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Modeling, Analysis, and Simulation of Discrete-Continuum Models of Step-Flow Epitaxy: Bunching Instabilities and Continuum Limits

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ABSTRACT OF DISSERTATION

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Modeling, Analysis, and Simulation of Discrete-Continuum Models of Step-Flow Epitaxy: Bunching Instabilities and Continuum Limits

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A dissertation submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in the College of Arts and Sciences at the University of Kentucky

By
Nicholas O. Kirby
Lexington, Kentucky

Director: Dr. Michel E. Jabbour, Professor of Mathematics
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Vicinal surfaces consist of terraces separated by atomic steps. In the step-flow regime, deposited atoms (adatoms) diffuse on terraces, eventually reaching steps where they attach to the crystal, thereby causing the steps to move. There are two main objectives of this work. First, we analyze rigorously the differences in qualitative behavior between vicinal surfaces consisting of infinitely many steps and nanowires whose top surface consists of a small number of steps bounded by a reflecting wall. Second, we derive the continuum model that describes the macroscopic behavior of vicinal surfaces from detailed microscopic models of step dynamics.

We use the standard theory of Burton–Cabrera–Frank (BCF) to show that in the presence of an Ehrlich–Schwoebel barrier, i.e., a preferential attachment of adatoms from the lower terraces, N-periodic step motions are stable with respect to step collisions. Nonetheless, for $N > 2$ step collisions may occur. Moreover, we consider a single perturbed terrace, in which we distinguish three cases: no attachment from the upper terraces (perfect ES barrier), no attachment from the lower terraces (perfect inverse ES barrier), and symmetric attachment. For a perfect ES barrier, steps never collide regardless of the initial perturbation. In contrast, for a perfect inverse ES barrier, collisions occur for any nonzero perturbation. Finally, for symmetric attachment, step collisions occur for sufficiently large outward perturbations.

To model nanowire growth, we consider rectilinear steps and concentric steps bounded by reflecting walls. In contrast to a vicinal surface with infinitely many steps, we prove analytically that the Ehrlich–Schwoebel barrier is destabilizing with respect to step collisions. We further consider nanowire growth with desorption, and prove that the initial conditions that lead to step collisions are characterized by a unique step motion trajectory.

We take as our starting point a thermodynamically consistent (TC) generalization of the BCF model to derive PDE that govern the evolution of the vicinal surface at the macroscale. Whereas the BCF model yields a fourth-order parabolic equation for the surface height, the TC model yields a system of coupled equations for the surface height and the surface chemical potential.

KEYWORDS: epitaxial crystal growth, step-flow, Ehrlich–Schwoebel barrier, Burton–Cabrera–Frank model, continuum limit

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Date: August 4, 2011

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By
Nicholas O. Kirby

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Date: August 4, 2011

RULES FOR THE USE OF DISSERTATIONS

DISSERTATION

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On the mathematics side, Dr. David Owen and Dr. William Williams introduced me to mathematical rigor in the Mathematical Studies program. Dr. Owen later agreed to teach me mathematical thermodynamics, and generously served as my research advisor for a summer undergraduate research fellowship. I learned quite a lot of continuum mechanics during the summer of my fellowship, but the lesson that has stayed with me was the example of the life of the mind that Dr. Owen provided, which convinced me that a career in academia was worth pursuing. As the person who introduced me to Dr. Man who kindly suggested that I take Dr. Jabbour as a mentor, I literally would not be here today without Dr. Owen.

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This thesis is dedicated to my parents Bill and Susan Kirby for showing me the importance of passion and humility, and to my wife Beth who has been an endless source of encouragement and empathy.

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1.1 Introduction

The defining feature of a crystal is the spatially periodic arrangement of its constituent atoms or molecules. We treat the surface of a single-component crystal for simplicity. The boundary between the crystal and its environment is called the crystal surface. A slight miscut with respect to a high-symmetry plane results in a vicinal surface consisting of terraces separated by steps of atomic height. The appropriate object of study (atoms, steps, or the surface itself) depends on the temperature of the crystal. At low temperatures, the relevant objects of study are the individual atoms, whereas at high temperatures (i.e., above the roughening temperature) steps are so numerous that the crystal surface is best viewed as a smooth surface. Between these two extremes there is a range of temperatures called the step-flow regime, in which steps are present and changes in the morphology of the crystal surface are due to the motion of these steps (Fig. 1.1 shows a silicon crystal at such a temperature). This chapter serves as a review of the standard Burton–Cabrera–Frank (BCF) model [2] of step-flow epitaxy. A vast amount of literature has been written on the topic of epitaxy and step dynamics, cf. Saito [3], Pimpinelli and Villain [4], Jeōng and Williams [5], Krug and Michely [6], and Krug [7].

The steps move as a result of the attachment or detachment of adsorbed atoms on the terrace, called adatoms. Mathematically, we model the steps as smoothly evolving curves projected onto a common plane parallel to the terraces endowed with a unit normal vector that points into the lower terrace.

We distinguish between two kinds of atoms. Crystallized atoms form the bulk, and adatoms located on the terrace that have not attached to a step. The primary difference between bulk atoms and adatoms is the number bonds such atoms have

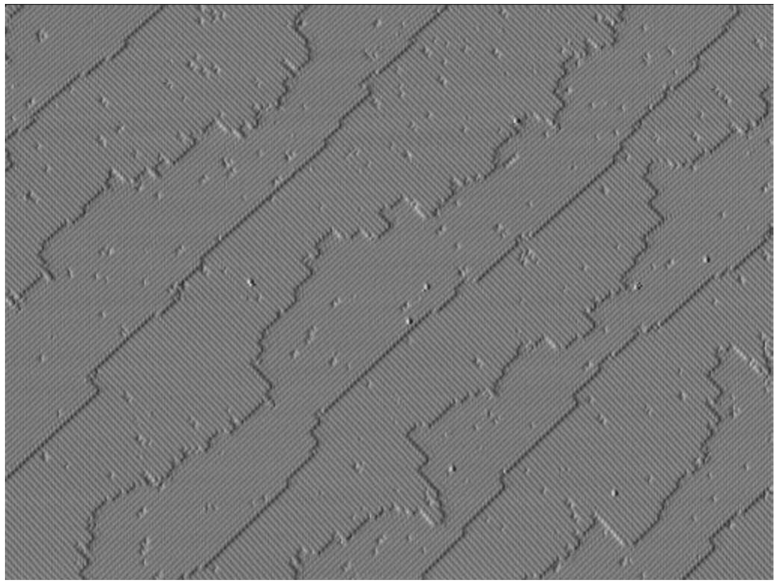

Figure 1.1: STM image of a silicon crystal showing steps on a vicinal surface, courtesy of B.S. Swartzentruber [1].

formed with other crystal atoms. In the step-flow regime, adatoms diffuse on the terraces via random walk. Steps move due the addition of adatoms into the bulk or the loss of bulk atoms onto the terrace.

In principle, if the adatoms diffuse on a terrace, there is some non-zero probability that two adatoms collide and form a bond (such an adatom pair is called a dimer). If the dimers remain bound for a sufficiently long time, they may combine to form an island of adatoms, thereby creating a new step at its boundary. This process is called island nucleation. We assume that the adatom mobility is sufficiently high that adatoms are more likely to reach a pre-existing step than to collide with each other to form dimers. As such, crystal growth occurs due to the motion of pre-existing steps.

At the atomic length scale, these steps are modeled as evolving, rectilinear paths (Fig. 1.2 shows a schematic of such a step separating an upper terrace from a lower terrace). These paths have kinks, which serve as absorption sites for adatoms to be incorporated into the bulk. Sufficiently long steps may be well-approximated by smooth, evolving curves in the plane. At this length scale, the position of individual

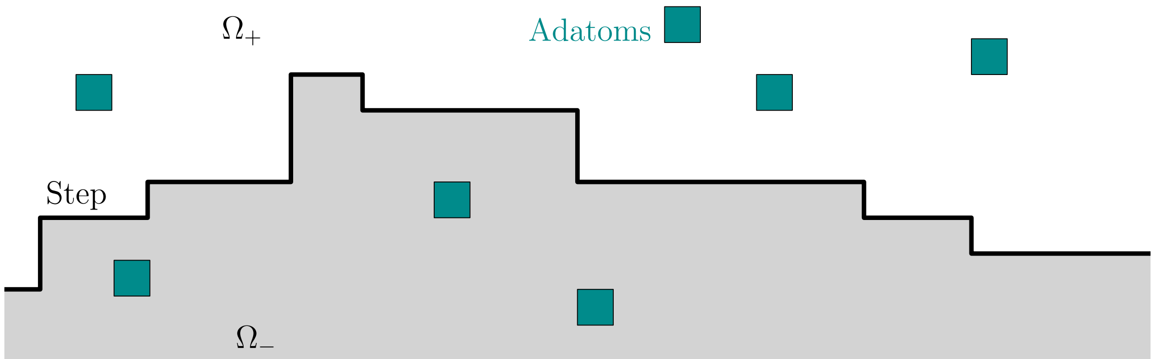

Figure 1.2: Top-down schematic of a step on a vicinal surface separating a lower terrace Ω_+ from an upper terrace Ω_-. The step consists of flat edges separated by kinks.

adatoms may be replaced by a continuous areal adatom number density ϱ, and we may apply the standard continuum mechanical treatment to the system. Given a step separating adjacent terraces, let ϱ^{b} denote the areal density[1] of crystallized adatoms within the monolayer immediately beneath the upper terrace.

We study the following modes of step-flow:

1. relaxation,

2. growth, and

3. growth with desorption.

During relaxation, desorption is negligible and there is no external source of crystalline atoms. Step-flow is, therefore, governed entirely by the diffusion of adatoms and the attachment/detachment process of adatoms to or from a step. We write $\mathbf{h}$ for the diffusive flux, J_+ for the rate of attachment of adatoms to the step from the lower terrace, and J_- for the rate of attachment of adatoms to the step from the upper terrace. Although the crystal surface may change in morphology during relaxation, with no external source of crystalline atoms, the crystal does not grow.

[1] The symbol ϱ^{b} is sometimes defined as the bulk atom volumetric density, and this difference may give rise to factors of a, the atomic diameter.

Indeed, for growth to occur, atoms must be deposited onto the terraces. We treat a model of deposition in which atoms attach uniformly to the terraces. This models molecular beam epitaxy (MBE), for example [3]. Other methods of crystal production may require the coupling of the three-dimensional diffusion process in the bulk of a fluid with the two-dimensional diffusion process of the adatoms; we do not address these here. A growth model incorporates only the processes of adatom diffusion and deposition.

Models with desorption account for the average time, τ, an adatom will diffuse on the vicinal surface before gaining enough energy to detach from the terrace to the vapor due to thermal fluctuations. Since bulk atoms are connected to the crystal by more bonds, the primary source of desorption is the detachment of terrace adatoms. The net rate of attachment and detachment is characterized by the adatom supply per unit area R. Models of growth with desorption include the processes of adatom diffusion, deposition, and desorption. For an extensive review of the literature on the modeling of steps on surfaces, see [5].

1.2 Derivation of the BCF model

Step-flow models track the motion of steps as evolving curves in the plane. Although one might more accurately say "the curve that corresponds to the step," we simply refer to the curve as "the step." We review terminology and basic facts regarding curves and evolving curves in the plane; an extensive discussion may be found in Gurtin [8]. A (plane) *curve* is a set $\mathcal{S}$ and a smooth map $\mathbf{r}$ from a sub-interval of the real line, $I \subset \mathbb{R}$, to $\mathbb{R}^2$ such that: $\mathcal{S}$ is the range of $\mathbf{r}$; $\frac{\mathrm{d}\mathbf{r}(p)}{\mathrm{d}p} \neq 0$ for all $p \in I$; I is either all of $\mathbb{R}$ or a bounded interval $[a, b]$; and if I is $\mathbb{R}$, then either $\mathbf{r}$ is periodic or $|\mathbf{r}(p)| \to \infty$ as $p \to \pm\infty$. A curve with a periodic parameterization is called *closed*. Curves with parameterizations such that $|\mathbf{r}(p)| \to \infty$ as $p \to \pm\infty$ are called *unbounded curves*. A curve is *simple* if it is an unbounded curve with an injective parameterization or if it is a closed curve such that the parameterization is injective on an interval of length equal to the minimal period of $\mathbf{r}$. By the Jordan curve theorem, a simple curve $(\mathcal{S}, \mathbf{r})$ divides the plane into two connected regions with each having boundary equal to $\mathcal{S}$. Because of this, we refer to simple curves as *boundary curves*.

We only consider steps that are simple curves. For a parameterization of a curve $\mathbf{r}$, the unit tangent vector $\mathbf{t} = (T_1, T_2)$ to the curve is defined by

$$\mathbf{t}(p) = \frac{1}{|\mathrm{d}\mathbf{r}/\mathrm{d}p|}\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}p}. \tag{1.2.1}$$

If $\mathbf{r}$ satisfies $\left|\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}p}\right| = 1$, then p is the arclength parameter, which we denote by s, and $\mathbf{r}$ is called an arclength parameterization of the curve. Then the normal vector $\mathbf{n}$ is the vector found upon rotating $\mathbf{t}$ counter-clockwise by $\pi/2$ radians. In particular, $\mathbf{n} = (-T_2, T_1)$. The curvature of a curve is defined by the Frenet formula:

$$\kappa = \frac{\mathrm{d}\mathbf{t}}{\mathrm{d}s} \cdot \mathbf{n}. \tag{1.2.2}$$

For a boundary curve, $\mathcal{S}$, with normal vector $\mathbf{n}$ and a function $u : \mathbb{R}^2 - \mathcal{S} \to \mathbb{R}^m$, we define the one-sided limits at a point on the curve $\mathbf{x}_0 \in \mathcal{S}$ by

$$u^+(\mathbf{x}_0) = \lim_{p\downarrow 0} u(\mathbf{x}_0 + p\mathbf{n}) \text{ and } u^-(\mathbf{x}_0) = \lim_{p\downarrow 0} u(\mathbf{x}_0 - p\mathbf{n}), \tag{1.2.3}$$

provided the limits exist.

An evolving interface, $(\mathcal{S}, \boldsymbol{\alpha})$ is a smooth family of boundary curves, such that for time $T > 0$, the function $\boldsymbol{\alpha}\colon \mathbb{R} \times [0, T) \to \mathbb{R}^2$ satisfies for each $t \in [0, T)$ the mapping $s \mapsto \boldsymbol{\alpha}(s, t)$ is a parameterization of a boundary curve. The normal velocity V of an evolving interface is the function defined by

$$V = \frac{\partial \boldsymbol{\alpha}}{\partial t} \cdot \mathbf{n}. \tag{1.2.4}$$

Evolution equations and jump conditions

We now provide a rational derivation of the Burton–Cabrera–Frank model, in which one must find an adatom density ϱ and a curve $\mathcal{S}$ with normal velocity V such that

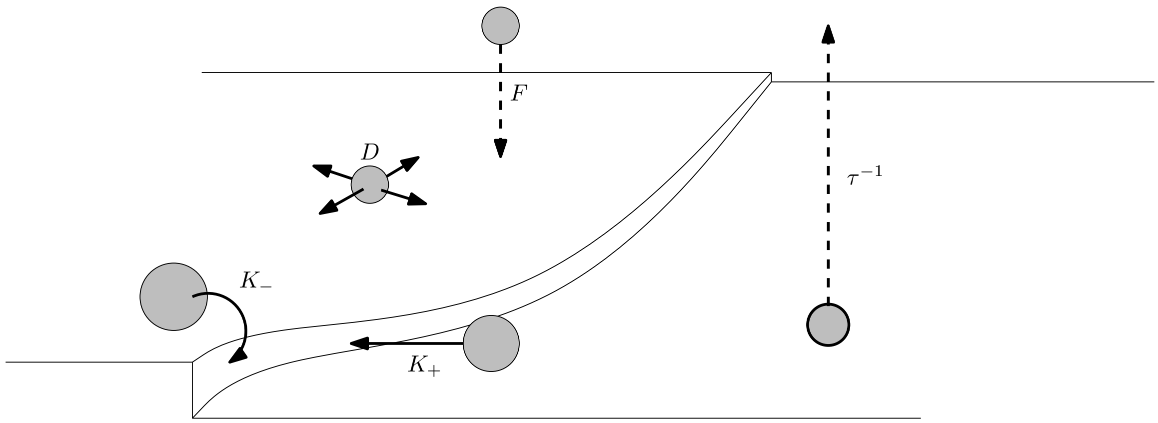

Figure 1.3: Schematic of adatom attachment ($K_\pm$), diffusion (D), desorption (τ^{-1}), and deposition (F).

the adatom density ϱ satisfies the partial differential equation (PDE)

$$\frac{\partial \varrho}{\partial t} = D\Delta\varrho - \tau^{-1}\varrho + F \qquad \text{on } \Omega_+ \cup \Omega_-, \tag{1.2.5}$$

with boundary conditions

$$\left.\begin{aligned} \varrho^+ V + D\nabla\varrho^+ \cdot \mathbf{n} &= K_+\left(\varrho^+ - \varrho_{\text{eq}} + \Gamma\kappa\right) \\ -\varrho^- V - D\nabla\varrho^- \cdot \mathbf{n} &= K_-\left(\varrho^- - \varrho_{\text{eq}} + \Gamma\kappa\right) \end{aligned} \quad \text{along } \mathcal{S}, \right\} \tag{1.2.6}$$

and

$$\varrho^{\text{b}} V = K_+\left(\varrho^+ - \varrho_{\text{eq}} + \Gamma\kappa\right) + K_-\left(\varrho^- - \varrho_{\text{eq}} + \Gamma\kappa\right), \tag{1.2.7}$$

where Ω_+ and Ω_- are time dependent open domains in $\mathbb{R}^2$ corresponding to a lower and upper terrace, respectively, and $\mathcal{S}$ is common boundary between them.

Let $\mathcal{R}$ be a regular subregion of $\Omega_+ \cup \Omega_-$. We denote the boundary of $\mathcal{R}$ by $\partial\mathcal{R}$, the upper and lower boundaries of $\mathcal{R}$ by $\partial\mathcal{R}_\pm = \partial\mathcal{R} \cap \Omega_\pm$, the portion of the step contained in $\mathcal{R}$ by $\Sigma = \mathcal{R} \cap \mathcal{S}$, the outward pointing normal to $\partial\mathcal{R}$ by $\mathbf{n}_{\partial\mathcal{R}}$, and the normal to $\mathcal{S}$ pointing into Ω_+ by $\mathbf{n}$. Recall that J_- is the attachment flux from the upper terrace, J_+ is the attachment flux from the lower terrace, and $\mathbf{h}$ is the diffusive flux of adatoms.

Mass balance in the upper and lower terrace requires that for any regular subregion $\mathcal{R}$ of Ω:

$$\underbrace{\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{R}_\pm} \varrho \,\mathrm{d}A}_{\substack{\text{rate of mass} \\ \text{production in } \mathcal{R}_\pm}} = \underbrace{\int_{\mathcal{R}_\pm} R \,\mathrm{d}A}_{\substack{\text{adsorption-desorption} \\ \text{onto } \mathcal{R}_\pm}} \underbrace{- \int_{\partial\mathcal{R}_\pm} \mathbf{h}\cdot\mathbf{n}_{\partial\mathcal{R}} \,\mathrm{d}s}_{\substack{\text{diffusion} \\ \text{across } \partial\mathcal{R}_\pm}} \underbrace{- \int_\Sigma J_\pm \,\mathrm{d}s}_{\substack{\text{attachment-detachment} \\ \text{from the } \Omega_\pm \text{ side of } \Sigma}} , \tag{1.2.8}$$

Let 1_{Ω_-} denote the characteristic function associated with the upper terrace,

$$1_{\Omega_-}(x) = \begin{cases} 1 & \text{if } x \in \Omega_-, \\ 0 & \text{otherwise.} \end{cases} \tag{1.2.9}$$

Mass balance for the entire region $\mathcal{R}$ requires that

$$\underbrace{\frac{\mathrm{d}}{\mathrm{d}t}\left(\int_{\mathcal{R}} \varrho + \varrho^{\mathrm{b}} 1_{\Omega_-} \,\mathrm{d}A\right)}_{\substack{\text{rate of mass production in } \mathcal{R} \\ \text{including mass absorbed into } \mathcal{R}_-}} = \underbrace{\int_{\mathcal{R}} R \,\mathrm{d}A}_{\substack{\text{adsorption-desorption} \\ \text{onto } \mathcal{R}}} \underbrace{- \int_{\partial\mathcal{R}} \mathbf{h}\cdot\mathbf{n}_{\partial\mathcal{R}} \,\mathrm{d}s}_{\substack{\text{diffusion} \\ \text{across } \partial\mathcal{R}}} . \tag{1.2.10}$$

We localize (1.2.8) away from the step to find that ϱ satisfies the equation

$$\frac{\partial \varrho}{\partial t} = -\operatorname{div}\mathbf{h} + R \qquad \text{in } \Omega_+ \cup \Omega_-. \tag{1.2.11}$$

Further, upon shrinking $\mathcal{R}_\pm \to \Sigma$ so that $\mathrm{vol}(\mathcal{R}_\pm) \to 0$, we find (1.2.8) implies that for any subcurve Σ of $\mathcal{S}$

$$\mp \int_\Sigma \varrho^\pm V \,\mathrm{d}s = \mp \int_\Sigma \mathbf{h}^\pm \cdot \mathbf{n} \,\mathrm{d}s - \int_\Sigma J_\pm \,\mathrm{d}s. \tag{1.2.12}$$

Thus, we deduce the jump condition

$$J_\pm = \pm\left(\varrho^\pm V - \mathbf{h}^\pm \cdot \mathbf{n}\right) \qquad \text{along } \mathcal{S}, \tag{1.2.13}$$

where V is the normal velocity of the step $\mathcal{S}$.

Similarly, shrinking $\mathcal{R} \to \Sigma$, mass balance (1.2.10) implies the jump condition

$$\varrho^{\mathrm{b}} V = [\![\varrho]\!] V - [\![\mathbf{h}]\!] \cdot \mathbf{n} \qquad \text{along } \mathcal{S}. \tag{1.2.14}$$

From (1.2.13) and (1.2.14), it follows that the velocity is proportional to the sum of the adatom fluxes $J_\pm$:

$$\varrho^{\mathrm{b}} V = J_+ + J_-. \tag{1.2.15}$$

Taken together, (1.2.11), (1.2.13), and (1.2.15) imply that the motion of the steps is governed by a moving boundary problem in which the adatom density ϱ solves the problem

$$\frac{\partial \varrho}{\partial t} = -\operatorname{div}\mathbf{h} + R \qquad \text{on } \Omega_+ \cup \Omega_-, \tag{1.2.16}$$

with boundary conditions

$$\left.\begin{aligned} \varrho^+ V - \mathbf{h}^+ \cdot \mathbf{n} &= J_+ \\ -\varrho^- V + \mathbf{h}^- \cdot \mathbf{n} &= J_- \end{aligned} \quad \text{along } \mathcal{S}, \right\} \tag{1.2.17}$$

and the normal velocity V of the step $\mathcal{S}$ is given by

$$\varrho^{\mathrm{b}} V = J_+ + J_-. \tag{1.2.18}$$

Constitutive assumptions

In order to study this problem (1.2.16)-(1.2.18), we must specify constitutive relations for $\mathbf{h}$, $J_\pm$, and R. The first constitutive assumption that we make is Fick's law, which states that the diffusive flux $\mathbf{h}$ is given by

$$\mathbf{h} = -D\nabla\varrho, \tag{1.2.19}$$

where D is a scalar constant. We say that the diffusion is isotropic when D is a scalar, as opposed to when D is a matrix that is not a multiple of the identity matrix, in which case we say the diffusion is anisotropic. Since D is a constant, we say that the diffusion occurs on a homogeneous medium.

The remaining prescription of R depends on the mechanism in which adatoms attach or detach from the terraces. A simple choice of R models uniform deposition of adatoms at a constant rate F, in which a typical adatom evaporates from the terrace after τ units of time. Then R is given by

$$R = F - \tau^{-1}\varrho. \tag{1.2.20}$$

The standard prescription for $J_\pm$ is based on an assumption that the limiting value of ϱ at the step is close to an equilibrium adatom density denoted by $\tilde{\varrho}_{\text{eq}}$. This adatom density corresponds to equilibrium, in the sense that if $\varrho^\pm = \tilde{\varrho}_{\text{eq}}$, then there is no attachment from below/above, i.e., $J_\pm = 0$. Moreover, it is assumed that $J_\pm$ is a function of only the deviation of the adatom density from its equilibrium value, $\varrho^\pm - \tilde{\varrho}_{\text{eq}}$. With these assumptions, it is natural to postulate a linear relation

$$J_\pm = K_\pm(\varrho^\pm - \tilde{\varrho}_{\text{eq}}), \tag{1.2.21}$$

where K_+ and K_- are attachment coefficients from below and from above, respectively. Local equilibrium means $K_\pm \to \infty$, so that $\varrho^\pm = \tilde{\varrho}_{\text{eq}}$.

To close this system one must specify $\tilde{\varrho}_{\text{eq}}$. The equilibrium adatom density is related to the step chemical potential μ^{s} by

$$\tilde{\varrho}_{\text{eq}} = \varrho_{\text{eq}} \exp\left(\frac{\mu^{\text{s}} - \mu_0^{\text{s}}}{k_B T}\right), \tag{1.2.22}$$

where k_B is the Boltzmann constant, T is the constant, homogeneous temperature, and ϱ_{eq} and μ_0^{s} are the equilibrium adatom density and the equilibrium step chemical potential, respectively, for a straight step that is isolated from other steps [3]. Implicit in the use of (1.2.22) is the assumption terrace adatoms behave collectively like a two-dimensional ideal lattice gas.

Let θ denote the step orientation, which may be identified with the angle between the unit normal $\mathbf{n}$ to the step and the x-axis. A step has an associated lineal free energy ψ^{s} which, due to the crystalline structure, is a function of the angle θ. For non-interacting steps, the Gibbs–Thomson relation relates the chemical potential of the step μ^{s} to the geometry of the step in the following way

$$\mu^{\mathrm{s}} - \mu_0^{\mathrm{s}} = -\frac{\kappa\tilde{\psi}^{\mathrm{s}}}{\varrho^{\mathrm{b}}}, \tag{1.2.23}$$

where $\tilde{\psi}^{\mathrm{s}}$ is the step stiffness

$$\tilde{\psi}^{\mathrm{s}} = \psi^{\mathrm{s}} + \frac{\mathrm{d}^2\psi^{\mathrm{s}}}{\mathrm{d}\theta^2}, \tag{1.2.24}$$

and we recall that κ is the curvature of the step (1.2.2).

Remark 1.2.1. *To account for step-step interactions, whether entropic, elastic, or electrostatic, additional terms are included in an ad hoc manner on the right-hand side of (1.2.23). In our treatment of BCF, such interactions are ignored. In Chapter 4, the thermodynamically consistent generalization of BCF supplies a modified Gibbs–Thomson relation, the consequence of which is a step-step interaction of a diffusive nature.*

For small departures from the rectilinear step configuration, the equilibrium adatom density is taken, in the absence of step-step interactions, to be

$$\tilde{\varrho}_{\mathrm{eq}} = \varrho_{\mathrm{eq}}\left(1 + \frac{\mu^{\mathrm{s}} - \mu_0^{\mathrm{s}}}{k_B T}\right) = \varrho_{\mathrm{eq}}\left(1 - \frac{\kappa\tilde{\psi}^{\mathrm{s}}}{\varrho^{\mathrm{b}} k_B T}\right). \tag{1.2.25}$$

We take ψ^{s} to be constant, in which case $\tilde{\psi}^{\mathrm{s}} = \psi^{\mathrm{s}}$ and (1.2.25) may be written as

$$\tilde{\varrho}_{\mathrm{eq}} = \varrho_{\mathrm{eq}} - \Gamma\kappa, \tag{1.2.26}$$

where

$$\Gamma = \frac{\varrho_{\mathrm{eq}}\psi^{\mathrm{s}}}{\varrho^{\mathrm{b}} k_B T}. \tag{1.2.27}$$

Taken together, (1.2.16)-(1.2.21) and (1.2.26) imply that the general BCF model is given by (1.2.5)-(1.2.7), as claimed.

Remark 1.2.2. *In their original work [2], Burton, Cabrera, and Frank do not treat the problem (1.2.16)-(1.2.18). In fact, they treat the steps as perfect sinks for adatoms,* *in which any deviation of $\varrho^{\pm}$ above $\tilde{\varrho}_{eq}$ leads to an immediate attachment to the step. This may be understood as a limiting model taking $K_{\pm} \to \infty$. If the prescription (1.2.21) is to hold as $K_{\pm} \to \infty$, then for a finite limiting attachment rate we must have $\varrho^{\pm} \to \tilde{\varrho}_{eq}$ in the limit. Therefore, using (1.2.14) directly, the model of step motion due to BCF is given by*

$$\frac{\partial \varrho}{\partial t} = D\Delta\varrho - \tau^{-1}\varrho + F \qquad \text{on } \Omega_{+} \cup \Omega_{-}, \tag{1.2.28}$$

with boundary conditions

$$\varrho^{-} = \varrho^{+} = \tilde{\varrho}_{eq} \qquad \text{along } \mathcal{S}, \tag{1.2.29}$$

and normal velocity given by

$$\varrho^{b} V = D[\![\nabla\varrho]\!] \cdot \mathbf{n}. \tag{1.2.30}$$

1.3 The Ehrlich–Schwoebel Effect

Ehrlich and Hudda observed experimentally that the attachment of an adatom from an upper terrace occurs less frequently than from a lower terrace [9]. In terms of the BCF model (1.2.5)-(1.2.7), this means that the kinetic coefficients K_{+} and K_{-} satisfy $K_{-} < K_{+}$. Soon after, Schwoebel and Shipsey [10] provided evidence that during growth conditions such preferential attachment from below leads to stability in the sense that steps perturbed away from uniform spacing return to uniform spacing. We call the assumption that $K_{-} < K_{+}$ a normal Ehrlich–Schwoebel (ES) barrier, and the reverse assumption that $K_{-} > K_{+}$ an inverse Ehrlich–Schwoebel (inverse ES) barrier.

The stability result may be understood intuitively by assuming that the attachment fluxes J_{+} and J_{-} may be approximated by

$$J_{+} = K_{+} j(l) \text{ and } J_{-} = K_{-} j(u), \tag{1.3.1}$$

where j are monotone increasing functions, l is the terrace width of the lower terrace, and u is the terrace width of the upper terrace. Consider a step profile with a narrow terrace of width w surrounded by two wide terraces of width W. Then assuming $K_- < K_+$ the net attachment at the left-most step is less than the net attachment at the right-most step, since

$$K_+ j(w) + K_- j(W) < K_+ j(W) + K_- j(w). \tag{1.3.2}$$

This causes the right-most step to move more quickly than the left-most step, which leads to the narrow terrace to become more broad [4].

1.4 Quasistatic approximation

A further reduction for the BCF problem (1.2.5)-(1.2.7) relies on a quasistatic approximation. The step motion is said to be quasistatic if the diffusive time scale is much shorter than that which characterizes step migration. In this case, we neglect the term $\frac{\partial \varrho}{\partial t}$ in (1.2.5) and the terms $\varrho^{\pm} V$ in (1.2.6). The quasistatic version of the BCF model is given by the PDE

$$D\Delta\varrho - \tau^{-1}\varrho + F = 0 \qquad \text{on } \Omega_+ \cup \Omega_-, \tag{1.4.1}$$

supplemented with boundary conditions

$$\left.\begin{aligned} D\nabla\varrho^+ \cdot \mathbf{n} &= K_+ \left(\varrho^+ - \varrho_{\mathrm{eq}} + \Gamma\kappa\right) \\ -D\nabla\varrho^- \cdot \mathbf{n} &= K_- \left(\varrho^- - \varrho_{\mathrm{eq}} + \Gamma\kappa\right) \end{aligned} \quad \text{along } \mathcal{S}, \right\} \tag{1.4.2}$$

where the normal velocity V must satisfy

$$\varrho^{\mathrm{b}} V = D[\![\nabla\varrho]\!] \cdot \mathbf{n}. \tag{1.4.3}$$

In the remainder, we make this simplifying assumption. We refer to (1.4.1)-(1.4.3) as the BCF, although the complete theory is contained in (1.2.5)-(1.2.7).

1.5 Roadmap for this thesis

In Chapters 1 and 2, we investigate initial configurations that lead to step collisions according to the BCF model (1.4.1)-(1.4.3). In Chapter 2, we consider a model of thin film growth, and in Chapter 3, we treat models of step motions in the growth of a nanowire. In both chapters, we study how the prevalence of step collisions depends on the kinetic coefficients $K_{\pm}$ and for the circular steps of Chapter 3, we consider the dependence on the line tension Γ. In Chapter 4, we reconsider the constitutive assumptions made in the BCF model, and present the generalization developed by Cermelli and Jabbour [11, 12]. This leads us to a thermodynamically consistent model of step-flow, which we call the TC model. In Chapters 5, 6, and 7, we find the continuum limit of the TC model in the context of rectilinear trains of steps in the manner of E and Yip [13] for the BCF model as well as concentric step profiles and profiles consisting of steps with slowly varying curvature in the manner of Margetis and Kohn [14] for the BCF model. In the work done here, a continuum limit is a PDE, or in our case a system of PDE, which governs a time dependent smooth surface called a height profile and a surface chemical potential. This height profile approximates the non-smooth vicinal surface consisting of flat terraces with discrete jumps of atomic height at the steps. In Chapter 8, we summarize the work and briefly state open problems and future directions for this research programme. There are two appendices which contain basic facts about Bessel functions and ordinary differential equations (Appendix A and Appendix B, respectively) that are used in Chapters 2 and 3.

2 Step collisions in the growth of infinite trains of rectilinear steps

2.1 Introduction

In this chapter, we study the stability of infinite trains of straight, parallel steps against step collisions. Since the physics of crystal growth is expected to be dramatically different for a surface with overhanging steps, we disallow such step configurations. If two steps move in such a way that they coincide, we say that there is a step collision.

We consider the quasistatic BCF model during growth (i.e., (1.4.1)-(1.4.3) with $\tau^{-1} = 0$). Schwoebel and Shipsey showed in [10] that for a model of crystal growth closely related to (1.4.1)-(1.4.3), a normal ES barrier ($K_- < K_+$) has asymptotically stable equilibria corresponding to step profiles with equal terrace widths (i.e., equally-spaced steps). We rigourously generalize these findings to two settings: N-terrace periodic step profiles and $l^2(\mathbb{Z};\mathbb{R})$ perturbed terraces.

For N-terrace periodic step profiles, the sequence of terrace widths repeats every Nth terrace. In the normal ES case ($K_- < K_+$), we find a Lyapunov function for each N. We also find that although step motions near uniform spacing tend asymptotically to uniform spacing, when $N \geq 3$ and $K_- > 0$, there are step motions that lead to step collisions. One of the points of emphasis in this chapter is that even though most cases that we consider admit uniform spacing as an asymptotically stable solution, there exist, nonetheless, initial step configurations that lead to step collisions. Indeed, besides the trivial 1-periodic case, only the 2-periodic case and a perfect ES barrier ($K_- = 0$) are such that step motions never lead to a step collision for N-terrace periodic step profiles.

For $l^2(\mathbb{Z};\mathbb{R})$ perturbed terrace, all but a few terraces have terrace width very close to 1. We consider two regimes for the attachment coefficients: symmetric attachment

($K_+ = K_-$) and perfect or perfect inverse ES barrier ($K_- = 0$ or $K_+ = 0$, respectively). For both cases we derive the general solution to the infinite dimensional system of ordinary differential equations. We then specialize and consider the case of a single perturbed terrace, in which the initial step profile has all but one terrace of equal width. In the symmetric attachment case ($K_+ = K_-$), if the perturbed terrace is smaller than the other terraces, then there is no step collision, but if the perturbed terrace is sufficiently wider than the others, then there is a step collision. For a perfect ES barrier ($K_- = 0$), we find there is no step collision in the case of a single perturbed terrace, and for a perfect inverse ES barrier ($K_+ = 0$), we find that any non-zero perturbation leads to a step collision.

Lyapunov functions

Let us recall some basic facts and definitions about autonomous systems of ordinary differential equations (ODE):

$$\dot{y} = f(y) \tag{2.1.1}$$

with $f : \mathbb{R}^n \to \mathbb{R}^n$ a smooth function.

Definition 2.1.1. *An* equilibrium point *of (2.1.1) is a point $y_0 \in \mathbb{R}^n$ such that $f(y_0) = 0$.*

Notice that the function $y(t) = y_0$ is a solution to (2.1.1) for any equilibrium point y_0.

Definition 2.1.2. *An equilibrium point y_0 is* stable *in the sense of Lyapunov if for every $\varepsilon > 0$ there exists a $\delta > 0$ such that when $|y_1 - y_0| < \delta$, the solution of the initial value problem (IVP)*

$$\left.\begin{aligned} \dot{y} &= f(y), \\ y(0) &= y_1 \end{aligned}\right\} \tag{2.1.2}$$

satisfies $|y(t) - y_0| < \varepsilon$ *for all* $t \geq 0$.

Definition 2.1.3. *An equilibrium point* y_0 *is* asymptotically stable *if* y_0 *is a stable equilibrium and there exists an open neighborhood* $\mathcal{O}$ *of* y_0 *such that for any* $y_1 \in \mathcal{O}$, *the solution* y *of (2.1.2) satisfies*

$$\lim_{t\to\infty} y(t) = y_0. \tag{2.1.3}$$

If y_0 is asymptotically stable and $\mathcal{O}$ is an open set as in the above definition, then we say that y_0 is asymptotically stable on $\mathcal{O}$.

