \frac{2r_{j+1}}{r_j + r_{j+1}} \left(\frac{a}{r_{j+1} - r_j} \right)^2, \quad (5)$$

where g is positive and measures the strength of the elastic dipoles arising from steps.

More generally, if U_j is the energy per length of step j , it has been shown by basic differential geometry [20] that

$$\mu_j = (\Omega/a)(\xi_\eta^{-1} \partial_{\eta_j} U_j + \kappa_j U_j), \quad (6)$$

where $\eta = \eta_j$ is a local curvilinear coordinate specifying step j , ξ_η is the associated metric coefficient, and κ_j is the step curvature. Thus, for the purpose of determining step motion, it is expedient to compute the quantity U_j in terms of step positions. This U_j includes the step line tension (energy to create a step), as well as entropic and elastic interactions.

2.2. Elastic step interactions in linear regime: a review

The simplest setting is a vicinal surface, which stems from cutting a crystal along a plane at a fixed, small angle with respect to one of crystal's high-symmetry planes. The resulting interface consists of regularly spaced, atomic-height steps. This configuration is not as favorable energetically as a perfectly flat interface, so the atoms at the surface 'react' to their missing bonds by undergoing small displacements. We can expect such displacements to induce an effective elastic force between adjacent steps (see footnote 4).

Alternatively, picture a step as a defect on a continuous elastic surface. In order to maintain this defect against the natural tendency of the medium to flatten out, a pair of oppositely-directed forces must be applied by the bulk of the crystal at distinct points of the step. Then the step itself applies equal and opposite forces on the bulk of the crystal, as depicted in figure 2. This *force dipole* introduces strain in the vicinity of the step. The resulting strain field causes elastic interactions between steps by displacing the intervening atoms. Although the existence of a force dipole is inferred from considerations of a *continuous* elastic surface, such a dipole can also be justified while respecting the discrete nature of a real crystal surface, as argued, e.g., in [25].

The question arises as to how the force distribution near a step is calculated. A proposal involving a pair of forces oriented normal to the step edge in the high-symmetry plane, as shown in figure 2, first appeared in a paper by Marchenko and Parshin [2] and has since been used as a core model. This (MP) model has one free parameter, which is related to the strength of the force dipole (see footnote 5).

⁴For a pictorial representation, consider the displacements calculated by atomistic simulations in [24].

⁵Note in passing that Prévot and Croset [26, 27] introduced a model of 'embedded dipoles', which describes the opposing forces by use of two free parameters rather than one. Accordingly, these authors were able to make predictions in close agreement with observed relaxations of atomistic simulations.

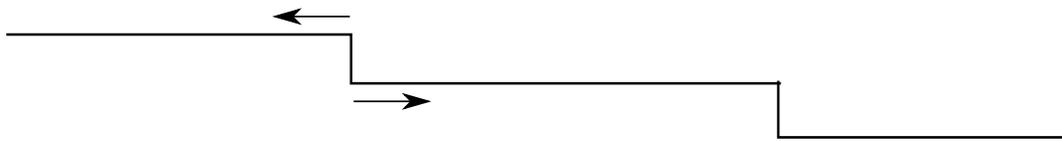


Figure 2. Schematic of a force dipole for to a step by the MP model [2]. The dipole moment is along the step edge and normal to the cross-sectional plane.

Pimpinelli and Villain [13] adopt the MP model, positing that the elastic strain field stems from a line of force dipoles normal to the step. It is tempting to resort to electrostatics for the field of an elastic force dipole. We do not pursue this analogy. It suffices to add that the scaling of the field strength as the inverse cube of distance is common to electric and elastic dipoles [28,29] (see footnote 6). For an explicit calculation of the linear response of elastic surface dipoles, the reader may consult the appendices in [13]. The nature of elastic step-step interactions implies that steps of the same sign (i.e., steps either descending or ascending) exert *repulsive* forces on each other. The situation is different, and more delicate, with steps of opposite sign [3].

Extensive discussions on defect interactions for crystal surfaces can be found in [2,13,24,25]. We appeal to the formulation in [13] to quantify the interaction energy of two force dipoles. In this work, the force dipole moments are defined as the mechanical moments, m_{bd} , stemming from forces \mathbf{F}_k acting at points \mathbf{R}_k [13]:

$$m_{bd} = \sum_k R_{k,b} F_{k,d} \quad (b, d = x, y, z),$$

where it is assumed that $\sum_k \mathbf{F}_k = 0$; (x, y, z) is a Cartesian coordinate system, z is the axis normal to the basal plane, and $Q_{k,b}$ is the b component of the vector \mathbf{Q}_k . For a cubic lattice, we adopt the formula [13]

$$m_{bd} = \delta_{bd}[(\delta_{bx} + \delta_{by})m + \delta_{bz}m_{zz}], \quad (7)$$

where δ_{bd} is Kronecker's delta. The interaction energy of two such force dipoles with moments m and m' is calculated to be [13]

$$W_{\text{int}}^{\text{dip}} = \frac{1 - \zeta^2}{\pi Y r^3} \left[mm' - \frac{\zeta}{1 - \zeta} (mm'_{zz} + m_{zz}m') + \left(\frac{\zeta}{1 - \zeta} \right)^2 m_{zz}m'_{zz} \right], \quad (8)$$

where Y is Young's modulus, ζ is the Poisson coefficient, and r is the distance between the dipoles; typically, $1/5 \leq \zeta < 1/2$ [30]. If the force dipoles lie in the high-symmetry plane as in the classic MP model (figure 2), then $m_{zz} = m'_{zz} = 0$. Alternatively, consider $|m_{zz}|, |m'_{zz}| \ll |m|$ and interpret our subsequent results as subject to corrections due to m_{zz} and m'_{zz} . So, we restrict attention to a truncated version of (8):

$$W_{\text{int}}^{\text{dip}} = \frac{1 - \zeta^2}{\pi Y r^3} mm'. \quad (9)$$

⁶Recall that the interaction energy of two electric dipoles with moments \mathbf{p}_A and \mathbf{p}_B at distance r_{AB} is [28] $W = \frac{1}{r_{AB}^3} [\mathbf{p}_A \cdot \mathbf{p}_B - 3(\mathbf{p}_A \cdot \mathbf{e}_{AB})(\mathbf{e}_{AB} \cdot \mathbf{p}_B)]$; \mathbf{e}_{AB} is the unit vector pointing from A to B .

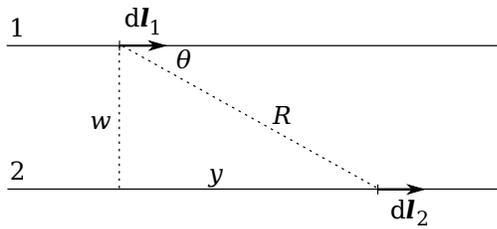


Figure 3. Geometry of straight steps.

Equation (9) forms our starting point. The moments m and m' are expressed in a fixed coordinate system. If the step segments are not parallel, the product mm' in (9) must be appropriately replaced by the dot product of the respective vector moments.

3. Reference cases: 1D step geometries

In this section, we illustrate the application of (9) to simple geometries describable in terms of a single spatial coordinate: straight steps and concentric circular steps.

3.1. Straight steps

Consider the case of two (infinite) straight steps shown in figure 3. The steps are aligned with the y -axis, and their distance equals w , the terrace width. To find the elastic interaction energy per unit length of step 1, we fix the line element dl_1 and integrate over step 2, summing up the contributions of interactions with the line elements dl_2 . Let \mathbf{R} be the vector along the line joining dl_1 and dl_2 , θ be the angle formed by \mathbf{R} and dl_1 , and $R = |\mathbf{R}|$. Choosing to integrate with respect to θ , we have

$$R = \frac{w}{\sin \theta}, \quad dl_2 = dy = \left| d \left(\frac{w}{\tan \theta} \right) \right| = \frac{w}{\sin^2 \theta} d\theta, \quad 0 \leq \theta \leq \pi.$$

The force dipoles, m and m' , are now proportional to the lengths of the associated step segments, dl_1 and dl_2 , with proportionality constant P , the dipole moment per unit length of a step. Thus, the interaction energy per length of step 1 due to step 2 is

$$V_{\text{int}} \equiv \frac{dW_{\text{int}}}{dl_1} = \frac{P^2}{w^2} \int_0^\pi \sin \theta d\theta = \frac{2P^2}{w^2}. \quad (10)$$

Note that we replaced the symbol $W_{\text{int}}^{\text{dip}}$ of (9) by $\frac{d^2 W_{\text{int}}}{dl_1 dl_2}$ and then integrated over dl_2 .

This example serves as a reference case. Indeed, the plausibility of later results can be checked by allowing the step curvature in respective geometries to approach zero.

3.2. Concentric circular steps

Next, we consider concentric circular steps, shown in figure 4. Our purpose is twofold. First, we aim to offer a streamline derivation and improvement of (5) for the interaction energy [14]. Second, we intend to clarify the role of a (assumed small) geometric parameter and demonstrate the use of the Mellin transform technique.

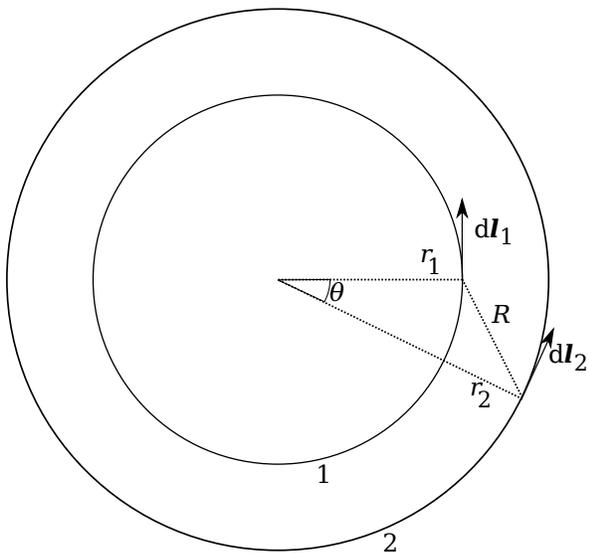


Figure 4. Geometry of concentric circular steps with radii r_1 and r_2 .

By figure 4, we fix our attention on the interaction between an infinitesimal element $d\mathbf{l}_1$ on the inner step (step 1) and the entire outer step (step 2). Recall formula (9), now written for two dipoles on circles 1 and 2. The product mm' is proportional to $d\mathbf{l}_1 \cdot d\mathbf{l}_2$ where $d\mathbf{l}_j$ is an infinitesimal tangential vector along step j ($j = 1, 2$). By use of Cartesian coordinates (x, y) , the dipoles are located at $(r_1, 0)$ and $(r_2 \cos \theta, r_2 \sin \theta)$.

If P is the dipole moment per unit length associated with each step, the interaction energy per unit length of step 1 is (see footnote 7)

$$V_{\text{int}} = \frac{dW_{\text{int}}}{dl_1} = P^2 \int_{-\pi}^{\pi} \frac{r_2 \cos \theta}{(r_1^2 + r_2^2 - 2r_1 r_2 \cos \theta)^{3/2}} d\theta. \quad (11)$$

This integral can be computed exactly in terms of a special function but the result is not particularly informative about the dependence on r_1 and r_2 (see appendix A).

To render (11) amenable to approximation, we identify a parameter expressing the property that the terrace width, $r_2 - r_1$, is sufficiently small. Thus, set $r_2 = r_1 + \rho$ and $r_1 = \epsilon^{-1}$, a large length scale, while $\epsilon\rho \ll 1$. We compute (11) by

$$V_{\text{int}} = \frac{dW_{\text{int}}}{dl_1} = 2P^2 \int_0^{\pi} \frac{r_2 \cos \theta}{[\rho^2 + 4(\epsilon^{-2} + \epsilon^{-1}\rho) \sin^2(\theta/2)]^{3/2}} d\theta. \quad (12)$$

By the change of variable $s = \sin(\theta/2)$ and the definition

$$\lambda^2 = 4(\epsilon^{-2} + \epsilon^{-1}\rho) = 4r_1 r_2 \Rightarrow \lambda \sim 2\epsilon^{-1}(1 + \epsilon\rho/2) = r_1 + r_2, \quad (13)$$

where λ is a macroscopic length parameter, integral (12) is recast to the form

$$V_{\text{int}}(\delta^2) = \frac{4P^2 r_2}{\lambda^3} \int_0^1 \frac{ds}{\sqrt{1-s^2}} \frac{1-2s^2}{(s^2 + \delta^2)^{3/2}} = \frac{4P^2 r_2}{\lambda^3} I(\delta^2). \quad (14)$$

Note that $I(\delta^2)$ diverges in the neighborhood of $s = 0$ as $\delta^2 \downarrow 0$.

⁷Because of rotational symmetry, the total interaction energy of steps 1 and 2 follows trivially.

3.2.1. Application of Mellin transform One may proceed by evaluating $V_{\text{int}}(\delta^2)$ exactly in terms of complete elliptic integrals; see (A.4) of appendix A. Instead, we apply the Mellin transform in δ^2 , which enables us to derive an asymptotic expansion for V_{int} if $\delta^2 \ll 1$ and is generalizable to cases without rotational symmetry. For a short review of the Mellin transform, see appendix B.