Definition 2.1.4. *A function* $\mathrm{V} : \mathbb{R}^n \to \mathbb{R}$ *is a Lyapunov function for the system (2.1.1) and the equilibrium point* $y_0 \in \mathbb{R}^n$, *provided* V *satisfies the following conditions for some domain* $\mathcal{O} \subset \mathbb{R}^n$ *containing* y_0*:*

1. $\mathrm{V}(y) > 0$ *for all* $y \in \mathcal{O} - \{y_0\}$ *and* $\mathrm{V}(y_0) = 0$*;*

2. $\nabla\mathrm{V}(y) \cdot f(y) < 0$ *for all* $y \in \mathcal{O} - \{y_0\}$*; and*

3. *there exists a (possibly infinite) constant* V_0 *such that for any* $y_0 \in \partial\mathcal{O}$ *we have* $\mathrm{V}(y) \to \mathrm{V}_0$ *as* $y \to y_0$.

A Lyapunov function is used to establish the asymptotic stability of solutions within the domain $\mathcal{O}$ by the following theorem [15].

Theorem 2.1.5. *The point* y_0 *is an asymptotically stable equilibrium within* $\mathcal{O}$, *if there exists a Lyapunov function for (2.1.1) on* $\mathcal{O}$.

2.2 Monotone trains of rectilinear steps

Monotone trains of rectilinear steps consist of countably many parallel steps in the plane that are either all step up or all step down (see Fig. 2.1). For such a configuration of steps, the BCF model reduces to a problem with a single spatial dimension.

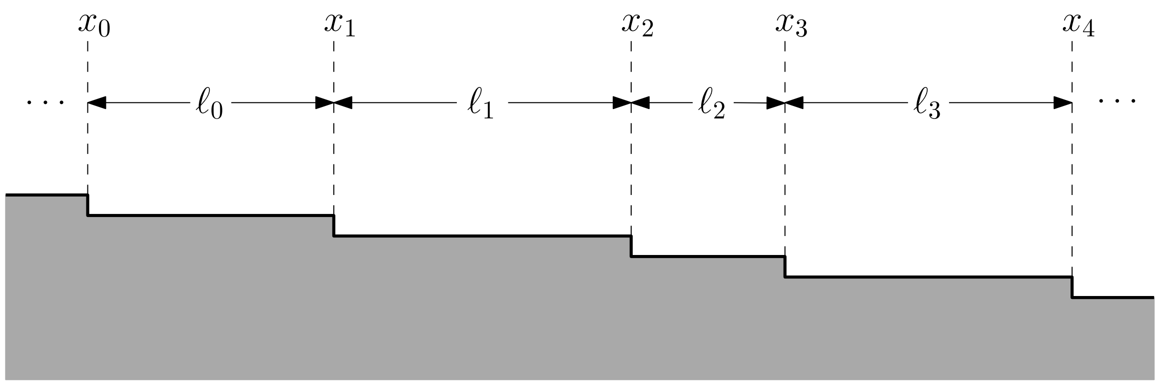

Figure 2.1: Side view of an infinite train of rectilinear steps.

A step $\mathcal{S}(T)$ at time T is specified by its position, $X(T)$, along the X-axis taken normal to the steps. Without loss of generality, we assume that the steps descend from left to right. We consider trains with infinitely many steps (in both directions) or trains consisting of only finitely many steps. Hence, we index the steps $\{\mathcal{S}_i(T)\}_{i\in I}$ by a set I such that $I = \mathbb{Z}$, in the first case, or $I = \{1, 2, \ldots, N\}$, in the second case. The position of $\mathcal{S}_i(T)$ is denoted by $X_i(T)$, and the index is chosen such that $X_i(T) \leq X_{i+1}(T)$.

Consistent with the above assumptions, the notation $u^{\pm}$ has its usual meaning since the limit of u approaching X_i from the lower terrace is

$$u|_{X_i}^{+} = \lim_{\varepsilon\downarrow 0} u(X_i + \varepsilon), \tag{2.2.1}$$

and the limit of u approaching X_i from the upper terrace is

$$u|_{X_i}^{-} = \lim_{\varepsilon\downarrow 0} u(X_i - \varepsilon). \tag{2.2.2}$$

Since the X-axis is normal to the steps, we have that

$$\nabla u \cdot \mathbf{n}^{\pm} = \frac{\mathrm{d}u}{\mathrm{d}X}^{\pm} \text{ and } V_i = \frac{\mathrm{d}X_i}{\mathrm{d}T}, \tag{2.2.3}$$

where V_i is the normal velocity of $\mathcal{S}_i$.

For rectilinear trains of steps, we treat collisions in step motions undergoing growth. Note that for rectilinear steps $\kappa = 0$, and therefore $\tilde{\varrho}_{\mathrm{eq}} = \varrho_{\mathrm{eq}}$. The quasistatic BCF problem (1.4.1)-(1.4.3) treating growth (taking $\tau^{-1} = 0$) reduces to the

ODE:

$$D\frac{\mathrm{d}^2\varrho_i}{\mathrm{d}X^2} + F = 0 \qquad \text{in } (X_i, X_{i+1}), \tag{2.2.4}$$

with boundary conditions

$$\left.\begin{aligned} D\frac{\mathrm{d}\varrho_i}{\mathrm{d}X} &= K_+(\varrho_i - \varrho_{\mathrm{eq}}) \quad \text{at } X = X_i, \\ -D\frac{\mathrm{d}\varrho_i}{\mathrm{d}X} &= K_-(\varrho_i - \varrho_{\mathrm{eq}}) \quad \text{at } X = X_{i+1}, \end{aligned}\right\} \tag{2.2.5}$$

supplemented with the velocity equation:

$$\varrho^{\mathrm{b}}\frac{\mathrm{d}X_i}{\mathrm{d}T} = D\left(\frac{\mathrm{d}\varrho_i}{\mathrm{d}X} - \frac{\mathrm{d}\varrho_{i-1}}{\mathrm{d}X}\right)\bigg|_{X=X_i}. \tag{2.2.6}$$

We make the boundary value problem (2.2.4)-(2.2.5) non-dimensional by choosing a length scale L, e.g., the average terrace width, and defining

$$x = \frac{X}{L},\ x_i = \frac{X_i}{L},\ t = \frac{FT}{2\varrho^{\mathrm{b}}},\ u = \frac{2D(\varrho - \varrho_{\mathrm{eq}})}{FL^2},\ \text{ and } k_\pm = \frac{K_\pm L}{D}. \tag{2.2.7}$$

Then the non-dimensional problem takes the form of the ODE

$$\frac{\mathrm{d}^2 u_i}{\mathrm{d}x^2} = -2 \qquad \text{in } (x_i, x_{i+1}), \tag{2.2.8}$$

with boundary conditions

$$\left.\begin{aligned} \frac{\mathrm{d}u_i}{\mathrm{d}x} &= k_+ u_i \quad \text{at } x = x_i, \\ -\frac{\mathrm{d}u_i}{\mathrm{d}x} &= k_- u_i \quad \text{at } x = x_{i+1}, \end{aligned}\right\} \tag{2.2.9}$$

and, for $\dot{x} := \mathrm{d}x/\mathrm{d}t$,

$$\dot{x}_i = \frac{\mathrm{d}u_i}{\mathrm{d}x} - \frac{\mathrm{d}u_{i-1}}{\mathrm{d}x}\bigg|_{x_i}. \tag{2.2.10}$$

The BVP (2.2.8)-(2.2.9) may be solved explicitly on each terrace (x_i, x_{i+1}). The solution and the velocity equation (2.2.10) combine as a system of ordinary differential equations (ODE) for x_i. Since we are interested in step collisions, we study the terrace widths, ℓ_i, defined by

$$\ell_i = x_{i+1} - x_i, \tag{2.2.11}$$

and, in particular, we consider the deviation of the terrace widths ε_i from unit width, i.e.,

$$\varepsilon_i = \ell_i - 1. \tag{2.2.12}$$

The system of ODE governing ℓ_i is found to be

$$\dot{\ell}_i = \ell_{i+1} - \ell_{i-1} + f(\ell_{i+1}) - 2f(\ell_i) + f(\ell_{i-1}), \tag{2.2.13}$$

where f is defined by

$$f(\ell) = \frac{(k_+ - k_-)\ell}{k_- k_+ \ell + k_- + k_+}. \tag{2.2.14}$$

Correspondingly, the system of ODE governing ε_i is given by

$$\dot{\varepsilon}_i = \varepsilon_{i+1} - \varepsilon_{i-1} + f(1+\varepsilon_{i+1}) - 2f(1+\varepsilon_i) + f(1+\varepsilon_{i-1}). \tag{2.2.15}$$

Remark 2.2.1. *For non-zero $k_\pm$, we may rewrite f in terms of the non-dimensional kinetic lengths*

$$l_\pm = \frac{1}{k_\pm}, \tag{2.2.16}$$

as

$$f(\ell) = \frac{(l_- - l_+)\ell}{\ell + l_- + l_+}. \tag{2.2.17}$$

We now turn to the analysis of these systems of ODE for ℓ_i with various types of normalized initial conditions

$$\{\ell_i(0)\}_{i\in\mathbb{Z}} = \{L_i\}_{i\in\mathbb{Z}}, \tag{2.2.18}$$

such that the mean terrace width is one, viz.:

$$\lim_{n\to\infty} \frac{1}{2n+1} \sum_{i=-n}^{n} L_i = 1. \tag{2.2.19}$$

In particular, we consider periodic initial profiles such that $L_{i+N} = L_i$. We show that periodic terrace step motions have constant mean terrace width, and therefore this serves as an appropriate length scale. Importantly, under these assumptions the infinite dimensional system (2.2.13) is reduced to a finite dimensional system.

We then treat perturbed initial conditions that satisfy

$$L_i = 1 + E_i, \text{ for } i \in \mathbb{Z} \tag{2.2.20}$$

with $E = \{E_i\} \in l^2(\mathbb{Z}; \mathbb{R})$ a square-summable sequence, i.e.,

$$\|E\|_{l^2(\mathbb{Z};\mathbb{R})} = \lim_{n\to\infty} \left(\sum_{i=-n}^{n} |E_i|^2 \right)^{1/2} < \infty. \tag{2.2.21}$$

We generally require that $L_i > 0$. This restricts the admissible E to those for which

$$\inf_{i \in \mathbb{Z}} E_i > -1. \tag{2.2.22}$$

2.3 N-terrace periodic step motions

We consider initial terrace widths $\{L_i\}$ that describe N-terrace periodic step profile. By (2.2.13), we have that the ℓ_i satisfy:

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\left(\sum_{i=1}^{N} \ell_i\right) &= \sum_{i=1}^{N} \dot{\ell}_i \\
&= \sum_{i=2}^{N+1} (\ell_i + f(\ell_i)) + \sum_{j=0}^{N-1} (-\ell_j + f(\ell_j)) - 2\sum_{k=1}^{N} f(\ell_k) \\
&= \ell_N + \ell_{N+1} - \ell_0 - \ell_1 \\
&\quad + f(\ell_N) + f(\ell_{N+1}) + f(\ell_0) + f(\ell_1) - 2f(\ell_1) - 2f(\ell_N) \\
&= 0.
\end{aligned} \tag{2.3.1}$$

Hence, the net width of N consecutive terraces is a constant for N-terrace periodic step profiles. For the average terrace width to be 1, the sum of the terrace widths of N consecutive terraces must be N.

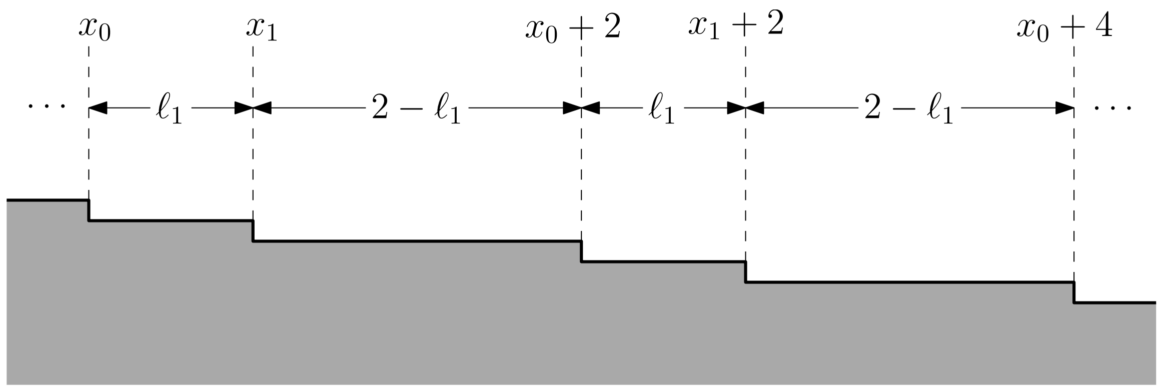

Figure 2.2: Side view of a 2-terrace periodic step profile.

Note that if $N > 2$ and $k_- > 0$, then an initial condition $\ell_3(0) = \cdots = \ell_N(0) = 0$ restricts the values of $\ell_1(0) = N - L$ and $\ell_2(0) = L$ for some $0 < L < N$, and initially, the time derivative of ℓ_3 is given by

$$\begin{aligned} \dot{\ell}_3(0) &= \ell_4(0) - \ell_2(0) + f(\ell_4(0)) - 2f(\ell_3(0)) + f(\ell_2(0)) = f(L) - L \\ &= -\frac{k_- L(2 + k_+)}{k_+ k_- L + k_- + k_-}. \end{aligned} \tag{2.3.2}$$

This is negative for any $k_- > 0$. It follows that if $k_- > 0$ and $N > 2$, then there exist step motions that lead to step collisions.

Step profiles with equally spaced steps, i.e., 1-terrace periodic step profiles, are stationary solutions to the terrace width problem (2.2.13).[1] We start our investigation of N-terrace periodic problems with 2-terrace periodic step motions.

2.4 2-terrace periodic step motions

For 2-terrace periodic step motions, the infinite dimensional system of ODE (2.2.13) reduces to a two dimensional system, for terrace widths ℓ_1 and ℓ_2:

$$\left. \begin{aligned} \dot{\ell}_1 &= 2(f(\ell_2) - f(\ell_1)), \\ \dot{\ell}_2 &= 2(f(\ell_1) - f(\ell_2)). \end{aligned} \right\} \tag{2.4.1}$$

[1]This should not be confused with solutions for which the *steps* are stationary.

Since $\ell_1(t) + \ell_2(t) = 2$ for all t, this system is further reduced to a single ODE. Put $\ell = \ell_1$, and we have that ℓ satisfies:

$$\begin{aligned} \dot{\ell} &= 2(f(2-\ell) - f(\ell)) \\ &= \frac{4(k_+ - k_-)(k_+ + k_-)(1-\ell)}{(k_+ + k_- + k_+k_-(2-\ell))(k_+ + k_- + k_+k_-\ell)}, \end{aligned} \tag{2.4.2}$$

where the terrace widths ℓ_1, ℓ_2 are both positive, if and only if $0 < \ell < 2$. Let $\operatorname{sgn} : \mathbb{R} \to \mathbb{R}$ be defined by

$$\operatorname{sgn}(x) = \begin{cases} 1 & \text{if } x > 0, \\ 0 & \text{if } x = 0, \\ -1 & \text{if } x < 0. \end{cases} \tag{2.4.3}$$

Then a solution ℓ of the problem (2.4.2) for which $0 < \ell < 2$ on its domain satisfies:

$$\operatorname{sgn}(\dot{\ell}) = \operatorname{sgn}(k_+ - k_-)\operatorname{sgn}(1-\ell). \tag{2.4.4}$$

Hence, $\ell \equiv 1$ is an asymptotically stable equilibrium of (2.4.2) if and only if $k_- < k_+$. If there is symmetric attachment, then the problem (2.4.2) reduces to $\dot{\ell} = 0$.

For $k_- > k_+$, the equilibrium $\ell \equiv 1$ is unstable. Indeed, if $\ell(0) > 1$, then $\dot{\ell} > 0$ and if $\ell(0) < 1$, then $\dot{\ell} < 0$. In fact, if $k_- > k_+$, then the map

$$\varphi(w) = 2(f(2-w) - f(w)) \tag{2.4.5}$$

is increasing. This follows from the fact that

$$\frac{\mathrm{d}\varphi(w)}{\mathrm{d}w} = -\frac{4(k_+ - k_-)(k_+ + k_-)((k_+k_- + k_+ + k_-)^2 + (k_+k_-)^2(w-1)^2)}{(k_+ + k_- + k_+k_-w)^2(k_+ + k_- + k_+k_-(2-w))^2}, \tag{2.4.6}$$

and, therefore,

$$\operatorname{sgn}\left(\frac{\mathrm{d}\varphi(w)}{\mathrm{d}w}\right) = \operatorname{sgn}(k_- - k_+). \tag{2.4.7}$$

It follows that if there is an inverse ES barrier, then for any initial terrace width $0 < w < 2$ such that $w \neq 1$, there exists a finite time $T_c > 0$ such that the solution

ℓ of (2.4.2) satisfies $0 < \ell(t) < 2$ for all $0 < t < T_c$ and $\ell(T_c) = 0$ or $\ell(T_c) = 2$, according to whether $w < 1$ or $w > 1$, respectively.

We conclude by summarizing our observations for any initial step width $0 < w < 2$ with $w \neq 1$. Step collisions never occur during 2-terrace periodic step motions for crystals with a normal ES barrier ($k_- < k_+$); moreover, $\ell(t) \to 1$ as $t \to \infty$. For crystals with an inverse ES barrier ($k_- > k_+$), on the other hand, for any initial condition with $\ell(0) \neq 1$ there is a step collision in finite time. If there is symmetric attachment ($k_+ = k_-$), then there are no step collisions, but the step profile does not approach equal spacing asymptotically.

2.5 3-terrace periodic step motions

For 3-terrace periodic step motions, the problem (2.2.13) reduces to the system for terrace widths ℓ_1, ℓ_2, and ℓ_3:

$$\left.\begin{aligned} \dot{\ell}_1 &= \ell_2 - \ell_3 + f(\ell_2) - 2f(\ell_1) + f(\ell_3), \\ \dot{\ell}_2 &= \ell_3 - \ell_1 + f(\ell_3) - 2f(\ell_2) + f(\ell_1), \\ \dot{\ell}_3 &= \ell_1 - \ell_2 + f(\ell_1) - 2f(\ell_3) + f(\ell_2). \end{aligned}\right\} \qquad (2.5.1)$$

As with the 2-terrace periodic system, we may reduce this problem to a system for ℓ_1 and ℓ_2, since $\ell_1(t) + \ell_2(t) + \ell_3(t) = 3$ for all t. The system for 3-terrace periodic step motions is given by

$$\left.\begin{aligned} \dot{\ell}_1 &= -3 + \ell_1 + 2\ell_2 + f(\ell_2) - 2f(\ell_1) + f(3 - \ell_1 - \ell_2), \\ \dot{\ell}_2 &= 3 - 2\ell_1 - \ell_2 + f(3 - \ell_1 - \ell_2) - 2f(\ell_2) + f(\ell_1). \end{aligned}\right\} \qquad (2.5.2)$$

In terms of the deviations $\varepsilon_k = \ell_k - 1$, we have

$$\left.\begin{aligned} \dot{\varepsilon}_1 &= \varepsilon_1 + 2\varepsilon_2 + f(1 + \varepsilon_2) - 2f(1 + \varepsilon_1) + f(1 - \varepsilon_1 - \varepsilon_2), \\ \dot{\varepsilon}_2 &= -2\varepsilon_1 - \varepsilon_2 + f(1 - \varepsilon_1 - \varepsilon_2) - 2f(1 + \varepsilon_2) + f(1 + \varepsilon_1), \end{aligned}\right\} \qquad (2.5.3)$$

where the terrace widths ℓ_1, ℓ_2, and ℓ_3 are positive only for $(\varepsilon_1, \varepsilon_2)$ in the set

$$\mathsf{T}_3 = \{(\varepsilon_1, \varepsilon_2) \in \mathbb{R}^2 \colon -1 < \varepsilon_1 < 2 \text{ and } -1 < \varepsilon_2 < 1 - \varepsilon_1\}. \tag{2.5.4}$$

In Section 2.6, we prove that

$$\mathrm{V}(\varepsilon_1, \varepsilon_2) = \frac{1}{2}\left(\varepsilon_1^2 + \varepsilon_2^2 + (\varepsilon_1 + \varepsilon_2)^2\right) \tag{2.5.5}$$

is a Lyapunov function for the system (2.5.3) for a normal ES barrier ($k_- < k_+$), but we first motivate this choice by studying the step motion with symmetric attachment ($k_- = k_+$).

Symmetric attachment

Suppose that $k_- = k_+$. Then $f(\ell) = 0$, and the system governing ε_i (2.5.3) reduces to the linear system:

$$\left.\begin{aligned} \dot{\varepsilon}_1 &= \quad \varepsilon_1 + 2\varepsilon_2, \\ \dot{\varepsilon}_2 &= \quad -2\varepsilon_1 - \varepsilon_2, \end{aligned}\right\} \tag{2.5.6}$$

which for initial conditions

$$\varepsilon_1(0) = E_1, \varepsilon_2(0) = E_2, \tag{2.5.7}$$

has solution

$$\begin{aligned} \varepsilon_1(t) &= E_1 \cos(\sqrt{3}t) + \frac{\sqrt{3}}{3}(E_1 + 2E_2)\sin(\sqrt{3}t), \\ \varepsilon_2(t) &= E_2 \cos(\sqrt{3}t) - \frac{\sqrt{3}}{3}(2E_1 + E_1)\sin(\sqrt{3}t). \end{aligned} \tag{2.5.8}$$

As seen in Fig. 2.3, the solution curves $(\varepsilon_1(t), \varepsilon_2(t))$ parameterize ellipses defined by

$$\varepsilon_1^2 + \varepsilon_1\varepsilon_2 + \varepsilon_2^2 = E_1^2 + E_1E_2 + E_2^2. \tag{2.5.9}$$

If

$$E_1^2 + E_1E_2 + E_2^2 > \frac{3}{4}, \tag{2.5.10}$$

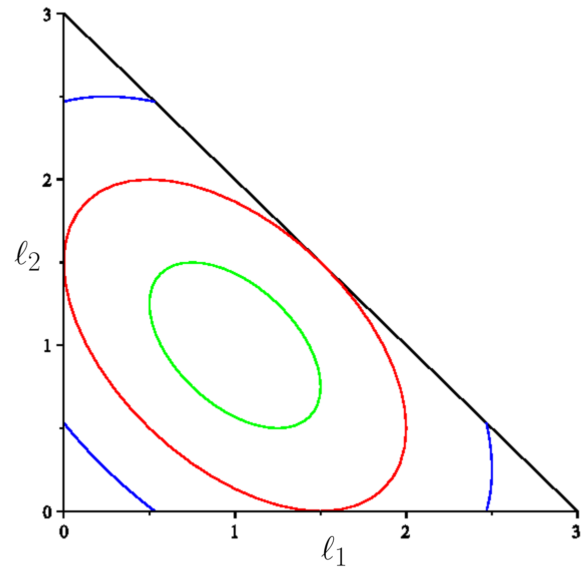

Figure 2.3: Step motions with symmetric attachment in the (ℓ_1, ℓ_2)-plane.

then the solution curve exits the triangle T_3, as defined in (2.5.4). Therefore, initial step deviations that satisfy (2.5.10) lead to step collisions in finite time. This is in contrast to the 2-terrace periodic step motions for which step collisions occur only in the presence of an inverse ES barrier ($k_- > k_+$). Step motions that lead to step collisions are said to be unstable with respect to collisions, and the set of initial conditions that lead to step collisions is called the unstable region, U.

Observe that for $\mathrm{V} : \mathsf{T}_3 \to \mathbb{R}$ defined by

$$\mathrm{V}(\varepsilon_1, \varepsilon_2) := \frac{1}{2}\left(\varepsilon_1^2 + \varepsilon_2^2 + (\varepsilon_1 + \varepsilon_2)^2\right), \tag{2.5.11}$$

we have that along a solution $(\varepsilon_1(t), \varepsilon_2(t))$ of (2.5.6),

$$\frac{\mathrm{d}\left(\mathrm{V}(\varepsilon_1(t), \varepsilon_2(t))\right)}{\mathrm{d}t} = 0. \tag{2.5.12}$$

Normal and inverse Ehrlich–Schwoebel barriers

Suppose now that $k_- \neq k_+$. Then for a solution $(\varepsilon_1, \varepsilon_2)$ of (2.5.3), we find that

$$\begin{aligned}\dot{\mathrm{V}}(\varepsilon_1,\varepsilon_2) &= \varepsilon_1\dot{\varepsilon}_1 + \varepsilon_2\dot{\varepsilon}_2 + (\varepsilon_1+\varepsilon_2)(\dot{\varepsilon}_1+\dot{\varepsilon}_2) \\ &= 3\varepsilon_1\left(f(1-\varepsilon_1-\varepsilon_2) - f(1+\varepsilon_1)\right) \\ &\quad + 3\varepsilon_2\left(f(1-\varepsilon_1-\varepsilon_2) - f(1+\varepsilon_2)\right) \\ &= \frac{3(k_-^2-k_+^2)\left[2(k_++k_-)P_1(\varepsilon_1,\varepsilon_2) + k_+k_-P_2(\varepsilon_1,\varepsilon_2)\right]}{Q(\varepsilon_1)Q(\varepsilon_2)Q(-\varepsilon_1-\varepsilon_2)},\end{aligned} \tag{2.5.13}$$

where P_1, P_2, and Q are defined by

$$\left.\begin{aligned} P_1(x,y) &= \tfrac{3}{4}(x+y)^2 + \tfrac{1}{4}(y-x)^2, \\ P_2(x,y) &= \tfrac{(1+x)(x+2y)^2}{3} + \tfrac{(1+y)(2x+y)^2}{3} + \tfrac{(1-x-y)(x-y)^2}{3}, \\ Q(x) &= k_+ + k_- + k_+k_-(1+x). \end{aligned}\right\} \tag{2.5.14}$$

It is clear as written that $\mathrm{sgn}(\dot{\mathrm{V}}(\varepsilon_1,\varepsilon_2)) = \mathrm{sgn}(k_- - k_+)$ on $\mathsf{T}_3 - \{(0,0)\}$ and V is positive definite. Therefore, by Theorem 2.1.5, we have that $(E_1, E_2) = (0,0)$ is an asymptotically stable equilibrium for the system (2.5.3) if and only if $k_- < k_+$. This calculation also provides a simple demonstration that for $k_- \neq k_+$ the only equilibrium point in T_3 is $(0,0)$. [2]

We have seen previously that if $k_- = k_+$, then the point $(E_1, E_2) = (0,0)$ is a stable equilibrium, but not asymptotically. If $k_- > k_+$, then the equilibrium point $(E_1, E_2) = (0,0)$ is unstable. In fact, we have that any initial step deviation $(E_1, E_2) \in \mathsf{T}_3 - \{(0,0)\}$ leads to step collision for $k_- > k_+$. It remains to describe the set of initial step deviations, $U \subset \mathsf{T}_3$ that lead to step collisions for $k_- < k_+$.

Since we expect the system governing the terrace widths (2.2.13) to be invariant under shift of index, it is natural that the system (2.5.1) is invariant with respect to the transformation $(\ell_1, \ell_2, \ell_3) \mapsto (\ell_3, \ell_1, \ell_2)$. Since $\ell_3 = 3 - \ell_1 - \ell_2$, the system (2.5.2) is invariant with respect to the transformation $(\ell_1, \ell_2) \mapsto (3 - \ell_1 - \ell_2, \ell_1)$.

[2] Otherwise, the equilibrium point (E_1, E_2) must satisfy $\dot{\mathrm{V}}(E_1, E_2) = 0$.

Theorem 2.5.1. *The system (2.5.3) is invariant with respect to the transformation* $(\varepsilon_1, \varepsilon_2) \mapsto (-\varepsilon_1 - \varepsilon_2, \varepsilon_1)$*. Moreover, the triangle* T_3 *is invariant under this transformation.*

Proof. Let a solution $(\varepsilon_1, \varepsilon_2)$ of (2.5.3) be given, and let (η_1, η_2) be defined by

$$\eta_1 = -\varepsilon_1 - \varepsilon_2 \text{ and } \eta_2 = \varepsilon_1. \tag{2.5.15}$$

Then, by (2.5.3), we have

$$\begin{aligned} \dot{\eta}_1 =& -\dot{\varepsilon}_1 - \dot{\varepsilon}_2 \\ &= \varepsilon_1 - \varepsilon_2 + f(1+\varepsilon_2) + f(1+\varepsilon_1) - 2f(1-\varepsilon_1-\varepsilon_2) \\ &= \eta_1 + 2\eta_2 + f(1-\eta_1-\eta_2) - 2f(1+\eta_2) + f(1+\eta_2), \end{aligned} \tag{2.5.16}$$

and

$$\begin{aligned} \dot{\eta}_2 =& \dot{\varepsilon}_1 \\ &= \varepsilon_1 + 2\varepsilon_2 + f(1+\varepsilon_2) - 2f(1+\varepsilon_1) + f(1-\varepsilon_1-\varepsilon_2) \\ &= -2\eta_1 - \eta_2 + f(1-\eta_1-\eta_2) - 2f(1+\eta_2) + f(1-\eta_1). \end{aligned} \tag{2.5.17}$$

Thus, (η_1, η_2) is a solution to (2.5.3).

We now show that the triangle T_3 is invariant under the transformation $(\eta_1, \eta_2) \mapsto (-\varepsilon_1 - \varepsilon_2, \varepsilon_1)$. To see this, note that for $(\varepsilon_1, \varepsilon_2) \in \mathsf{T}_3$, we have

$$\begin{aligned} \eta_1 =& -\varepsilon_1 - \varepsilon_2 < 2, \\ \eta_1 =& -\varepsilon_1 - \varepsilon_2 > -\varepsilon_1 - 1 + \varepsilon_1 = -1, \\ \eta_2 =& \varepsilon_1 > -1, \end{aligned}$$

and since $1 + \varepsilon_2 > 0$, we have that

$$\eta_2 = \varepsilon_1 < 1 + \varepsilon_1 + \varepsilon_2 = 1 - \eta_1.$$

This completes our proof. □

Notice that the right-hand side of the step deviation problem (2.5.3) is smooth in T_3. Let $\mathbf{N}$ denote the outward pointing normal vector to the boundary of T_3. It suffices to find the points along the boundary of T_3 at which $(\dot{\varepsilon}_1, \dot{\varepsilon}_2) \cdot \mathbf{N} > 0$, to find the solution trajectories that exit T_3. In fact, by Theorem 2.5.1, it is sufficient to investigate the behavior of trajectories for the system (2.5.3) along a particular edge of T_3 to characterize the set of trajectories that exit T_3.

Consider the system (2.5.3) along $\{(\varepsilon_1, \varepsilon_2)\colon \varepsilon_1 = -1 \text{ and } -1 < \varepsilon_2 < 2\}$. Let $\mathbf{v} = (v_1, v_2)$ denote the vector field associated with the system (2.5.3),

$$\left.\begin{aligned} v_1(\varepsilon_1, \varepsilon_2) = &\quad \varepsilon_1 + 2\varepsilon_2 + f(1+\varepsilon_2) - 2f(1+\varepsilon_1) + f(1-\varepsilon_1-\varepsilon_2), \\ v_2(\varepsilon_1, \varepsilon_2) = &\quad -2\varepsilon_1 - \varepsilon_2 + f(1-\varepsilon_1-\varepsilon_2) - 2f(1+\varepsilon_2) + f(1+\varepsilon_1). \end{aligned}\right\} \tag{2.5.18}$$

The curve that forms the part of the boundary between the stable region and the unstable region is called a separatrix. The separatrix is also a solution to (2.5.3).

Theorem 2.5.2. *If $0 < k_- < k_+$, then there exists a unique $-1 < \varepsilon_s < 2$ such that*

$$\operatorname{sgn}\left(\mathbf{v}(-1, \varepsilon) \cdot (-1, 0)\right) = \operatorname{sgn}(\varepsilon_s - \varepsilon). \tag{2.5.19}$$

It follows that there is a unique separatrix with trajectory $(\varepsilon_1, \varepsilon_2)$ tangent to T_3 at the point $(\varepsilon_1, \varepsilon_2) = (-1, \varepsilon_s)$.

Proof. By (2.5.18),

$$\begin{aligned} \mathbf{v}(-1, \varepsilon) \cdot (-1, 0) &= -v_1(-1, \varepsilon) \\ &= 1 - 2\varepsilon - f(1+\varepsilon) - f(2-\varepsilon). \end{aligned} \tag{2.5.20}$$

Let $g : [-1, 2] \to \mathbb{R}$ be defined by

$$g(\varepsilon) = 1 - 2\varepsilon - f(1+\varepsilon) - f(2-\varepsilon). \tag{2.5.21}$$

Observe that since $k_- > 0$

$$\left.\begin{aligned} g(-1) = &\quad 3 - f(3) = \tfrac{3(3k_-k_+ + 2k_-)}{3k_+k_- + k_+ + k_-} > 0, \\ g(2) = &\quad -3 - f(3) = -\tfrac{3(3k_-k_+ + 2k_+)}{3k_+k_- + k_+ + k_-} < 0. \end{aligned}\right\} \tag{2.5.22}$$

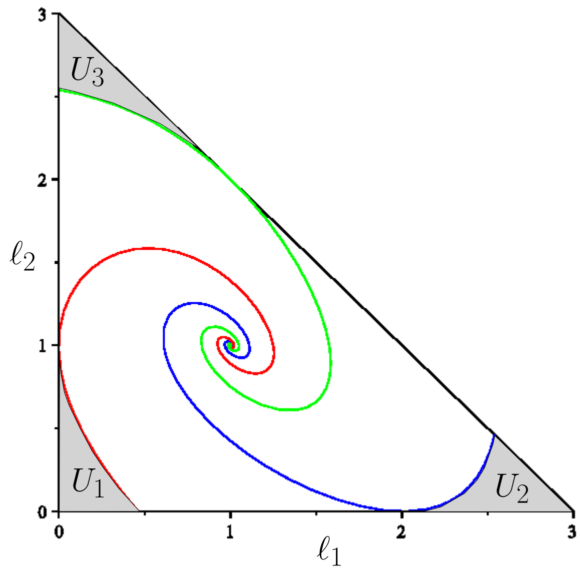

Figure 2.4: The separatrices for a 3-terrace periodic train with a normal Ehrlich–Schwoebel barrier, which divide the region of admissible step widths into four regions: the stable region and U_1, U_2, U_3 forming parts of the unstable region.

Moreover,

$$g'(\varepsilon) = -2 - \frac{k_+k_-(k_+ - k_-)(k_+ + k_-)(2(k_- + k_+) + 3k_+k_-)(1-2\varepsilon)}{(k_+k_-(1+\varepsilon) + k_+ + k_-)^2(k_+k_-(2-\varepsilon) + k_+ + k_-)^2}. \qquad (2.5.23)$$

Since $k_+ - k_- > 0$, $g'(\varepsilon) < 0$ for $-1 < \varepsilon < \frac{1}{2}$. Thus, there is at least one root of $g(\varepsilon)$ in the interval $(-1, 2)$, and there is at most one root in the interval $(-1, 1/2)$. To complete our proof, we note that for $\varepsilon \in (1/2, 2)$, we have that

$$g(\varepsilon) = 1 - 2\varepsilon - f(1+\varepsilon) - f(2-\varepsilon) < -f(1+\varepsilon) - f(2-\varepsilon) < 0, \qquad (2.5.24)$$

since $f(\ell) > 0$ for any $\ell > 0$ as is clear from the definition (2.2.14) of f. Taken together, we have that there is exactly one root ε_s of $g(\varepsilon)$ in the interval $(-1, 2)$. Moreover, $-1 < \varepsilon_s < \frac{1}{2}$, and $g(\varepsilon) > 0$ for all $0 < \varepsilon < \varepsilon_s$ and $g(\varepsilon) < 0$ for all $\varepsilon_s < \varepsilon < 2$. □

We end this section by showing a typical plot of these separatrices in the (ℓ_1, ℓ_2)-plane in Fig. 2.4.

2.6 N-terrace periodic step motions, revisited

We return to our discussion of N-terrace periodic step motions to establish the existence of a Lyapunov function for the system governing the deviations ε_i:

$$\dot{\varepsilon}_i = \varepsilon_{i+1} - \varepsilon_{i-1} + f(\varepsilon_{i+1}+1) - 2f(\varepsilon_i+1) + f(\varepsilon_{i-1}+1). \tag{2.6.1}$$

For each N, let V_N be defined by

$$\mathrm{V}_N(\{\varepsilon_i\}_{i=1}^N) = \frac{1}{2}\sum_{i=1}^N \varepsilon_i^2. \tag{2.6.2}$$

For the sake of notational convenience, given a set $\{a_i\}_{i=1}^N$, define $a_{i-N} = a_{i+N} = a_i$ for each $i \in \{1, 2, \ldots, N\}$.

Theorem 2.6.1. *The positive definite function* V_N *is a Lyapunov function for the system (2.2.15) for* N*-terrace periodic step motions assuming a normal ES barrier.*

Proof. Note that $\mathrm{V}_N(\{\varepsilon_i\}) \geq 0$, with $\mathrm{V}_N(\{\varepsilon_i\}) = 0$ if and only if $\varepsilon_i = 0$ for all $i = 1, 2, \ldots, N$.