The Mellin-transformed integral of (14) reads

$$\hat{I}(\zeta) = \int_0^\infty I(\delta^2)(\delta^2)^{-\zeta} d\delta^2 = \int_0^1 \frac{ds(1-2s^2)}{\sqrt{1-s^2}} \left(\int_0^\infty \frac{(\delta^2)^{-\zeta}}{(s^2+\delta^2)^{3/2}} d\delta^2 \right),$$

by interchange of the order of integrations. The integral for $\hat{I}(\zeta)$ converges for $-\frac{1}{2} < \text{Re}\zeta < 0$ and can be evaluated in terms of the Gamma function [31]:

$$\begin{aligned} \hat{I}(\zeta) &= \frac{\Gamma(1-\zeta)\Gamma(\zeta+\frac{1}{2})}{\Gamma(\frac{3}{2})} \int_0^1 d(s^2) \frac{(s^2)^{-\zeta-1/2}}{\sqrt{1-s^2}} (1-2s^2) \\ &= -\frac{1}{2} \frac{\Gamma(1-\zeta)^2 \Gamma(\frac{1}{2}+\zeta) \Gamma(\frac{1}{2})}{\Gamma(\frac{1}{2}-\zeta) \Gamma(\frac{3}{2})} \left(\frac{1}{\zeta} + \frac{2}{\frac{1}{2}-\zeta} \right); \end{aligned} \quad (15)$$

recall that the sole singularities of $\Gamma(\omega)$ are simple poles at $\omega = -n = 0, -1, -2, \dots$

We invert (15) by summing over residues from poles that lie in the right half-plane and are closest to the fundamental strip; this sum yields the desired expansion for $\delta \ll 1$. We write

$$I(\delta^2) = \frac{1}{2\pi i} \int_{\nu-i\infty}^{\nu+i\infty} (\delta^2)^{\zeta-1} \hat{I}(\zeta) d\zeta, \quad -\frac{1}{2} < \nu < 0, \quad (16)$$

by definition 2 in appendix B. By shifting the contour to the right, the *leading-order term* in (16) comes from the residue at $\zeta = 0$. Thus, we approximate [31]

$$(\delta^2)^{\zeta-1} \hat{I}(\zeta) \sim -\frac{1}{2\delta^2} \frac{\Gamma(\frac{1}{2})}{\Gamma(\frac{3}{2})} \frac{1}{\zeta} = -\frac{1}{\delta^2} \frac{1}{\zeta} \quad \text{as } \zeta \rightarrow 0.$$

The respective residue at $\zeta = 0$ is $1/\delta^2$. Thus, by (14) we find

$$I(\delta^2) \sim \frac{1}{\delta^2} \Rightarrow U_{\text{int}} \sim \frac{4P^2 r_2}{\lambda^3 \delta^2} \quad \text{as } \delta^2 \downarrow 0. \quad (17)$$

To leading order in δ^2 the interaction energy per unit length of step 1 is written as

$$V_{\text{int}} \sim \frac{1}{2} \sqrt{\frac{r_2}{r_1}} \left(\frac{2P}{r_2 - r_1} \right)^2 \sim \frac{1}{2} \left(\frac{2r_2}{r_1 + r_2} \right) \left(\frac{2P}{r_2 - r_1} \right)^2, \quad \frac{r_2 - r_1}{r_1} \ll 1, \quad (18)$$

where we used $\lambda = 2\sqrt{r_1 r_2} \sim r_1 + r_2$ and $\delta = \rho/\lambda$. Formula (18) is in agreement with (5) via the definition $2P =: a\sqrt{2g}$ [14, 17]. By setting $\rho = r_2 - r_1 \equiv w$ (fixed) with $r_1 = \epsilon^{-1}$ and $r_2 = \epsilon^{-1} + \rho$, we recover the straight-step interaction energy (10) as $\epsilon \downarrow 0$.

Corrections to (18) can originate from residues at the poles $\zeta = 1, 2, \dots$ of $\hat{I}(\zeta)(\delta^2)^{\zeta-1}$. In particular, the residue at $\zeta = 1$ is found via expansions in $\tilde{\zeta} = 1 - \zeta$. Using the recursive relation $\omega\Gamma(\omega) = \Gamma(\omega + 1)$ [31] where necessary, we have

$$\hat{I}(\zeta) \sim \frac{1}{4} \left[-\frac{3}{\tilde{\zeta}^2} - \frac{6\psi(1) - 3\psi(3/2) - 3\psi(-1/2) + 7}{\tilde{\zeta}} \right] \quad \text{as } \tilde{\zeta} \rightarrow 0,$$

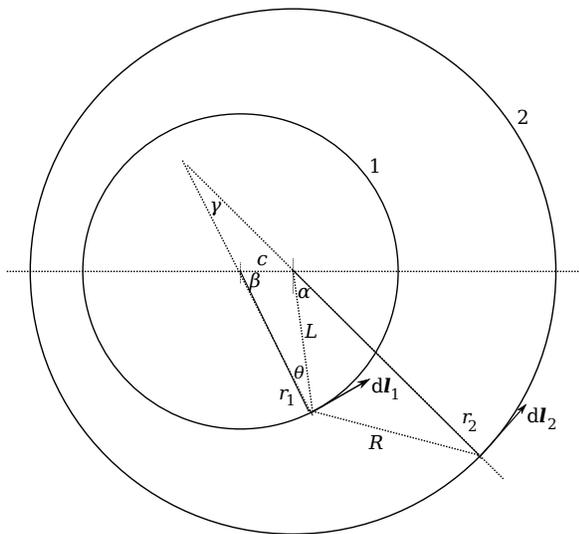


Figure 5. Geometry of non-concentric circular steps of radii r_1 and r_2 .

where $\psi(\omega) = \frac{d}{d\omega} \ln \Gamma(\omega)$ [31]. Thus, $(\delta^2)^{\zeta-1} \hat{I}(\zeta)$ has the residue $\frac{1}{4}(-3 \ln \frac{16}{\delta^2} + 5)$ at $\zeta = 1$. Accordingly, we obtain a *logarithmic correction*:

$$V_{\text{int}} \sim P^2 r_2 \left[\frac{4}{\lambda} \frac{1}{\rho^2} - \frac{3}{\lambda^3} \ln \left(\frac{16\lambda^2}{\rho^2} \right) + \frac{5}{\lambda^3} \right], \quad \frac{\rho}{\lambda} \ll 1. \quad (19)$$

Further corrections in this context may be questionable, since these may be comparable in magnitude to terms omitted from our starting point, equation (8). Our computation demonstrates the contributions of force dipole moments *parallel to step edges on the basal plane*.

4. Non-concentric circular steps

In this section, we consider two circular steps of different centers. This geometry forms a deviation from the radial case (section 3.2). The energy of interest is still exactly calculable in terms of elliptic integrals and also amenable to asymptotics by the Mellin transform. Specifying the shape of step 1 is not necessary since attention is focused on the interaction energy per unit length. In the end, we indicate the computation of the total elastic interaction energy for the two steps.

The geometry is depicted in figure 5. Let the x -axis join the two centers, which are offset by a distance c . The circles radii are r_1 and r_2 . The centers and the fixed point of interest on the inner circle (step 1) form a triangle of sides with lengths c , r_1 and L . The dipole $d\mathbf{l}_1$ along step 1 is located at a point at angle β with the x -axis (see footnote 8). The dipole $d\mathbf{l}_2$ on the outer circle is located at angle α with the side of length L . We also define the angles γ and θ , and the distance R between the two dipoles as in

⁸For the interaction energy per unit length, it suffices to take $d\mathbf{l}_1$ in a fixed (say, y -) axis. Here, we choose to also give a formula for the total energy, so β is needed to parametrize the position of $d\mathbf{l}_1$.

figure 5. Clearly, we have the relations $R^2 = L^2 + r_2^2 - 2Lr_2 \cos \alpha$ and

$$\alpha = \theta + \gamma, \quad \cos \gamma = \sqrt{1 - \left(\frac{c}{L} \sin \beta\right)^2} \cos \alpha + \frac{c}{L} \sin \beta \sin \alpha.$$

We compute the elastic interaction energy per unit length of step 1 with step 2 via an integral over α . So, fix $d\mathbf{l}_1$, L and β . By $d\mathbf{l}_1 \cdot d\mathbf{l}_2 = (dl_1)(r_2 d\alpha) \cos \gamma$, we find

$$V_{\text{int}} = \frac{dW_{\text{int}}}{dl_1} = P^2 r_2 \int_{-\pi}^{\pi} \frac{\cos \alpha \sqrt{1 - \left(\frac{c}{L} \sin \beta\right)^2} + \frac{c}{L} \sin \alpha \sin \beta}{(L^2 + r_2^2 - 2r_2 L \cos \alpha)^{3/2}} d\alpha.$$

This integral is recast to a form analogous to the radial case (section 3.2). Let $s = \sin(\alpha/2)$; accordingly,

$$V_{\text{int}}(\beta) = \frac{4P^2 r_2}{\lambda^3} \sqrt{1 - \left(\frac{c}{L} \sin \beta\right)^2} I(\delta^2), \quad \delta = \rho/\lambda, \quad (20)$$

where $L^2 = L(\beta)^2 = r_1^2 + c^2 - 2r_1 c \cos \beta$, $\rho = r_2 - L$, $\lambda = 2\sqrt{r_2 L}$ and $I(\delta^2)$ is defined by (12); in the radial case, $c = 0$ and $L = r_1$.

Hence, we wind up with the *same* integral, $I(\delta^2)$, as in the case with *concentric* circular steps. By (17), the leading-order approximation for the interaction energy with step 2 per unit length of step 1 is

$$V_{\text{int}}(\beta) \sim \frac{1}{2} \sqrt{\frac{r_2}{L}} \sqrt{1 - \left(\frac{c}{L} \sin \beta\right)^2} \left(\frac{2P}{r_2 - L}\right)^2 \quad \text{if } r_2 - L \ll \sqrt{r_2 L}, \quad (21)$$

i.e., provided dipole 1 does not lie too close to the center of step 2 and the radii difference is small compared to $\sqrt{r_1 r_2}$. Formula (21) reduces to approximation (18) of the radial case if $c \rightarrow 0$. Correction terms to (21) follow from the higher-order terms in the expansion for $I(\delta^2)$; see end of section 3.2.

We note in passing that an approximation for the *total* elastic interaction energy of steps 1 and 2 stems from integrating (21) with respect to β , where $dl_1 = r_1 d\beta$:

$$V_{\text{int}}^{\text{tot}} \sim r_1 \int_0^\pi \sqrt{\frac{r_2}{L(\beta)}} \sqrt{1 - \left(\frac{c}{L(\beta)} \sin \beta\right)^2} \left(\frac{2P}{r_2 - L(\beta)}\right)^2 d\beta.$$

5. Perturbation of circular step

In this section we address the computation of the interaction energy, V_{int} , per unit length of a step with another non-circular step. The latter step has a shape that forms perturbation of a circle. Our main assumption is that the polar coordinates r_1 and r_2 for the two steps are sufficiently close, by direct analogy with the radial case (section 3.2). We derive leading-order and correction (logarithmic) terms for V_{int} .

The Mellin transform technique could have been bypassed in favor of elliptic integrals and their asymptotic expansions, if our only focus in this paper was the energies of circular steps. The worth of the Mellin transform may be better demonstrated by indicating how it can be applied to the integral for elastic-dipole interactions between steps of other smooth shapes. From the viewpoint of our analysis, the ensuing integrals

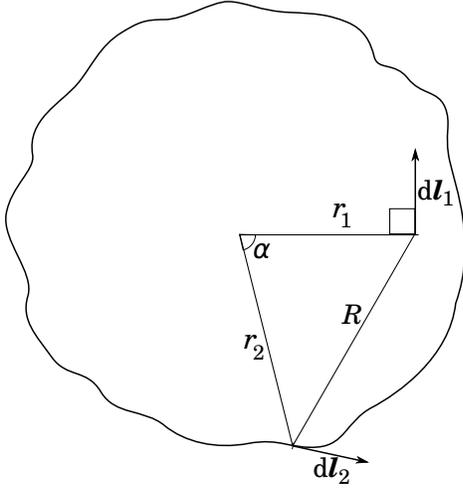


Figure 6. Force dipole moment $Pd\mathbf{l}_1$ and neighboring perturbed (non-circular) step.

are amenable to approximations if a coordinate system can be specified such that $|r_1 - r_2|$ is small compared to r_1 and r_2 (uniformly in the assorted angle variables).

The geometry is shown in figure 6. The system consists of: (i) a fixed force dipole $d\mathbf{l}_1 = (dl_1)e_y$ (along the y -axis) located at $(x, y) = (r_1, 0)$; and (ii) a step described by the polar graph $(r_2(\alpha), \alpha)$ where $r_2(\alpha)$ is smooth and $-\pi < \alpha \leq \pi$. The force dipole along the latter step is $d\mathbf{l}_2$, at distance R from dipole $d\mathbf{l}_1$. Since we focus on the interaction energy per unit length of step 1, the overall shape of this step does not enter our discussion. We can assume that the position of dipole 1 is parametrized so that the element $d\mathbf{l}_1$ lies on some prescribed smooth curve (see footnote 9). Consider

$$r_2(\alpha) = r_1 + r(s), \quad r(s) = \rho[1 + s\bar{r}(s)]; \quad s = \sin(\alpha/2), \quad (22)$$

where $\bar{r}(s)$ is smooth, $\mathcal{O}(1)$ and signifies the breaking of rotational symmetry.

By analogy with the radial case (section 3.2), the distance R here is given by

$$R(s)^2 = r_1^2 + r_2^2 - 2r_1r_2 \cos(\alpha) = \lambda^2\{s^2 + \delta^2[1 + sA(s)]\} =: \lambda^2\mathcal{Q}(s; \delta^2),$$

where

$$\lambda^2 = 4r_1(r_1 + \rho), \quad \delta^2 = \rho^2/\lambda^2, \quad A(s) = \bar{r}(s)[2 + s\bar{r}(s) + 4s^2r_1/\rho]; \quad (23)$$

$A(s) \equiv 0$ in the radial case ($\bar{r} \equiv 0$). In general, $A(s)$ depends on δ via r_1 and ρ . In using the Mellin transform, we treat $A(s)$ as δ -independent. So, the coefficients of the expansion can be functions of δ ; this feature does not raise any concerns (see footnote 10).

We now proceed with the calculation of the elastic-dipole interaction energy, noting that $d\mathbf{l}_1 \cdot d\mathbf{l}_2 = [r_2'(\alpha) \sin \alpha + r_2 \cos \alpha]d\alpha dl_1$ where the prime here denotes differentiation. Thus, we obtain the formula

$$\frac{dW_{\text{int}}}{dl_1} = \frac{2P^2}{\lambda^3} [(r_1 + \rho)I_0 + 2\rho I_1 + \rho I_{21} - 2(r_1 + \rho)I_{22} - 3\rho I_3 - \rho I_4], \quad (24)$$

⁹More generally, we can assume that the polar graph of step 1, not shown in figure 6, is $(r_1(\beta), \beta)$; thus, ρ as well as λ and δ (to be defined below) are β -dependent.