In terms of the terrace widths $\ell_i = 1 + \varepsilon_i$, we have that

$$\mathrm{V}_N(\{\varepsilon_i\}_{i=1}^N) = \frac{1}{2}\sum_{i=1}^N(\ell_i - 1)^2 = \frac{1}{2}\sum_{i=1}^N \ell_i^2 - \sum_{i=1}^N \ell_i + \frac{N}{2}. \tag{2.6.3}$$

Therefore, since we have established that the net terrace width is constant, we have that

$$\begin{aligned}
\dot{\mathrm{V}}_N &= \frac{1}{2}\sum_{i=1}^N \frac{\mathrm{d}}{\mathrm{d}t}\left(\ell_i^2\right) \\
&= \sum_{i=1}^N \ell_i\dot{\ell}_i \\
&= \sum_{i=1}^N \ell_i(\ell_{i+1} - \ell_{i-1}) + \sum_{i=1}^N \ell_i\left(f(\ell_{i+1}) - 2f(\ell_i) + f(\ell_{i-1})\right) \qquad (2.6.4)\\
&= \sum_{i=1}^N \ell_{i+1}\ell_i - \sum_{i=1}^N \ell_{i+1}\ell_i + \sum_{i=1}^N \ell_i\left(f(\ell_{i+1}) - 2f(\ell_i) + f(\ell_{i-1})\right) \\
&= \sum_{i=1}^N \ell_i\left(f(\ell_{i+1}) - 2f(\ell_i) + f(\ell_{i-1})\right),
\end{aligned}$$

where we have applied the periodicity of the terrace widths. Define the constants ϖ^k, σ^k, and δ^k by

$$\varpi^k = k_+ k_-, \; \sigma^k = k_+ + k_-, \; \text{ and } \delta^k = k_+ - k_-. \tag{2.6.5}$$

Then

$$f(\ell) = \frac{\delta^k \ell}{\varpi^k \ell + \sigma^k}. \tag{2.6.6}$$

Hence,

$$\dot{\mathrm{V}}_N = \sum_{i=1}^{N} \frac{\delta^k \wp_{i-1,i,i+1} \ell_i}{\wp} \left[h(\ell_{i+1}, \ell_{i-1}, \ell_i) - 2h(\ell_i, \ell_{i+1}, \ell_{i-1}) \; + h(\ell_{i-1}, \ell_i, \ell_{i+1}) \right], \tag{2.6.7}$$

where

$$\begin{aligned} h(x, y, z) =& x(\varpi^k y + \sigma^k)(\varpi^k z + \sigma^k), \\ \wp_{i-1,i,i+1} =& \prod_{\substack{j=1,2,\ldots,N \\ j \neq i-1, i, \text{ or } i+1}} (\varpi^k \ell_j + \sigma^k), \\ \wp =& \prod_{j=1}^{N} (\varpi^k \ell_j + \sigma^k). \end{aligned} \tag{2.6.8}$$

Note that

$$\begin{aligned} & h(z, x, y) - 2h(y, z, x) + h(x, y, z) \\ & \qquad = (z - y)(\sigma^k + \varpi^k x) + (x - y)(\sigma^k + \varpi^k z). \end{aligned} \tag{2.6.9}$$

Therefore,

$$\begin{aligned} \dot{\mathrm{V}}_N =& \frac{\delta^k}{\wp} \left(\sum_{i=1}^{N} \wp_{i-1,i,i+1} \ell_i (\ell_{i+1} - \ell_i)(\sigma^k + \varpi^k \ell_{i-1}) \right. \\ & \left. + \sum_{i=1}^{N} \wp_{i-1,i,i+1} \ell_i (\ell_{i-1} - \ell_i)(\sigma^k + \varpi^k \ell_{i+1}) \right) \\ =& \frac{\delta^k}{\wp} \left(\sum_{i=1}^{N} \wp_{i,i+1} \ell_i (\ell_{i+1} - \ell_i) - \sum_{i=1}^{N} \wp_{i-1,i} \ell_i (\ell_i - \ell_{i-1}) \right), \end{aligned} \tag{2.6.10}$$

where

$$\wp_{i,i+1} = \prod_{\substack{j=1,2,\ldots,N \\ j\neq i \text{ or } i+1}} (\varpi^k \ell_j + \sigma^k). \tag{2.6.11}$$

By N-terrace periodicity, we have that

$$\dot{\mathrm{V}}_N = -\frac{\delta^k}{\wp}\left(\sum_{i=1}^{N} \wp_{i,i+1}(\ell_{i+1}-\ell_i)^2\right) < 0, \tag{2.6.12}$$

provided that $\delta^k > 0$, as assumed, and $\varpi^k \ell_i + \sigma^k > 0$. The latter inequality follows trivially from $\ell_i > 0$ and $k_\pm \geq 0$ with $k_+ \neq 0$ or $k_- \neq 0$. □

2.7 Step motions for $l^2(\mathbb{Z};\mathbb{R})$ perturbed terraces with symmetric attachment

We say that a step profile has $l^2(\mathbb{Z};\mathbb{R})$ perturbed terraces if the terrace deviations $\{\varepsilon_i\}_{i\in\mathbb{Z}}$ are in $l^2(\mathbb{Z};\mathbb{R})$. Assume that there is symmetric attachment, i.e., take $k_- = k_+$. Then for f as defined in (2.2.14), $f(\ell) = 0$. Let $\Phi : l^2(\mathbb{Z};\mathbb{R}) \to l^2(\mathbb{Z};\mathbb{R})$ be defined by

$$\Phi(\{\varepsilon_k\}_{k\in\mathbb{Z}}) = \{\varepsilon_{k+1} - \varepsilon_{k-1}\}_{k\in\mathbb{Z}}. \tag{2.7.1}$$

Then system of ODE (2.2.15) with symmetric attachment may be reframed as an initial value problem for a function taking values in $l^2(\mathbb{Z};\mathbb{R})$ and may be written as

$$\left.\begin{aligned} \frac{\mathrm{d}\varepsilon}{\mathrm{d}t} &= \Phi(\varepsilon), \\ \varepsilon(0) &= E, \end{aligned}\right\} \tag{2.7.2}$$

where $E \in l^2(\mathbb{Z};\mathbb{R})$. The purpose of this section is to derive the general solution of this IVP. In the next section we specialize to the case in which E consists of zeroes in all but one entry.

Schwoebel and Schipsey derive the solution of (2.7.2) by finding the Taylor series for each ε_i. We present a different method for finding the solution of (2.7.2) as an alternative to the approach of Schwoebel and Schipsey [10]. It is a formal calculation, in that we do not concern ourselves with convergence or the validity of the term-wise differentiation or integration and arrive at functions $\{\varepsilon_i\}_{i\in\mathbb{Z}}$. Once we have the proposed solutions, we verify that they indeed solve the problem (2.7.2).

Since for each time $t \geq 0$ the terrace deviations $\varepsilon(t)$ is in $l^2(\mathbb{Z};\mathbb{R})$, we may view them as coefficients for a Fourier series of a function $U(t) \in L^2(0, 2\pi)$. Specifically, let $U : \mathbb{R} \times [0, \infty) \to \mathbb{C}$ be defined by

$$U(x,t) = \sum_{k=-\infty}^{\infty} \varepsilon_k(t)e^{ikx}, \tag{2.7.3}$$

for an $l^2(\mathbb{Z};\mathbb{R})$ solution $\varepsilon = \{\varepsilon_k\}_{k\in\mathbb{Z}}$ to (2.7.2). Then differentiating term-wise, we find that U satisfies

$$\begin{aligned} \frac{\partial U(x,t)}{\partial t} &= \sum_{k=-\infty}^{\infty} \dot{\varepsilon}_k(t)e^{ikx} \\ &= \sum_{k=-\infty}^{\infty} \varepsilon_{k+1}(t)e^{ikx} - \sum_{k=-\infty}^{\infty} \varepsilon_{k-1}(t)e^{ikx} \\ &= -(e^{ix} - e^{-ix})U(x,t) \\ &= -2i\sin(x)U(x,t), \end{aligned} \tag{2.7.4}$$

and with initial value

$$U(x,0) = U_0(x) = \sum_{k=-\infty}^{\infty} E_k e^{ikx}. \tag{2.7.5}$$

From (2.7.4) and (2.7.5), we have that

$$U(x,t) = U_0(x)e^{-2i\sin(x)t}. \tag{2.7.6}$$

The Fourier coefficients of $U(t)$ are given by

$$\varepsilon_n(t) = \frac{1}{2\pi}\int_0^{2\pi} \sum_{k=-\infty}^{\infty} E_k e^{i((k-n)x-2\sin(x)t)}\,\mathrm{d}x. \tag{2.7.7}$$

It follows that [3]

$$\begin{aligned}\varepsilon_n(t) &= \sum_{k=-\infty}^{\infty} E_k \left(\frac{1}{2\pi} \int_0^{2\pi} e^{-i((n-k)x-(-2t)\sin(x))}\, \mathrm{d}x \right) \\ &= \sum_{k=-\infty}^{\infty} E_k J_{n-k}(-2t) \\ &= E_n J_0(2t) + \sum_{k=1}^{\infty} (E_{n+k} + (-1)^k E_{n-k}) J_k(2t),\end{aligned} \tag{2.7.8}$$

where $J_n(x)$ is the Bessel function of the first kind of order n. We have used the properties of Bessel functions [17]:

$$J_{-n}(x) = (-1)^n J_n(x), \quad J_n(-x) = (-1)^n J_n(x), \tag{2.7.9}$$

and the integral representation of J_n:

$$J_n(z) = \frac{1}{2\pi} \int_0^{2\pi} e^{in\theta + iz\sin\theta}\, \mathrm{d}\theta. \tag{2.7.10}$$

We now verify that $\{\varepsilon_n\}$ as defined in (2.7.8) solves (2.7.2) by proving uniform and absolute convergence of the series in (2.7.8). Indeed, uniform convergence allows us to differentiate the series for $\varepsilon_i(t)$ in (2.7.8) term-wise and the absolute convergence allows us to rearrange as necessary, and we find

$$\begin{aligned}\dot{\varepsilon}_n(t) &= \sum_{k=-\infty}^{\infty} -2E_k J'_{n-k}(-2t) \\ &= \sum_{k=-\infty}^{\infty} E_k (J_{n+1-k}(-2t) - J_{n-1-k}(-2t)) \\ &= \sum_{k=-\infty}^{\infty} E_k J_{n+1-k}(-2t) - \sum_{k=-\infty}^{\infty} E_k J_{n-1-k}(-2t) \\ &= \varepsilon_{n+1}(t) - \varepsilon_{n-1}(t).\end{aligned} \tag{2.7.11}$$

Moreover, since $J_0(0) = 1$ and $J_n(0) = 0$ for $n > 0$, we have that $\varepsilon_n(0) = E_n$.

[3] Series representation (2.7.8) of ε_n, i.e., a series of the form $\sum_{k=0}^{\infty} a_k J_k(t)$, is called a Neumann's expansion. Historically, such series have also been referred to as Neumann series [16], but the latter term has come to mean the generalization of a geometric series for linear operators. Both names honor the mathematician Carl Neumann (1832-1925), and not John von Neumann (1903-1957), as it is often assumed.

Theorem 2.7.1. *For* $\{E_k\}_{k\in\mathbb{Z}} \in l^2(\mathbb{Z};\mathbb{R})$ *and for each* $n \in \mathbb{Z}$ *the series*

$$\varepsilon_n(t) = E_n J_0(2t) + \sum_{k=1}^{\infty}(E_{n+k} + (-1)^k E_{n-k})J_k(2t) \qquad (2.7.12)$$

is absolutely and uniformly convergent.

Proof. Let $n \in \mathbb{Z}$ and $T > 0$ be given. It suffices to prove that the sequence of partial sums

$$w_N(t) = |E_n||J_0(2t)| + \sum_{k=1}^{N} |(E_{n+k} + (-1)^k E_{n-k})||J_k(2t)|, \qquad (2.7.13)$$

is uniformly Cauchy, that is, given any $\eta > 0$ there exists an M such that if $i, j \geq M$, then $|w_j(t) - w_i(t)| < \eta$. For any $i < j$, we have

$$\begin{aligned} |w_j(t) - w_i(t)| &= \left| \sum_{k=i+1}^{j} |E_{n+k} + (-1)^k E_{n-k}||J_k(2t)| \right| \\ &\leq \sum_{k=i+1}^{j} (|E_{n+k}| + |E_{n-k}|)|J_k(2t)| \\ &\leq \left(\sum_{k=i+1}^{j} |J_k(2t)|^2 \right)^{1/2} \\ &\quad \times \left\{ \left(\sum_{k=i+1}^{j} |E_{n+k}|^2 \right)^{1/2} + \left(\sum_{k=i+1}^{j} |E_{n-k}|^2 \right)^{1/2} \right\} \\ &= \left(\sum_{k=i+1}^{j} |J_k(2t)|^2 \right)^{1/2} \\ &\quad \times \left\{ \left(\sum_{k=n+i+1}^{n+j} |E_k|^2 \right)^{1/2} + \left(\sum_{k=n-j}^{n-i-1} |E_k|^2 \right)^{1/2} \right\}, \end{aligned} \qquad (2.7.14)$$

where Hölder's inequality is applied twice. For all $z \in \mathbb{R}$, Bessel functions have the property that (see [16]),

$$J_0(z)^2 + 2\sum_{k=1}^{\infty} J_k(z)^2 = 1. \qquad (2.7.15)$$

Choose $M_1 > 0$ sufficiently large such that

$$\left(\sum_{k=-\infty}^{-M_1} |E_k|^2 + \sum_{k=i}^{M_1} |E_k|^2 \right) < \frac{\eta^2}{2}. \qquad (2.7.16)$$

Let $M = M_1 + |n|$, then, for $M \le i < j$ we have

$$n + i + 1 \ge n + M_1 + |n| + 1 > M_1 + 1,$$
$$n - i - 1 \le n - M_1 - |n| - 1 < -M_1 - 1.$$

Therefore, for such $M \le i < j$:

$$\begin{aligned} |w_j(t) - w_i(t)| &\le \frac{\sqrt{2}}{2}\left(\sum_{k=n+i+1}^{n+j} |E_k|^2\right)^{1/2} + \left(\sum_{k=n-j}^{n-i-1} |E_{n-k}|^2\right)^{1/2} \\ &\le \frac{\sqrt{2}}{2}\left(\sum_{k=M_1+1}^{\infty} |E_k|^2\right)^{1/2} + \left(\sum_{k=-\infty}^{-M_1-1} |E_{n-k}|^2\right)^{1/2} \\ &\le \eta. \end{aligned}$$

This is what we wanted to show. □

2.8 Step motions for a perturbed terrace with symmetric attachment

We now suppose that a single terrace is initially perturbed. That is, we consider the initial value problem:

$$\left.\begin{aligned} \frac{\mathrm{d}\varepsilon}{\mathrm{d}t} &= \Phi(\varepsilon), \\ \varepsilon_0(0) &= E_0, \\ \varepsilon_n(0) &= 0 \qquad \text{if } n \neq 0, \end{aligned}\right\} \tag{2.8.1}$$

where $E_0 \in \mathbb{R}$. This corresponds to an initial step profile in which all but one (namely, the terrace with width ℓ_0) of the terraces have unit length and $\ell_0(0) = 1 + E_0$. Then from (2.7.8) for each $n \in \mathbb{Z}$

$$\varepsilon_n(t) = E_0 J_n(-2t). \tag{2.8.2}$$

A step collision of the nth and $(n+1)$th step occurs at time t, if $\varepsilon_n(t) = -1$. We consider the minimal minimum, m, and the maximal maximum, M, defined by

$$m = \min_{n\in\mathbb{Z}} \min_{x\in[0,\infty)} J_n(-x), \quad M = \max_{n\in\mathbb{Z}} \max_{x\in[0,\infty)} J_n(-x). \tag{2.8.3}$$

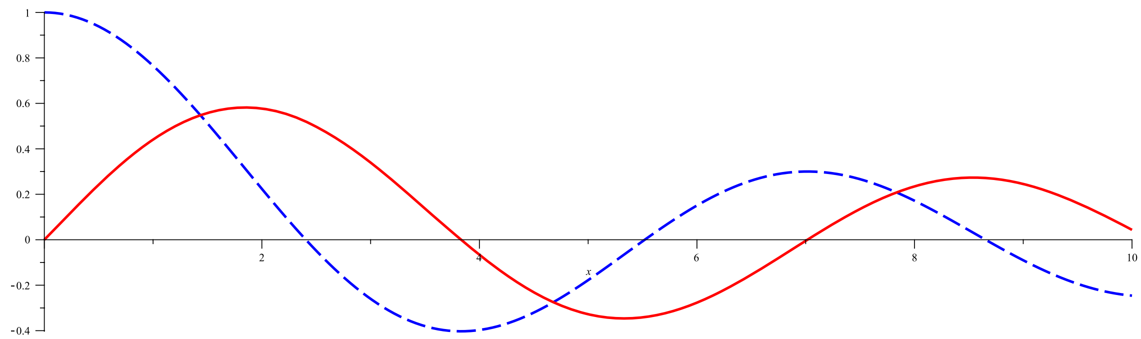

Figure 2.5: Graphs of J_0, the dashed curve, and J_1, the solid curve.

If E_0 is between $\frac{-1}{M}$ and $-\frac{1}{m}$, then there are no step collisions. Otherwise, there are step collisions. Since we assume no overhang in the initial conditions, we consider only $E_0 > -1$. By [18], for $n \geq 0$, the range of $J_n|_{[0,\infty)}$ is given by a closed interval $[a_n, b_n]$ such that the sequence of intervals are nested, i.e.,

$$[a_0, b_0] \subset [a_1, b_1] \subset [a_2, b_2] \subset \cdots, \tag{2.8.4}$$

and the values a_n and b_n are the left-most local minimum and the left-most local maximum of J_n on $[0, \infty)$ (the first few positive extrema of J_0 and J_1 are shown in Fig. 2.5). Since $J_n(-x) = (-1)^n J_n(x)$ and $J_n(x) = (-1)^n J_{-n}(x)$ we have that

$$\begin{aligned} m &= \min_{n\in\mathbb{Z}} \min_{x\in[0,\infty)} (-1)^n J_n(x) \\ &= \min\left(\min_{k\in\mathbb{Z}} \min_{x\in[0,\infty)} J_{2k}(x), -\max_{k\in\mathbb{Z}} \max_{x\in[0,\infty)} J_{2k+1}(x) \right) \\ &= \min\left(\min_{k\in\mathbb{N}} \min_{x\in[0,\infty)} J_{2k}(x), -\max_{k\in\mathbb{N}} \max_{x\in[0,\infty)} J_{2k+1}(x), \min_{k\in\mathbb{N}} \min_{x\in[0,\infty)} J_{2k+1}(x) \right) \\ &= \min\left(\min_{n\in\mathbb{N}} \min_{x\in[0,\infty)} J_n(x), -\max_{k\in\mathbb{N}} \max_{x\in[0,\infty)} J_{2k+1}(x) \right). \end{aligned} \tag{2.8.5}$$

Hence, by (2.8.4)

$$m = \min(a_0, -b_1). \tag{2.8.6}$$

Similarly,

$$M = \max\left(\max_{n\in\mathbb{N}} \max_{x\in[0,\infty)} J_n(x), -\min_{k\in\mathbb{N}} \min_{x\in[0,\infty)} J_{2k+1}(x) \right) = \max(b_0, -a_1). \tag{2.8.7}$$

Since $J_0(0) = 1$, and $|J_n(x)| \leq 1$ for all n, we have that $M = b_0 = 1$. On the other hand, we find numerically that $b_1 \cong 0.581$ and $a_0 \cong -0.403$, and so $m = -b_1$. Therefore, there are no step collisions if and only if $-1 < E_0 < b_1^{-1} \cong 1.72$. In particular, inward perturbations of a single terrace never lead to a step collision, and step collisions only occur if the terrace is outwardly perturbed such that its initial length is nearly three times that of all the others.

2.9 Step motions for $l^2(\mathbb{Z};\mathbb{R})$ perturbed terraces with perfect asymmetric attachment

As in Section 2.7, we find the solution to the system (2.2.15) with $l^2(\mathbb{Z};\mathbb{R})$ initial data and assuming now that either $k_- = 0$ or $k_+ = 0$. We say that the attachment process is a perfect ES barrier or a perfect inverse ES barrier if $k_- = 0$ or $k_+ = 0$, respectively, and we refers to either case as perfect asymmetric attachment. For perfect ES attachment, $f(\ell) = \ell$, and for a perfect inverse ES barrier $f(\ell) = -\ell$. Hence, for a perfect ES barrier, (2.2.15) may be written as

$$\dot{\varepsilon}_k = 2(\varepsilon_{k+1} - \varepsilon_k) \tag{2.9.1}$$

and for a perfect ES barrier, (2.2.15) may be written as

$$\dot{\varepsilon}_k = 2(\varepsilon_k - \varepsilon_{k-1}). \tag{2.9.2}$$

Notice that if $\{\varepsilon_k\}_{k\in\mathbb{Z}}$ is a solution to (2.9.1) then the functions $\{\eta_k\}_{k\in\mathbb{Z}}$ defined by

$$\eta_k(t) = \varepsilon_{-k}(-t) \tag{2.9.3}$$

solve (2.9.2).

Proceeding as before, for a solution $\{\varepsilon_k\}_{k\in\mathbb{Z}}$ of the initial value problem problem (2.9.1) with initial data $\varepsilon_k(0) = E_k$ for $\{E_k\}_{k\in\mathbb{Z}} \in l^2(\mathbb{Z};\mathbb{R})$ we define

$$U(x,t) = \sum_{k=-\infty}^{\infty} \varepsilon_k(t) e^{ikx}. \tag{2.9.4}$$

Then U is the solution to the initial value problem:

$$\left.\begin{aligned} \frac{\partial U}{\partial t}(x,t) = &\quad 2(e^{-ix}-1)U(x,t), \\ U(x,0) = &\quad U_0(x) = \sum_{k=-\infty}^{\infty} E_k e^{ikx}. \end{aligned}\right\} \tag{2.9.5}$$

Hence, U is given by

$$U(x,t) = \sum_{k=-\infty}^{\infty} E_k e^{i(kx-2t\sin(x))+2t(\cos(x)-1)}, \tag{2.9.6}$$

and therefore, ε_n is found to be

$$\begin{aligned} \varepsilon_n(t) &= \frac{1}{2\pi}\int_0^{2\pi} \sum_{k=-\infty}^{\infty} E_k e^{i((k-n)x-2t\sin(x))+2t(\cos(x)-1)}\,\mathrm{d}x \\ &= \sum_{k=-\infty}^{\infty} E_k e^{-2t}\frac{1}{2\pi}\int_0^{2\pi}\left(e^{-ix}\right)^{n-k}\exp(2te^{-ix})\,\mathrm{d}x. \end{aligned} \tag{2.9.7}$$

Let $\mathcal{C} = \{z \in \mathbb{C} : |z| = 1\}$ with positive orientation (i.e., parameterized in the counter-clockwise direction). Note that the each term in the series is the product of $E_k e^{-2t}$ and an expression of the form

$$\begin{aligned} \frac{1}{2\pi}\int_0^{2\pi}(e^{-ix})^{n-k}\exp(2te^{-ix})\,\mathrm{d}x &= \frac{1}{2\pi i}\int_0^{2\pi}(e^{ix})^{n-k-1}\exp(2te^{ix})ie^{ix}\,\mathrm{d}x \\ &= \frac{1}{2\pi i}\int_{\mathcal{C}} z^{n-k-1}e^{2tz}\,\mathrm{d}z. \end{aligned} \tag{2.9.8}$$

By the residue theorem

$$\frac{1}{2\pi i}\int_{\mathcal{C}} z^{n-k-1}e^{2tz}\,\mathrm{d}z = \begin{cases} \frac{(2t)^{k-n}}{(k-n)!} & \text{if } k \geq n \\ 0 & \text{otherwise.} \end{cases} \tag{2.9.9}$$

Hence, we have that for a perfect ES barrier, ε_n is given by

$$\varepsilon_n(t) = \sum_{k=n}^{\infty} E_k e^{-2t}\frac{(2t)^{k-n}}{(k-n)!} = e^{-2t}\sum_{k=0}^{\infty} E_{n+k}\frac{(2t)^k}{k!}. \tag{2.9.10}$$

Moreover, for a perfect inverse ES barrier, ε_n is given by

$$\varepsilon_n(t) = e^{2t}\sum_{k=0}^{\infty}(-1)^k E_{k-n}\frac{(2t)^k}{k!}. \tag{2.9.11}$$

To verify that the functions defined in (2.9.10) solve (2.9.1), we show that for each n the series

$$S(t) = \sum_{k=0}^{\infty} E_{n+k} \frac{(2t)^k}{k!} \tag{2.9.12}$$

is absolutely and uniformly convergent on intervals $[0, T]$ for all $T > 0$.

Theorem 2.9.1. *For all $n \in \mathbb{Z}$, the series (2.9.12) is absolutely and uniformly convergent on intervals $[0, T]$ for all $T > 0$.*

Proof. We use the same method as in the proof of Theorem 2.7.1. Let $n \in \mathbb{Z}$ and $\eta, T > 0$ be given. Let S_i denote the ith partial sum

$$S_i(t) = \sum_{k=0}^{i} |E_{n+k}| \frac{(2t)^k}{k!}. \tag{2.9.13}$$

For any $i < j$, we have for any $t \in [0, T]$

$$\begin{aligned}(S_j(t) - S_i(t))^2 &= \left(\sum_{k=i}^{j} |E_{n+k}| \frac{(2t)^k}{k!} \right)^2 \\ &\leq \left(\sum_{k=i}^{j} |E_{n+k}|^2 \right) \left(\sum_{k=i}^{j} \frac{(2t)^2 k}{(k!)^2} \right) \\ &\leq \|E\|^2_{l^2(\mathbb{Z};\mathbb{R})} \sum_{k=i}^{\infty} \frac{(2T)^{2k}}{k!}.\end{aligned} \tag{2.9.14}$$

Since $e^{4T^2} = \sum_{k=0}^{\infty} \frac{(2T)^{2k}}{k!}$, we may choose an M sufficiently large that

$$\sum_{k=i}^{\infty} \frac{(2T)^{2k}}{k!} < \eta^2 / \|E\|^2_{l^2(\mathbb{Z};\mathbb{R})}, \tag{2.9.15}$$

for $i > M$. Then, we have

$$(S_j(t) - S_i(t))^2 < \eta^2 \text{ or } |S_j(t) - S_i(t)| < \eta, \tag{2.9.16}$$

for all $i, j \geq M$. □

2.10 Step motions for a perturbed terrace with totally asymmetric attachment

As with Section 2.8, we consider the problem of a perturbed terrace, in that the initial data is:

$$\varepsilon_0(0) = E, \text{ and } \varepsilon_n(0) = 0, \text{ for } n \neq 0. \tag{2.10.1}$$

The main result of this section is that for a perfect ES barrier, step collisions do not occur, and for a perfect inverse ES barrier, any deviation from uniform spacing leads to a step collision.

A perfect ES barrier

According to (2.9.10), in the case of a perfect ES barrier the step deviations $\varepsilon_n(t)$ with initial conditions (2.10.1), are given by [4]

$$\varepsilon_n(t) = \begin{cases} Ee^{-2t\frac{(2t)^{-n}}{(-n)!}} & \text{if } n \leq 0 \\ 0 & \text{otherwise.} \end{cases} \tag{2.10.2}$$

Note that for $n \geq 0$, the function p_n defined by

$$p_n(t) = e^{-2t}\frac{(2t)^n}{n!}. \tag{2.10.3}$$

has maximum

$$\max_{t\in[0,\infty)} (p_n(t)) = p_n\left(\frac{n}{2}\right) = \frac{e^{-n}n^n}{n!}. \tag{2.10.4}$$

Put $a_0 = 1$ and $a_n = e^{-n}n^n/n!$ for $n > 0$, then we have that for $n \geq 0$

$$\frac{a_{n+1}}{a_n} = e^{-1}\left(1 + \frac{1}{n}\right)^n = e^{-1}b_n. \tag{2.10.5}$$

[4] The fact that only the terraces with negative index vary in time can be understood intuitively by noting that for a perfect ES barrier (i.e., no attachment from the terrace to the left of the step), a step only "feels" the effect of the terraces to the right.

The sequence b_n is a monotone increasing sequence tending to e. Therefore $e^{-1}b_n < 1$, and it follows that a_n is a monotone decreasing sequence. By Stirling's formula, we have that

$$\lim_{n\to\infty} a_n = \lim_{n\to\infty} \frac{e^{-n}n^n\sqrt{2\pi n}}{n!}\frac{1}{\sqrt{2\pi n}} = \lim_{n\to\infty} \frac{e^{-n}n^n\sqrt{2\pi n}}{n!} \lim_{n\to\infty} \frac{1}{\sqrt{2\pi n}} = 0. \qquad (2.10.6)$$

It follows that in the case of a perfect ES barrier, for any initial terrace deviation $E > -1$, the terrace deviations decay to 0 as $t \to \infty$, with no step collisions.

Perfect inverse ES barrier

According to (2.9.11), in the case of a perfect inverse ES barrier the step deviations $\varepsilon_n(t)$ with initial data (2.10.1) are given by

$$\varepsilon_n(t) = \begin{cases} \frac{Ee^{2t}(-2t)^n}{n!} & \text{if } n \geq 0, \\ 0 & \text{otherwise.} \end{cases} \qquad (2.10.7)$$

For any non-zero initial terrace deviation $E > -1$, there is a minimal time t_c and at least one index N such that $\varepsilon_n(t) > -1$ for all n and $0 \leq t < t_c$ and $\varepsilon_N(t_c) = -1$. In particular, for even indices n, we have

$$\varepsilon_n(t) = \frac{Ee^{2t}(2t)^n}{n!} > 0 \qquad (2.10.8)$$

for all $t \geq 0$, but for odd indices n, we have

$$\varepsilon_n(t) = -\frac{Ee^{2t}(2t)^n}{n!}. \qquad (2.10.9)$$

If $E > 0$ or $E < 0$, then for odd indices $n \in \mathbb{N}$ or even indices $n \in \mathbb{N}$, respectively, the step deviation $\varepsilon_n(t) \searrow -\infty$ as $t \to \infty$. Therefore, for each such index there is a time $t_n \geq 0$ such that $\varepsilon_n(t_n) = -1$. Let

$$a_n = 2t_n, \qquad (2.10.10)$$

then a_n is the unique solution to the equation

$$e^{a_n} {a_n}^n = \frac{n!}{|E|}. \tag{2.10.11}$$

We want to show that

$$\inf_{\substack{n\in\mathbb{N} \\ n \text{ is odd}}} \{a_n/2\} > 0 \text{ and } \inf_{\substack{n\in\mathbb{N} \\ n \text{ is even}}} \{a_n/2\} > 0, \tag{2.10.12}$$

but it suffices to show that for n sufficiently large, the solutions of the relation (2.10.11) are monotone increasing in n. Since the function $\varphi_n = x \mapsto e^x x^n$ is positive and increasing, it suffices to show that the ratio $\varphi_n(a_{n+1})/\varphi_n(a_n) > 1$, for sufficiently large n. From (2.10.11), we have that

$$a_{n+1}\varphi_n(a_{n+1}) = e^{a_{n+1}} {a_{n+1}}^{n+1} = \frac{(n+1)!}{E} = (n+1)\frac{n!}{E} = (n+1)\varphi_n(a_n). \tag{2.10.13}$$

Therefore,

$$\frac{\varphi_n(a_{n+1})}{\varphi_n(a_n)} = \frac{n+1}{a_{n+1}}. \tag{2.10.14}$$

The right hand side is greater than 1 if and only if $a_{n+1} < n+1$. Since $\varphi_n(x)$ is continuous, increasing, and has range containing $[0, \infty)$, the equation $\varphi_n(x_n) = n!/|E|$ has a solution such that $x_n < n$ if and only if $n!/|E| < \varphi_n(n)$. In particular, we require that for sufficiently large n

$$\frac{1}{|E|} < \frac{\varphi_n(n)}{n!} = \frac{e^n n^n}{n!}, \tag{2.10.15}$$

but this follows from the fact that

$$\lim_{n\to\infty} \frac{e^n n^n}{n!} = \infty. \tag{2.10.16}$$

3 Step collisions in nanowire growth

3.1 Introduction

Understanding the causes of step collisions is important in the modeling of growth, due to their potential use in the production nanostructured wires. In Chapter 2, we see that a normal ES barrier is stabilizing against step collisions during growth of an infinite trains of steps. Nonetheless, step collisions do occur in that context for certain initial step profiles. For the growth of a nanowire upon which there is a small number of steps, we find that a normal ES barrier is destabilizing with respect to step collisions.

Golovin, Davis, and Voorhees [19] provide numerical evidence for facts similar to those established in the present chapter. They study a model of crystal growth in which a spherical droplet of a liquid catalyst is set upon a cylindrical nanotube; this requires a vapor-liquid-solid (VLS) model. For such a model there is a coupling of diffusion on the terraces and diffusion through the liquid. Specifically, Golovin et al. treat two concentric steps forming a valley on this circular nanotube and consider a fixed initial outer radius r_2 and choose various initial values of the inner radius r_1. They find that there is a critical radius of r_1 above which step motions lead to step collisions, and below which the inner circle collapses to a point before the outer circle. This critical radius depends on the kinetic coefficients K_+ and K_-, in such a way that increasing the Schwoebel barrier (i.e., increasing K_+ while keeping K_- fixed or decreasing K_- while keeping K_+ fixed) decreases the critical radius, which means that there are more initial step configurations that lead to step collisions.

In the present chapter, we consider the flow of two concentric steps bounded by a reflecting wall, which serves as a model for the growth of a nanowire. For simplicity, we consider standard quasistatic BCF model (1.4.1)-(1.4.3) with a concentric reflecting wall. Our choice to treat the most basic version of the BCF model (1.4.1)-(1.4.3) allows us to clarify in a rigorous fashion the mechanisms responsible for the reversal of stability with respect to step bunching during nanowire growth by VLS as numerically predicted by Golovin et al. Specifically, to illustrate that this phenomenon is not due to the geometry of the steps being circles, we consider first two rectilinear steps bounded by two rectilinear reflecting walls. Moreover, since this dependence of stability on K_+ and K_- occurs even with the quasistatic BCF model, i.e., in the absence of coupling between the stepped top surface of the nanowire and a catalyst liquid phase, it cannot be due to the coupling of diffusion processes in the VLS model. Indeed, this behavior is the result of the presence of the boundaries.