¹⁰This situation is somewhat analogous to seeking an expansion for, e.g., $[1 - b(\delta^2)\delta^2]^{-1}$ for $\delta^2 \ll 1$ where $b(u) = o(1)$ as $u \downarrow 0$. One can treat b as independent of δ and finally account for $b = b(\delta^2)$.

where, with $\mathcal{Q}(s; \delta^2) = s^2 + \delta^2[1 + sA(s)]$, the associated integrals are defined by

$$\begin{aligned} I_0(\delta^2) &= \int_{-1}^1 \frac{ds}{\sqrt{1-s^2}} \mathcal{Q}(s; \delta^2)^{-3/2}, & I_1(\delta^2) &= \int_{-1}^1 \frac{ds}{\sqrt{1-s^2}} \frac{s\bar{r}(s)}{\mathcal{Q}(s; \delta^2)^{3/2}}, \\ I_{21}(\delta^2) &= \int_{-1}^1 \frac{ds}{\sqrt{1-s^2}} \frac{\bar{r}'(s) s^2}{\mathcal{Q}(s; \delta^2)^{3/2}}, & I_{22}(\delta^2) &= \int_{-1}^1 \frac{ds}{\sqrt{1-s^2}} \frac{s^2}{\mathcal{Q}(s; \delta^2)^{3/2}}, \\ I_3(\delta^2) &= \int_{-1}^1 \frac{ds}{\sqrt{1-s^2}} \frac{\bar{r}(s) s^3}{\mathcal{Q}(s; \delta^2)^{3/2}}, & I_4(\delta^2) &= \int_{-1}^1 \frac{ds}{\sqrt{1-s^2}} \frac{\bar{r}'(s) s^4}{\mathcal{Q}(s; \delta^2)^{3/2}}. \end{aligned}$$

Evidently, these integrals are classified according to the explicit power of s appearing in their integrands. As $\delta^2 \downarrow 0$, the most singular integral is $I_0(\delta^2)$, which reduces precisely to the integral of the radial case if $\bar{r}(s) \equiv 0$. By contrast, the integrals $I_3(\delta^2)$ and $I_4(\delta^2)$ remain finite, yielding (δ -independent) constants.

In appendix C, the above integrals are approximated for small δ^2 ($\delta^2 \ll 1$) by use of the Mellin transform. The main idea is to single out the contributions of the underlying divergencies (as $\delta^2 \downarrow 0$) in the form of appropriate residues of a complex-valued function. Our results, up to (and including) logarithmic corrections, are summarized as follows:

$$I_0(\delta^2) \sim \frac{2}{\delta^2} + \frac{1}{2} \ln \frac{16}{\delta^2} - \frac{1}{2} [2A'(0) - A(0)^2 + 3], \quad (25)$$

$$I_1(\delta^2) \sim \bar{r}(0)A(0) + \bar{r}'(0) \left(\ln \frac{16}{\delta^2} - 2 \right) + \mathcal{C}_1, \quad (26)$$

$$I_{21}(\delta^2) \sim \bar{r}'(0) \left(\ln \frac{16}{\delta^2} - 2 \right) + \mathcal{C}_2, \quad I_{22}(\delta^2) \sim \ln \frac{16}{\delta^2} - 2, \quad (27)$$

$$I_3(\delta^2) \sim \mathcal{C}_3 = \int_{-1}^1 \frac{ds}{\sqrt{1-s^2}} \bar{r}(s) \operatorname{sgn}(s), \quad (28)$$

$$I_4(\delta^2) \sim \mathcal{C}_4 = \int_{-1}^1 \frac{ds}{\sqrt{1-s^2}} \bar{r}'(s) |s|, \quad (29)$$

where $\operatorname{sgn}(s) = -1$ if $s < 0$ and $\operatorname{sgn}(s) = 1$ if $s > 0$, and

$$\mathcal{C}_1 = \int_{-1}^1 \frac{ds}{\sqrt{1-s^2}} \left[\frac{\bar{r}(s) - \bar{r}(0)}{s} - \bar{r}'(0) \right] |s|^{-1}, \quad (30)$$

$$\mathcal{C}_2 = \int_{-1}^1 \frac{ds}{\sqrt{1-s^2}} [\bar{r}'(s) - \bar{r}'(0)] |s|^{-1}, \quad (31)$$

$$A(0) = 2\bar{r}(0), \quad A'(0) = 2\bar{r}'(0) + \bar{r}(0)^2. \quad (32)$$

Note that ρ does not appear in the values $A(0)$ and $A'(0)$ to these orders of approximation; see appendix C for more details.

The corresponding expansion for $V_{\text{int}} = dW_{\text{int}}/dl_1$ follows from combination of (24) with (25)–(29). By neglect of $\mathcal{O}(\delta)$ terms, this expansion reads

$$\begin{aligned} \frac{dW_{\text{int}}}{dl_1} &\sim \frac{4P^2}{\lambda^3} (r_1 + \rho) \left\{ \frac{1}{\delta^2} - \frac{3}{4} \left[1 - 2 \frac{\rho}{r_1 + \rho} \bar{r}'(0) \right] \ln \frac{16}{\delta^2} \right. \\ &\quad \left. + \frac{1}{4} [5 + 2\bar{r}(0)^2 - 4\bar{r}'(0)] \right\}. \end{aligned} \quad (33)$$

For $\bar{r}(s) \equiv 0$ (radial case), this dW_{int}/dl_1 reduces to formula (19). For a non-circular step 2, the logarithmic correction in (33) involves the derivative of $\bar{r}(s)$ at $s = 0$, a geometric dependence not seen in the leading-order term of the same formula.

A few more remarks on the results of this section are in order.

Remark 1. In the context of the BCF-type step flow, (33) can be used in order to express the step chemical potential, μ_1 , at any point of step 1 (where $d\mathbf{l}_1$ is located); recall formula (6). The curve representing step 1, and thus the position of the dipole on step 1, must be parametrized accordingly, e.g., by use of an angle variable. For the validity of our approximation, impose $|r_1 - r_2| \ll \sqrt{r_1 r_2}$.

Remark 2. In principle, higher-order terms of the asymptotic expansion for dW_{int}/dl_1 involve higher derivatives of $\bar{r}(s)$ at $s = 0$. This means that knowing these asymptotic terms to arbitrary order in principle amounts to extracting information about the local shape of step 2 (assuming $\bar{r}(s)$ is smooth).

Remark 3. The leading-order term in (33) is consistent with the geometric factor based on local coordinates in [20]. This is not surprising since the present geometry is a (regular) perturbation of concentric circles.

Remark 4. We reiterate that the magnitude of corrections to (33) relative to terms omitted in (8) is not known a priori. Adding corrections from other residues here might not be enough to ensure overall accuracy. Estimating the contribution of cross-terms in (8), which stem from dipole moments perpendicular to the basal plane, lies beyond our present purposes.

6. Conclusion

We began this investigation in an attempt to verify, and possibly improve, a previously used formula for the elastic-dipole interaction energy between two concentric circular steps. To this end, we applied the Mellin transform with respect to a parameter expressing the relative magnitude of the step distance and the step radii of curvature. This technique singles out the most important contributions to integration over the step circumference in the form of appropriate residues of poles in the complex plane for the transformed integral. Our derivation offered a refinement of the previous formula in two respects: the leading-order term is slightly more accurate; and a logarithmic correction is added.

In the course of our derivation, we extended the calculation of the interaction energy to a class of smooth 2D steps. In our model, these steps form perturbations of circles. The leading-order behavior of their interaction energy is consistent with physical intuition: the elastic energy per unit length between the steps decays as the inverse square of their separation, as measured along the appropriate *local normal*. This property was invoked by Weeks et al [7] for perturbations of straight steps. Here, we generalized this result to other geometries and also derived corrections; these may become important for a certain range of interstep distances and material parameters.

Previous numerical studies of step flow with circular steps [15, 17] made use of the interaction energy formula from [14], which we now understand to be valid when step separations are sufficiently small compared to the step radii ($\delta^2 \ll 1$ in our notation). A more precise regime of validity of this formula should stem by considering limitations of classical elasticity as well; for example, the starting elastic-dipole formula becomes inadequate if the step distance becomes comparable to a few atomic lengths [24].

The extended formulas of this paper express effects of rotational symmetry breaking through logarithmic corrections. These involve local geometric features of the step curve.

Our analysis has limitations. For example, we did not address contributions of dipole moments perpendicular to the basal plane; nor did we compute corrections due to elastic-multipole interactions. Our goal was to demonstrate the use of an analytical tool (Mellin transform) in simple yet physically relevant geometries, rather than embark on lengthy computations. In cases of multipole interactions, the associated integrals have a similar algebraic structure with some modifications, e.g., the denominators of the integrands involve higher powers. Such energies are amenable to the Mellin transform as well and are the subject of work in progress.

Acknowledgements

We are indebted to T L Einstein for discussions. The first author's (John Quah's) research was supported by NSF-MRSEC under grant DMR-0520471 during the spring of 2009. The work of the second author (Li Peng Liang) was supported by the NSF-MRSEC REU via grant DMR-0520471 at the University of Maryland. The third author's (Dionisios Margetis's) research was supported by NSF under grant DMS-0847587.

Appendix A. On elliptic integrals

In this appendix, we compute the integral $V_{\text{int}}(\delta^2)$ of the radial case, equation (14), in terms of complete elliptic integrals [32].

By (14), we express $V_{\text{int}}(\delta^2)$ as

$$V_{\text{int}}(\delta^2) = \frac{4P^2r_2}{\lambda^3} \left[-2(2\delta^2 + 1) \frac{d}{d(\delta^2)} - 2 \right] I_c(\delta^2) \quad (\text{A.1})$$

where

$$I_c(\delta^2) = \int_0^1 \frac{ds}{\sqrt{1-s^2}} \frac{1}{\sqrt{s^2 + \delta^2}}. \quad (\text{A.2})$$

With $s = \cos \theta$ in (A.2), we find

$$I_c(\delta^2) = \int_0^{\pi/2} \frac{d\theta}{\sqrt{\delta^2 + 1 - \sin^2 \theta}} = \frac{1}{\sqrt{1 + \delta^2}} \mathbb{K}(1/\sqrt{1 + \delta^2}) \quad (\text{A.3})$$

where $\mathbb{K}(\varpi) = \int_0^{\pi/2} d\theta (1 - \varpi^2 \sin^2 \theta)^{-1/2}$ is the complete elliptic integral of the first kind [32]. Thus, by (A.1) and $\varpi = (1 + \delta^2)^{-1/2}$, we obtain

$$V_{\text{int}}(\delta^2) = \frac{4P^2r_2}{\lambda^3} \varpi \left[\frac{2 - \varpi^2}{1 - \varpi^2} \mathbb{E}(\varpi) - 2\mathbb{K}(\varpi) \right]; \quad (\text{A.4})$$

$\mathbb{E}(\varpi) = \int_0^{\pi/2} \sqrt{1 - \varpi^2 \sin^2 \theta} d\theta$ is the complete elliptic integral of the second kind [32].

This result is compatible with the asymptotic expansion of section 3.2. In particular, by expanding $(1 + \delta^2)^{-1/2}$ about $\delta = 0$ and using an expansion of $\mathbb{K}(\varpi)$ about $\varpi = 1$ [32], we recover $I_c \sim \ln(16/\delta^2)$ and the assorted correction terms as $\delta \downarrow 0$.

Appendix B. Review of Mellin transform

In this appendix, we review elements of the Mellin integral transform. For a more thorough discussion including other applications, the reader may consult, e.g., [10–12, 33–35]. We include only technical elements that serve our present purposes.

Definition 1 *The Mellin transform of $F(x) : \mathbb{R}_+ \rightarrow \mathbb{R}$ (\mathbb{R} : set of reals) is defined as*

$$\hat{F}(\zeta) = \int_0^\infty F(x)x^{-\zeta} dx, \quad (\text{B.1})$$

where ζ lies in some vertical strip, \mathbb{S}_0 , of the complex plane so that the integral converges.

Note that, once defined via (B.1) for $\zeta \in \mathbb{S}_0$, the function $\hat{F}(\zeta)$ can in principle be continued analytically to the whole complex plane, \mathbb{C} .

Definition 2 *The inverse Mellin transform of $\hat{F}(\zeta) : \mathbb{C} \rightarrow \mathbb{C}$ is defined by*

$$(\hat{F})^\sim(x) = \frac{1}{2\pi i} \int_{\nu-i\infty}^{\nu+i\infty} \hat{F}(\zeta)x^{\zeta-1} d\zeta \quad (i^2 = -1), \quad (\text{B.2})$$

where, for appropriate ν , the contour of integration must lie in $\mathbb{S}_0 \subset \mathbb{C}$.

Under reasonably general assumptions on $F(x)$, we henceforth take $F(x) = (\hat{F})^\sim(x)$ (almost everywhere). In the following, we motivate formulas (B.1) and (B.2) with recourse to a (presumably more familiar) variant of the Fourier transform.

For a function $f : \mathbb{R} \rightarrow \mathbb{R}$, the *two-sided Laplace transform* is

$$\mathcal{L}(f)(\sigma) = \int_{-\infty}^\infty f(t)e^{-\sigma t} dt, \quad (\text{B.3})$$

which follows from the Fourier transform [33]. By reasonably general conditions, f is recovered from $\mathcal{L}(f)$ via the inversion formula

$$f(t) = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} \mathcal{L}(f)(\sigma)e^{\sigma t} d\sigma, \quad (\text{B.4})$$

where the integration path lies in the region of convergence of the integral for $\mathcal{L}(f)(\sigma)$.

The Mellin transform ensues from (B.3) by $x = e^t$. Formally, this yields

$$\mathcal{L}(f)(\sigma) = \int_0^\infty f(\ln x)x^{-\sigma-1} dx, \quad (\text{B.5})$$

which leads to (B.1) via the definitions $F(x) = f(\ln x)$, $\zeta = \sigma + 1$, and $\hat{F}(\zeta) = \mathcal{L}(f)(\zeta - 1)$. The inverse Mellin transform (B.2) with $(\hat{F})^\sim = F$ follows from (B.4).