3.2 Rectilinear steps between walls during growth

We use the quasistatic version of the BCF model of growth, with the same boundary conditions and velocity equations at the two rectilinear steps as (1.4.1)-(1.4.3), but we neglect desorption (i.e., $\tau \to \infty$). As before, the fact that the steps and walls are parallel lines allows us to reduce to a problem with one spatial dimension. We consider walls at locations $X = 0$ and $X = L$ and two descending steps with positions X_1 and X_2 between 0 and L with $X_1 < X_2$. The boundary conditions for ϱ at the reflecting walls are

$$\left.\frac{\mathrm{d}\varrho}{\mathrm{d}X}\right|_{X=0}^{+} = \left.\frac{\mathrm{d}\varrho}{\mathrm{d}X}\right|_{X=L}^{-} = 0, \tag{3.2.1}$$

which ensure that there is no adatom source or attachment at the walls. Non-dimensionalizing as in (2.2.7), the step motion is governed by:

$$\frac{\mathrm{d}^2 u}{\mathrm{d}x^2} = -2 \qquad \text{in } (0, x_1) \cup (x_1, x_2) \cup (x_2, 1), \tag{3.2.2}$$

$$\left.\begin{aligned} \frac{\mathrm{d}u^{\pm}}{\mathrm{d}x} &= \pm k_{\pm} u^{\pm} \qquad \text{at } x = x_1 \text{ and } x = x_2, \\ \left.\frac{\mathrm{d}u}{\mathrm{d}x}\right|_{x=0}^{+} &= \left.\frac{\mathrm{d}u}{\mathrm{d}x}\right|_{x=1}^{-} = 0, \end{aligned}\right\} \tag{3.2.3}$$

with the velocities given by:

$$\dot{x}_i = \left[\!\left[\frac{\mathrm{d}u}{\mathrm{d}x} \right]\!\right]_{x=x_i} \qquad \text{for } i = 1, 2. \tag{3.2.4}$$

The system (3.2.2)-(3.2.3) is solved explicitly and the equations for the motion of the steps (3.2.4) take the form

$$\left.\begin{aligned} \dot{x}_1 &= \frac{k_-k_+(x_2+x_1)(x_2-x_1)+2(k_+x_2+k_-x_1)}{k_-k_+(x_2-x_1)+k_-+k_+}, \\ \dot{x}_2 &= \frac{k_-k_+(2-x_2-x_1)(x_2-x_1)+2(k_+(1-x_2)+k_-(1-x_1))}{k_-k_+(x_2-x_1)+k_-+k_+}. \end{aligned}\right\} \tag{3.2.5}$$

To make easier the comparison with the concentric step case treated in the next sections, we write the system (3.2.5) for the distances of the steps from the right-most wall:

$$\ell_1 = 1 - x_2 \text{ and } \ell_2 = 1 - x_1. \tag{3.2.6}$$

The requirement that there are no overhanging steps implies that $x_1 < x_2$, which in turn implies $\ell_1 < \ell_2$. The domain T of admissible (ℓ_1, ℓ_2) is defined by

$$\mathsf{T} = \{(\ell_1, \ell_2) \in \mathbb{R}^2 \colon 0 < \ell_1 < \ell_2 < 1\}. \tag{3.2.7}$$

Then for a given initial step profile $(\Lambda_1, \Lambda_2) \in \mathsf{T}$, the functions ℓ_1 and ℓ_2 satisfy:

$$\left.\begin{aligned} \dot{\ell}_1 &= -\frac{k_-k_+(\ell_2+\ell_1)(\ell_2-\ell_1)+2(k_-\ell_2+k_+\ell_1)}{k_-k_+(\ell_2-\ell_1)+k_-+k_+}, \\ \dot{\ell}_2 &= -\frac{k_-k_+(2-\ell_1-\ell_2)(\ell_2-\ell_1)+2(k_-(1-\ell_2)+k_+(1-\ell_1))}{k_-k_+(\ell_2-\ell_1)+k_-+k_+}, \\ \ell_1(0) &= \Lambda_1 \quad \text{and } \ell_2(0) = \Lambda_2. \end{aligned}\right\} \tag{3.2.8}$$

Let $\mathbf{v} = (v_1, v_2)$ be defined by

$$\left.\begin{aligned} v_1(\ell_1, \ell_2) &= -\frac{k_-k_+(\ell_2+\ell_1)(\ell_2-\ell_1)+2(k_-\ell_2+k_+\ell_1)}{k_-k_+(\ell_2-\ell_1)+k_-+k_+}, \\ v_2(\ell_1, \ell_2) &= -\frac{k_-k_+(2-\ell_1-\ell_2)(\ell_2-\ell_1)+2(k_-(1-\ell_2)+k_+(1-\ell_1))}{k_-k_+(\ell_2-\ell_1)+k_-+k_+}. \end{aligned}\right\} \tag{3.2.9}$$

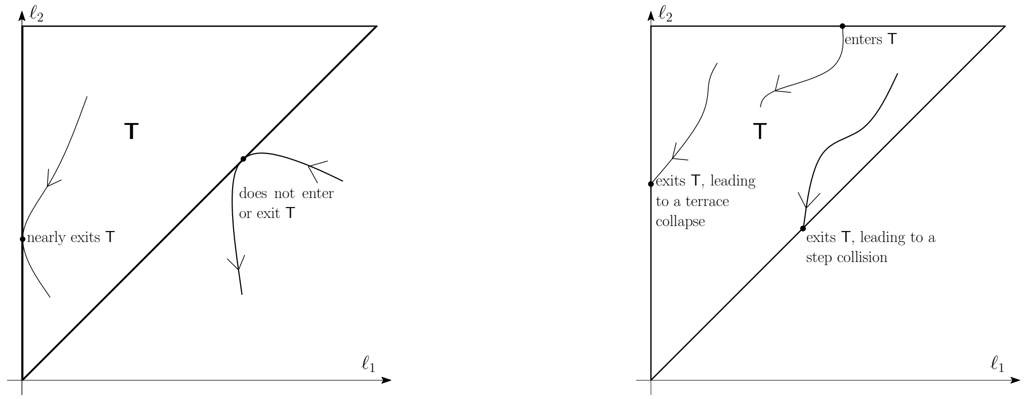

Figure 3.1: On the left, we see examples of Scenarios 1 and 2: of a boundary point at which a trajectory nearly exits the triangle T, as well as a boundary point at which a trajectory does not enter or exit the triangle T. On the right, we see examples of Scenarios 3 (of each kind) and 4: two boundary points at which a trajectory exits the triangle T, as well as a boundary point at which a trajectory enters the triangle T

The vector field $\mathbf{v}$ is smooth in an open set $\mathcal{O} \subset \mathbb{R}^2$ such that $\mathsf{T} \subset\subset \mathcal{O}$ (that is, T is compactly contained in $\mathcal{O}$). Therefore, we have existence and uniqueness in $\mathcal{O}$ for any initial value problem (3.2.8), with $(\Lambda_1, \Lambda_2) \in \mathsf{T} \cup \partial\mathsf{T}$. This implies that for each $(B_1, B_2) \in \partial\mathsf{T}$ there is exactly one solution $(\ell_1, \ell_2) : (a, b) \to \mathcal{O}$ solving (3.2.8), where (a, b) is the maximal interval of existence with $a < 0 < b$, where a may be $-\infty$ and b may be $+\infty$. There are four possible scenarios for this solution, with each case illustrated in Fig. 3.1:

Scenario 1 There exists a time $T > 0$ such that for all $t \in (-T, T)$ the solution $(\ell_1(t), \ell_2(t)) \in \mathsf{T}$. In this case, we say that (ℓ_1, ℓ_2) *nearly exits* T at the point (B_1, B_2).

Scenario 2 For every $\varepsilon > 0$, there exist times $0 < t' < \varepsilon$ and $-\varepsilon < t'' < 0$ such that $(\ell_1(t'), \ell_2(t'))$ and $(\ell_1(t''), \ell_2(t'')) \notin \mathsf{T}$. In this case, we say that there is *no step motion entering or exiting* T at the point (B_1, B_2).

Scenario 3 For every $\varepsilon > 0$, there exists a time $0 < t' < \varepsilon$ such that $(\ell_1(t'), \ell_2(t')) \notin \mathsf{T}$, but for some time $T > 0$, the solution $(\ell_1(t), \ell_2(t)) \in \mathsf{T}$ for all $t \in (-T, 0)$. In this case, we say that (ℓ_1, ℓ_2) *exits* T at the point (B_1, B_2). An initial condition (Λ_1, Λ_2) *leads to a step collision* if the trajectory (ℓ_1, ℓ_2) through (Λ_1, Λ_2) exits T at a point of the form (B, B), where $0 < B < 1$. An initial condition (Λ_1, Λ_2) *leads to a terrace collapse (with the trailing terrace of length B)* if the trajectory (ℓ_1, ℓ_2) through (Λ_1, Λ_2) exits T at a point of the form $(0, B)$ where $0 < B < 1$.

Scenario 4 For every $\varepsilon > 0$, there exists a time $-\varepsilon < t' < 0$ such that $(\ell_1(t'), \ell_2(t')) \notin \mathsf{T}$, but for some $T > 0$, the solution $(\ell_1(t), \ell_2(t)) \in \mathsf{T}$ for all $t \in (0, T)$. In this case, we say that (ℓ_1, ℓ_2) *enters* T at the point (B_1, B_2).

Given a non-vertex boundary point $(B_1, B_2) \in \partial\mathsf{T} - \{(0,0), (0,1), (0,1)\}$, let $\mathbf{N}$ be the outward pointing normal vector to $\partial\mathsf{T}$ at the point (B_1, B_2) and let (ℓ_1, ℓ_2) be the solution to (3.2.8) through (B_1, B_2). If $\mathbf{v}(B_1, B_2) \cdot \mathbf{N} > 0$, then the solution (ℓ_1, ℓ_2) exits T at (B_1, B_2). If $\mathbf{v}(B_1, B_2) \cdot \mathbf{N} < 0$, then the solution (ℓ_1, ℓ_2) enters T at (B_1, B_2).

By (3.2.9), we have that for any $0 < B < 1$:

$$\left.\begin{aligned} \mathbf{v}(0,B) \cdot (-1,0) &= \frac{Bk_-(k_+B+2)}{k_-k_+B + k_- + k_+}, \\ \mathbf{v}(B,1) \cdot (0,1) &= -\frac{k_-k_+(1-B)^2 + 2k_+(1-B)}{k_-k_+(1-B) + k_- + k_+}, \\ \mathbf{v}(B,B) \cdot (1,-1) &= 2(1-2B). \end{aligned}\right\} \tag{3.2.10}$$

Therefore, assuming $k_\pm > 0$,

- by $(3.2.10)_1$, we have that $\mathbf{v} \cdot \mathbf{N} > 0$ along the edge $\ell_1 = 0$ and $0 < \ell_2 \leq 1$, from which it follows that there are trajectories for which the right-most terrace collapses with the left-most terrace of length B for any $0 < B < 1$;

- by $(3.2.10)_2$, $\mathbf{v} \cdot \mathbf{N} < 0$ along the edge $0 < \ell_1 < 1$ and $\ell_2 = 1$, from which it follows that no step motions lead to a step configuration of the form $(B, 1)$ for any $0 < B < 1$ (indeed, trajectories enter T at those points); and

- by $(3.2.10)_3$, there are step motions for which a step collision occurs at (B, B) for any $0 < B < \frac{1}{2}$ but there are no such collisions at points (B, B) if $\frac{1}{2} < B < 1$.

We partition the domain T into three parts:

$$\left.\begin{aligned} \mathsf{U} = &\quad \{(\Lambda_1, \Lambda_2) \in \mathsf{T} \colon (\Lambda_1, \Lambda_2) \text{ leads to a step collision}\}, \\ \mathsf{S} = &\quad \{(\Lambda_1, \Lambda_2) \in \mathsf{T} \colon (\Lambda_1, \Lambda_2) \text{ leads to a terrace collapse}\}, \\ \mathsf{R} = &\quad \mathsf{T} - (\mathsf{U} \cup \mathsf{S}). \end{aligned}\right\} \tag{3.2.11}$$

Before we prove that R consists of the trajectory that exits T at $(0, 0)$, we state the following useful theorem, which is proven in Appendix B.

Theorem B.2.4 (Functions that exit compact sets of a bounded domain and are monotone in their coordinates exit the domain)**.** *Let* T *be a bounded open subset of* $\mathbb{R}^n$*. Suppose* $x\colon (\alpha, \beta) \to \mathsf{T}$ *is a differentiable function,* $x(t) = (x_1(t), x_2(t), \ldots, x_n(t))$*, with the properties that*

- *for any compact subset* K *of* T *and* $\varepsilon > 0$*, there exists a sequence* t_k *such that* $t_k \to \beta$ *and* $x(t_k) \in \mathsf{T} - K$ *as* $k \to \infty$*,*
- x_i *is monotone for each* $i = 1, 2, \ldots, n$*.*

Then the limit $\lim_{t \to \beta} x(t) = X$ *exists with* X *an element of the boundary of* T*.*

With this theorem, we are ready to prove that the region R separating the stable and unstable regions consists of a single trajectory.

Theorem 3.2.1. *The set* R *consists of the trajectory exiting* T *at the point* $(0, 0)$*.*

Proof. It is easy to see that $v_1(\ell_1, \ell_2)$ and $v_2(\ell_1, \ell_2) < 0$ for all $(\ell_1, \ell_2) \in \mathsf{T}$. Hence, there is no equilibrium point of the system (3.2.8) in T.

For any solution (ℓ_1, ℓ_2) of (3.2.8), the component functions ℓ_1, ℓ_2 are monotonically decreasing in t. Therefore, by Theorem B.2.4, any solution (ℓ_1, ℓ_2) must enter at some point and must exit at some point on the boundary $\partial\mathsf{T}$. Since there are no trajectories which exit T at points $(B,1)$ with $0<B<1$,

$$\mathsf{R} \subset \{\text{trajectories through the points } (0,0),\ (0,1),\ \text{or } (1,1)\}. \tag{3.2.12}$$

Since a solution (ℓ_1,ℓ_2) to (3.2.8) must be monotonically decreasing in each component, no trajectory exits T at the point $(1,1)$ or $(0,1)$.

Let A_2 be any positive number less than $\frac{1}{2}$. Since solutions (ℓ_1,ℓ_2) are strictly monotone in time, points of the form (A,A_2) lie on distinct trajectories for $0<A<A_2$. Each of these trajectories must exit T at points in the set

$$\mathsf{V} = \{\mathbf{b}\in\mathbb{R}^2 \colon \mathbf{b}=(0,B) \text{ or } (B,B) \text{ for } 0\le B<A_2\}. \tag{3.2.13}$$

Each trajectory exiting at such points must enter T at points of the form $(A,1)$ or (A',A') such that $0\le A\le 1$ and $\frac{1}{2}\le A'<1$. It follows that there is a map $\varphi:(0,A_2)\to\mathsf{V}$ such that

$$\varphi(A) = (B_1,B_2), \tag{3.2.14}$$

where (B_1,B_2) is the unique point at which the trajectory through (A,A_2) exits T.

Let $\psi:(0,1)\to\mathsf{V}$ be the parameterization defined by

$$\psi(s) = \begin{cases} (0, A_2 - 2A_2 s) & \text{if } 0<s<\frac{1}{2} \\ (2A_2 s - A_2, 2A_2 s - A_2) & \text{if } \frac{1}{2}<s<1. \end{cases} \tag{3.2.15}$$

Then by uniqueness and the intermediate value theorem, we have that the map $\psi^{-1}\circ\varphi$ is monotone increasing. If a monotone increasing function has a discontinuity, then it must be a jump discontinuity. Since $\left(0,\frac{1}{2}\right)\cup\left(\frac{1}{2},1\right)\subset(\psi^{-1}\circ\varphi)(0,A_2)\subset(0,1)$, it follows that there is no jump discontinuity and 0.5 lies in the image of $\psi^{-1}\circ\varphi$. This proves that there is a point (A,A_2) lying on a trajectory that exits T at $(0,0)$. $\square$

By the monotonicity in time of the solutions ℓ_1 and ℓ_2 to (3.2.8), the set R is the graph of a function $\tilde{\ell}_2$. In particular, there exists a number $\frac{1}{2}<\delta\le 1$ and a unique solution $\tilde{\ell}_2$ to the initial value problem

$$\left.\begin{aligned} \frac{\mathrm{d}\tilde{\ell}_2}{\mathrm{d}\ell_1} &= \frac{v_2(\ell_1,\tilde{\ell}_2)}{v_1(\ell_1,\tilde{\ell}_2)}, \\ \tilde{\ell}_2(0) &= 0, \end{aligned}\right\} \tag{3.2.16}$$

which has the property that

$$\mathsf{R} = \left\{(\ell_1,\ell_2) \in \mathbb{R}^2 \colon\ 0 < \ell_1 < \delta \text{ and } \ell_2 = \tilde{\ell}_2(\ell_1)\right\}, \tag{3.2.17}$$

where $\delta > 0$ is the unique smallest value such that either $\tilde{\ell}_2(\delta) = \delta$ or $\delta = 1$.

Definition 3.2.2. *The solution separating the stable region and the unstable region and its graph are called* the separatrix*.*

Parameter dependence of the unstable region

To characterize the dependence of the sizes of U and S on the attachment rates (k_-, k_+), we need only characterize the dependence of the solution $\tilde{\ell}_2$ of (3.2.16) on (k_-, k_+), since

$$\begin{aligned} \mathsf{U} &= \left\{(\ell_1,\ell_2) \in \mathsf{T} \colon \ell_1 \geq \delta \text{ or } 0 < \ell_1 < \delta \text{ and } \ell_2 < \tilde{\ell}_2(\ell_1)\right\}, \\ \mathsf{S} &= \left\{(\ell_1,\ell_2) \in \mathsf{T} \colon 0 < \ell_1 < \delta \text{ and } \ell_2 > \tilde{\ell}_2(\ell_1)\right\}. \end{aligned} \tag{3.2.18}$$

Let $f : (0,1) \times (0,1) \to \mathbb{R}^2$ be defined by

$$f(t,y) = \frac{v_2(t,y)}{v_1(t,y)} = -1 - \frac{2(k_+k_-(y-t) + k_- + k_+)}{k_+k_-(y+t)(y-t) + 2(k_-y + k_+t)}. \tag{3.2.19}$$

We apply the following result, which is proved in Appendix B.

Corollary B.1.2. *If, for $i = 1$ and 2, $f_i \colon (0,a) \times (0,b) \to \mathbb{R}$ are two functions such that $f_i(t,y)$ are decreasing in y and such that there exists a solution, y_i, to the problems*

$$\left.\begin{aligned} y' &= f_i(t,y), \\ y(0) &= 0, \end{aligned}\right\}$$

and $f_1(t,y) \leq f_2(t,y)$, then $y_1(t) \leq y_2(t)$ for all $0 < t < a$.

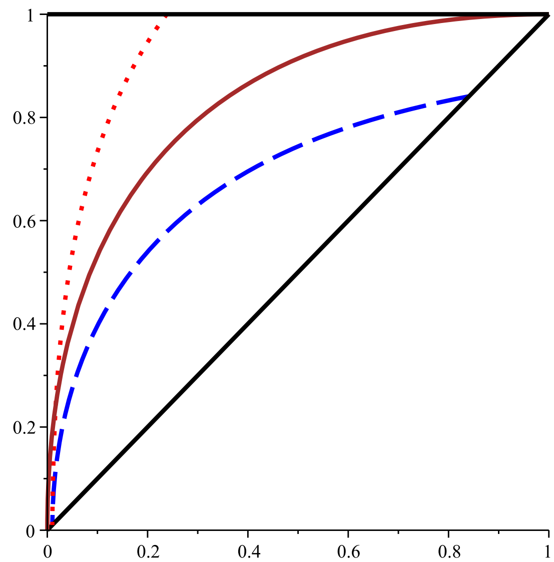

Figure 3.2: The dotted curve shows the separatrix for a normal Ehrlich–Schwoebel barrier ($k_- = 1$ and $k_+ = 10$); the solid curve shows the separatrix when there is symmetric attachment; and the dashed curve shows the separatrix for an inverse Ehrlich–Schwoebel barrier ($k_- = 10$ and $k_+ = 1$).

With this result, we prove the following theorem.

Theorem 3.2.3. *The family of solutions $\tilde{\ell}_2(\ell_1)$ to (3.2.16) is decreasing in k_- and increasing k_+. Consequently, increasing k_- decreases the size of the unstable region, whereas increasing k_+ increases the size of the unstable region.*

Proof. With the intention of applying Corollary B.1.2, we first verify that f is, indeed, decreasing in y in T:

$$\frac{\partial f(t,y)}{\partial y} = -\frac{4k_-(k_- + k_+) + 2(k_-k_+)^2(y-t)^2 + 4(y-t)k_-k_+(k_- + k_+)}{(k_+k_-(y+t)(y-t) + 2(k_-y + k_+t))^2}, \quad (3.2.20)$$

which is negative for $(t, y) \in \mathsf{T}$ and $k_- > 0$. Hence, by Corollary B.1.2, the set U depends monotonically on k_- and k_+, if f depends monotonically on k_- and k_+ in T. We find that

$$\begin{aligned} \frac{\partial(f(t,y))}{\partial k_-} &= -\frac{2(y-t)^2k_+^2 + 4(y-t)k_+}{(k_+k_-(y+t)(y-t) + 2(k_-y + k_+t))^2}, \\ \frac{\partial(f(t,y))}{\partial k_+} &= \frac{2(y-t)^2k_-^2 + 4(y-t)k_-}{(k_+k_-(y+t)(y-t) + 2(k_-y + k_+t))^2}. \end{aligned} \quad (3.2.21)$$

Hence, U grows with k_+ and shrinks with k_-. □

To finish our analysis, we consider the case of symmetric attachment $k_- = k_+$. The system (3.2.8) reduces to

$$\left.\begin{aligned} \dot{\ell}_1 = &\quad -\ell_1 - \ell_2, \\ \dot{\ell}_2 = &\quad -2 + \ell_2 + \ell_1, \\ \ell_1(0) = &\quad \Lambda_1 \text{ and } \ell_2(0) = \Lambda_2. \end{aligned}\right\} \tag{3.2.22}$$

The general solution to this system is

$$\ell_1(t) = t(t - \Lambda_2) + \Lambda_1(1-t), \quad \ell_2(t) = t(\Lambda_1 - 2 - t) + \Lambda_2(t+1). \tag{3.2.23}$$

Notice that if $\Lambda_1 = \Lambda_2 = 1$, then $\ell_1(t) = (1-t)^2$ and $\ell_2(t) = (1-t^2)$. Assuming $k_- = k_+$, the trajectory of this solution forms the separatrix. In particular, the separatrix is the graph of

$$\ell_2 = 2\sqrt{\ell_1} - \ell_1. \tag{3.2.24}$$

Any separatrix with a normal ES barrier ($k_- < k_+$) has an unstable region U which is larger than (i.e., a superset of) the region in T below the graph of (3.2.24). Moreover, any separatrix with an inverse ES barrier ($k_- > k_+$) has an unstable region which is smaller than this region (see Fig. 3.2). Physically, this means that there are more step collisions for materials with a larger normal ES barrier.

3.3 Concentric steps

We now consider two circular steps with common center bounded by a concentric wall (see Fig. 3.3). Such a small number of steps is realistic for the growth of nanowires (see e.g. [20]) We investigate:

- step motion during growth,

- step motion during growth with desorption.

In the case of growth, we establish the existence and uniqueness of a step motion that has trajectory which bounds the stable and unstable regions of initial step configurations. We then show that when the step line tension is negligible, i.e., for $\Gamma = 0$, the dependence of the size of the unstable region with respect to the parameters $K_\pm$ is the same as in the case straight steps between two walls found in the previous section. If $\Gamma > 0$, we establish that both fixing either Γ and K_+ and decreasing K_- or, alternately, fixing K_+ and K_- and decreasing Γ increases the size of the unstable region.

The remainder of the chapter is spent establishing the existence and uniqueness of the separatrix for the growth with desorption case with $\Gamma = 0$. Existence is proven in the same manner as for the straight steps, but uniqueness requires an argument based on monotonicity. Establishing the claimed monotonicity forms the bulk of the section on the growth with desorption case, and requires some information about modified Bessel functions.

Let the radial variable and the radii of the inner and outer circular steps be denoted by $\bar{r}$, $\bar{r}_1$, and $\bar{r}_2$, respectively, and let the radius of the wall be denoted by $\bar{R}$. Let $\bar{t}$ denote the time variable. We treat the models of growth and of growth with desorption, although we restrict ourselves to parameters such that the dominant process is deposition. In particular, we assume

$$\mathtt{F}_{\text{ed}} := F\tau - \varrho_{\text{eq}} > 0. \tag{3.3.1}$$

Recall that τ is the average evaporation time for an adatom on a terrace and F is a deposition flux. The assumption (3.3.1) may be regarded as an assumption on any of the parameters F, τ, or ϱ_{eq}, although the deposition flux is the parameter directly controllable in the experimental setting.

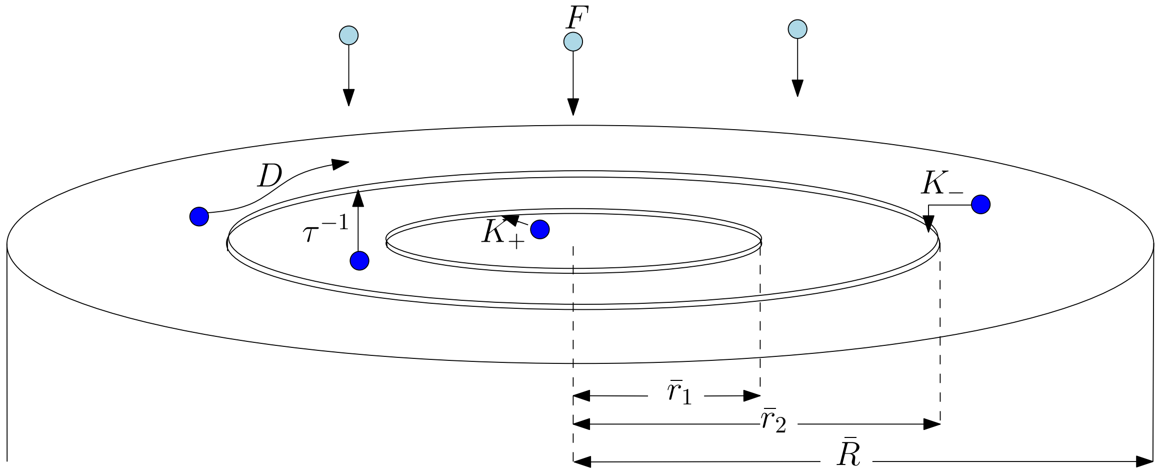

Figure 3.3: Schematic view of a nanowire where the crystal surface consists of concentric steps bounded by a wall.

The radial symmetry of the steps and wall allows us to consider the following model of growth: ϱ solves the ODE

$$0 = \frac{D}{\bar{r}}\frac{\partial}{\partial \bar{r}}\left(\bar{r}\frac{\partial \varrho}{\partial \bar{r}}\right) + F \qquad \text{in } (0, \bar{r}_1) \cup (\bar{r}_1, \bar{r}_2) \cup (\bar{r}_2, \bar{R}), \tag{3.3.2}$$

with boundary conditions

$$\left.\begin{array}{rcll} -D\dfrac{\partial \varrho^+}{\partial \bar{r}} & = & K_+\left(\varrho^+ - \varrho_{\text{eq}} + \dfrac{\Gamma}{\bar{r}}\right) & \text{at } \bar{r} = \bar{r}_n,\ n = 1, 2, \\ D\dfrac{\partial \varrho^-}{\partial \bar{r}} & = & K_-\left(\varrho^- - \varrho_{\text{eq}} + \dfrac{\Gamma}{\bar{r}}\right) & \\ \varrho(0) & < & \infty, & \\ \dfrac{\partial \varrho^+}{\partial \bar{r}} & = & 0 & \text{at } \bar{r} = \bar{R}, \end{array}\right\} \tag{3.3.3}$$

and the radii are governed by

$$\varrho^{\mathrm{b}}\frac{\mathrm{d}\bar{r}_n}{\mathrm{d}\bar{t}} = D\left[\!\!\left[\frac{\partial \varrho}{\partial \bar{r}}\right]\!\!\right]_{\bar{r}=\bar{r}_n}, \qquad \text{for } n = 1, 2, \tag{3.3.4}$$

and model of growth with desorption: ϱ solves the ODE

$$0 = \frac{D}{\bar{r}}\frac{\partial}{\partial \bar{r}}\left(\bar{r}\frac{\partial \varrho}{\partial \bar{r}}\right) - \tau^{-1}\varrho + F \qquad \text{in } (0, \bar{r}_1) \cup (\bar{r}_1, \bar{r}_2) \cup (\bar{r}_2, \bar{R}), \tag{3.3.5}$$

with boundary conditions

$$\left.\begin{aligned} -D\frac{\partial \varrho^+}{\partial \bar{r}} &= K_+\left(\varrho^+ - \varrho_{\text{eq}} + \frac{\Gamma}{\bar{r}}\right) && \text{at } \bar{r} = \bar{r}_n,\ n = 1, 2, \\ D\frac{\partial \varrho^-}{\partial \bar{r}} &= K_-\left(\varrho^- - \varrho_{\text{eq}} + \frac{\Gamma}{\bar{r}}\right) && \\ \varrho(0) &< \infty, && \\ \frac{\partial \varrho^+}{\partial \bar{r}} &= 0 && \text{at } \bar{r} = \bar{R}, \end{aligned}\right\} \tag{3.3.6}$$

with the radii governed by

$$\varrho^{\text{b}}\frac{\mathrm{d}\bar{r}_n}{\mathrm{d}\bar{t}} = D\left[\!\!\left[\frac{\partial \varrho}{\partial \bar{r}}\right]\!\!\right]_{\bar{r}=\bar{r}_n} \qquad \text{for } n = 1, 2. \tag{3.3.7}$$

Remark 3.3.1. *It is important to keep in mind that the notation u^+ and u^- means the limiting value from the lower terrace side and from the upper terrace side, which in the present case means that the notation is in conflict with the usual meaning in terms of the radial variable. In particular, for circular steps forming a valley:*

$$u^+(r_n) = \lim_{\varepsilon\downarrow 0} u(r_n - \varepsilon) \ \textit{and}\ u^-(r_n) = \lim_{\varepsilon\downarrow 0} u(r_n + \varepsilon). \tag{3.3.8}$$

For the case of growth, we choose the non-dimensional variables defined by

$$r = \frac{\bar{r}}{\bar{R}},\ t = \frac{F\bar{t}}{4\varrho^{\text{b}}},\ u = \frac{4D(\varrho - \varrho_{\text{eq}})}{F\bar{R}^2}, k_\pm = \frac{K_\pm \bar{R}}{D},\ \text{and } \mathtt{g}_{\text{d}} = \frac{4D\Gamma}{F\bar{R}^3}. \tag{3.3.9}$$

Then the boundary value problem (3.3.2)-(3.3.3) reduces to the ODE

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) + 4{=}0 \qquad \text{in } (0, r_1) \cup (r_1, r_2) \cup (r_2, 1), \tag{3.3.10}$$

with boundary conditions

$$\left.\begin{aligned} -\frac{\partial u^+}{\partial r} &= k_+\left(u^+ + \frac{\mathtt{g}_{\text{d}}}{r}\right) && \text{at } r = r_1, r_2, \\ \frac{\partial u^-}{\partial r} &= k_-\left(u^- + \frac{\mathtt{g}_{\text{d}}}{r}\right) && \\ u(0) &< \infty, && \\ \frac{\partial u^+}{\partial r} &= 0 && \text{at } r = 1, \end{aligned}\right\} \tag{3.3.11}$$

and (3.3.4) reduces to

$$\dot{r}_n = \left[\!\left[\frac{\partial u}{\partial r}\right]\!\right]_{r=r_n} \qquad \text{for } n = 1, 2. \tag{3.3.12}$$

For the case of growth with desorption, we choose the non-dimensional variables:

$$r = \frac{\bar{r}}{\sqrt{D\tau}},\ R = \frac{\bar{R}}{\sqrt{D\tau}},\ t = \frac{\bar{t}}{\tau\varrho^{\mathrm{b}}},\ u = \frac{\varrho - \varrho_{\mathrm{eq}}}{\mathtt{F}_{\mathrm{ed}}},\ k_{\pm} = \sqrt{\frac{\tau}{D}}K_{\pm}, \\ \text{and } \mathtt{g}_{\mathrm{ed}} = \frac{\Gamma}{\mathtt{F}_{\mathrm{ed}}\sqrt{D\tau}}. \tag{3.3.13}$$

Then the boundary value problem problem (3.3.5)-(3.3.6) reduces to the ODE

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) - u = -1 \qquad \text{in } (0, r_1) \cup (r_1, r_2) \cup (r_2, 1), \tag{3.3.14}$$

with boundary conditions

$$\left.\begin{aligned} -\frac{\partial u^+}{\partial r} &= k_+\left(u^+ + \frac{\mathtt{g}_{\mathrm{ed}}}{r}\right) \\ \frac{\partial u^-}{\partial r} &= k_-\left(u^- + \frac{\mathtt{g}_{\mathrm{ed}}}{r}\right) \end{aligned}\quad \text{at } r = r_1, r_2, \\ \begin{aligned} u(0) &< \infty, \\ \frac{\partial u^+}{\partial r} &= 0 \qquad\qquad \text{at } r = R, \end{aligned}\right\} \tag{3.3.15}$$

and (3.3.7) reduces to

$$\dot{r}_n = \left[\!\left[\frac{\partial u}{\partial r}\right]\!\right]_{r=r_n} \qquad \text{for } n = 1, 2. \tag{3.3.16}$$

In both cases the boundary value problem only has a solution for degenerate step configurations (i.e., where $r_1 = 0$ or $r_2 = R$) if either $k_- = 0$ or $k_+ = 0$. Therefore, we assume that $k_\pm > 0$.

3.4 Concentric steps: motion under growth conditions

In this section we show that there is a unique separatrix, which depends on the parameters such that the unstable region U grows if $\Gamma = 0$ and K_+ is increased or if $\Gamma \geq 0$ and K_- is decreased; or if Γ is decreased. This means that larger normal ES barriers have more initial conditions which lead to step collisions, and that increasing the effect of line tension causes there to be less initial conditions that lead to step collisions.

The boundary value problem (3.3.10)-(3.3.11) may be solved explicitly so that the velocity equations (3.3.12) reduce to the system

$$\left.\begin{aligned} \dot{r}_1 &= f_1^{\mathrm{d}}(r_1, r_2), \\ \dot{r}_2 &= f_2^{\mathrm{d}}(r_1, r_2), \end{aligned}\right\} \tag{3.4.1}$$

where

$$\begin{aligned} f_1^{\mathrm{d}}(r_1, r_2) &= -\frac{\Xi(r_1, r_2)}{r_1}, \\ f_2^{\mathrm{d}}(r_1, r_2) &= \frac{\Xi(r_1, r_2) - 2}{r_2}, \end{aligned} \tag{3.4.2}$$

with Ξ defined by

$$\Xi(r_1, r_2) = \frac{k_+ k_- \left(r_2 - r_1\right)\left(r_1 r_2 (r_2 + r_1) + \mathsf{g}_{\mathrm{d}}\right) + 2 r_1 r_2 (k_- r_2 + k_+ r_1)}{k_+ r_2 + k_- r_1 + k_+ k_- r_1 r_2 \ln\left(\frac{r_2}{r_1}\right)}. \tag{3.4.3}$$

Numerical solutions for various initial conditions are found in Fig. 3.4 for two different choices of the parameters k_-, k_+, and g_{d}: $k_- = 1$, $k_+ = 10$, and $\mathsf{g}_{\mathrm{d}} = 0.1$ and $k_- = 10$, $k_+ = 1$, and $\mathsf{g}_{\mathrm{d}} = 0.1$. For both cases, Fig. 3.4 shows step motions with initial outer radius $r_2 = 0.8$ and various initial inner radii. It is clear that step collisions occur for initial radii sufficiently close, and they do not occur for initial radii sufficiently separated. Moreover, it appears that for a strong barrier, reversing the barrier from inverse ES ($k_- > k_+$) to normal ES ($k_- < k_+$) tends to destabilize in the sense that more step collisions occur (i.e., for larger initial separations), but also in the sense that step collisions occur more quickly. These observations are conjectural, since we do not establish how the separatrix depends on k_+ when $\mathsf{g}_{\mathrm{d}} > 0$, and we do not show any results regarding the rate of step collisions as a function of the parameters $k_\pm$.

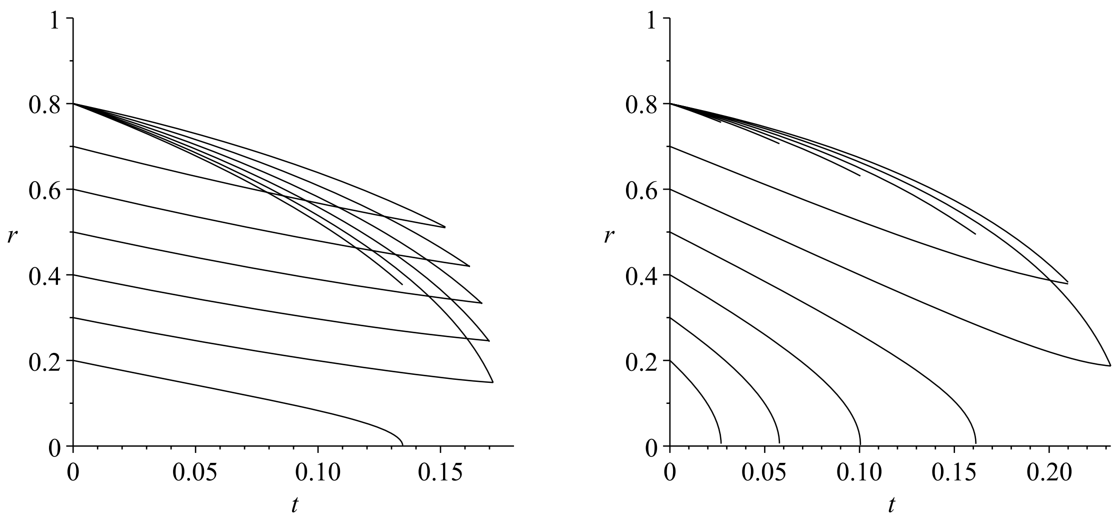

Figure 3.4: On the left, step motions for BCF model during growth and parameters $k_- = 1, k_+ = 10$, and $\mathsf{g}_\mathrm{d} = 0.1$. On the right, step motions for the BCF model without desorption for parameters $k_- = 10, k_+ = 1$, and $\mathsf{g}_\mathrm{d} = 0.1$.

Existence

We now prove the existence of a separatrix. The domain of admissible step positions is the same as in the straight step section:

$$\mathsf{T} = \{(r_1, r_2) \in \mathbb{R}^2 \colon 0 < r_1 < r_2 < 1\}. \tag{3.4.4}$$

Trajectories which exit T along $r_1 = r_2$ are said to lead to step collisions, whereas the inner terrace is said to collapse if a trajectory exits T along the edge $r_1 = 0$.

Note that $f_1^\mathrm{d}(r_1, r_2) < 0$ for all $(r_1, r_2) \in \mathsf{T}$. This means that during growth, the inner circle always moves inward. The same cannot be said of the outer step. Indeed, if $\mathsf{g}_\mathrm{d} k_- - 2 > 0$, then

$$\lim_{r_1 \to 0} f_2^\mathrm{d}(r_1, r_2) = \frac{\mathsf{g}_\mathrm{d} k_- - 2}{r_2} > 0, \tag{3.4.5}$$

and, by continuity of f_2^d away from $(0, 0)$, it is clear that if $\mathsf{g}_\mathrm{d} k_- - 2 > 0$, then $\dot{r}_2 > 0$ for some step configurations (r_1, r_2). On the other hand, for $0 < r < 1$,

$$f_2^\mathrm{d}(r, r) = -\frac{2(1 - r^2)}{r} < 0. \tag{3.4.6}$$

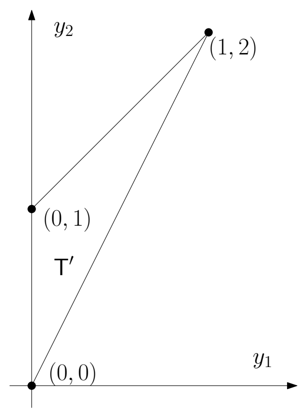

Figure 3.5: T' is the relevant domain for the (y_1, y_2) problem (3.4.8) associated with the (r_1, r_2) problem (3.4.1)

In general, then, f_2^{d} is not strictly positive or strictly negative in a neighborhood of $(0,0)$ in T. Hence, we cannot apply Theorem B.2.4 to show that all trajectories of (3.4.1) enter and exit T. Nonetheless, we may establish the following technical fact about our system.

Lemma 3.4.1. *Any trajectory of (3.4.1) must enter at some point on $\partial \mathsf{T}$ and must exit at some point on $\partial \mathsf{T}$.*

Proof. Given a solution (r_1, r_2) to the problem (3.4.1) in T, the functions

$$y_1 = r_1^2 \text{ and } y_2 = r_1^2 + r_2^2 \tag{3.4.7}$$

solve

$$\left.\begin{aligned} \dot{y}_1 &= 2\sqrt{y_1} f_1^{\mathrm{d}}(\sqrt{y_1}, \sqrt{y_2 - y_1}), \\ \dot{y}_2 &= -4, \end{aligned}\right\} \tag{3.4.8}$$

in the triangle T', shown in Fig. 3.4,

$$\mathsf{T}' = \{(y_1, y_2) \in \mathbb{R}^2 \colon 0 < y_1 < 1 \text{ and } 2y_1 < y_2 < 1 + y_1\}, \tag{3.4.9}$$

and given a solution (y_1, y_2) of (3.4.8) in T', the functions $r_1 = \sqrt{y_1}$ and $r_2 = \sqrt{y_2 - y_1}$ solve (3.4.1) in T.

For any solution (y_1, y_2) to the system (3.4.8), the function y_1 is monotone increasing in time and the function y_2 is monotone decreasing in time. Since we also have that there is no equilibrium point in T' for this system, every trajectory of (3.4.8) must enter at some point on $\partial\mathsf{T}'$ and must exit at some point on $\partial\mathsf{T}$. This completes our proof. □

We now show that there exists at least one step motion trajectory for which the inner and the outer steps collide at the moment both have zero radius. We then establish that this trajectory is unique.

Lemma 3.4.2. *There exists at least one solution of the terminal value problem*

$$\left.\begin{aligned} \dot{r}_1 = &\quad f_1^d(r_1, r_2), \\ \dot{r}_2 = &\quad f_2^d(r_1, r_2), \end{aligned}\right\} \tag{3.4.10}$$

such that for some $0 < T \leq \infty$*, the following limit holds:*

$$\lim_{t \to T} (r_1(t), r_2(t)) = (0, 0); \tag{3.4.11}$$

and $(r_1(t), r_2(t)) \in \mathsf{T}$ *for all* $0 < t < T$*.*

Proof. We may analyze the behavior of the right hand side of (3.4.8) to determine the points at which trajectories enter or exit T'. The outward pointing normal vectors to the sides $\{(y_1, y_2) \colon y_1 = 0,\ 0 < y_2 < 1\}$; $\{(y_1, y_2) \colon 0 < y_1 < 1 \text{ and } y_2 = 1 + y_1\}$; and $\{(y_1, y_2) \colon 0 < y_1 < 1 \text{ and } y_2 = 2y_1\}$ are $(-1, 0)$; $(-1, 1)$; and $(2, -1)$, respectively. Our concern is only the behavior near $(0, 0)$. Hence, we consider, for $0 < y < 1$, the signs of

$$-2 \lim_{\substack{(y_1,y_2) \to (0,y) \\ (y_1,y_2) \in \mathsf{T}'}} \sqrt{y_1} f_1^{\mathrm{d}}(\sqrt{y_1}, \sqrt{y_2 - y_1})$$

and

$$2\sqrt{y} f_1^{\mathrm{d}}(\sqrt{y}, \sqrt{y}) - 2\sqrt{y} f_2^{\mathrm{d}}(\sqrt{y}, \sqrt{y}).$$

We find that the limit along the edge $y_1 = 0$ is given by

$$-2 \lim_{\substack{(y_1,y_2)\to(0,y) \\ (y_1,y_2)\in\mathsf{T}'}} \sqrt{y_1} f_1^{\mathrm{d}}(\sqrt{y_1}, \sqrt{y_2 - y_1}) = 2k_{-}\mathsf{g}_{\mathrm{d}} > 0, \tag{3.4.12}$$

and along the edge $y_2 = 2y_1$, we find

$$2\sqrt{y} f_1^{\mathrm{d}}(\sqrt{y}, \sqrt{y}) - 2\sqrt{y} f_2^{\mathrm{d}}(\sqrt{y}, \sqrt{y}) = \frac{2(1-2y)}{\sqrt{y}}. \tag{3.4.13}$$

Hence, we have that for each point $(0, y)$ such that $0 < y < 1$, there exists a trajectories that exits T' at that point. Moreover, from the expression (3.4.13), we have that if $0 < y < \frac{1}{2}$, then there exists a trajectory that exits T' at the point (y, y). Let $0 < Y_2 < \frac{1}{2}$. Since a solution (y_1, y_2) has $\dot{y}_2 < 0$, any trajectory containing a point of the form (y, Y), with $0 < y < Y/2$, exits T' at a point in the set

$$\mathsf{V}' = \{\mathbf{y} \in \mathbb{R}^2 \colon \mathbf{y} = (0, y) \text{ or } (y, y/2) \text{ for } 0 < y < Y\}. \tag{3.4.14}$$

As argued previously, since

- trajectories do not cross within T',
- each trajectory (y_1, y_2) containing a point of the form $(y, Y) \in \mathsf{T}'$ exits at a point in V', and
- there exists a trajectory (y_1, y_2) through a point of the form $(y, Y) \in \mathsf{T}'$, such that (y_1, y_2) exits at (Y_1, Y_2) for each $(Y_1, Y_2) \in \mathsf{V}' - \{(0, 0)\}$,

there exists at least one trajectory that exits T' at the point $(0, 0)$. This completes our proof. □

Uniqueness

We now show that such a trajectory is unique. For this, we consider the system governing $z_1 = r_1^2$ and $z_2 = r_2^2$, which is

$$\left.\begin{aligned} \dot{z}_1 &= \tilde{f}_1^{\mathrm{d}}(z_1, z_2), \\ \dot{z}_2 &= \tilde{f}_2^{\mathrm{d}}(z_1, z_2), \end{aligned}\right\} \tag{3.4.15}$$

where

$$\begin{aligned}\tilde{f}_1^{\mathrm{d}}(z_1, z_2) &= 2\sqrt{z_1} f_1^{\mathrm{d}}(\sqrt{z_1}, \sqrt{z_2}),\\ \tilde{f}_2^{\mathrm{d}}(z_1, z_2) &= 2\sqrt{z_2} f_2^{\mathrm{d}}(\sqrt{z_1}, \sqrt{z_2}),\end{aligned} \tag{3.4.16}$$

and the system is, also, defined on T. The existence of a trajectory of (3.4.1) through $(0, 0)$ implies the existence of a trajectory of (3.4.15) through $(0, 0)$, and the uniqueness in T of the trajectory of (3.4.15) implies the uniqueness of the trajectory of (3.4.1). Since $\tilde{f}_1^{\mathrm{d}}, \tilde{f}_2^{\mathrm{d}}$ are smooth in T, trajectories do not cross in T. Therefore, we need only establish that there is a unique trajectory exiting at $(0, 0)$ in a neighborhood $U \cap \mathsf{T}$ for any open set $U \subset \mathbb{R}^2$ containing $(0, 0)$. Moreover, any trajectory of (3.4.15) through $(0, 0)$ forms the graph of a solution to the integral equation:

$$z_2(z_1) = \int_0^{z_1} \frac{\tilde{f}_2^{\mathrm{d}}(\zeta, z_2(\zeta))}{\tilde{f}_1^{\mathrm{d}}(\zeta, z_2(\zeta))} \,\mathrm{d}\zeta, \tag{3.4.17}$$

since $\tilde{f}_1^{\mathrm{d}}$ is strictly positive in T. Hence, it suffices to show that (3.4.17) has a unique solution. The following uniqueness theorem suits our purpose.

Theorem B.1.1 (Peano's uniqueness theorem for integral equations)**.** *Suppose $f : \mathbb{R}^2 \to \mathbb{R}$ is non-increasing in its second argument. Then the integral equation*

$$y(x) = \int_0^x f(t, y(t))\ dt$$

has at most one solution.

By Theorem B.1.1, if for some $\varepsilon > 0$ and each $0 < z_1 < \varepsilon$ the mapping $z_2 \mapsto (\tilde{f}_2^{\mathrm{d}}/\tilde{f}_1^{\mathrm{d}})(z_1, z_2)$ is monotone decreasing, then there is at most one solution to the integral equation (3.4.17). We find that

$$\frac{\partial(\tilde{f}_2^{\mathrm{d}}/\tilde{f}_1^{\mathrm{d}})(z_1, z_2)}{\partial z_2} = -\frac{\alpha(z_1, z_2)}{\beta(z_1, z_2)}, \tag{3.4.18}$$

where

$$\begin{aligned}\alpha(z_1,z_2) &= k_-\sqrt{z_1}\left(\alpha_0(z_1,z_2)+\mathsf{g}_{\mathrm{d}}\alpha_1(z_1,z_2)\right),\\ \alpha_0(z_1,z_2) &= k_+k_-\sqrt{z_1}\left\{k_+\sqrt{z_2}\left(z_1+\ln\left(\frac{z_2}{z_1}\right)\right)+(z_2-z_1)+\ln\left(\frac{z_2}{z_1}\right)\right\}\\ &\qquad + 2k_+\left\{k_+\sqrt{z_2}(z_2-z_1)+z_2+z_1\right\}+k_-\sqrt{z_1z_2}(4-k_+^2z_2),\\ \alpha_1(z_1,z_2) &= k_+\left\{k_+k_-\left(\sqrt{z_1}+\sqrt{z_1}\ln\left(\sqrt{\frac{z_2}{z_1}}\right)\right)+k_-+k_+(1-k_-\sqrt{z_2})\right\},\\ \beta(z_1,z_2) &= \sqrt{z_2}\left\{k_+k_-(\sqrt{z_2}-\sqrt{z_1})[\mathsf{g}_{\mathrm{d}}+\sqrt{z_1z_2}(\sqrt{z_1}+\sqrt{z_2})]\right.\\ &\qquad \left.+2\sqrt{z_1z_2}(k_-\sqrt{z_2}+k_+\sqrt{z_1})\right\}^2.\end{aligned} \tag{3.4.19}$$

It is clear that $\beta(z_1,z_2)>0$ in T. Moreover, only the last terms in the expressions for $\alpha_0(z_1,z_2)$ and $\alpha_1(z_1,z_2)$ are not strictly positive for all $(z_1,z_2)\in\mathsf{T}$ and all choices of $k_+,k_-\geq 0$ with at least one parameter non-zero. However, these terms are indeed positive for $(z_1,z_2)\in\mathsf{T}$ sufficiently close to $(0,0)$. In particular, $\alpha(z_1,z_2)$ is positive for $(z_1,z_2)\in\mathsf{T}$ such that

$$0<z_2<\min\left(\frac{4}{k_+^2},\frac{1}{k_-^2}\right). \tag{3.4.20}$$

Hence, we have that the integral equation (3.4.17) has a unique solution as existence was shown in Lemma 3.4.2, and we have the following theorem.

Theorem 3.4.3. *There exists a unique trajectory, $(\tilde{r}_1,\tilde{r}_2)$, of (3.4.1) that exits T at the point $(0,0)$. Moreover, all trajectories leading to step collisions are bounded above by this trajectory and the (potentially empty) line segment*

$$\{(r,1)\in\mathbb{R}^2\colon R_1<r<1\}. \tag{3.4.21}$$

where R_1 is defined by

$$\lim_{t\to t_0}(\tilde{r}_1(t),\tilde{r}_2(t))=(R_1,1) \tag{3.4.22}$$

if such a t_0 exists and 1, otherwise.

Proof. We have shown the first statement. The second statement may be argued as follows. Since $f_1^{\mathrm{d}}(r_1, r_2) < 0$, any trajectory $(\bar{r}_1, \bar{r}_2)$ parameterizes the graph of a continuous function $r_2 = R_2(r_1)$, each of which do not intersect the others. Let $\tilde{R}_2$ denote the corresponding function for the separatrix $(\tilde{r}_1, \tilde{r}_2)$. Then any trajectory that exits T at a point (r, r) must satisfy $R_2(r) = r < \tilde{R}_2(r)$ or r is not in the domain of $\tilde{R}_2$, which entails that $\tilde{R}_2(r_0) = 1$ for some $r_0 < r$. □

Dependence of the unstable region on parameters

We now consider the dependence of the separatrix on the parameters $\mathsf{g}_{\mathrm{d}}, k_+$, and k_-, from which we deduce the dependence of the unstable region on those parameters. To do this we again consider the integral equation (3.4.17). Dependence of the separatrix on the parameters is illustrated in Fig. 3.6. Notice that increasing g_{d} is stabilizing, since the solid curve of the left is lower than the dotted curve on the left. Moreover, although in the infinite train case discussed in the previous chapter, a normal ES barrier ($k_- < k_+$) is stabilizing againt step collisions, in the figure on the right, it is clear that a large normal ES barrier corresponds to a large unstable region, and may be made larger by increasing the normal ES barrier.

Theorem 3.4.4. *If $\mathsf{g}_{d} = 0$, then for $k_+, k_- > 0$ the solution to the integral equation (3.4.17) is pointwise increasing in k_+ and decreasing in k_-. In general, for $\mathsf{g}_{d}, k_+, k_- > 0$, the solution is pointwise decreasing in k_- as well as g_{d}.*

Proof. For all $\mathsf{g}_{\mathrm{d}}, k_\pm \geq 0$ with at least one of $k_\pm$ non-zero, the integral equation (3.4.17) has right-hand side non-decreasing in the dependent variable z_2. Hence, Corollary B.1.2 found in Appendix B is potentially applicable. It suffices to show that for all $(z_1, z_2) \in \mathsf{T}$:

- if $\mathsf{g}_{\mathrm{d}} = 0$, then the function $\tilde{f}_2^{\mathrm{d}}/\tilde{f}_1^{\mathrm{d}}(z_1, z_2)$ is monotone increasing in k_+ and monotone decreasing in k_-, and

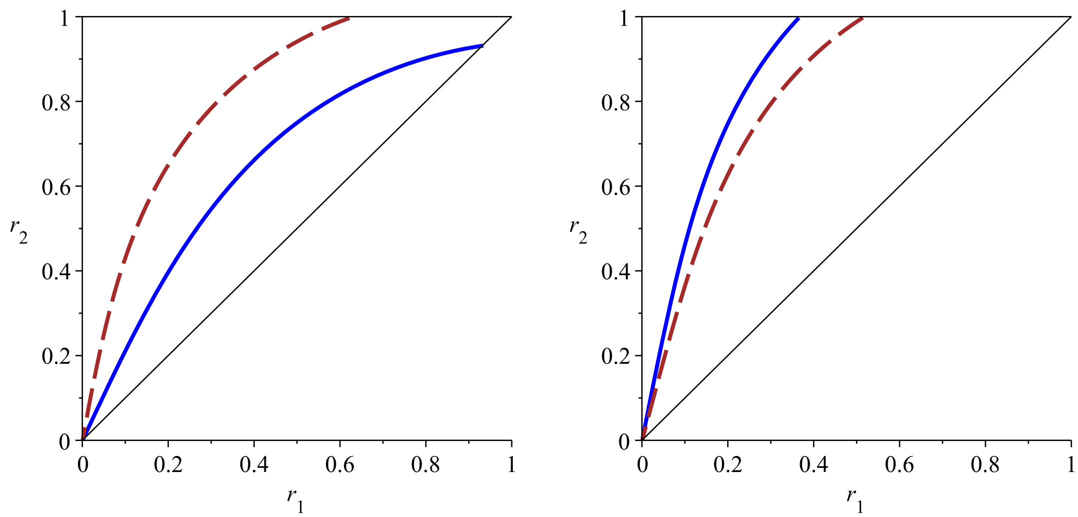

Figure 3.6: On the left, the dashed curve is the separatrix for $k_- = k_+ = 1$ and $\mathsf{g}_{\text{d}} = 0.1$; the solid curve is the separatrix for $k_- = k_+ = 1$ and $\mathsf{g}_{\text{d}} = 1$. On the right, the dashed curve is the separatrix for $k_- = 2$, $k_+ = 10$, and $\mathsf{g}_{\text{d}} = 0.1$; the solid curve is the separatrix for $k_- = 1$, $k_+ = 10$, and $\mathsf{g}_{\text{d}} = 0.1$. The unstable region is the set of points to the right of the separatrices.

- if $\mathsf{g}_{\text{d}} > 0$, then the function $\tilde{f}_2^{\text{d}}/\tilde{f}_1^{\text{d}}(z_1, z_2)$ is monotone decreasing in g_{d} and monotone decreasing in k_-.

As such, we compute the partial derivatives with respect to these parameters, and we find that for any $\mathsf{g}_{\text{d}} \geq 0$ at $(z_1, z_2) \in \mathsf{T}$:

$$
\begin{aligned}
\frac{\partial(\tilde{f}_2^{\text{d}}/\tilde{f}_1^{\text{d}})}{\partial k_+} &= \frac{2k_-\sqrt{z_1}}{\Upsilon^2}\Bigg\{2\sqrt{z_2}(z_2 - z_1) \\
&\quad + k_-\sqrt{z_1 z_2^3}\left(\frac{z_1}{z_2} - 1 - \ln\left(\frac{z_1}{z_2}\right)\right) - k_-\mathsf{g}_{\text{d}}(\sqrt{z_2} - \sqrt{z_1})\Bigg\}, \\
\frac{\partial(\tilde{f}_2^{\text{d}}/\tilde{f}_1^{\text{d}})}{\partial k_-} &= -\frac{2k_+\sqrt{z_2}}{\Upsilon^2}\Bigg\{2\sqrt{z_1}(z_2 - z_1) \\
&\quad + k_+\sqrt{z_1^3 z_2}\left(\frac{z_2}{z_1} - 1 - \ln\left(\frac{z_2}{z_1}\right)\right) + k_+\mathsf{g}_{\text{d}}(\sqrt{z_2} - \sqrt{z_1})\Bigg\}, \\
\frac{\partial(\tilde{f}_2^{\text{d}}/\tilde{f}_1^{\text{d}})}{\partial \mathsf{g}_{\text{d}}} &= -\frac{2k_+k_-(\sqrt{z_2} - \sqrt{z_1})}{\Upsilon^2} \\
&\quad \times \left(k_+\sqrt{z_2} + k_-\sqrt{z_1} + k_+k_-\sqrt{z_2 z_1}\ln\left(\sqrt{\frac{z_2}{z_1}}\right)\right),
\end{aligned}
\tag{3.4.23}
$$

where

$$\Upsilon = 2\sqrt{z_2 z_1}(k_+\sqrt{z_1} + k_-\sqrt{z_2}) + k_+k_-(\sqrt{z_2} - \sqrt{z_1})(z_1\sqrt{z_2} + \sqrt{z_1}z_2 + \mathsf{g}_{\mathrm{d}}). \quad (3.4.24)$$

As written, it is clear that $\partial(\tilde{f}^{\mathrm{d}}{}_2/\tilde{f}^{\mathrm{d}}{}_1(z_1, z_2))/\partial \mathsf{g}_{\mathrm{d}} > 0$ for all $(z_1, z_2) \in \mathsf{T}$. Note that

$$t - 1 - \ln t > 0, \quad (3.4.25)$$

for all $t > 0$ since ln is a concave function and $y = t - 1$ is a tangent line to $y = \ln t$. Hence, $\partial(\tilde{f}^{\mathrm{d}}{}_2/\tilde{f}^{\mathrm{d}}{}_1(z_1, z_2))/\partial k_- < 0$ for all $\mathsf{g}_{\mathrm{d}} \geq 0$ and that $\partial(\tilde{f}^{\mathrm{d}}{}_2/\tilde{f}^{\mathrm{d}}{}_1(z_1, z_2))/\partial k_+ > 0$ if $\mathsf{g}_{\mathrm{d}} = 0$, where $k_\pm \geq 0$ with at least one $k_\pm$ nonzero, for all $(z_1, z_2) \in \mathsf{T}$. This completes the proof. □

The above theorem implies that increasing a Schwoebel barrier (by decreasing k_-) tends to increase the prevalence of step collisions. Moreover, the line tension g_{d} is stabilizing. This is not surprising, since the line tension is acting more strongly to shrink the step with high curvature, which is the inner step.

3.5 Concentric steps: growth with desorption

Recall that the boundary value problem (3.3.14)-(3.3.15) incorporates the effect of desorption, in contrast to the previous section. Here we neglect the effect of line tension, and study step motion governed by:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) - u + 1 = 0 \qquad \text{in } (0, r_1) \cup (r_1, r_2) \cup (r_2, 1), \quad (3.5.1)$$

with boundary conditions

$$\left.\begin{array}{rcll} -\dfrac{\partial u^+}{\partial r} &=& k_+u^+ & \text{at } r = r_1, r_2, \\ \dfrac{\partial u^-}{\partial r} &=& k_-u^- & \text{at } r = r_1, r_2, \\ u(0) &<& \infty, & \\ \dfrac{\partial u^+}{\partial r} &=& 0 & \text{at } r = R, \end{array}\right\} \quad (3.5.2)$$

and

$$\dot{r}_n = \left[\!\left[\frac{\partial u}{\partial r} \right]\!\right]_{r=r_n} \qquad \text{for } n = 1, 2. \tag{3.5.3}$$

The main result of this section is that there exists a unique separatrix, for the step motions governed by (3.5.1)-(3.5.2) and (3.5.3) forming the boundary of the stable and unstable regions, S and U in the region of admissible step positions

$$\mathsf{T}(R) = \{(r_1, r_2) \in \mathbb{R}^2 \colon 0 < r_1 < r_2 < R\}. \tag{3.5.4}$$

We showed similar facts in the preceding sections.

The general solution to the ODE (3.5.1) is a linear combination of the modified Bessel functions, and, therefore, the velocity equations involve I_0, I_1, K_0, and K_1.[1] For the sake of notational brevity, we introduce the following functions:

$$\left.\begin{aligned} \sigma_1(x,y) = &\quad K_1(x)I_1(y) - I_1(x)K_1(y), \\ \sigma_2(x,y) = &\quad I_0(x)K_1(y) + K_0(x)I_1(y), \\ \sigma_3(x,y) = &\quad I_1(x)K_0(y) + K_1(x)I_0(y), \\ \sigma_4(x,y) = &\quad K_0(x)I_0(y) - I_0(x)K_0(y). \end{aligned}\right\} \tag{3.5.6}$$

Note that $\sigma_3(x,y) = \sigma_2(y,x)$. Some useful facts about these functions are discussed in Appendix A, but we note the following:

$$\frac{\sigma_3(x,y)}{K_1(x)} = I_0(y) + \frac{I_1(x)K_0(y)}{K_1(x)} \geq 1 \text{ for all } x, y > 0, \tag{3.5.7}$$

[1]By Abramowitz and Stegun [21],

$$\begin{aligned} I_0(x) &= \sum_{j=0}^{\infty} \left(\frac{(x/2)^j}{j!} \right)^2, \quad I_1(x) = \frac{\mathrm{d}I_0(x)}{\mathrm{d}x}, \\ K_0(x) &= -\left(\ln\left(\frac{x}{2}\right) + \gamma\right) I_0(x) + \sum_{j=1}^{\infty} \left(\sum_{k=1}^{j} \frac{1}{k} \right) \left(\frac{(z/2)^j}{j!} \right)^2, \\ K_1(x) &= -\frac{\mathrm{d}K_0(x)}{\mathrm{d}x}, \end{aligned} \tag{3.5.5}$$

where γ is Euler's constant defined by $\gamma = \lim_{n\to\infty} \sum_{k=1}^{n} \frac{1}{k} - \ln n$.

since modified Bessel functions are positive on $(0,\infty)$ and I_0 is increasing with $I_0(0) = 1$.

Solving (3.3.14)-(3.3.15) explicitly and using this solution in (3.3.16), we find the step radii r_1 and r_2 satisfy

$$\left.\begin{aligned} \dot{r}_1 &= f_1^{\mathrm{ed}}(r_1, r_2), \\ \dot{r}_2 &= f_2^{\mathrm{ed}}(r_1, r_2), \end{aligned}\right\} \tag{3.5.8}$$

where

$$\left.\begin{aligned} f_1^{\mathrm{ed}}(r_1,r_2) &= f_{11}^{\mathrm{ed}}(r_1,r_2) + f_{12}^{\mathrm{ed}}(r_1,r_2), \\ f_2^{\mathrm{ed}}(r_1,r_2) &= f_{21}^{\mathrm{ed}}(r_1,r_2) + f_{22}^{\mathrm{ed}}(r_1,r_2), \\ f_{11}^{\mathrm{ed}}(r_1,r_2) &= \frac{-k_+ I_1(r_1)}{I_1(r_1) + k_+ I_0(r_1)}, \\ f_{12}^{\mathrm{ed}}(r_1,r_2) &= \frac{-(k_-\sigma_1(r_1,r_2) + k_+k_-\left(\sigma_3(r_1,r_2) - \sigma_3(r_1,r_1)\right))}{\sigma_1(r_1,r_2) + k_-\sigma_2(r_1,r_2) + k_+\sigma_3(r_1,r_2) + k_+k_-\sigma_4(r_1,r_2)}, \\ f_{21}^{\mathrm{ed}}(r_1,r_2) &= \frac{-(k_+\sigma_1(r_1,r_2) + k_+k_-(\sigma_2(r_1,r_2) - \sigma_2(r_2,r_2)))}{\sigma_1(r_1,r_2) + k_-\sigma_2(r_1,r_2) + k_+\sigma_3(r_1,r_2) + k_+k_-\sigma_4(r_1,r_2)}, \\ f_{22}^{\mathrm{ed}}(r_1,r_2) &= \frac{-k_-\sigma_1(r_2,R)}{k_-\sigma_2(r_2,R) + \sigma_1(r_2,R)}, \end{aligned}\right\} \tag{3.5.9}$$

where the functions σ_k for $k = 1, 2, 3,$ and 4 are defined in (3.5.6). The right-hand sides f_1^{ed} and f_2^{ed} of (3.5.8) are negative in $\mathsf{T}(R)$. This is a consequence of the following:

- I_0, I_1 are positive on $(0,\infty)$;
- on the domain $\mathsf{T}(R)$, the functions σ_k are positive for $k = 1, 2, 3,$ and 4 (see Appendix A);
- σ_2 is decreasing in its first argument;
- σ_3 is increasing in its second argument.

In particular, there are no equilibrium points of the system (3.5.8), and solutions (r_1, r_2) in $\mathsf{T}(R)$ are monotone decreasing in t, and therefore for each trajectory there exists points (A_1, A_2) and (B_1, B_2) on the boundary $\partial\mathsf{T}(R)$ at which the trajectories enter and exit, respectively.

Existence

So far, we have seen only that any trajectory through $\mathsf{T}(R)$ must enter and exit at boundary points. We show that there exist trajectories that exit at boundary points of the form (r,r) or $(0,r)$ for $0<r<\varepsilon$, provided that $\varepsilon>0$ is sufficiently small. As a first step toward establishing this, we first show that for a continuous extension of $(f_1^{\mathrm{ed}}, f_2^{\mathrm{ed}})$ to $\mathbb{R}^2$, there exist trajectories through any point on the boundary of $\mathsf{T}(R)$. This amounts to proving that there exists a continuous extension of $(f_1^{\mathrm{ed}}, f_2^{\mathrm{ed}})$ to $\mathbb{R}^2$ by Peano's existence theorem.

Theorem 3.5.1 (Peano's existence theorem)**.** *If $f:(-\infty,\infty)\times \mathsf{D}\to \mathsf{D}$ is continuous for a domain $\mathsf{D}\subset\mathbb{R}^n$, then for any $y_0\in \mathsf{D}$ there exists at least one solution to the initial value problem*

$$\left.\begin{aligned} \frac{dy}{dt} &= f(t,y), \\ y(0) &= y_0. \end{aligned}\right\} \tag{3.5.10}$$

We apply Peano's existence theorem to points on the boundary of $\mathsf{T}(R)$. Hence, we prove that $(f_1^{\mathrm{ed}}, f_2^{\mathrm{ed}})$ may be continuously extended to $\mathbb{R}^2$. To do this we first prove the following lemma.

Lemma 3.5.2. *For any $r\geq 0$, we have the following limits:*

$$\left.\begin{aligned} \lim_{\substack{(x,y)\to(0,r)\\(x,y)\in\mathsf{T}(R)}} \frac{\sigma_1(x,y)}{K_1(x)} &= I_1(r), \\ \lim_{\substack{(x,y)\to(0,r)\\(x,y)\in\mathsf{T}(R)}} \frac{\sigma_3(x,y)}{K_1(x)} &= I_0(r), \\ \lim_{\substack{(x,y)\to(0,r)\\(x,y)\in\mathsf{T}(R)}} \frac{\sigma_4(x,y)}{K_1(x)} &= 0. \end{aligned}\right\} \tag{3.5.11}$$

Moreover, for any $r>0$, we have

$$\lim_{\substack{(x,y)\to(0,r)\\(x,y)\in\mathsf{T}(R)}} \frac{\sigma_2(x,y)}{K_1(x)} = 0. \tag{3.5.12}$$

Proof. By Abramowitz and Stegun [21], the small-argument asymptotics for K_0 and K_1 are given by

$$\left.\begin{aligned} K_0(x) &\sim -\ln x, && \text{as } x \downarrow 0, \\ K_1(x) &\sim \frac{1}{x}, && \text{as } x \downarrow 0, \end{aligned}\right\} \tag{3.5.13}$$

where $f \sim g$ as $x \downarrow 0$ means

$$\lim_{x\downarrow 0} \frac{f(x)}{g(x)} = 1. \tag{3.5.14}$$

Hence, we have

$$\lim_{x\downarrow 0} \frac{K_0(x)}{K_1(x)} = \frac{\left(\lim\limits_{x\downarrow 0} -\dfrac{K_0(x)}{\ln x}\right)\left(\lim\limits_{x\downarrow 0} -x\ln x\right)}{\lim\limits_{x\downarrow 0} \dfrac{K_1(x)}{1/x}} = 0. \tag{3.5.15}$$

Since $K_1(x) \to \infty$, $I_0(x) \to 1$, and $I_1(x) \to 0$ as $x \downarrow 0$, it is clear that

$$\lim_{x\downarrow 0} \frac{I_0(x)}{K_1(x)} = \lim_{x\downarrow 0} \frac{I_1(x)}{K_1(x)} = 0. \tag{3.5.16}$$

1. We now prove $(3.5.11)_1$. For any $r \geq 0$,

$$\begin{aligned} \lim_{\substack{(x,y)\to(0,r)\\(x,y)\in\mathsf{T}(R)}} \frac{\sigma_1(x,y)}{K_1(x)} &= \lim_{\substack{(x,y)\to(0,r)\\(x,y)\in\mathsf{T}(R)}} I_1(y) - K_1(y)\frac{I_1(x)}{K_1(x)} \\ &= I_1(r) - \lim_{\substack{(x,y)\to(0,r)\\(x,y)\in\mathsf{T}(R)}} \frac{K_1(y)}{K_1(x)} I_1(x). \end{aligned} \tag{3.5.17}$$

   Since K_1 is monotone decreasing, we have that $0 < \frac{K_1(y)}{K_1(x)} < 1$ for any $0 < x < y$. Therefore, given any $\varepsilon > 0$, we may chose $\delta > 0$ such that if $0 < x < \delta$, then $0 < I_1(x) < \varepsilon$ (since I_1 is continuous with $I_1(0) = 0$), and therefore for any $(x,y) \in \mathsf{T}(R)$ with $x < \delta$:

$$0 < \frac{K_1(y)}{K_1(x)} I_1(x) < \varepsilon. \tag{3.5.18}$$

   Hence, we have

$$\lim_{\substack{(x,y)\to(0,r)\\(x,y)\in\mathsf{T}(R)}} \frac{\sigma_1(x,y)}{K_1(x)} = I_1(r). \tag{3.5.19}$$

2. Similarly, to establish $(3.5.11)_{2,3}$, note that we have for any $r \geq 0$,

$$\lim_{\substack{(x,y)\to(0,r)\\(x,y)\in\mathsf{T}(R)}} \frac{\sigma_3(x,y)}{K_1(x)} = \lim_{\substack{(x,y)\to(0,r)\\(x,y)\in\mathsf{T}(R)}} I_0(y) + I_1(x)\frac{K_0(y)}{K_1(x)} \tag{3.5.20}$$

and

$$\lim_{\substack{(x,y)\to(0,r)\\(x,y)\in\mathsf{T}(R)}} \frac{\sigma_4(x,y)}{K_1(x)} = \lim_{\substack{(x,y)\to(0,r)\\(x,y)\in\mathsf{T}(R)}} I_0(y)\frac{K_0(x)}{K_1(x)} - I_0(x)\frac{K_0(y)}{K_1(x)}. \tag{3.5.21}$$

Since for any $0 < x < y$,

$$0 < \frac{K_0(y)}{K_1(x)} \leq \frac{K_0(x)}{K_1(x)} \to 0 \text{ as } x \downarrow 0, \tag{3.5.22}$$

the limits $(3.5.11)_{2,3}$ follow.

3. Finally, for any $r > 0$,

$$\begin{aligned}\lim_{\substack{(x,y)\to(0,r)\\(x,y)\in\mathsf{T}(R)}} \frac{\sigma_2(x,y)}{K_1(x)} &= \lim_{x\to 0} \frac{I_0(x)}{K_1(x)} \lim_{y\to r} K_1(y) + \lim_{x\to 0} \frac{K_0(x)}{K_1(x)} \lim_{y\to r} I_1(y) \\ &= 0.\end{aligned} \tag{3.5.23}$$

This proves (3.5.12).

□

With this lemma, we turn to proving that $(f_1^{\text{ed}}, f_2^{\text{ed}})$ may be continuously extended to $\mathbb{R}^2$, and we then show that solutions through points on the boundary of $\mathsf{T}(R)$ either enter or exit.

Lemma 3.5.3. *There exist continuous extensions of (f_1^{ed}, f_2^{ed}) to all of $\mathbb{R}^2$. For any such continuous extension, there exist trajectories of (3.5.8) through any point in $\mathbb{R}^2$, and in particular, through any point on $\partial\mathsf{T}(R)$.*

Proof. The second statement follows from the first directly according to Peano's existence theorem.

Let $\overline{\mathsf{T}}(R)$ denote the closure of $\mathsf{T}(R)$. Note that any continuous function $\mathbf{f}$: $\overline{\mathsf{T}}(R) \to \mathbb{R}^2$ may be continuously extended to a function $\tilde{\mathbf{f}} : \mathbb{R}^2 \to \mathbb{R}^2$, with the following definition

$$\tilde{\mathbf{f}}(x,y) = \begin{cases} \mathbf{f}(0,R) & \text{if } x \le 0 \text{ and } y \ge R, \\ \mathbf{f}(0,y) & \text{if } x \le 0 \text{ and } 0 \le y \le R, \\ \mathbf{f}(0,0) & \text{if } x \le 0 \text{ and } y \le 0, \\ \mathbf{f}(x,R) & \text{if } 0 \le x \le R \text{ and } y \ge R, \\ \mathbf{f}(x,y) & \text{if } 0 \le x \le y \ge R, \\ \mathbf{f}(x,x) & \text{if } 0 \le x \le R \text{ and } y \le x, \\ \mathbf{f}(R,R) & \text{if } x \ge R. \end{cases} \tag{3.5.24}$$

Hence, it suffices to show that $(f_1^{\text{ed}}, f_2^{\text{ed}})$ may be continuously extended to the boundary $\partial\mathsf{T}(R)$.

It is clear from the definition in (3.5.9) that the function f_{11}^{ed} is continuous in $\overline{\mathsf{T}}(R)$, noting that $I_0(0) = 1$ and $I_1(0) = 0$. From the definition (3.5.9), we see that f_{22}^{ed} is continuous on $\overline{\mathsf{T}}(R) - \{(0,0)\}$, and

$$\begin{aligned} \lim_{\substack{(x,y)\to(0,0) \\ (x,y)\in\mathsf{T}(R)}} f_{22}^{\text{ed}}(x,y) &= -\frac{k_-\left(\lim_{y\downarrow 0}\frac{\sigma_1(y,R)}{K_1(y)}\right)}{\lim_{y\downarrow 0}\frac{k_-\sigma_2(y,R)}{K_1(y)} + \frac{\sigma_1(y,R)}{K_1(y)}} \\ &= -k_-. \end{aligned} \tag{3.5.25}$$

Hence, there exists a continuous extension of f_{22}^{ed} to $\overline{\mathsf{T}}(R)$.

From the definitions of f_{12}^{ed} and f_{21}^{ed} it is clear that these functions are continuous up to the edges $\{(x,R) \in \mathbb{R}^2 \colon 0 < x \le R\}$ and $\{(x,x) \colon 0 < x \le R\}$. We establish the existence of the limits approaching the edge $\{(0,y) \colon 0 < y \le R\}$ and the point $(0,0)$.