We add a note on convergence. For arbitrary yet fixed $c > 0$, split integral (B.1) as

$$\hat{F}(\zeta) = \left(\int_0^c + \int_c^\infty \right) F(x)x^{-\zeta} dx, \quad (\text{B.6})$$

and assume that $F(x)$ is summable on any finite $(c_1, c_2) \subset (0, \infty)$ where $c_1 > 0$, $F(x) = \mathcal{O}(x^{p_2-1})$ as $x \downarrow 0$ and $F(x) = \mathcal{O}(x^{p_1-1})$ as $x \rightarrow \infty$. The first integral converges provided $\text{Re}\zeta < p_2$, while the second one converges if $p_1 < \text{Re}\zeta$. Thus, if $p_1 < p_2$, $\hat{F}(\zeta)$ is originally defined (as a convergent integral) in the *fundamental strip* $p_1 < \text{Re}\zeta < p_2$.

Appendix C. Asymptotics for integrals of non-circular step

In this appendix, we evaluate approximately the integrals $I_\ell(\delta^2)$ ($\ell = 0, 1, 21, 22, 3, 4$) of section 4 by use of their Mellin transforms, $\hat{I}_\ell(\zeta)$. Each $\hat{I}_\ell(\zeta)$ is a meromorphic function and, although not exactly calculable in terms of tractable special functions, it can be written as a Laurent series in the vicinity of every pole. By starting with the definition of the Mellin transform in the fundamental strip, we derive terms of the Laurent series by *analytic continuation*. So, the respective residues can be computed to yield an asymptotic expansion in δ with coefficients containing details of the step curve.

Integral I_0 . The leading-order term for the energy stems from $I_0(\delta^2)$. We compute

$$\hat{I}_0(\zeta) = \frac{\Gamma(1-\zeta)\Gamma(\frac{1}{2}+\zeta)}{\Gamma(\frac{3}{2})} \int_{-1}^1 \frac{ds}{\sqrt{1-s^2}} [1+sA(s)]^{\zeta-1} (s^2)^{-\zeta-1/2}, \quad (\text{C.1})$$

with fundamental strip $-1/2 < \text{Re}\zeta < 0$. To single out the *simple* pole $\zeta = 0$, we write

$$\int_{-1}^1 \frac{ds}{\sqrt{1-s^2}} [1+sA(s)]^{\zeta-1} (s^2)^{-\zeta-1/2} = 2 \int_0^1 \frac{ds}{\sqrt{1-s^2}} (s^2)^{-\zeta-1/2} + \mathcal{O}(1)$$

as $\zeta \rightarrow 0$, where $\mathcal{O}(1)$ is bounded. The last integral equals $\Gamma(-\zeta)\Gamma(1/2)/\Gamma(1/2-\zeta)$; thus,

$$\hat{I}_0(\zeta) \sim -2/\zeta \quad \text{as } \zeta \rightarrow 0, \quad (\text{C.2})$$

which yields the first term in (25). In the same vein, we find *zero* residue at $\zeta = 1/2$ and thus no contribution $\mathcal{O}(1/\delta)$ to $I_0(\delta^2)$.

Regarding the *double* pole of $\hat{I}_0(\zeta)$ at $\zeta = 1$, we write

$$[1+sA(s)]^{\zeta-1} = 1 + s^2[\Lambda_0(s; \zeta) - \Lambda_0(0; \zeta)] + s^2\Lambda_0(0, \zeta) + \mathcal{K}_0(\zeta) s,$$

where

$$\Lambda_0(s; \zeta) = s^{-1} \left\{ \frac{[1+sA(s)]^{\zeta-1} - 1}{s} - \mathcal{K}_0(\zeta) \right\},$$

$$\mathcal{K}_0(\zeta) = \lim_{s \rightarrow 0} \frac{[1+sA(s)]^{\zeta-1} - 1}{s}.$$

As $\tilde{\zeta} = 1-\zeta \rightarrow 0$, we have $\mathcal{K}_0(\zeta) \sim -\tilde{\zeta}A(0)$ and $\Lambda_0(s; \zeta) \sim -\tilde{\zeta}\{\ln[1+sA(s)] - sA(0)\}/s^2$ uniformly in s ; hence, $\Lambda(0; \zeta) \sim -\tilde{\zeta}[A'(0) - \frac{1}{2}A(0)^2]$. By integration (in s), we obtain

$$\hat{I}_0(\zeta) \sim \frac{1}{2} \left[\frac{1}{\tilde{\zeta}^2} - \frac{2A'(0) - A(0)^2 - 1 + \psi(\frac{3}{2}) + \psi(-\frac{1}{2}) - 2\psi(1)}{\tilde{\zeta}} \right]. \quad (\text{C.3})$$

The residue for $\hat{I}_0(\zeta)(\delta^2)^{\zeta-1}$ at $\tilde{\zeta} = 0$ yields the remaining terms in (25); $\ln \delta^2$ appears.

Integral I_1 . The Mellin transform of $I_1(\delta^2)$ reads

$$\hat{I}_1(\zeta) = \frac{\Gamma(1-\zeta)\Gamma(\frac{1}{2}+\zeta)}{\Gamma(\frac{3}{2})} \int_{-1}^1 \frac{ds}{\sqrt{1-s^2}} s\bar{r}(s)[1+sA(s)]^{\zeta-1}(s^2)^{-\zeta-1/2}$$

with fundamental strip $-1/2 < \text{Re}\zeta < 1/2$. Because of the factor s here, we conclude by analytic continuation that $\zeta = 1/2$ is a ‘removable singularity’. Next, consider the *double* pole at $\zeta = 1$; $\tilde{\zeta} = 1 - \zeta$. For analytic continuation, apply the splitting

$$\bar{r}(s)[1+sA(s)]^{\zeta-1} = s[\Lambda_1(s; \zeta) - \Lambda_1(0; \zeta)] + s\Lambda_1(0; \zeta) + \bar{r}(0) ,$$

where

$$\Lambda_1(s; \zeta) = \frac{\bar{r}(s)[1+sA(s)]^{\zeta-1} - \bar{r}(0)}{s} .$$

Notice that $\Lambda_1(s; \zeta) \sim s^{-1}\{\bar{r}(s) - \bar{r}(0) - \tilde{\zeta}\bar{r}(s)\ln[1+sA(s)]\}$ as $\tilde{\zeta} \rightarrow 0$, uniformly in s ; in particular, $\lim_{s \rightarrow 0} \Lambda_1(s; \zeta) \sim \bar{r}'(0) - \tilde{\zeta}\bar{r}(0)A(0)$. By integration in s , we find

$$\hat{I}_1(\zeta) \sim \frac{\bar{r}'(0)}{\tilde{\zeta}^2} + \frac{\mathcal{C}_1 + [2\psi(1) - \psi(\frac{1}{2}) - \psi(\frac{3}{2})]\bar{r}'(0) + \bar{r}(0)A(0)}{\tilde{\zeta}} , \quad (\text{C.4})$$

as $\tilde{\zeta} \rightarrow 0$; the constant \mathcal{C}_1 is defined by (30). The expansion for $\hat{I}_1(\zeta)(\delta^2)^{\zeta-1}$ as $\zeta \rightarrow 1$ yields (26).