Let $0 < r \le R$ be given. Then

$$\lim_{\substack{(x,y)\to(0,r)\\(x,y)\in\mathsf{T}(R)}} f_{12}^{\text{ed}}(x,y) = \lim_{\substack{(x,y)\to(0,r)\\(x,y)\in\mathsf{T}(R)}} -\frac{k_-\frac{\sigma_1(x,y)}{K_1(x)} + k_+k_-\left(\frac{\sigma_3(x,y)}{K_1(x)} - \frac{\sigma_3(x,x)}{K_1(x)}\right)}{\frac{\sigma_1(x,y)}{K_1(x)} + k_-\frac{\sigma_2(x,y)}{K_1(x)} + k_+\frac{\sigma_3(x,y)}{K_1(x)} + k_+k_-\frac{\sigma_4(x,y)}{K_1(x)}}$$
$$= -\frac{k_+I_1(r) + k_+k_-(I_0(r)-1)}{I_1(r) + k_+I_0(r)}, \tag{3.5.26}$$

and

$$\lim_{\substack{(x,y)\to(0,r)\\(x,y)\in\mathsf{T}(R)}} f_{21}^{\text{ed}}(x,y) = \lim_{\substack{(x,y)\to(0,r)\\(x,y)\in\mathsf{T}(R)}} -\frac{k_+\frac{\sigma_1(x,y)}{K_1(x)} + k_+k_-\left(\frac{\sigma_2(x,y)}{K_1(x)} - \frac{\sigma_2(y,y)}{K_1(x)}\right)}{\frac{\sigma_1(x,y)}{K_1(x)} + k_-\frac{\sigma_2(x,y)}{K_1(x)} + k_+\frac{\sigma_3(x,y)}{K_1(x)} + k_+k_-\frac{\sigma_4(x,y)}{K_1(x)}}$$
$$= -\frac{k_+I_1(r)}{I_1(r) + k_+I_0(r)}. \tag{3.5.27}$$

Finally, we show that

$$\lim_{\substack{(x,y)\to(0,0)\\(x,y)\in\mathsf{T}(R)}} f_{12}^{\text{ed}}(x,y) = \lim_{\substack{(x,y)\to(0,0)\\(x,y)\in\mathsf{T}(R)}} f_{21}^{\text{ed}}(x,y) = 0. \tag{3.5.28}$$

Note that by (3.5.7) and the fact that $\sigma_k(x,y) > 0$ for all $(x,y) \in \mathsf{T}(R)$, we have that

$$\frac{\sigma_1(x,y)}{K_1(x)} + k_-\frac{\sigma_2(x,y)}{K_1(x)} + k_+\frac{\sigma_3(x,y)}{K_1(x)} + k_+k_-\frac{\sigma_4(x,y)}{K_1(x)} \ge k_+. \tag{3.5.29}$$

Let $\varepsilon > 0$ be given. Since

- I_0 is continuous on $[0,1]$ with $I_0(0) = 1$,
- I_1 is continuous at 0 with $I_1(0) = 0$, and
- $K_0(x)/K_1(x) \to 0$ as $x \downarrow 0$,

we may choose $\delta > 0$ such that: for all $y, x > 0$ such that $0 < x < y < \delta$, we have

$$|I_0(y) - I_0(x)|, \frac{K_0(x)}{K_1(x)} < \frac{\varepsilon}{3k_-} \text{ and } I_1(x) < \min\left(\frac{\varepsilon}{3}\left(1 + \frac{k_-}{k_+}\right)^{-1}, 1\right). \tag{3.5.30}$$

Then for $(x,y) \in \mathsf{T}(R)$ with $0 < x < y < \delta$, it follows that

$$|f_{12}^{\text{ed}}(x,y)| = \frac{k_-I_1(x)\left(1 - \frac{K_1(y)}{K_1(x)}\right) + k_+(I_1(y) - I_1(x)) + k_+k_-\frac{\sigma_3(x,y)-\sigma_3(x,x)}{K_1(x)}}{\frac{\sigma_1(x,y)}{K_1(x)} + k_-\frac{\sigma_2(x,y)}{K_1(x)} + k_+\frac{\sigma_3(x,y)}{K_1(x)} + k_+k_-\frac{\sigma_4(x,y)}{K_1(x)}}$$
$$\le \frac{k_-I_1(x)\left[1 - \frac{K_1(y)}{K_1(x)}\right]}{k_+} + (I_1(y) - I_1(x)) + \frac{k_-(\sigma_3(x,y) - \sigma_3(x,x))}{K_1(x)}. \tag{3.5.31}$$

By the monotonicity of K_1, I_1, and σ_3, we have that

$$0 < 1 - K_1(y)/K_1(x) < 1, \quad 0 < I_1(y) - I_1(x) < I_1(y), \tag{3.5.32}$$

and

$$\begin{aligned}
\frac{\sigma_3(x,y) - \sigma_3(x,x)}{K_1(x)} &= \left|\frac{\sigma_3(x,y) - \sigma_3(x,x)}{K_1(x)}\right| \\
&= \left|I_0(y) - I_0(x) + I_1(x)\left[\frac{K_0(y)}{K_1(x)} - \frac{K_0(x)}{K_1(x)}\right]\right| \\
&\le I_0(y) - I_0(x) + I_1(x)\left|\frac{K_0(y) - K_0(x)}{K_1(x)}\right| \\
&= I_0(y) - I_0(x) + I_1(x)\frac{K_0(x) - K_0(y)}{K_1(x)} \\
&\le I_0(y) - I_0(x) + I_1(x)\frac{K_0(x)}{K_1(x)}.
\end{aligned} \tag{3.5.33}$$

Hence, for $0 < x < y < \delta$, by (3.5.30) we have

$$\begin{aligned}
|f_{12}^{\text{ed}}(x,y)| &\le \frac{k_-}{k_+}I_1(x) + I_1(y) + k_-\left(I_0(y) - I_0(x) + I_1(x)\frac{K_0(x)}{K_1(x)}\right) \\
&< \frac{\varepsilon}{3} + \frac{\varepsilon}{3} + k_-\frac{K_0(x)}{K_1(x)} < \varepsilon.
\end{aligned} \tag{3.5.34}$$

We argue similarly for f_{21}^{ed}. By (3.5.29), for any $(x,y) \in \mathsf{T}(R)$ we have that

$$\begin{aligned}
|f_{21}^{\text{ed}}(x,y)| &= \frac{k_+\frac{\sigma_1(x,y)}{K_1(x)} + k_+k_-\left(\frac{\sigma_2(x,y)}{K_1(x)} - \frac{\sigma_2(y,y)}{K_1(x)}\right)}{\frac{\sigma_1(x,y)}{K_1(x)} + k_-\frac{\sigma_2(x,y)}{K_1(x)} + k_+\frac{\sigma_3(x,y)}{K_1(x)} + k_+k_-\frac{\sigma_4(x,y)}{K_1(x)}} \\
&\le \frac{\sigma_1(x,y)}{K_1(x)} + k_-\left(\frac{\sigma_2(x,y)}{K_1(x)} - \frac{\sigma_2(y,y)}{K_1(x)}\right) \\
&\le I_1(y) + k_-\left(I_1(y)\frac{K_0(y)}{K_1(x)}I_0(y) - I_0(x)\right) \to 0
\end{aligned} \tag{3.5.35}$$

as $(x,y) \to (0,0)$ and $(x,y) \in \mathsf{T}(R)$.

This proves that $(f_1^{\text{ed}}, f_2^{\text{ed}})$ may be continuously extended to the closure of $\mathsf{T}(R)$ and, therefore, to all of $\mathbb{R}^2$. □

We now record some observations about the continuous extension $\tilde{\mathbf{f}} = (f_1, f_2)$ of $\mathbf{f} = (f_1^{\text{ed}}, f_2^{\text{ed}})$ to $\mathbb{R}^2$ as defined in (3.5.24). Observe that

1. $f_1 = f_1^{\text{ed}} < 0$ and $f_2 = f_2^{\text{ed}} < 0$ on $\mathsf{T}(R)$;

2. for $0 < r \leq R$,

$$\begin{aligned} f_1(0,r) = &-\frac{k_+ I_1(r) + k_+ k_-(I_0(r)-1)}{I_1(r) + k_+ I_0(r)} < 0, \\ f_2(0,r) \leq &-\frac{k_+ I_1(r)}{I_1(r) + k_+ I_0(r)} < 0; \end{aligned} \tag{3.5.36}$$

3. and for $0 < r < R$,

$$\begin{aligned} f_1(r,R) \leq &-\frac{k_+ I_1(r)}{I_1(r) + k_+ I_0(r)} < 0, \\ f_2(r,R) = &-\frac{k_+\sigma_1(r,R) + k_+ k_-(\sigma_2(r,R) - \sigma_2(R,R))}{\sigma_1(r,R) + k_-\sigma_2(r,R) + k_+\sigma_3(r,R) + k_+ k_-\sigma_4(r,R)} < 0. \end{aligned} \tag{3.5.37}$$

Therefore, the functions f_1 and f_2 are negative on $\{(x,y) : 0 \leq x < R \text{ and } x < y \leq R\}$.

Since $f_1(0,r) < 0$ for all $0 < r < R$, it is clear that any trajectory through $(0,r)$ in $\mathbb{R}^2$ contains a trajectory in $\mathsf{T}(R)$ that exits at the point $(0,r)$. Since $f_2(r,R) < 0$ for all $0 < r < R$, it is also clear that any trajectory through (r,R) in $\mathbb{R}^2$ contains a trajectory in $\mathsf{T}(R)$ that enters at the point (r,R). To determine if there are trajectories which enter or exit at points of the form (r,r) for $0 < r < R$, we consider the sign of $f_1(r,r) - f_2(r,r)$: if it is positive, then a trajectory exits $\mathsf{T}(R)$ at (r,r); whereas if it is negative, then a trajectory enters $\mathsf{T}(R)$ at (r,r).

Lemma 3.5.4. *There exists a unique* $0 < r_0 < R$ *such that* $f_1(r,r) - f_2(r,r) > 0$ *for* $0 < r < r_0$ *and* $f_1(r,r) - f_2(r,r) < 0$ *for* $r_0 < r < R$. *It follows that there exist trajectories that exit* $\mathsf{T}(R)$ *at points of the form* (r,r) *if* $0 < r < r_0$ *and there exist trajectories that enter* $\mathsf{T}(R)$ *at points of the form* (r,r) *if* $r_0 < r < R$.

This lemma implies the following fact about step motions. For each $0 < r < R$, consider initial step configurations $0 < r_1^{(n)} < r_2^{(n)} < R$ such that $r_1^{(n)}, r_2^{(n)} \to r$ as $n \to \infty$. On the one hand, if $r > r_0$, the step motions with initial position $r_1^{(n)}$ and $r_2^{(n)}$ initially spread so as to make the middle terrace wider, if n is large enough. On the other hand, if $r < r_0$, the step motions move together leading to a step collision, if n is large enough.

The proof of this lemma requires facts about log-convex functions.

Definition 3.5.5. *A function,* $f : D \to \mathbb{R}$*, where* $D \subset \mathbb{R}$ *is* log-convex *if* $x \mapsto \ln(f(x))$ *is convex. Equivalently,* f *is log-convex if for every* x, y *and* $0 < \lambda < 1$*, we have*

$$f(\lambda x + (1-\lambda)y) \leq f(x)^{\lambda} f(y)^{1-\lambda}. \tag{3.5.38}$$

It is easy to see that f is convex if it is log-convex, since $f(x) = e^{\ln(f(x))}$. Moreover, the sum of two log-convex functions is also log-convex. This follows from Hölder's inequality.

Specifically, let f and g be two log-convex functions with convex common domain and let x, y be two points in that domain and $0 < \lambda < 1$. For $p = 1/\lambda$ and $q = 1/(1-\lambda)$, we have that $p, q > 0$ and $\frac{1}{p} + \frac{1}{q} = 1$. Put

$$a_1 = f(x)^{1/p},\ a_2 = g(x)^{1/p},\ b_1 = f(x)^{1/q},\ \text{ and } b_2 = g(y)^{1/q}.$$

Then

$$\begin{aligned}
(f+g)(\lambda x + (1-\lambda)y) &\leq f(x)^{\lambda} f(y)^{1-\lambda} + g(x)^{\lambda} g(y)^{1-\lambda} \\
&= a_1 b_1 + a_2 b_2 \\
&\leq (a_1^p + a_2^p)^{1/p} (b_1^q + b_2^q)^{1/q} \\
&= (f(x) + g(x))^{\lambda} (f(y) + g(y))^{1-\lambda}.
\end{aligned}$$

We now prove Lemma 3.5.4.

Proof. Note that for all $0 < r < R$,

$$\begin{aligned}
f_1(r,r) - f_2(r,r) &= f_{11}(r,r) - f_{22}(r,r) \\
&= -\frac{k_+ I_1(r)}{I_1(r) + k_+ I_0(r)} + \frac{k_- \sigma_1(r,R)}{k_- \sigma_2(r,R) + \sigma_1(r,R)}.
\end{aligned} \tag{3.5.39}$$

Since

$$f_1(R,R) - f_2(R,R) = -\frac{k_+ I_1(R)}{I_1(R) + k_+ I_0(R)} < 0 \tag{3.5.40}$$

and

$$f_1(0,0) - f_2(0,0) = k_- > 0, \tag{3.5.41}$$

it suffices to show that $f_1(r,r) - f_2(r,r)$ is monotone decreasing in r for $0 < r < R$. In particular, we show that $f_{11}(r,r)$ is monotone decreasing and $f_{22}(r,r)$ is monotone increasing in r. Recall that $I_0'(r) = I_1(r)$. Therefore,

$$f_{11}(r,r) = -\frac{k_+ I_0'(r)}{I_0'(r) + k_+ I_0(r)}. \tag{3.5.42}$$

Since I_0 is strictly log-convex [22], we have that $I_0'' I_0 - I_0'^2 > 0$. Hence, for all $0 < r \leq R$,

$$\frac{\mathrm{d} f_{11}(r,r)}{\mathrm{d}r} = -\frac{k_+^2}{(I_0'(r) + k_+ I_1(r))^2} \left(I_0''(r) I_0(r) - (I_0'(r))^2 \right) < 0. \tag{3.5.43}$$

Note that since

$$\frac{\partial \sigma_2(r_1, r_2)}{\partial r_1} = -\sigma_1(r_1, r_2), \tag{3.5.44}$$

the expression $f_{22}(r,R)$ may be re-written as

$$f_{22}(r,r) = \frac{k_- S_2'(r)}{k_- S_2(r) - S_2'(r)}, \tag{3.5.45}$$

where

$$S_2(r) = \sigma_2(r,R). \tag{3.5.46}$$

Therefore, $f_{22}(r,r)$ is increasing in r if and only if

$$\frac{\mathrm{d}(f_{22}(r,r))}{\mathrm{d}r} = \frac{k_-^2 (S_2''(r) S_2(r) - (S_2'(r))^2)}{(k_- S_2(r) - S_2'(r))^2} > 0. \tag{3.5.47}$$

This inequality (3.5.47) is equivalent to the requirement that $S_2''(r) S_2(r) - (S_2'(r))^2 > 0$, which in turn is equivalent to the function S_2 being a C^2 log-convex function. Since $K_1(R), I_1(R) > 0$ for $R > 0$ and I_0 and K_0 are log-convex (see [23]), we have that

$$S_2(r) = K_1(R) I_0(r) + I_1(R) K_0(r) \tag{3.5.48}$$

is a log-convex function, since S_2 is a sum two log-convex functions $K_1(R) I_0$ and $I_1(R) K_0$. □

Since trajectories of (3.5.8) inside $\mathsf{T}(R)$ exit the region at points of the form $(0, r)$ with $0 < r < R$ and at points of the form (r, r) with $0 < r < \min(r_0, R)$ for some $0 < r_0$, and since $f_2^{\text{ed}}, f_1^{\text{ed}}$ are negative on $\mathsf{T}(R)$, it follows, as in the previous cases, that there is at least one trajectory that exits $\mathsf{T}(R)$ at the point $(0, 0)$.

Uniqueness

The remainder of this section is devoted to showing the uniqueness of the separatrix, which is the trajectory exiting $\mathsf{T}(R)$ at $(0, 0)$. This is equivalent to the uniqueness of the solution to the integral equation:

$$\tilde{r}_2(r_1) = \int_0^{r_1} \frac{f_2(r, \tilde{r}_2(r))}{f_1(r, \tilde{r}_2(r))} \, \mathrm{d}r. \tag{3.5.49}$$

Since f_2/f_1 is smooth within $\mathsf{T}(R)$, it suffices to show that there is a unique solution on $[0, \eta)$ for some $\eta > 0$.

The continuous extension $\tilde{\mathbf{f}}$ in (3.5.24) is defined in such a way that if f_k^{ed} is monotone increasing or decreasing in its second variable, then the extension f_k is also monotone increasing or decreasing in its second variable. By Theorem B.1.1, it suffices to show that $f_2^{\text{ed}}/f_1^{\text{ed}}$ is monotone decreasing in its second argument for $0 < r_1 < r_2 < \eta$ and some $\eta > 0$. Since f_1^{ed} and f_2^{ed} are negative for $0 < r_1 < r_2$, we may show that f_1^{ed} is monotone decreasing and f_2^{ed} is monotone increasing in their second arguments on $0 < r_1 < r_2 < \eta$ for some $\eta > 0$. To do this, we first prove the following inequalities.

Lemma 3.5.6. *There exists an $\eta > 0$ such that for any $0 < r_1 < r_2 < \eta$,*

$$\left.\begin{aligned} \sigma_3(r_1, r_2) - \frac{\sigma_1(r_1, r_2)}{r_2} &> 0, \\ \sigma_2(r_1, r_2)\sigma_3(r_1, r_2) - \sigma_1(r_1, r_2)\sigma_4(r_1, r_2) &> 0, \\ \sigma_3(r_1, r_1) - \frac{\sigma_1(r_1, r_2)}{r_2} &> 0, \\ \sigma_1(r_1, r_2)\sigma_4(r_1, r_2) - \sigma_2(r_1, r_2)(\sigma_3(r_1, r_2) - \sigma_3(r_1, r_1)) &> 0. \end{aligned}\right\} \tag{3.5.50}$$

Proof. To prove $(3.5.50)_1$ and $(3.5.50)_3$, we show that the limit as $(r_1, r_2) \to (0,0)$ within $\mathsf{T}(R)$ of each left-hand side divided by $K_1(r_1)$ is positive. By [21], we have that

$$I_1(r) \sim \frac{r}{2} \text{ as } r \downarrow 0, \tag{3.5.51}$$

which is equivalent to

$$\lim_{r \downarrow 0} \frac{I_1(r)}{r} = \frac{1}{2}. \tag{3.5.52}$$

Hence,

$$\begin{aligned}
\lim_{\substack{(r_1,r_2)\to(0,0)\\(r_1,r_2)\in\mathsf{T}(R)}} \frac{\sigma_3(r_1,r_2)}{K_1(r_1)} - \frac{\sigma_1(r_1,r_2)}{r_2 K_1(r_1)} &= \lim_{\substack{(r_1,r_2)\to(0,0)\\(r_1,r_2)\in\mathsf{T}(R)}} \left(\frac{I_1(r_1)K_0(r_2)}{K_1(r_1)} + I_0(r_2) \right. \\
&\qquad \left. - \frac{I_1(r_2)}{r_2} + \frac{I_1(r_1)K_1(r_2)}{r_2 K_1(r_1)} \right) \\
&\geq \lim_{\substack{(r_1,r_2)\to(0,0)\\(r_1,r_2)\in\mathsf{T}(R)}} I_0(r_2) - \frac{I_2(r_2)}{r_2} \\
&= \frac{1}{2},
\end{aligned} \tag{3.5.53}$$

and, similarly,

$$\begin{aligned}
\lim_{\substack{(r_1,r_2)\to(0,0)\\(r_1,r_2)\in\mathsf{T}(R)}} \frac{\sigma_3(r_1,r_1)}{K_1(r_1)} - \frac{\sigma_1(r_1,r_2)}{r_2 K_1(r_1)} &\geq \lim_{\substack{(r_1,r_2)\to(0,0)\\(r_1,r_2)\in\mathsf{T}(R)}} I_0(r_1) - \frac{I_2(r_2)}{r_2} \\
&= \frac{1}{2}.
\end{aligned} \tag{3.5.54}$$

For brevity, put[2]

$$\psi_{20}(r_1,r_2) = \sigma_2(r_1,r_2)\sigma_3(r_1,r_2) - \sigma_1(r_1,r_2)\sigma_4(r_1,r_2),$$

$$\psi_{22}(r_1,r_2) = \sigma_1(r_1,r_2)\sigma_4(r_1,r_2) - \sigma_2(r_1,r_2)(\sigma_3(r_1,r_2) - \sigma_3(r_1,r_1)).$$

Establishing $(3.5.50)_2$ is a matter of algebra and recalling the fact that I_n, K_n are positive on $(0,\infty)$. Specifically,

$$\begin{aligned}
\psi_{20}(r_1,r_2) = K_0(r_1)I_1(r_1)\left[K_0(r_2)I_1(r_2) + K_1(r_2)I_0(r_2)\right] \\
+ K_1(r_1)I_0(r_1)\left[K_1(r_2)I_0(r_2) + K_0(r_2)I_1(r_2)\right] > 0.
\end{aligned} \tag{3.5.55}$$

[2]The rationale for this notation is found in (3.5.58).

Choose $\eta > 0$ sufficiently small so that for any $0 < r_1 < r_2 < \eta$ the inequalities $(3.5.50)_1$ and $(3.5.50)_3$ hold. To prove $(3.5.50)_4$, we note that

$$\psi_{22}(r,r) = \sigma_1(r,r)\sigma_4(r,r) = 0, \tag{3.5.56}$$

and

$$\begin{aligned}\frac{\partial \psi_{22}(r_1,r_2)}{\partial r_2} &= \sigma_4(r_1,r_2)\left(\sigma_3(r_1,r_1) - \frac{\sigma_1(r_1,r_2)}{r_2}\right) \\ &\quad + \frac{\sigma_2(r_1,r_2)}{r_2}(\sigma_3(r_1,r_2) - \sigma_3(r_1,r_1)).\end{aligned} \tag{3.5.57}$$

Since the first term is the product of $\sigma_4(r_1,r_2)$ and the left hand side of $(3.5.50)_3$ each of which is strictly positive for $0 < r_1 < r_2 < \eta$, and since σ_3 is increasing in its second argument, we have that ψ_{22} is strictly increasing in its second argument. Therefore, $\psi_{22}(r_1,r_2) > 0$ for any $0 < r_1 < r_2 < \eta$. □

We use Lemma 3.5.6 to show the monotonicity of f_1^{ed} and f_2^{ed} in the second argument.

Lemma 3.5.7. *There exists an $\varepsilon > 0$ such that for each $0 < r_1 < \varepsilon$:*

- *the function $r \mapsto f_1^{ed}(r_1, r)$ is decreasing for $r_1 < r < \varepsilon$, and*
- *the function $r \mapsto f_2^{ed}(r_1, r)$ is increasing for $r_1 < r < \varepsilon$.*

Proof. We show that for sufficiently small $\varepsilon > 0$, if $0 < r_1 < r_2 < \varepsilon$, then

$$\frac{\partial f_1^{\text{ed}}(r_1,r_2)}{\partial r_2} < 0 \text{ and } \frac{\partial f_2^{\text{ed}}(r_1,r_2)}{\partial r_2} > 0.$$

Since f_{11}^{ed} is constant in r_2, we have that

$$\frac{\partial f_1^{\text{ed}}(r_1,r_2)}{\partial r_2} = \frac{\partial f_{12}^{\text{ed}}(r_1,r_2)}{\partial r_2} = -\frac{\displaystyle\sum_{m,n=0}^{2} k_-^m k_+^n \psi_{mn}(r_1,r_2)}{(q^{\text{ed}}(r_1,r_2))^2}, \tag{3.5.58}$$

where

$$\left.\begin{aligned}
q^{\text{ed}}(r_1,r_2) = &\ \sigma_1(r_1,r_2) + k_-\sigma_2(r_1,r_2) + k_+\sigma_3(r_1,r_2) + k_+k_-\sigma_4(r_1,r_2),\\
\psi_{00} = &\ \psi_{01} = \psi_{02} = \psi_{10} \equiv 0,\\
\psi_{11}(r_1,r_2) = &\ \sigma_3(r_1,r_1)\left(\sigma_3(r_1,r_2) - \frac{\sigma_1(r_1,r_2)}{r_2}\right),\\
\psi_{12}(r_1,r_2) = &\ \sigma_1(r_1,r_2)\sigma_3(r_1,r_1),\\
\psi_{20}(r_1,r_2) = &\ \sigma_2(r_1,r_2)\sigma_3(r_1,r_2) - \sigma_1(r_1,r_2)\sigma_4(r_1,r_2),\\
\psi_{21}(r_1,r_2) = &\ \sigma_4(r_1,r_2)\left(\sigma_3(r_1,r_1) - \frac{\sigma_1(r_1,r_2)}{r_2}\right)\\
&+\frac{\sigma_2(r_1,r_2)}{r_2}(\sigma_3(r_1,r_2) - \sigma_3(r_1,r_1)),\\
\psi_{22}(r_1,r_2) = &\ \sigma_1(r_1,r_2)\sigma_4(r_1,r_2) - \sigma_2(r_1,r_2)(\sigma_3(r_1,r_2) - \sigma_3(r_1,r_1)).
\end{aligned}\right\} \quad (3.5.59)$$

Each of these $\psi_{nm}(r_1,r_2)$ is non-negative for $0 < r_1 < r_2 < \eta$ by Lemma 3.5.6 and Theorem A.2.1. This shows that f_1^{ed} is decreasing in its second argument for $0 < r_1 < r_2 < \eta$ where $\eta > 0$ is prescribed by Lemma 3.5.6.

To show that there exists an $\varepsilon_0 > 0$ such that f_2^{ed} is increasing in its second argument for $0 < r_1 < r_2 < \varepsilon_0$, we show that for some $\varepsilon_0 > 0$ and a constant $C < 0$, if $0 < r_1 < r_2 < \varepsilon_0$, then

$$\frac{\partial f_{21}^{\text{ed}}(r_1,r_2)}{\partial r_2} \geq C, \quad (3.5.60)$$

as well as the fact that

$$\lim_{\substack{(r_1,r_2)\to(0,0)\\(r_1,r_2)\in\mathsf{T}(R)}} \frac{\partial f_{22}(r_1,r_2)}{\partial r_2} = +\infty. \quad (3.5.61)$$

This implies that for some $\varepsilon_1 > 0$ the partial derivative $\frac{\partial f_2^{\text{ed}}(r_1,r_2)}{\partial r_2} > 0$ for all $0 < r_1 < r_2 < \varepsilon_1$.

Let p^{ed} be defined by

$$p^{\text{ed}}(r_1,r_2) = \sigma_1(r_1,r_2) + k_-(\sigma_2(r_1,r_2) - \sigma_2(r_2,r_2)), \quad (3.5.62)$$

so that for q^{ed} defined in (3.5.59)

$$f_{21}^{\text{ed}}(r_1, r_2) = -\frac{k_+ p^{\text{ed}}(r_1, r_2)}{q^{\text{ed}}(r_1, r_2)}. \tag{3.5.63}$$

Recall that by (3.5.29), we have for all $0 < r_1 < r_2$,

$$\frac{q^{\text{ed}}(r_1, r_2)}{K_1(r_1)} > 1. \tag{3.5.64}$$

Since

$$\frac{\partial f_{21}^{\text{ed}}(r_1, r_2)}{\partial r_2} = -k_+ \left(\frac{\frac{\partial p^{\text{ed}}(r_1, r_2)}{\partial r_2}}{q^{\text{ed}}(r_1, r_2)} - \frac{p^{\text{ed}}(r_1, r_2)\frac{\partial q^{\text{ed}}(r_1, r_2)}{\partial r_2}}{q^{\text{ed}}(r_1, r_2)^2} \right), \tag{3.5.65}$$

to show (3.5.60), it suffices to show that there exist $\varepsilon_1, C_1, C_2 > 0$ such that for $0 < r_1 < r_2 < \varepsilon_1$,

$$\frac{\frac{\partial p^{\text{ed}}(r_1, r_2)}{\partial r_2}}{q^{\text{ed}}(r_1, r_2)} \leq C_1 \text{ and } \frac{p^{\text{ed}}(r_1, r_2)\frac{\partial q^{\text{ed}}(r_1, r_2)}{\partial r_2}}{q^{\text{ed}}(r_1, r_2)^2} \geq -C_2. \tag{3.5.66}$$

Since $q^{\text{ed}}(r_1, r_2)/K_1(r_1) \geq k_+$ and

$$\begin{aligned} \frac{\partial p^{\text{ed}}(r_1, r_2)}{\partial r_2} &= k_- \left[\sigma_1(r_2, r_2) + \frac{\sigma_2(r_2, r_2) - \sigma_2(r_1, r_2)}{r_2} \right] \\ &\quad + k_- \left(\sigma_4(r_1, r_2) - \sigma_4(r_2, r_2) \right) + \sigma_3(r_1, r_2) \\ &\leq k_- \left[\sigma_1(r_2, r_2) + \frac{\sigma_2(r_2, r_2) - \sigma_2(r_1, r_2)}{r_2} + \sigma_4(r_1, r_2) \right] \\ &\quad + \sigma_3(r_1, r_2), \end{aligned} \tag{3.5.67}$$

we have

$$\frac{\frac{\partial p^{\text{ed}}(r_1, r_2)}{\partial r_2}}{q^{\text{ed}}(r_1, r_2)} \leq \frac{k_- \left(\sigma_1(r_2, r_2) + \frac{\sigma_2(r_2, r_2) - \sigma_2(r_1, r_2)}{r_2} + \sigma_4(r_1, r_2) + \frac{\sigma_3(r_1, r_2)}{k_-} \right)}{k_+ K_1(r_1)}, \tag{3.5.68}$$

where we have used

$$k_- \left(\frac{\sigma_1(r_2, r_2)}{K_1(r_1)} + \frac{\sigma_2(r_2, r_2) - \sigma_2(r_1, r_2)}{r_2 K_1(r_1)} + \frac{\sigma_4(r_1, r_2)}{K_1(r_1)} \right) + \frac{\sigma_3(r_1, r_2)}{K_1(r_1)} > 0 \tag{3.5.69}$$

on $\mathsf{T}(R)$. From Lemma 3.5.2, we see that $\sigma_1/K_1, \sigma_3/K_1$, and σ_4/K_1 are continuous functions on the compact set $\overline{\mathsf{T}}(R)$. Hence, we need only bound the term involving σ_2.

Given $\varepsilon_1 > 0$ and $0 < r_1 < r_2 < \varepsilon_1$, we may choose $r_1 < r < r_2$ such that $I_0(r_2) - I_0(r_1) = I_1(r)(r_2 - r_1)$, by the mean value theorem. Moreover, we have seen that

$$\lim_{t\downarrow 0} \frac{I_1(t)}{t} = \frac{1}{2} \text{ and } \lim_{t\downarrow 0} \frac{K_0(t)}{K_1(t)} = 0, \tag{3.5.70}$$

and therefore there is a bound M such that $|I_1(t)/t|, |K_0(t)/K_1(t)| < M$ for $t \in [0, \varepsilon_1]$. Hence, since $K_1(r_2)/K_1(r_1) < 1$ for $0 < r_1 < r_2$,

$$\begin{aligned}
\frac{\sigma_2(r_2, r_2) - \sigma_2(r_1, r_2)}{r_2 K_1(r_1)} &= \frac{I_0(r_2) - I_0(r_1)}{r_2} \frac{K_1(r_2)}{K_1(r_1)} + \frac{I_1(r_2)\left[\frac{K_0(r_2)}{K_1(r_2)} - \frac{K_0(r_1)}{K_1(r_1)}\right]}{r_2} \\
&\leq \frac{I_0(r_2) - I_0(r_1)}{r_2} + \frac{I_1(r_2)}{r_2} \frac{K_0(r_2)}{K_1(r_2)} \\
&= I_1(r) \frac{r_2 - r_1}{r_2} + \frac{I_1(r_2)}{r_2} \frac{K_0(r_2)}{K_1(r_2)} \\
&\leq I_1(\varepsilon_1) + M^2.
\end{aligned} \tag{3.5.71}$$

We have used the fact that I_1 is increasing and $0 < \frac{r_2 - r_1}{r_2} < 1$ for $(r_1, r_2) \in \mathsf{T}(R)$. This proves the first inequality in $(3.5.66)_1$.

We now show the second inequality $(3.5.66)_2$. Appealing to the differential relations (A.1.1) found in Appendix A, we find that

$$\begin{aligned}
\frac{\partial q^{\text{ed}}(r_1, r_2)}{\partial r_2} = &\left(k_+ - 1\frac{1}{r_2}\right) \sigma_1(r_1, r_2) + \left(1 - \frac{k_-}{r_2}\right) \sigma_2(r_1, r_2) \\
&+ \sigma_3(r_1, r_2) + k_- \sigma_4(r_1, r_2) \\
\geq &- \frac{\sigma_1(r_1, r_2)}{r_2} - k_- \frac{s_2(r_1, r_2)}{r_2}.
\end{aligned} \tag{3.5.72}$$

Since $p^{\text{ed}}(r_1, r_2) > 0$ on $\mathsf{T}(R)$,

$$\begin{aligned}
\frac{\frac{\partial q^{\text{ed}}(r_1, r_2)}{\partial r_2} p^{\text{ed}}(r_1, r_2)}{q^{\text{ed}}(r_1, r_2)^2} &\geq -\frac{1}{k_+^2} \left(\frac{\sigma_1(r_1, r_2)}{r_2 K_1(r_1)} + k_- \frac{\sigma_2(r_1, r_2)}{r_2 K_1(r_1)}\right) \frac{p^{\text{ed}}(r_1, r_2)}{K_1(r_1)} \\
&= -\frac{1}{k_+^2} \left(\frac{\sigma_1(r_1, r_2)}{K_1(r_1)} + k_- \frac{\sigma_2(r_1, r_2)}{K_1(r_1)}\right) \frac{p^{\text{ed}}(r_1, r_2)}{r_2 K_1(r_1)}.
\end{aligned} \tag{3.5.73}$$

We note

$$\begin{aligned}
0 < \frac{p^{\text{ed}}(r_1, r_2)}{r_2 K_1(r_1)} &= \frac{\sigma_1(r_1, r_2)}{r_2 K_1(r_1)} + k_- \frac{\sigma_2(r_1, r_2) - \sigma_2(r_2, r_2)}{r_2 K_1(r_1)} \\
&\leq \frac{I_1(r_2)}{r_2} + k_- \frac{\sigma_2(r_1, r_2) - \sigma_2(r_2, r_2)}{r_2 K_1(r_1)},
\end{aligned} \tag{3.5.74}$$

which is bounded since $I_1(t)/t \to \frac{1}{2}$ as $t \downarrow 0$ and inequality (3.5.71). If necessary, increase M, as defined after (3.5.70), to be larger than this bound. Then the boundedness from below of $\frac{\frac{\partial q^{\mathrm{ed}}(r_1,r_2)}{\partial r_2} p^{\mathrm{ed}}(r_1,r_2)}{q^{\mathrm{ed}}(r_1,r_2)^2}$ for $0 < r_1 < r_2 < \varepsilon_1$ follows from the fact that

$$\begin{aligned}
\frac{\frac{\partial q^{\mathrm{ed}}(r_1,r_2)}{\partial r_2} p^{\mathrm{ed}}(r_1,r_2)}{q^{\mathrm{ed}}(r_1,r_2)^2} &\geq -\frac{1}{k_+^2}\left(\frac{\sigma_1(r_1,r_2)}{K_1(r_1)} + k_- \frac{\sigma_2(r_1,r_2)}{K_1(r_1)}\right)\frac{p^{\mathrm{ed}}(r_1,r_2)}{r_2 K_1(r_1)} \\
&\geq -\frac{M}{k_+^2}\left[I_1(r_2) + k_-\left(\frac{I_0(r_1)K_1(r_2)}{K_1(r_1)} + \frac{I_1(r_2)K_0(r_1)}{K_1(r_2)}\right)\right] \\
&\geq -\frac{M}{k_+^2}\left(I_1(\varepsilon_1) + k_-\left(I_0(\varepsilon_1) + M^2\right)\right).
\end{aligned} \tag{3.5.75}$$

This proves the bound (3.5.60).

Finally, we show the limit (3.5.61) by Lemma 3.5.2:

$$\begin{aligned}
\lim_{\substack{(r_1,r_2)\to(0,0)\\(r_1,r_2)\in\mathsf{T}(R)}} \frac{\partial f_{22}^{\mathrm{ed}}(r_1,r_2)}{\partial r_2} &= \lim_{r_2\downarrow 0} k_-^2 \frac{\sigma_2(r_2,R)^2 - \sigma_1(r_2,R)^2 + \frac{\sigma_1(r_2,R)\sigma_2(r_2,R)}{r_2}}{(k_-\sigma_2(r_2,R) + \sigma_1(r_2,R))^2} \\
&= -\frac{k_-}{I_1(R)} + \frac{k_-}{I_1(R)} \lim_{r_2\downarrow 0} \frac{\sigma_2(r_2,R)}{r_2 K_1(r_2)}.
\end{aligned} \tag{3.5.76}$$

Explicitly,

$$\begin{aligned}
\lim_{r_2\downarrow 0} \frac{\sigma_2(r_2,R)}{r_2 K_1(r_2)} &= \lim_{r_2\downarrow 0} K_1(R)\frac{I_0(r_2)}{r_2 K_1(r_2)} + I_1(R)\frac{K_0(r_2)}{r_2 K_1(r_2)} \\
&\geq I_1(R) \lim_{r_2\downarrow 0} \frac{K_0(r_2)}{r_2 K_1(r_2)} \\
&= I_1(R) \lim_{r_2\downarrow 0} (-\ln r_2) \\
&= \infty,
\end{aligned} \tag{3.5.77}$$

by $(3.5.13)_1$ and $(3.5.13)_2$.

This completes our proof. □

4 A thermodynamically consistent step-flow model of epitaxial growth

4.1 Introduction

In Chapter 1, the derivation of the BCF model does not explicitly address compatibility with the laws of thermodynamics. In the present chapter, we adopt the perspective that the first and second laws of thermodynamics restrict the class of admissible constitutive relations. In particular, constitutive relations should be chosen such that the resulting dissipation inequality holds trivially. We review the development provided by Cermelli and Jabbour [11, 12], and take their model as the starting point for Chapters 5, 6, and 7.

The key result of this chapter is that the step chemical potential μ^{s} satisfies a modified Gibbs–Thomson relation:

$$\mu^{\mathrm{s}} = \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} - \frac{\tilde{\psi}^{\mathrm{s}}\kappa}{\varrho^{\mathrm{b}}} - \frac{[\![\omega]\!]}{\varrho^{\mathrm{b}}}, \tag{4.1.1}$$

where μ^{s} is the step chemical potential, Ψ^{b} is the bulk free energy per unit area, ϱ^{b} is the areal density of crystallized adatoms, $\tilde{\psi}^{\mathrm{s}}$ is the step stiffness, κ is the curvature of the step, and ω is grand canonical potential associated with the terrace adatoms. In contrast with the classical Gibbs–Thomson relation (1.2.23), the modified Gibbs–Thomson relation couples the adatom diffusion on adjacent terraces through boundary conditions that involve the jump in the grand canonical potential. The resulting step-flow model is called the TC model. It is consistent with the first and second laws of thermodynamics, holds away from equilibrium, and accounts explicitly for the dissipation that accompanies the diffusion of adatoms on terraces and the migration of steps that results from the attachment and detachment of adatoms to step edges. We then compare the BCF and TC models, and show that the BCF model may be viewed as a first-order approximation to the TC model, when the equilibrium coverage

$$\Theta = \frac{\varrho_{\mathrm{eq}}}{\varrho^{\mathrm{b}}} \tag{4.1.2}$$

is small. Finally, we state the simplifying assumptions that provide the starting point for the continuum limits derived in the subsequent chapters.

4.2 Mass balance including step adatom density

We return now to the derivation of the step-flow model, but modify the constitutive assumptions made in Section 1.2 so that step motions automatically satisfy the second law of thermodynamics. Recall that in Section 1.2, we found that mass balance localizes to

$$\left.\begin{aligned} \frac{\partial \varrho}{\partial t} &= -\operatorname{div}\mathbf{h} + R \qquad \text{in } \Omega_+ \cup \Omega_-, \\ \varrho^+ V - \mathbf{h}^+ \cdot \mathbf{n} &= J_+ \\ -\varrho^- V + \mathbf{h}^- \cdot \mathbf{n} &= J_- \qquad \text{along } \mathcal{S}, \\ \varrho^{\mathrm{b}} V &= J_+ + J_-. \end{aligned}\right\} \tag{4.2.1}$$

We parameterize $\mathcal{S}$ by a smooth function $\boldsymbol{\alpha} : \mathbb{R} \times [0, T) \to \mathbb{R}^2$ with $s \mapsto \boldsymbol{\alpha}(s, t)$ an arclength parameterization at each $t \in [0, T)$. For a subcurve Σ of $\mathcal{S}$, let $\boldsymbol{\alpha}(S_1(t), t) = \mathbf{R}_1(t)$ and $\boldsymbol{\alpha}(S_2(t), t) = \mathbf{R}_2(t)$ denote the endpoints of $\Sigma(t)$ such that

$$\Sigma(t) = \{\boldsymbol{\alpha}(s, t)\colon S_1(t) \leq s \leq S_2(t)\}. \tag{4.2.2}$$

For such a subcurve, we define the endpoint velocity $\mathfrak{v}_{\partial\Sigma}$ and its tangential $\mathfrak{v}_{\partial\Sigma(\tan)}$ by

$$\mathfrak{v}_{\partial\Sigma}(S_k) = \frac{\mathrm{d}\mathbf{R}_k}{\mathrm{d}t} \text{ and } \mathfrak{v}_{\partial\Sigma(\tan)}(S_k) = \frac{\mathrm{d}\mathbf{R}_k}{\mathrm{d}t} \cdot \mathbf{t}, \tag{4.2.3}$$

for $k = 1$ and 2. Note that by the chain rule, it is easy to see for $k = 1$ and 2 that $\frac{\mathrm{d}\mathbf{R}_k}{\mathrm{d}t} \cdot \mathbf{n} = V$, since $\mathbf{t} \cdot \mathbf{n} = 0$.

Given a time $t_0 \in [0, T)$ and an arclength parameter value $s_0 \in \mathbb{R}$ in the domain of $\mathbf{r}$, let S be a function defined in a neighborhood of t_0 such that $S(t_0) = s_0$. The function S is a normal arclength trajectory through s_0 at time t_0 if

$$\mathbf{t}(S(t), t) \cdot \frac{\mathrm{d}\left(\boldsymbol{\alpha}(S(t), t)\right)}{\mathrm{d}t} = 0. \tag{4.2.4}$$

For neighborhoods I of s_0 and J of t_0, the normal time derivative $\mathring{u}$ of a function $u : I \times J \to \mathbb{R}^n$ is defined by

$$\mathring{u}(s_0, t_0) = \left.\frac{\mathrm{d}(u(S(t), t))}{\mathrm{d}t}\right|_{t=t_0}. \tag{4.2.5}$$

Then,

$$\mathring{u}(s, t) = \frac{\partial u(s, t)}{\partial t} - \left(\frac{\partial \boldsymbol{\alpha}(s, t)}{\partial t} \cdot \mathbf{t}(s, t)\right) \frac{\partial u(s, t)}{\partial s}. \tag{4.2.6}$$

Let θ denote the angle between the unit normal $\mathbf{n}$ to $\mathcal{S}$ pointing into the lower terrace and the x-axis, i.e, θ is chosen such that

$$\mathbf{n} = (\cos\theta, \sin\theta). \tag{4.2.7}$$

Then we have the following result (see, e.g. [8]):

Proposition 4.2.1. *The angle θ satisfies the following*

$$\frac{\partial \theta}{\partial s} = \kappa \text{ and } \mathring{\theta} = \frac{\partial V}{\partial s}, \tag{4.2.8}$$

where s is the arclength parameter.

Proof. By Frenet's theorem, the curvature, κ, of a plane curve satisfies

$$\frac{\partial \mathbf{t}}{\partial s} = \kappa \mathbf{n} \text{ and } \frac{\partial \mathbf{n}}{\partial s} = -\kappa \mathbf{t}. \tag{4.2.9}$$

Recall that in Chapter 1 we defined the unit normal $\mathbf{n}$ in terms of the unit tangent vector $\mathbf{t} = (T_1, T_2)$ by $\mathbf{n} = (-T_2, T_1)$. Therefore, $\mathbf{t}$ is given by

$$\mathbf{t} = (\sin\theta, \cos\theta). \tag{4.2.10}$$

By (4.2.7), we have that

$$\frac{\partial \mathbf{t}}{\partial s} = \frac{\partial(\sin\theta, -\cos\theta)}{\partial s} = \frac{\partial \theta}{\partial s}(\cos\theta, \sin\theta) = \frac{\partial \theta}{\partial s}\mathbf{n}. \tag{4.2.11}$$

This proves $(4.2.8)_1$.

To show $(4.2.8)_2$, we calculate $\overset{\circ}{\mathbf{t}}$ in two ways. First, we note that

$$\begin{aligned}\overset{\circ}{\mathbf{t}} &= \frac{\partial \mathbf{t}}{\partial t} - \left(\frac{\partial \boldsymbol{\alpha}}{\partial t} \cdot \mathbf{t}\right)\frac{\partial \mathbf{t}}{\partial s} \\ &= (\cos\theta, \sin\theta)\left(\frac{\partial \theta}{\partial t} - \left(\frac{\partial \boldsymbol{\alpha}}{\partial t} \cdot \mathbf{t}\right)\frac{\partial \theta}{\partial s}\right) \\ &= \overset{\circ}{\theta}\mathbf{n}.\end{aligned} \tag{4.2.12}$$

Next, since $\mathbf{t} = \frac{\partial \boldsymbol{\alpha}}{\partial s}$, we have that

$$\overset{\circ}{\theta}\mathbf{n} = \overset{\circ}{\mathbf{t}} = \frac{\partial^2 \boldsymbol{\alpha}}{\partial t \partial s} - \left(\frac{\partial \boldsymbol{\alpha}}{\partial t} \cdot \mathbf{t}\right)\frac{\partial \mathbf{t}}{\partial s}, \tag{4.2.13}$$

which is equivalent to

$$\overset{\circ}{\theta} = \frac{\partial^2 \boldsymbol{\alpha}}{\partial t \partial s} \cdot \mathbf{n} - \left(\frac{\partial \boldsymbol{\alpha}}{\partial t} \cdot \mathbf{t}\right)\frac{\partial \mathbf{t}}{\partial s} \cdot \mathbf{n}. \tag{4.2.14}$$

We calculate $\frac{\partial V}{\partial s}$, and find that

$$\frac{\partial V}{\partial s} = \frac{\partial}{\partial s}\left(\frac{\partial \boldsymbol{\alpha}}{\partial t} \cdot \mathbf{n}\right) = \frac{\partial^2 \boldsymbol{\alpha}}{\partial s \partial t} \cdot \mathbf{n} + \frac{\partial \boldsymbol{\alpha}}{\partial t} \cdot \frac{\partial \mathbf{n}}{\partial s} = \frac{\partial^2 \boldsymbol{\alpha}}{\partial t \partial s} \cdot \mathbf{n} + \frac{\partial \boldsymbol{\alpha}}{\partial t} \cdot \frac{\partial \mathbf{n}}{\partial s}, \tag{4.2.15}$$

since $\boldsymbol{\alpha}$ is smooth. We solve (4.2.15) for $\frac{\partial^2 \boldsymbol{\alpha}}{\partial t \partial s} \cdot \mathbf{n}$ and substituting into (4.2.14), we arrive at

$$\begin{aligned}\overset{\circ}{\theta} &= \frac{\partial V}{\partial s} - \frac{\partial \boldsymbol{\alpha}}{\partial t} \cdot \frac{\partial \mathbf{n}}{\partial s} - \left(\frac{\partial \boldsymbol{\alpha}}{\partial t} \cdot \mathbf{t}\right)\frac{\partial \mathbf{t}}{\partial s} \cdot \mathbf{n} \\ &= \frac{\partial V}{\partial s} + \kappa\left(\frac{\partial \boldsymbol{\alpha}}{\partial t} \cdot \mathbf{t}\right) - \kappa\left(\frac{\partial \boldsymbol{\alpha}}{\partial t} \cdot \mathbf{t}\right)(\mathbf{n} \cdot \mathbf{n}) \\ &= \frac{\partial V}{\partial s}.\end{aligned} \tag{4.2.16}$$

where in the penultimate equality we have applied Frenet's theorem (4.2.9). This proves $(4.2.8)_2$. □

In this chapter, we consider smoothly evolving subregions $\mathcal{R}(t)$ of Ω. We denote the unit tangent and normal vectors to the boundary $\partial\mathcal{R}$ by $\mathbf{t}_{\partial\mathcal{R}}$ and $\mathbf{n}_{\partial\mathcal{R}}$, respectively; the velocity of the boundary $\partial\mathcal{R}$ by $\boldsymbol{w}$; and the velocity's tangential and normal components by $w_{\parallel} = \boldsymbol{w}\cdot\mathbf{t}_{\partial\mathcal{R}}$ and $w_{\perp} = \boldsymbol{w}\cdot\mathbf{n}_{\partial\mathcal{R}}$, respectively.

For any scalar or vector field f defined along $\mathcal{S}$ we define:

$$\int_{\partial\Sigma} f := f(S_2) - f(S_1) = \int_{\Sigma} \frac{\partial f}{\partial s}\,\mathrm{d}s. \tag{4.2.17}$$

We generalize the BCF model to account for step edge diffusion introducing a tangential step adatom flux $h^{\mathrm{s}} = \mathbf{h}^{\mathrm{s}}\cdot\mathbf{t}$, but assume the edge adatom density is negligible. This leaves the terrace mass balance (1.2.8) unchanged, and therefore leaves $(4.2.1)_{1,2,3}$ unaltered. However, the mass balance is augmented as the requirement that

$$\begin{aligned}\underbrace{\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{R}}\left(\varrho+\varrho^{\mathrm{b}}1_{\Omega_-}\right)\mathrm{d}A}_{\text{rate of mass production}} = &\underbrace{\int_{\mathcal{R}} R\,\mathrm{d}A}_{\substack{\text{rate of mass}\\ \text{adsorption onto }\mathcal{R}}} \underbrace{-\int_{\partial\mathcal{R}}\mathbf{h}\cdot\mathbf{n}_{\partial\mathcal{R}}\,\mathrm{d}s}_{\substack{\text{diffusion}\\ \text{into }\partial\mathcal{R}}} \\ &+\underbrace{\int_{\partial\mathcal{R}}(\varrho+\varrho^{\mathrm{b}}1_{\Omega_-})\boldsymbol{w}\cdot\mathbf{n}_{\partial\mathcal{R}}\,\mathrm{d}s}_{\substack{\text{rate of mass flow}\\ \text{due to the motion of }\mathcal{R}}} \underbrace{-\int_{\partial\Sigma} h^{\mathrm{s}}}_{\substack{\text{edge diffusion}\\ \text{into }\partial\Sigma}},\end{aligned} \tag{4.2.18}$$

where 1_{Ω_-} is the characteristic function associated with Ω_- as defined in (1.2.9). for any moving control region $\mathcal{R}(t)$ and $\Sigma(t) = \mathcal{R}(t)\cap\mathcal{S}(t)$.

Letting the area shrink to a subcurve of $\Sigma(t)$ of $\mathcal{S}(t)$, this global mass balance (4.2.18) implies that

$$\int_{\Sigma(t)}\left([\![\mathbf{h}\cdot\mathbf{n} - (\varrho+\varrho^{\mathrm{b}}1_{\Omega_-})V]\!] - \frac{\partial h^{\mathrm{s}}}{\partial s}\right)\mathrm{d}s = 0. \tag{4.2.19}$$

Localizing (4.2.19) we arrive at

$$[\![\mathbf{h}\cdot\mathbf{n} - (\varrho+\varrho^{\mathrm{b}}1_{\Omega_-})V]\!] - \frac{\partial h^{\mathrm{s}}}{\partial s} = 0, \tag{4.2.20}$$

and by $(4.2.1)_{2,3}$, we have that

$$\varrho^{\mathrm{b}}V + \frac{\partial h^{\mathrm{s}}}{\partial s} = J_+ + J_-. \tag{4.2.21}$$

4.3 Configurational force balance

The migration of steps is relative to the underlying crystalline bulk. Hence, rather than being material curves, steps should be viewed as defects of the sort studied by Eshelby [24, 25, 26]. The evolution of such defects—which include vacancies, dislocations, grain boundaries, and phase interfaces—is driven by configurational forces (as opposed to standard, i.e., Newtonian, forces that accompany material deformations). In Eshelby's approach, the configurational force acting on a defect is defined as the variational derivative of an appropriate free-energy functional with respect to the configuration of the defect. [1]

Eshelby's work, being variational, (*i.*) allows only for small departures from equilibrium, (*ii.*) is predicated on the a priori constitutive prescription of the free energy, and (*iii.*) cannot account for dissipative mechanisms that typically accompany the motion of defects. An alternative framework, one that circumvents the shortcomings of the variational approach, was developed by Gurtin [27, 28], see also Gurtin and Struthers [29]. It distinguishes between basic laws, such as mass balance, which hold for large classes of materials, and constitutive relations, such as Fick's law, that differentiate between materials. In it, configurational forces are treated as primitive fields that obey a separate balance. Moreover, power expenditures associated with the motion of defects are accounted for properly in the energy balance and the second law of thermodynamics (or entropy imbalance) serves to impose physically meaningful restrictions on constitutive relations, as we shall see below.

Gurtin's ideas has been applied to the study of crack propagation [30], solidification [31], fluid-fluid phase transitions [32], solid-state phase transformations [33], and liquid crystals [34, 35]. Herein, we use this approach to derive the dynamical equations that govern the nonequilibrium motion of steps during epitaxial growth. In

[1] In the present setting, the driving force on a step is associated with the change in a free energy comprising contributions from the step, the adjacent terraces, and the layer of crystallized adatoms beneath the upper terrace, upon altering the position of the step.

doing so, we ensure that the resulting step-flow model holds away from equilibrium and that all constitutive relations are compatible with the dissipation inequality.

Let $\mathbf{C}$ be the terrace configurational stress, $\boldsymbol{l}$ the terrace configurational internal force, $\boldsymbol{g}$ the configurational internal force at the step, and $\mathbf{c}$ the step configurational traction. The configurational force balance requires that

$$\int_{\partial\mathcal{R}} \mathbf{C}\mathbf{n}_{\partial\mathcal{R}}\,\mathrm{d}s + \int_{\mathcal{R}} \boldsymbol{l}\,\mathrm{d}A + \int_{\Sigma} \boldsymbol{g}\,\mathrm{d}s + \int_{\partial\Sigma} \mathbf{c} = 0, \tag{4.3.1}$$

for any region $\mathcal{R}$ and $\Sigma = \mathcal{R} \cap \mathcal{S}$. Localizing away from the step, this force balance implies that

$$\operatorname{div}\mathbf{C} + \boldsymbol{l} = 0 \quad \text{in } \Omega_+ \cup \Omega_-, \tag{4.3.2}$$

and at the step

$$[\![\mathbf{C}]\!]\mathbf{n} + \frac{\partial \mathbf{c}}{\partial s} + \boldsymbol{g} = 0 \quad \text{along } \mathcal{S}. \tag{4.3.3}$$

Putting

$$\mathbf{c} = \gamma\mathbf{t} + \sigma\mathbf{n} \text{ and } g = \boldsymbol{g}\cdot\mathbf{n}, \tag{4.3.4}$$

we find the normal component of (4.3.3)

$$\mathbf{n}\cdot[\![\mathbf{C}]\!]\mathbf{n} + \frac{\partial\sigma}{\partial s} + \gamma\kappa + g = 0. \tag{4.3.5}$$

4.4 Consistency with the first and second law of thermodynamics

Let Ψ be the terrace free energy per unit area, Ψ^{b} the free energy per unit area of the layer of atoms beneath the upper terrace, and ψ^{s} the step free energy per unit length. Further, let μ be the terrace adatom chemical potential per unit area, μ^{b} the chemical potential per unit area of the atoms in the layer beneath the upper terrace, and μ^{s} the step chemical potential per unit length. Following Gurtin and Voorhees [33], we view these chemical potentials as primitive fields accounting for the energy from the transported atoms.

Assuming that step motion occurs isothermally, the first and second law yield a dissipation inequality: for any subregion compactly contained in a single terrace, i.e., $\mathcal{R} \subset\subset \Omega_+$:

$$\underbrace{\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{R}} \Psi \,\mathrm{d}A}_{\substack{\text{rate of free}\\ \text{energy production}\\ \text{in } \mathcal{R}}} \leq -\underbrace{\int_{\partial\mathcal{R}} \mu \mathbf{h}\cdot\mathbf{n}_{\partial\mathcal{R}}\,\mathrm{d}s}_{\substack{\text{energy flow}\\ \text{due to diffusion}\\ \text{through } \partial\mathcal{R}}} + \underbrace{\int_{\mathcal{R}} \mu R \,\mathrm{d}A}_{\substack{\text{energy flow}\\ \text{due to deposition}\\ \text{on } \mathcal{R}}}, \tag{4.4.1}$$

and for any moving subregion $\mathcal{R}(t)$ of Ω that intersects a step $\mathcal{S}(t)$ at $\Sigma(t)$, which has endpoints $\boldsymbol{\alpha}(S_1(t), t) = \mathbf{R}_1(t)$ and $\boldsymbol{\alpha}(S_2(t), t) = \mathbf{R}_2(t)$ at time t,

$$\underbrace{\frac{\mathrm{d}}{\mathrm{d}t}\left(\int_{\mathcal{R}} (\Psi + \Psi^{\mathrm{b}} 1_{\Omega_-})\,\mathrm{d}A + \int_{\Sigma} \psi^{\mathrm{s}}\,\mathrm{d}s\right)}_{\substack{\text{rate of free}\\ \text{energy production}\\ \text{in } \mathcal{R} \text{ and on } \Sigma}} \leq -\underbrace{\int_{\partial\mathcal{R}} \mu \mathbf{h}\cdot\mathbf{n}_{\partial\mathcal{R}}\,\mathrm{d}s}_{\substack{\text{energy flow}\\ \text{due to diffusion}\\ \text{through } \partial\mathcal{R}}} + \underbrace{\int_{\mathcal{R}} \mu R \,\mathrm{d}A}_{\substack{\text{energy flow}\\ \text{due to deposition}\\ \text{on } \mathcal{R}}}$$
$$+ \underbrace{\int_{\partial\mathcal{R}} (\mu\varrho + \mu^{\mathrm{b}}\varrho^{\mathrm{b}} 1_{\Omega_-})\boldsymbol{w}\cdot\mathbf{n}_{\partial\mathcal{R}}\,\mathrm{d}s}_{\substack{\text{energy flow due to}\\ \text{the motion of } \mathcal{R}}} - \underbrace{\int_{\partial\Sigma} \mu^{\mathrm{s}} h^{\mathrm{s}}}_{\substack{\text{energy flow}\\ \text{due to diffusion}\\ \text{along the step } \Sigma}}$$
$$+ \underbrace{\int_{\partial\Sigma} \mathbf{c}\cdot\mathfrak{v}_{\partial\Sigma} + \int_{\partial\mathcal{R}} \mathbf{C}\mathbf{n}_{\partial\mathcal{R}}\cdot\boldsymbol{w}\,\mathrm{d}s}_{\text{work due to configurational forces}}. \tag{4.4.2}$$

The following proposition follows from this dissipation inequality (cf. [31]).

Proposition 4.4.1. *Given that (4.4.2) holds for any moving subregion $\mathcal{R}(t)$, the terrace configurational stress $\mathbf{C}$ satisfies*

$$\mathbf{C} = (\omega + \omega^b 1_{\Omega_-})\mathbf{1}, \tag{4.4.3}$$

where ω and ω^b are the terrace and bulk grand canonical potentials

$$\omega = \Psi - \mu\varrho \text{ and } \omega^b = \Psi^b - \mu^b\varrho^b. \tag{4.4.4}$$

Proof. For moving subregions $\mathcal{R}(t)$ compactly contained in the upper or lower terrace, the dissipation inequality (4.4.2) implies that

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\int_{\mathcal{R}} (\Psi + \Psi^{\mathrm{b}} 1_{\Omega_-})\,\mathrm{d}A\right) \leq \int_{\mathcal{R}} \mu R \,\mathrm{d}A$$
$$+ \int_{\partial\mathcal{R}} -\mu\mathbf{h}\cdot\mathbf{n}_{\partial\mathcal{R}} + (\mu\varrho + \mu^{\mathrm{b}}\varrho^{\mathrm{b}} 1_{\Omega_-})\boldsymbol{w}\cdot\mathbf{n}_{\partial\mathcal{R}} + \boldsymbol{w}\cdot\mathbf{C}\mathbf{n}_{\partial\mathcal{R}}\,\mathrm{d}s. \tag{4.4.5}$$

For brevity, let $\tilde{\Psi} = \Psi + \Psi^{\mathrm{b}} 1_{\Omega_-(t)}$. By the divergence theorem and the transport theorem, we have that (4.4.5)

$$\int_{\mathcal{R}} \frac{\partial \tilde{\Psi}}{\partial t} \, \mathrm{d}A + \int_{\partial\mathcal{R}} \tilde{\Psi} w_\perp \, \mathrm{d}s \le \int_{\mathcal{R}} \mu R - \operatorname{div}(\mu \mathbf{h}) \, \mathrm{d}A$$
$$+ \int_{\partial\mathcal{R}} (\mu\varrho + \mu^{\mathrm{b}} \varrho^{\mathrm{b}} 1_{\Omega_-} + (\mathbf{C}\mathbf{n}_{\partial\mathcal{R}}) \cdot \mathbf{n}_{\partial\mathcal{R}}) w_\perp + (\mathbf{C}\mathbf{n}_{\partial\mathcal{R}} \cdot \mathbf{t}_{\partial\mathcal{R}}) \, w_\parallel \, \mathrm{d}s, \quad (4.4.6)$$

recalling that $\boldsymbol{w} = w_\perp \mathbf{n}_{\partial\mathcal{R}} + w_\parallel \mathbf{t}_{\partial\mathcal{R}}$. Since for any $\mathcal{R}$ we may parameterize $\partial\mathcal{R}$ in such a way as to make $w_\parallel$ arbitrarily large and positive or negative without changing the region $\mathcal{R}$ or its normal velocity, it follows that the term in (4.4.6) multiplying $w_\parallel$ must be zero, i.e., $\mathbf{C}\mathbf{n}_{\partial\mathcal{R}} \cdot \mathbf{t}_{\partial\mathcal{R}} = 0$. Since $\mathbf{n}_{\partial\mathcal{R}}$ is orthogonal to $\mathbf{t}_{\partial\mathcal{R}}$, we have, in this two dimensional setting, that $\mathbf{C}\mathbf{n}_{\partial\mathcal{R}} = k\mathbf{n}_{\partial\mathcal{R}}$. This holds for any subregion $\mathcal{R}$ compactly contained in an upper or lower terrace. At any point in the upper or lower terrace and any unit vector $\mathbf{a}$, there exists a region compactly contained in that terrace with unit normal vector equal to $\mathbf{a}$. Hence, every vector $\mathbf{a}$ is an eigenvector of $\mathbf{C}$, which implies that $\mathbf{C}$ is a multiple of the identity matrix $\mathbf{1}$, say $\mathbf{C} = \lambda\mathbf{1}$. Then, we may write the dissipation inequality (4.4.6) in the following form:

$$\int_{\mathcal{R}} \frac{\partial \tilde{\Psi}}{\partial t} \; - \; \mu R \; + \; \operatorname{div}(\mu \mathbf{h}) \, \mathrm{d}A \quad \le \quad \int_{\partial\mathcal{R}} \left(\mu\varrho + \mu^{\mathrm{b}} \varrho^{\mathrm{b}} 1_{\Omega_-} + \lambda - \tilde{\Psi} \right) w_\perp \, \mathrm{d}s. \quad (4.4.7)$$

It suffices to note that given a region $\mathcal{R}_0$ compactly contained in the upper or lower terrace at time t_0 and a smooth scalar field w defined on boundary $\partial\mathcal{R}_0$, there exists a moving region $\mathcal{R}$ compactly contained in the upper or lower terrace defined on a time interval containing t_0 for which $\mathcal{R}(t_0) = \mathcal{R}_0$ and the normal velocity, $w_\perp$ of $\partial\mathcal{R}$ at time $t = t_0$ satisfies $w_\perp = w$ at time t_0. Therefore, the term multiplying $w_\perp$ in integrand on the right-hand side of (4.4.7) must be identically zero. Specifically, we have that

$$\lambda = \tilde{\Psi} - \mu\varrho - \mu^{\mathrm{b}} \varrho^{\mathrm{b}} 1_{\Omega_-}, \quad (4.4.8)$$

and since $\mathbf{C} = \lambda\mathbf{1}$, we have proven our proposition. □

Localizing (4.4.1), we find that

$$\frac{\partial \Psi}{\partial t} + \operatorname{div}(\mu \mathbf{h}) - \mu R \leq 0. \tag{4.4.9}$$

It follows from $(4.2.1)_1$ that

$$\frac{\partial \Psi}{\partial t} - \mu \frac{\partial \varrho}{\partial t} + \nabla \mu \cdot \mathbf{h} \leq 0. \tag{4.4.10}$$

Extending the procedure introduced by Coleman and Noll [36], we assume $\Psi = \Psi(\varrho)$ and that this dissipation inequality (4.4.10) holds for any process, it follows that

$$\frac{\partial \varrho}{\partial t}\left(\frac{\partial \Psi}{\partial \varrho} - \mu\right) + \nabla \mu \cdot \mathbf{h} \leq 0, \tag{4.4.11}$$

and since $\frac{\partial \varrho}{\partial t}$ may be chosen arbitrarily and assuming the other quantities do not depend on $\frac{\partial \varrho}{\partial t}$, it follows that

$$\mu = \frac{\partial \Psi}{\partial \varrho}. \tag{4.4.12}$$

Hence, the dissipation inequality for points within a terrace reduces to

$$\nabla \mu \cdot \mathbf{h} \leq 0. \tag{4.4.13}$$

A linear constitutive assumption that makes (4.4.13) trivially satisfied is:

$$\mathbf{h} = -M \nabla \mu \tag{4.4.14}$$

for positive M. Note that R is not restricted by entropy imbalance. We consider the linear relation

$$R = -\breve{\sigma} \mu + F \tag{4.4.15}$$

Again, considering (4.4.2) applied to subregions $\mathcal{R}(t)$ shrinking to a subcurve Σ of the step $\mathcal{S}$, we find [8]

$$\int_{\Sigma}\left(\overset{\circ}{\psi}{}^{\mathrm{s}} - \psi^{\mathrm{s}}\kappa V + [\![\mu(\mathbf{h}\cdot\mathbf{n} - \varrho V)]\!] + \mu^{\mathrm{b}}\varrho^{\mathrm{b}} V - \mathbf{n}\cdot[\![\mathbf{C}]\!]\mathbf{n}V\right) \mathrm{d}s \\ + \int_{\partial\Sigma}\left(\psi^{\mathrm{s}}\mathfrak{v}_{\partial\Sigma(\tan)} + \mu^{\mathrm{s}} h^{\mathrm{s}} - \mathbf{c}\cdot\mathfrak{v}_{\partial\Sigma}\right) \leq 0, \tag{4.4.16}$$

where the last terms of (4.4.16) may be written as

$$\begin{aligned}\int_{\partial\Sigma(t)} \mu^{s} h^{s} &= \int_{\Sigma(t)} h^{s}\frac{\partial \mu^{s}}{\partial s} + \mu^{s}\frac{\partial h^{s}}{\partial s}\,\mathrm{d}s \\ &= \int_{\Sigma(t)} h^{s}\frac{\partial \mu^{s}}{\partial s} + \mu^{s}\left(J_{+} + J_{-} - \varrho^{b} V\right)\mathrm{d}s\end{aligned} \tag{4.4.17}$$

and

$$\begin{aligned}\int_{\partial\Sigma} \mathbf{c}\cdot\mathfrak{v}_{\partial\Sigma} &= \int_{\partial\Sigma} \sigma V + \gamma \mathfrak{v}_{\partial\Sigma(\tan)} \\ &= \int_{\Sigma} \frac{\partial(\sigma V)}{\partial s}\,\mathrm{d}s + \int_{\partial\Sigma} \gamma \mathfrak{v}_{\partial\Sigma(\tan)} \\ &= \int_{\Sigma} -\mathbf{n}\cdot[\![\mathbf{C}]\!]\mathbf{n}V - \gamma\kappa V - gV + \sigma\overset{\circ}{\theta}\,\mathrm{d}s + \int_{\partial\Sigma} \gamma \mathfrak{v}_{\partial\Sigma(\tan)}.\end{aligned} \tag{4.4.18}$$

It follows that for any subcurve Σ of $\mathcal{S}$

$$\begin{aligned}\int_{\Sigma}\Big(&\overset{\circ}{\psi}{}^{s} + (\gamma - \psi^{s})\kappa V + [\![\mu(\mathbf{h}\cdot\mathbf{n} - \varrho V)]\!] + (\mu^{b}\varrho^{b} + g)V - \sigma\overset{\circ}{\theta} \\ &+ \frac{\partial \mu^{s}}{\partial s} h^{s} + \mu^{s}\left(J_{+} + J_{-} - \varrho^{b} V\right)\Big)\,\mathrm{d}s + \int_{\partial\Sigma} (\psi^{s} - \gamma)\mathfrak{v}_{\partial\Sigma(\tan)} \le 0.\end{aligned} \tag{4.4.19}$$

By [8], we have the following lemma:

Lemma 4.4.2. *Let φ and ω be interfacial fields and suppose that*

$$\int_{\Sigma} \varphi\, ds + \int_{\partial\Sigma} \omega \mathfrak{v}_{\partial\Sigma(tan)} \le 0 \tag{4.4.20}$$

for all evolving subcurves of Σ of $\mathcal{S}$. Then $\varphi \le 0$ and $\omega = 0$.

Hence, we have that

$$\left.\begin{aligned} 0 \ge\ & \overset{\circ}{\psi}{}^{s} + [\![\mu(\mathbf{h}\cdot\mathbf{n} - \varrho V)]\!] + (\mu^{b}\varrho^{b} + g)V - \sigma\overset{\circ}{\theta} + \tfrac{\partial \mu^{s}}{\partial s} h^{s} \\ & + \mu^{s}\left(J_{+} + J_{-} - \varrho^{b} V\right), \\ \gamma =\ & \psi^{s}. \end{aligned}\right\} \tag{4.4.21}$$

In particular, this establishes, in the present context, that the step line tension is the same as the step free energy.

Appealing to $(4.2.1)_{2,3}$, we find

$$\overset{\circ}{\psi}{}^{s} - \sigma\overset{\circ}{\theta} + J_{+}(\mu^{s} - \mu^{+}) + J_{-}(\mu^{s} - \mu^{-}) + (\varrho^{b}(\mu^{b} - \mu^{s}) + g)V + \frac{\partial \mu^{s}}{\partial s} h^{s} \le 0 \tag{4.4.22}$$

Let $G = \varrho^{\rm b}(\mu^{\rm s} - \mu^{\rm b}) - g$. Then $(4.4.21)_1$ reduces to

$$0 \leq (\sigma\overset{\circ}{\theta} - \overset{\circ}{\psi}{}^{\rm s}) + J_+(\mu^+ - \mu^{\rm s}) + J_-(\mu^- - \mu^{\rm s}) + GV - \frac{\partial \mu^{\rm s}}{\partial s} h^{\rm s}. \tag{4.4.23}$$

Recalling that $\psi^{\rm s}$ is a function of θ, we find that

$$0 \leq \left(\sigma - \frac{\partial \psi^{\rm s}}{\partial \theta}\right)\overset{\circ}{\theta} + J_+(\mu^+ - \mu^{\rm s}) + J_-(\mu^- - \mu^{\rm s}) + GV - \frac{\partial \mu^{\rm s}}{\partial s} h^{\rm s}. \tag{4.4.24}$$

Since the normal time derivative of θ may be specified arbitrarily (in particular, arbitrarily large and negative or positive) independently of θ it follows that

$$\frac{\partial \psi^{\rm s}}{\partial \theta} = \sigma. \tag{4.4.25}$$

This reduces our dissipation inequality to:

$$0 \leq J_+(\mu^+ - \mu^{\rm s}) + J_-(\mu^- - \mu^{\rm s}) + GV - \frac{\partial \mu^{\rm s}}{\partial s} h^{\rm s}, \tag{4.4.26}$$

We choose linear prescriptions for J_+, J_-, G, and $h^{\rm s}$ such that the above inequality (4.4.26) holds trivially; namely, we assume for some positive constants C_+, C_-, β and D^s

$$\left.\begin{aligned} J_+ &= \quad C_+(\mu^+ - \mu^{\rm s}), \\ J_- &= \quad C_-(\mu^- - \mu^{\rm s}), \\ G &= \quad \beta V, \\ h^{\rm s} &= \quad -D^s \tfrac{\partial \mu^{\rm s}}{\partial s}. \end{aligned}\right\} \tag{4.4.27}$$

Appealing to (4.4.25), we have

$$\frac{\partial \sigma}{\partial s} = \frac{\partial^2 \psi^{\rm s}}{\partial s \partial \theta} = \frac{\partial^2 \psi^{\rm s}}{\partial \theta^2}\frac{\partial \theta}{\partial s} = \kappa \frac{\partial^2 \psi^{\rm s}}{\partial \theta^2}. \tag{4.4.28}$$

Hence, by (4.4.3), (4.3.5), $(4.4.21)_2$, and (4.4.28) the normal configurational force balance (4.3.5) reduces to

$$[\![\omega]\!] - \omega^{\rm b} + \left(\psi^{\rm s} + \frac{\partial^2 \psi^{\rm s}}{\partial \theta^2}\right)\kappa + \varrho^{\rm b}\mu^{\rm s} - \varrho^{\rm b}\mu^{\rm b} = \beta V. \tag{4.4.29}$$

We assume local equilibrium, i.e., $\beta = 0$, and since $\omega^{\mathrm{b}} = \Psi^{\mathrm{b}} - \varrho^{\mathrm{b}}\mu^{\mathrm{b}}$, it follows that

$$\mu^{\mathrm{s}} = \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} - \frac{\tilde{\psi}^{\mathrm{s}}\kappa}{\varrho^{\mathrm{b}}} - \frac{[\![\omega]\!]}{\varrho^{\mathrm{b}}}, \tag{4.4.30}$$

where

$$\tilde{\psi}^{\mathrm{s}} = \psi^{\mathrm{s}} + \frac{\partial^2 \psi^{\mathrm{s}}}{\partial \theta^2}. \tag{4.4.31}$$

This is the modified Gibbs–Thomson relation (1.2.23).