Integrals I_{21} , I_{22} . The Mellin transforms of $I_{21}(\delta^2)$ and $I_{22}(\delta^2)$ read

$$\hat{I}_{21}(\zeta) = \frac{\Gamma(1-\zeta)\Gamma(\frac{1}{2}+\zeta)}{\Gamma(\frac{3}{2})} \int_{-1}^1 \frac{ds}{\sqrt{1-s^2}} [1+sA(s)]^{\zeta-1}\bar{r}'(s)(s^2)^{-\zeta+1/2}, \quad (\text{C.5})$$

$$\hat{I}_{22}(\zeta) = \frac{\Gamma(1-\zeta)\Gamma(\frac{1}{2}+\zeta)}{\Gamma(\frac{3}{2})} \int_{-1}^1 \frac{ds}{\sqrt{1-s^2}} [1+sA(s)]^{\zeta-1}(s^2)^{-\zeta+1/2} , \quad (\text{C.6})$$

with fundamental strip $-1/2 < \text{Re}\zeta < 1$. Each of the above functions has a double pole at $\zeta = 1$. We analytically continue each function to $1 \leq \text{Re}\zeta < 3/2$ via the splitting

$$\Lambda_2(s; \zeta) \equiv [1+sA(s)]^{\zeta-1}q(s) = [\Lambda_2(s; \zeta) - \Lambda_2(0; \zeta)] + \Lambda_2(0; \zeta) ,$$

where $q(s) = \bar{r}'(s)$ or 1 . Note that $\Lambda_2(s; \zeta) \sim \{1 - \tilde{\zeta}\ln[1+sA(s)]\}q(s)$ as $\tilde{\zeta} \rightarrow 0$, uniformly in s . After substitution in (C.5) and (C.6), and further algebra, we find

$$\hat{I}_{21}(\zeta) \sim \frac{\bar{r}'(0)}{\tilde{\zeta}^2} + \frac{\mathcal{C}_2 + \bar{r}'(0)[2\psi(1) - \psi(\frac{1}{2}) - \psi(\frac{3}{2})]}{\tilde{\zeta}} , \quad (\text{C.7})$$

$$\hat{I}_{22}(\zeta) \sim \frac{1}{\tilde{\zeta}^2} + \frac{2\psi(1) - \psi(\frac{1}{2}) - \psi(\frac{3}{2})}{\tilde{\zeta}} , \quad (\text{C.8})$$

where the constant \mathcal{C}_2 is defined by (31). The expansions of $\hat{I}_{21}(\zeta)(\delta^2)^{\zeta-1}$ and $\hat{I}_{22}(\zeta)(\delta^2)^{\zeta-1}$ at $\zeta = 1$ ($\tilde{\zeta} = 0$) and computation of residues lead to formulas (27).

Integrals I_3 , I_4 . By contrast to $I_\ell(\delta^2)$ for $\ell = 0, 1, 21, 22$, the integrals $I_3(\delta^2)$ and $I_4(\delta^2)$ remain convergent as $\delta^2 \downarrow 0$. Thus, by continuity in δ , we have $I_3(\delta^2) \sim I_3(0)$ and $I_4(\delta^2) \sim I_4(0)$ as $\delta^2 \downarrow 0$. These assertions readily yield (28) and (29).

References

- [1] Jeong H-C and Williams E D 1999 *Surf. Sci. Rep.* **34** 171
- [2] Marchenko V I and Parshin A Ya 1980 *Soviet Phys. JETP* **52** 129
- [3] Kukta R V, Peralta A, and Kouris D 2002 *Phys. Rev. Lett.* **88** 186102
- [4] Léonard F, Bartelt N C, and Kellogg G L 2005, *Phys. Rev. B* **71** 045416
- [5] Huang G-Y and Yu S-W 2007 *J. Appl. Mech.* **74** 821
- [6] Burton W K, Cabrera N and Frank F C 1951 *Phil. Trans. R. Soc. A* **243** 299
- [7] Weeks J D, Liu D-J, and Jeong H-C 1997 in *Dynamics of Crystal Surfaces and Interfaces* eds P M Duxbury and T J Pence (New York: Plenum Press) p 199
- [8] Bonzel H P 2003 *Phys. Rep.* **385** 1
- [9] Giesen M 2001 *Prog. Surf. Sci.* **68** 1
- [10] Sasiela R J and Shelton J D 1993 *J. Math. Phys.* **34** 2572
- [11] Margetis D and Fikioris G 2000 *J. Math. Phys.* **41** 6130
- [12] Cheng H and Wu T T 1987 *Expanding Protons: Scattering at High Energies* (Cambridge, MA: MIT Press)
- [13] Pimpinelli A and Villain J 1998 *Physics of Crystal Growth* (Cambridge: Cambridge University Press)
- [14] Tanaka S, Bartelt N C, Umbach C C, Tromp R M and Blakely J M 1997 *Phys. Rev. Lett.* **78** 3342
- [15] Fok P-W 2006 PhD thesis (Cambridge, MA: Massachusetts Institute of Technology)
- [16] Israeli N and Kandel D 1998 *Phys. Rev. Lett.* **80** 3300
- [17] Israeli N and Kandel D 1999 *Phys. Rev. B* **60** 5946
- [18] Margetis D, Aziz M J and Stone H 2005 *Phys. Rev. B* **71** 165432
- [19] Uwaha M and Watanabe K 2000 *J. Phys. Soc. Japan* **69** 497
- [20] Margetis D and Kohn R V 2006 *Multisc. Model. Simul.* **5** 729
- [21] Paulin S, Gillet F, Pierre-Louis O and Misbah C 2001 *Phys. Rev. Lett.* **86** 5538
- [22] Quah J and Margetis D 2008 *J. Phys. A: Math. and Theor.* **41** 235004
- [23] Krug J 2005 *Multiscale Modeling of Epitaxial Growth* ed A Voigt (Basel, Switzerland: Birkhäuser) p 69
- [24] Najafabadi R and Srolovitz D J 1994 *Surf. Sci.* **317** 221
- [25] Eshelby J D 1956 *Solid State Phys.* **3** 79
- [26] Prévot G and Croset B 2004 *Phys. Rev. Lett.* **92** 256104
- [27] Prévot G and Croset B 2006 *Phys. Rev. B* **74** 235410
- [28] Jackson J D 1999 *Classical Electrodynamics* (New York: Wiley)
- [29] Kubo R and Nagamiya T 1969 *Solid State Physics* ed R S Knox (New York: McGraw Hill)
- [30] Mott P H and Roland C M 2009 arXiv:0909.4697, Los Alamos, preprint
- [31] Bateman Manuscript Project 1953 *Higher Transcendental Functions* vol I ed A Erdélyi (New York: McGraw-Hill)
- [32] Bateman Manuscript Project 1953 *Higher Transcendental Functions* vol II ed A Erdélyi (New York: McGraw-Hill)
- [33] Carrier G F, Krook M, and Pearson C E 1966 *Functions of a Complex Variable: Theory and Technique* (New York: McGraw-Hill)
- [34] Bleistein N and Handelsman R A 1986 *Asymptotic Expansions of Integrals* (New York: Dover)
- [35] Fikioris G 2006 *IEEE Trans. Antennas Propagat.* **54** 3895