Using our constitutive assumptions (4.4.14), (4.4.15), and (4.4.27) in mass balance (4.2.1), we have

$$\left.\begin{aligned}
\frac{\partial \varrho}{\partial t} &= \operatorname{div}(M\nabla\mu) + F - \breve{\sigma}\mu && \text{in } \Omega_+ \cup \Omega_-,\\
\varrho^+ V + M\nabla\mu^+ \cdot \mathbf{n} &= C_+(\mu^+ - \mu^{\mathrm{s}}) && \text{along } \mathcal{S},\\
-\varrho^- V - M\nabla\mu^- \cdot \mathbf{n} &= C_-(\mu^- - \mu^{\mathrm{s}}) && \text{along } \mathcal{S},\\
\varrho^{\mathrm{b}} V - \frac{\partial}{\partial s}\left(D^s \frac{\partial \mu^{\mathrm{s}}}{\partial s}\right) &= C_+(\mu^+ - \mu^{\mathrm{s}}) + C_-(\mu^- - \mu^{\mathrm{s}}) && \text{along } \mathcal{S}.
\end{aligned}\right\} \tag{4.4.32}$$

We call this, together with modified Gibbs–Thomson relation (4.4.30), the general TC model. To study this system, one must prescribe $\Psi, \Psi^{\mathrm{b}}, \varrho^{\mathrm{b}}, \psi^{\mathrm{s}}, C_{\pm}, M$, F and $\breve{\sigma}$, but in the remaining we make several simplifying approximations.

4.5 The TC model as a generalization of the BCF model

Suppose $\Psi(\varrho)$ is second continuously differentiable, convex, and satisfies $\Psi(0) = 0$ and $\Psi(\varrho) > 0$ for $\varrho > 0$. Since $\mu = \frac{\partial \Psi}{\partial \varrho}$ and Ψ is convex, we have that μ is an increasing function of ϱ. Therefore, the grand canonical potential $\omega(\varrho) = \Psi(\varrho) - \varrho\mu(\varrho)$ satisfies $\omega(0) = 0$ and

$$\frac{\partial \omega}{\partial \varrho} = \mu - \mu - \varrho\frac{\partial \mu}{\partial \varrho} = -\varrho\frac{\partial \mu}{\partial \varrho} < 0 \tag{4.5.1}$$

on $(0, \infty)$. Hence, for $\varrho_{\mathrm{eq}} > 0$, we have that

$$\begin{aligned}
\mu(\varrho) &= \mu(\varrho_{\mathrm{eq}}) + \mu'(\varrho_{\mathrm{eq}})(\varrho - \varrho_{\mathrm{eq}}) + O((\varrho - \varrho_{\mathrm{eq}})^2),\\
\omega(\varrho) &= \omega(\varrho_{\mathrm{eq}}) - \varrho_{\mathrm{eq}}\mu'(\varrho_{\mathrm{eq}})(\varrho - \varrho_{\mathrm{eq}}) + O((\varrho - \varrho_{\mathrm{eq}})^2).
\end{aligned} \tag{4.5.2}$$

Choose $\varrho_{\rm eq}$ such that $\mu(\varrho_{\rm eq}) = \frac{\Psi^{\rm b}}{\varrho^{\rm b}}$, and set $D^s = 0$. We keep up to first-order terms in $\varrho - \varrho_{\rm eq}$, and find that $(4.4.32)_1$ reduces to

$$\frac{\partial \varrho}{\partial t} = \operatorname{div}(D\nabla\varrho) + F - \tau^{-1}\varrho + O((\varrho - \varrho_{\rm eq})^2) \text{ in } \Omega, \tag{4.5.3}$$

the boundary conditions $(4.4.32)_{2,3}$ reduce to

$$\begin{aligned} \pm\varrho^{\pm}V \pm D\nabla\varrho^{\pm}\cdot\mathbf{n} = K_{\pm}\left(\varrho^{\pm} - \varrho_{\rm eq} + \Gamma\kappa - \frac{\varrho_{\rm eq}}{\varrho^{\rm b}}[\![\varrho]\!]\right) \\ + O((\varrho - \varrho_{\rm eq})^2) \text{ along } \mathcal{S}, \end{aligned} \tag{4.5.4}$$

where

$$D = \mu'(\varrho_{\rm eq})M,\; F = \mathsf{F} + \breve{\sigma}\left(\mu'(\varrho_{\rm eq})\varrho_{\rm eq} - \frac{\Psi^{\rm b}}{\varrho^{\rm b}}\right),\; \tau^{-1} = \breve{\sigma}\mu'(\varrho_{\rm eq}), \tag{4.5.5}$$

and the velocity equation $(4.4.32)_4$ takes the form

$$\begin{aligned} \varrho^{\rm b}V = K_{+}\left(\varrho^{+} - \varrho_{\rm eq} + \Gamma\kappa - \Theta[\![\varrho]\!]\right) + K_{-}\left(\varrho^{-} - \varrho_{\rm eq} + \Gamma\kappa - \Theta[\![\varrho]\!]\right) \\ + O((\varrho - \varrho_{\rm eq})^2) \text{ along } \mathcal{S}, \end{aligned} \tag{4.5.6}$$

where

$$\Theta = \frac{\varrho_{\rm eq}}{\varrho^{\rm b}} \tag{4.5.7}$$

is the (equilibrium) adatom coverage relative to the bulk density and

$$K_{\pm} = C_{\pm}\mu'(\varrho_{\rm eq}) \text{ and } \Gamma = \frac{\tilde{\psi}^{\rm s}}{\mu'(\varrho_{\rm eq})\varrho^{\rm b}}. \tag{4.5.8}$$

If we assume that the adatom coverage, Θ, and the departure of adatom density, ϱ, from the equilibrium density of an isolated straight step, $\varrho_{\rm eq}$, are negligible, we recover the BCF model (1.2.5)-(1.2.7).

4.6 Simplifying approximations

We assume, as in the preceding section, that $\Psi(\varrho)$ is a convex function with $\Psi(0) = 0$. Since μ is increasing, we have that μ is an invertible function, with inverse function

$\mu^{-1}(\mu)$. Moreover, for all ϱ such that $\frac{\partial\mu(\varrho)}{\partial\varrho} \neq 0$,

$$\frac{\partial\omega}{\partial\mu} = \frac{\partial\omega}{\partial\varrho}\frac{\partial\mu^{-1}}{\partial\mu} = -\varrho\frac{\partial\mu}{\partial\varrho}\left(\frac{\partial\mu}{\partial\varrho}\right)^{-1} = -\varrho. \tag{4.6.1}$$

Hence, assuming ω is a second-continuously differentiable function of μ,

$$\omega(\mu) = \omega_0 - \varrho_{\text{eq}}\mu + O((\mu - \mu_{\text{eq}})^2) \tag{4.6.2}$$

where

$$\mu_{\text{eq}} = \mu(\varrho_{\text{eq}}) \text{ and } \omega_0 = \omega(\mu_{\text{eq}}) + \varrho_{\text{eq}}\mu_{\text{eq}}. \tag{4.6.3}$$

Let Θ denote the adatom coverage, and let γ be the line tension ,

$$\Theta = \frac{\varrho_{\text{eq}}}{\varrho^{\text{b}}} \text{ and } \gamma = \frac{1}{\varrho^{\text{b}}}\left(\psi^{\text{s}} + \frac{\partial\psi^{\text{s}}}{\partial\theta}\right). \tag{4.6.4}$$

Neglecting terms of order $(\mu - \mu_{\text{eq}})^2$ or higher, the modified Gibbs–Thomson relation (4.4.30) reduces to

$$\mu^{\text{s}} = \frac{\Psi^{\text{b}}}{\varrho^{\text{b}}} - \gamma\kappa + \Theta[\![\mu]\!]. \tag{4.6.5}$$

When the step motion occurs on a time scale that is much larger than the time scale of diffusion, we use the quasistatic version of (4.4.32), in which μ solves the PDE

$$0 = \operatorname{div}(M\nabla\mu) + F - \breve{\sigma}\mu \qquad \text{in } \Omega_+ \cup \Omega_-, \tag{4.6.6}$$

with boundary conditions

$$\left.\begin{aligned} M\nabla\mu^+ \cdot \mathbf{n} &= C_+(\mu^+ - \mu^{\text{s}}) \\ -M\nabla\mu^- \cdot \mathbf{n} &= C_-(\mu^- - \mu^{\text{s}}) \end{aligned} \quad \text{along } \mathcal{S}, \right\} \tag{4.6.7}$$

and the normal velocity V satisfies

$$\varrho^{\text{b}}V = C_+(\mu^+ - \mu^{\text{s}}) + C_-(\mu^- - \mu^{\text{s}}) + \frac{\partial}{\partial s}\left(D^{\text{s}}\frac{\partial\mu^{\text{s}}}{\partial s}\right) \qquad \text{along } \mathcal{S}. \tag{4.6.8}$$

In the remaining, we take M, F, $\breve{\sigma}$, $C_{\pm}$, $\frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}}$, and Θ to be constants, i.e., independent of θ, and let $D^{s} = 0$.

In conclusion, the TC model ensures consistency with thermodynamics assuming small departures from μ_{eq}. We now turn to finding the continuum limit of this model, (4.6.6)-(4.6.8) and (4.6.5).

5 Thermodynamically consistent continuum limit of step-flow epitaxial growth in one spatial dimension

5.1 Introduction: What is a continuum limit?

For both the BCF and the TC models, one must track the motion of steps which form plane curves. The adatom density is required to solve a PDE, and must satisfy some boundary conditions at the steps (see (4.6.6)-(4.6.7)). Once the adatom density is specified, the motion of the steps is determined (see (4.6.8)). The steps are discrete objects in that there are finitely or countably-infinitely many steps and not a continuum of them. This interplay between the continuum theory of the adatom density and the discrete theory of the steps gives rise to the terminology of discrete-continuum models.

As a practical matter, tracking a large number of curves is computationally expensive. Discrete-continuum models are not the only construct. Indeed, there are continuum models of epitaxial growth, wherein a PDE governs the motion of a smooth surface, specified by the graph at each time t

$$z = h(x, y, t), \tag{5.1.1}$$

of a function h called the height function. As in Chapter 1, the (x, y)-plane is assumed to be parallel to the terraces.

There is no consensus, however, as to what the PDE for the continuum model ought to be. To address this, there are many attempts in connecting discrete-continuum models and coarse-grained continuum models of epitaxy (e.g. [37], [38], [39], [40]). E and Yip [13] find that if one allows for step diffusion, the continuum limit consists of a coupled system of PDE, which accounts for surface densities at the macroscale. Margetis and Kohn [14] and Quah and Margetis [41] show that even in the absence of anisotropy in the discrete continuum model, if there is a small deviation away from radially symmetric steps, then the continuum equations contain a mobility that is tensorial in nature.

The process of finding continuum equations that are consistent with the discrete-continuum equations falls under the general heading of finding a continuum limit. We do not attempt to provide the most general definition a continuum limit, but describe continuum limits in the present context of step-flow epitaxy. The basic idea is to find a continuum theory that arises from considering what happens when we fix a step location x and take the step height a to 0, while keeping the slope $\frac{a}{\ell} = O(1)$ where ℓ is the terrace width.

To find a continuum limit of our discrete-continuum model (4.6.6)-(4.6.8), we assume that each step $\mathcal{S}$, forms a level set of $h(x, y, t)$ at each time t with adjacent steps corresponding to level sets with h value differing by the step height a. We assume that steps are sufficiently non-oscillatory and close to each other that for a point $\mathbf{x}$ on a step $\mathcal{S}_k$, there are terrace widths $\ell^+, \ell^- > 0$ such that $\mathbf{x} + \ell^+\mathbf{n} \in \mathcal{S}_{k+1}$ and $\mathbf{x} - \ell^-\mathbf{n} \in \mathcal{S}_{k-1}$, and, moreover, that h is monotone in the normal direction. This means that for each $t \in [0, T)$ and $\mathbf{x} \in \mathcal{S}(t)$ the map $p \mapsto h(\mathbf{x} + p\mathbf{n}(\mathbf{x}), t)$ is decreasing on $[-\ell^-(\mathbf{x}), \ell^+(\mathbf{x})]$. In this case, we may let the step $\mathcal{S}_0$ to be at 0 height, and for any given step $\mathcal{S}_k$

$$\mathcal{S}_k(t) = \{(x, y) \in \mathbb{R}^2 : h(x, y, t) = -ak\}. \tag{5.1.2}$$

Since ∇h points in the direction of greatest increase and is normal to the level set of h, but our choice of $\mathbf{n}$ to point into the *lower* terrace (i.e., in the direction of decrease in h), we have that

$$\mathbf{n} = -\frac{\nabla h}{|\nabla h|} \quad \text{and} \quad \frac{\partial h}{\partial n} = \nabla h \cdot \mathbf{n} = -|\nabla h|. \tag{5.1.3}$$

Next, we approximate $\ell^+(a)$ and $\ell^-(a)$ for small a, and, in particular, use second-order Taylor polynomials of $\ell^{\pm}$ about $a = 0$. For each t,[1]

$$h(\mathbf{x} + \ell^{+}(a)\mathbf{n}, t) = -a + h(\mathbf{x}, t) \text{ and } h(\mathbf{x} - \ell^{-}(a)\mathbf{n}, t) = a + h(\mathbf{x}, t). \tag{5.1.4}$$

Therefore, since $p \mapsto h(\mathbf{x} + p\mathbf{n}, t)$ is monotone decreasing, it follows that $\ell^{-}(0) = \ell^{+}(0) = 0$. Moreover, since we assume that $\mathbf{x}$, t, and $\mathcal{S}(t)$ are independent of a, by (5.1.4), we have that

$$\mp 1 = \frac{\mathrm{d}\left(h(\mathbf{x} \pm \ell^{\pm}(a)\mathbf{n}, t)\right)}{\mathrm{d}a} = \pm \frac{\partial h(\mathbf{x} \pm \ell^{\pm}(a)\mathbf{n}, t)}{\partial n} \frac{\mathrm{d}\ell^{\pm}(a)}{\mathrm{d}a}, \tag{5.1.5}$$

and

$$0 = \frac{\partial^2 h(\mathbf{x} \pm \ell^{\pm}(a)\mathbf{n}, t)}{\partial n^2} \left(\frac{\mathrm{d}\ell^{\pm}(a)}{\mathrm{d}a}\right)^2 \pm \frac{\partial h(\mathbf{x} \pm \ell^{\pm}(a)\mathbf{n}, t)}{\partial n} \frac{\mathrm{d}^2\ell^{\pm}(a)}{\mathrm{d}a^2}. \tag{5.1.6}$$

Appealing to (5.1.3), (5.1.5), and (5.1.6), we have

$$\frac{\mathrm{d}\ell^{\pm}(0)}{\mathrm{d}a} = \frac{1}{|\nabla h(\mathbf{x}, t)|}, \tag{5.1.7}$$

and

$$\frac{\mathrm{d}^2\ell^{\pm}(0)}{\mathrm{d}a} = \mp \frac{\frac{\partial^2 h(\mathbf{x},t)}{\partial n^2}}{\left(\frac{\partial h(\mathbf{x},t)}{\partial n}\right)^3} = \pm \frac{\frac{\partial}{\partial n}\left[\left(\frac{\partial h(\mathbf{x},t)}{\partial n}\right)^{-1}\right]}{\left(\frac{\partial h(\mathbf{x},t)}{\partial n}\right)} = \pm \frac{\frac{\partial}{\partial n}\left(\frac{1}{|\nabla h(\mathbf{x},t)|}\right)}{|\nabla h(\mathbf{x}, t)|}. \tag{5.1.8}$$

In the remaining, we use the following notation:

$$f \overset{n}{\approx} g \text{ if and only if } f - g = O(a^n) \text{ as } a \to 0. \tag{5.1.9}$$

Then,

$$\left.\begin{aligned} \ell^{+}(a) &\overset{3}{\approx} \frac{a}{|\nabla h(\mathbf{x}, t)|} + \frac{a}{|\nabla h(\mathbf{x}, t)|} \frac{\partial}{\partial n}\left(\frac{a}{|\nabla h(\mathbf{x}, t)|}\right), \\ \ell^{-}(a) &\overset{3}{\approx} \frac{a}{|\nabla h(\mathbf{x}, t)|} - \frac{a}{|\nabla h(\mathbf{x}, t)|} \frac{\partial}{\partial n}\left(\frac{a}{|\nabla h(\mathbf{x}, t)|}\right). \end{aligned}\right\} \tag{5.1.10}$$

[1] Reversing one's perspective can help in understanding the process of finding a continuum limit. Indeed, the approximations made are easily understood if we ask ourselves: Given the height function h, find an approximation of the distance in the normal direction between (or more generally, change in normal parameter) level sets on which h is incremented by a small value a.

Moreover, if $\boldsymbol{\alpha} : (-\infty, \infty) \times [0, T) \to \mathbb{R}^2$ parameterizes a step, then

$$0 = \frac{\mathrm{d}(h(\boldsymbol{\alpha}(s,t),t))}{\mathrm{d}t} = \nabla h(\boldsymbol{\alpha}(s,t),t) \cdot \frac{\partial \boldsymbol{\alpha}(s,t)}{\partial t} + \frac{\partial h(\boldsymbol{\alpha}(s,t),t)}{\partial t}. \tag{5.1.11}$$

Hence, the normal velocity of a step is found to be

$$V = \frac{1}{|\nabla h|} \frac{\partial h}{\partial t}. \tag{5.1.12}$$

We first solve the PDE (4.6.6)-(4.6.7) for the adatom chemical potential μ_j by taking μ^{s}_{j-1}, μ^{s}_j, and μ^{s}_{j+1} to be constants, and in so doing set aside the modified Gibbs–Thomson. Then, the velocity equation takes the form

$$\varrho^{\mathrm{b}} V_j = \mathfrak{F}(\mathbf{x}_j, \ell^+_j, \ell^-_j, \mu^{\mathrm{s}}_{j-1}, \mu^{\mathrm{s}}_j, \mu^{\mathrm{s}}_{j+1}, C_+, C_-, \cdots), \tag{5.1.13}$$

and the modified Gibbs–Thomson relation takes the form

$$\mu^{\mathrm{s}}_j = \mathfrak{G}(\mathbf{x}_j, \ell^+_j, \ell^-_j, \mu^{\mathrm{s}}_{j-1}, \mu^{\mathrm{s}}_j, \mu^{\mathrm{s}}_{j+1}, C_+, C_-, \cdots). \tag{5.1.14}$$

We then find continuum versions of (5.1.13) and (5.1.14), by which we mean that we

- take μ^{s}_k to be the value of a macroscale function $\tilde{\mu}^{\mathrm{s}}(\mathbf{x}_k)$ for $k = j-1$, j and $j+1$, and writing $\mathbf{x}_{j\pm1} = \mathbf{x}_j \pm \ell^{\pm}_j \mathbf{n}$;
- make the replacements (5.1.10) and (5.1.12);
- substitute $M/C_{\pm} = a l_{\pm}$ with $l_{\pm}$ constant in a; and
- Taylor expand the right-hand sides of (5.1.13) and (5.1.14) to order a^2 about $a = 0$.

5.2 TC model for rectilinear trains of steps and its continuum limit

The remainder of the chapter is devoted to finding the continuum limit of the TC model for an infinite train of steps with positions $\{x_j\}_{j\in\mathbb{Z}}$. We assume that $C_+, C_- > 0$

and that they are inversely proportional to the step height a, such that the length scales associated with the attachment kinetics satisfies

$$\frac{M}{C_\pm} = L_\pm = a l_\pm, \tag{5.2.1}$$

with M and $l_\pm$ independent of a. This ensures that the length scales associated with the attachment kinetics, $L_\pm$, decrease as we decrease the terrace widths and the step height, so that the ratio of the $L_\pm$ and the step height is fixed as a decreases to 0.

For descending steps, we find the continuum limit for the equations:

$$\left.\begin{aligned}
0 &= M\frac{\partial^2 \mu_j}{\partial x^2} + F && \text{in } (x_j, x_{j+1}),\\
M\frac{\partial \mu_j}{\partial x} &= C_+\left(\mu_j - \mu_j^{\mathrm{s}}\right) && \text{at } x = x_j,\\
M\frac{\partial \mu_j}{\partial x} &= -C_-\left(\mu_j - \mu_{j+1}^{\mathrm{s}}\right) && \text{at } x = x_{j+1},\\
\mu_j^{\mathrm{s}} &= \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} + \Theta[\![\mu]\!]_j = \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} + \Theta\left(\mu_j - \mu_{j-1}\right) && \text{at } x = x_j,\\
\varrho^{\mathrm{b}} V_j &= C_+\left(\mu_j - \mu_j^{\mathrm{s}}\right) + C_-\left(\mu_{j-1} - \mu_j^{\mathrm{s}}\right) && \text{at } x = x_j.
\end{aligned}\right\} \tag{5.2.2}$$

The main result of this section is that the continuum limit takes the form of a coupled system of PDE. Specifically, letting $h_x = \frac{\partial h}{\partial x}$ and $h_t = \frac{\partial h}{\partial t}$, upon taking the continuum limit of the velocity equation $(5.2.2)_5$, we find h satisfies

$$\varrho^{\mathrm{b}} h_t - aF = a\frac{\partial}{\partial x}\left\{\alpha(|h_x|)\left[M\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial x} + \frac{aF(l_- - l_+)}{2}\right]\right\}, \tag{5.2.3}$$

where α is defined by[2]

$$\alpha(|\nabla h|) = \frac{1}{1 + (l_- + l_+)|\nabla h|}. \tag{5.2.4}$$

This equation is complemented by the continuum limit of the modified Gibbs–Thomson relation $(5.2.2)_4$

$$\tilde{\mu}^{\mathrm{s}} = \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} + a(l_+ + l_-)\Theta\alpha(|h_x|)\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial x} - \frac{a^2(l_- - l_+)\Theta}{2|h_x|}\left\{\frac{\partial}{\partial x}\left[\alpha(|h_x|)\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial x}\right] + \frac{F\alpha(|h_x|)}{M}\right\}. \tag{5.2.5}$$

[2]We have written as $\alpha(|\nabla h|)$ as this effective mobility arises again in the context of circular steps and then in general step steps with slowly varying curvature.

We assume $h_x(x,t), h_t(x,t)$, and, therefore, $\alpha(|h_x(x)|)$ are independent of a. As discussed in Section 5.3, if we neglect terms of order higher than a, this continuum limit may be understood as a coupled system in which (5.2.3) is a mass balance, and (5.2.5) is a configurational force balance, in the small slope limit.

Finding the continuum limit

Solving the boundary value problem $(5.2.2)_{1-3}$ for μ_j on each interval (x_j, x_{j+1}), we find that

$$\mu_j(x) = -\frac{F}{2M}x^2 + A_j x + B_j, \tag{5.2.6}$$

where A_j and B_j are prescribed in terms of μ_j^{s} and μ_{j+1}^{s} using $(5.2.2)_{2,3}$, and, in particular, A_j is given by

$$A_j = \frac{\mu_{j+1}^{\mathrm{s}} - \mu_j^{\mathrm{s}}}{\ell_j + L_+ + L_-} + \frac{F}{M}\left(x_j + \frac{L_-\ell_j + \frac{\ell_j^2}{2}}{\ell_j + L_+ + L_-}\right), \tag{5.2.7}$$

where ℓ_j denotes the terrace width defined by

$$\ell_j = x_{j+1} - x_j. \tag{5.2.8}$$

Define the adatom attachment flux J_j by

$$J_j(x) = -M\frac{\partial \mu_j(x)}{\partial x}. \tag{5.2.9}$$

Then appealing to (5.2.1), (5.2.6), and (5.2.7), we have that

$$J_j(x_j) = -\frac{M(\mu_{j+1}^{\mathrm{s}} - \mu_j^{\mathrm{s}})}{\ell_j + L_+ + L_-} - \frac{F\left(L_-\ell_j + \frac{\ell_j^2}{2}\right)}{\ell_j + L_+ + L_-}, \tag{5.2.10}$$

$$J_j(x_{j+1}) = J_j(x_j) + F\ell_j. \tag{5.2.11}$$

Moreover, the modified Gibbs–Thomson relation $(5.2.2)_4$ may be written in terms of J_j and J_{j-1} as

$$\mu_j^{\mathrm{s}} = \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} - \Theta\left(\frac{J_j(x_j)}{C_+} + \frac{J_{j-1}(x_j)}{C_-}\right), \tag{5.2.12}$$

and the velocity equation $(5.2.2)_5$ is equivalent to

$$\varrho^{\mathrm{b}} V_j = -J_j(x_j) + J_{j-1}(x_j). \tag{5.2.13}$$

This means that finding a continuum limit is reduced to finding the appropriate approximations of $J_j(x_j)$ and $J_{j-1}(x_j)$ in terms of x_j, a, $h_x(x_j)$, and the parameters: the mobility M, the deposition flux F, and the attachment coefficients $C_\pm$. To do so, we first find the order a^2 approximation for $J_j(x_j)$.

Approximating the diffusive flux J_j at the jth step

We use the approximation of the terrace widths

$$\ell_j \overset{3}{\approx} \frac{a}{|h_x(x_j)|} + \frac{a}{2|h_x(x_j)|}\frac{\partial}{\partial x}\left(\frac{a}{|h_x(x_j)|}\right), \tag{5.2.14}$$

as stated in $(5.1.10)_1$, and assume that in the continuum limit $\mu^{\mathrm{s}}_j = \tilde{\mu}^{\mathrm{s}}(x_j)$ is a smooth function of x. Further, we approximate μ^{s}_{j+1} by the Taylor polynomial of $\tilde{\mu}^{\mathrm{s}}$ centered at x_j, i.e.,

$$\mu^{\mathrm{s}}_{j+1} \overset{3}{\approx} \tilde{\mu}^{\mathrm{s}}(x_j) + \ell_j \frac{\partial \tilde{\mu}^{\mathrm{s}}(x_j)}{\partial x} + \frac{\ell_j^2}{2}\frac{\partial^2 \tilde{\mu}^{\mathrm{s}}(x_j)}{\partial x^2}. \tag{5.2.15}$$

By (5.2.10)-(5.2.11) and (5.2.15), we have that

$$J_j(x_j) \overset{2}{\approx} -\frac{M\left(\ell_j \frac{\partial \tilde{\mu}^{\mathrm{s}}(x_j)}{\partial x} + \frac{\ell_j^2}{2}\frac{\partial^2 \tilde{\mu}^{\mathrm{s}}(x_j)}{\partial x^2}\right)}{\ell_j + L_+ + L_-} - \frac{F\left(L_-\ell_j + \frac{\ell_j^2}{2}\right)}{\ell_j + L_+ + L_-}. \tag{5.2.16}$$

Let $\tilde{M}$ be defined by

$$\tilde{M}(x) = M\alpha(|h_x(x)|) = \frac{\frac{aM}{|h_x(x)|}}{\frac{a}{|h_x(x)|} + L_+ + L_-}. \tag{5.2.17}$$

Since $\alpha(|h_x(x)|)$, $M = O(1)$, we have that $\tilde{M}(x) = O(1)$.

Note that

$$
\begin{aligned}
\frac{M\ell_j}{\ell_j + L_+ + L_-} &\overset{2}{\approx} \frac{M\left(\frac{a}{|h_x(x_j)|} + \frac{a}{2|h_x(x_j)|}\frac{\partial}{\partial x}\left(\frac{a}{|h_x(x_j)|}\right)\right)}{\frac{a}{|h_x(x_j)|} + \frac{a}{2|h_x(x_j)|}\frac{\partial}{\partial x}\left(\frac{a}{|h_x(x_j)|}\right) + L_+ + L_-} \\
&\overset{2}{\approx} \frac{\frac{aM}{|h_x(x_j)|}}{\frac{a}{|h_x(x_j)|} + L_+ + L_-} + \frac{a}{2|h_x(x_j)|}\frac{\partial}{\partial x}\left(\frac{\frac{aM}{|h_x(x_j)|}}{\frac{a}{|h_x(x_j)|} + L_+ + L_-}\right) \\
&= \tilde{M}(x_j) + \frac{a}{2|h_x(x_j)|}\frac{\partial \tilde{M}(x_j)}{\partial x},
\end{aligned}
\tag{5.2.18}
$$

and, furthermore,

$$
\frac{\frac{\ell_j^2}{2}}{\ell_j + L_+ + L_-} \overset{2}{\approx} \frac{a\tilde{M}(x_j)}{2|h_x(x_j)|M}. \tag{5.2.19}
$$

Hence, applying (5.2.18) and (5.2.19) to (5.2.16) and recalling that $L_- = al_-$, we find

$$
\begin{aligned}
J_j(x_j) \overset{2}{\approx} & -\frac{\partial \tilde{\mu}^{s}(x_j)}{\partial x}\left(\tilde{M}(x_j) + \frac{a}{2|h_x(x_j)|}\frac{\partial \tilde{M}(x_j)}{\partial x}\right) \\
& - \frac{a\tilde{M}(x_j)}{2|h_x(x_j)|}\frac{\partial^2 \tilde{\mu}^{s}(x_j)}{\partial x^2} - \frac{aF l_- \tilde{M}(x_j)}{M} \\
& - \frac{aF\tilde{M}(x_j)}{2|h_x(x_j)|M}.
\end{aligned}
\tag{5.2.20}
$$

This approximation (5.2.20) may be re-arranged to yield

$$
\begin{aligned}
J_j(x_j) \overset{2}{\approx} & -\tilde{M}(x_j)\frac{\partial \tilde{\mu}^{s}(x_j)}{\partial x} - \frac{aF\left(l_- - l_+\right)\tilde{M}(x_j)}{2M} \\
& - \frac{a}{2|h_x(x_j)|}\left(F + \frac{\partial}{\partial x}\left(\tilde{M}(x_j)\frac{\partial \tilde{\mu}^{s}(x_j)}{\partial x}\right)\right).
\end{aligned}
\tag{5.2.21}
$$

Let $\mathcal{J}_0$ and$\mathcal{J}_1$ be defined by

$$
\begin{aligned}
\mathcal{J}_0 &:= -\tilde{M}\frac{\partial \tilde{\mu}^{s}}{\partial x}, \\
\mathcal{J}_1 &:= -\frac{aF(l_- - l_+)\tilde{M}}{2M} - \frac{a}{2|h_x|}\left(F + \frac{\partial}{\partial x}\left(\tilde{M}\frac{\partial \tilde{\mu}^{s}}{\partial x}\right)\right).
\end{aligned}
\tag{5.2.22}
$$

Let $\mathcal{J}_2 = O(a^2)$ be a function such that the function $\mathcal{J}$ be defined by

$$
\mathcal{J}(x) = \mathcal{J}_0(x) + \mathcal{J}_1(x) + \mathcal{J}_2(x) \tag{5.2.23}
$$

satisfies

$$J_j(x_j) \overset{3}{\approx} \mathcal{J}(x_j). \tag{5.2.24}$$

An example of such a $\mathcal{J}_2$ may be found explicitly in the same manner that we found $\mathcal{J}_0$ and $\mathcal{J}_1$, i.e., Taylor expanding to order a^2. However, the particular form of $\mathcal{J}_2$ does not enter into the order a^2 continuum equations.

Approximating the diffusive flux J_{j-1} at the jth step

We now find the order a^2 approximation of $J_{j-1}(x_j)$. Then, using $(5.1.10)_2$,

$$\ell_{j-1} \overset{3}{\approx} \frac{a}{|h_x(x_j)|} - \frac{a}{2|h_x(x_j)|}\frac{\partial}{\partial x}\left(\frac{a}{|h_x(x_j)|}\right), \tag{5.2.25}$$

we have from (5.2.11) that

$$\begin{aligned} J_{j-1}(x_j) &= J_{j-1}(x_{j-1}) + F\ell_{j-1} \\ &\overset{3}{\approx} \mathcal{J}(x_{j-1}) + F\left(\frac{a}{|h_x(x_j)|} - \frac{a}{2|h_x(x_j)|}\frac{\partial}{\partial x}\left(\frac{a}{|h_x(x_j)|}\right)\right). \end{aligned} \tag{5.2.26}$$

Expanding $\mathcal{J}(x_{j-1})$ about x_j, (5.2.26) yields

$$\begin{aligned} J_{j-1}(x_j) &\overset{3}{\approx} \mathcal{J}(x_j) - \ell_{j-1}\frac{\partial \mathcal{J}(x_j)}{\partial x} + \frac{\ell_{j-1}^2}{2}\frac{\partial^2 \mathcal{J}(x_j)}{\partial x^2} \\ &\quad + F\left(\frac{a}{|h_x(x_j)|} - \frac{a}{2|h_x(x_j)|}\frac{\partial}{\partial x}\left(\frac{a}{|h_x(x_j)|}\right)\right) \\ &\overset{3}{\approx} \mathcal{J} + \frac{a}{|h_x|}\left\{F + +\frac{\partial}{\partial x}\left[\frac{a}{2|h_x|}\frac{\partial \mathcal{J}_0}{\partial x} - \mathcal{J}_0 - \mathcal{J}_1 - \frac{aF}{2|h_x|}\right]\right\}\Bigg|_{x=x_j}, \end{aligned} \tag{5.2.27}$$

where we first Taylor expand $\mathcal{J}(x_{j-1})$ about x_j, and then use our approximation for ℓ_{j-1} (5.2.25). We may simplify the last term of (5.2.27) as

$$\frac{a}{2|h_x|}\frac{\partial \mathcal{J}_0}{\partial x} - \mathcal{J}_0 - \mathcal{J}_1 - \frac{aF}{2|h_x|} = \tilde{M}\frac{\partial \tilde{\mu}^s}{\partial x} + \frac{a(l_- - l_+)\tilde{M}F}{2M}. \tag{5.2.28}$$

Hence, (5.2.27) is equivalent to

$$J_{j-1}(x_j) \overset{3}{\approx} \mathcal{J}(x_j) + \frac{a}{|h_x|}\left\{F + \frac{\partial}{\partial x}\left(\tilde{M}\frac{\partial \tilde{\mu}^s}{\partial x}\right) + \frac{aF\,(l_- - l_+)}{2M}\frac{\partial \tilde{M}}{\partial x}\right\}\Bigg|_{x=x_j}. \tag{5.2.29}$$

Continuum limit

In the continuum limit, we have $V_j = \dfrac{h_t(x_j)}{|h_x(x_j)|}$. Therefore, applying (5.2.24) and (5.2.29) to (5.2.13) we find:

$$\varrho^{\mathrm{b}} h_t = a\mathcal{F} + \frac{a^2\mathcal{F}}{2M}(l_- - l_+)\frac{\partial \tilde{M}}{\partial x} + a\frac{\partial}{\partial x}\left(\tilde{M}\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial x}\right). \tag{5.2.30}$$

Appealing to $(5.2.2)_{2,3,4}$, the modified Gibbs–Thomson relation may be written in terms of $J_j(x_j)$ and $J_{j-1}(x_j)$ as

$$\frac{\mu_j^{\mathrm{s}} - \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}}}{\Theta} = \mu_{x_j}^+ - \mu_{x_j}^- = -\left(\frac{J_j(x_j)}{C_+} + \frac{J_{j-1}(x_j)}{C_-}\right). \tag{5.2.31}$$

Since $C_\pm = O(1/a)$, we have that

$$\frac{\mu_j^{\mathrm{s}} - \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}}}{\Theta} \overset{3}{\approx} -\frac{\mathcal{J}_0(x_j) + \mathcal{J}_1(x_j)}{C_+} - \frac{\mathcal{J}_0(x_j) + \mathcal{J}_1(x_j) + \frac{a}{|h_x|}\left(\mathcal{F} + \frac{\partial}{\partial x}\left[\tilde{M}(x_j)\frac{\partial \tilde{\mu}^{\mathrm{s}}(x_j)}{\partial x}\right]\right)}{C_-}. \tag{5.2.32}$$

Hence, in the continuum limit (5.2.32) requires that

$$\begin{aligned}\frac{\tilde{\mu}^{\mathrm{s}} - \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}}}{\Theta} &= \left(\frac{1}{C_+} + \frac{1}{C_-}\right)\tilde{M}\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial x} + \frac{a}{2|h_x|}\left(\frac{1}{C_+} - \frac{1}{C_-}\right) \\ &\quad\times\left(\frac{-\mathcal{F}L_+ + L_-\frac{|h_x|}{a}}{1 + (L_+ + L_-)\frac{|h_x|}{a}} + \mathcal{F} + \frac{\partial}{\partial x}\left(\tilde{M}\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial x}\right)\right) \\ &= \left(\frac{1}{C_+} + \frac{1}{C_-}\right)\tilde{M}\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial x} + \frac{a}{2|h_x|}\left(\frac{1}{C_+} - \frac{1}{C_-}\right) \\ &\quad\times\left(\frac{\mathcal{F}\tilde{M}}{M} + \frac{\partial}{\partial x}\left(\tilde{M}\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial x}\right)\right)\end{aligned} \tag{5.2.33}$$

Upon rearrangement and use of $l_\pm$, (5.2.33) reduces to

$$\tilde{\mu}^{\mathrm{s}} = \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} + a\Theta\left\{(l_+ + l_-)\frac{\tilde{M}}{M}\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial x} - \frac{a}{2|h_x|}(l_- - l_+)\left(\frac{\mathcal{F}\tilde{M}}{M^2} + \frac{\partial}{\partial x}\left(\frac{\tilde{M}}{M}\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial x}\right)\right)\right\}. \tag{5.2.34}$$

Since $\tilde{M} = M\alpha(|h_x|)$, (5.2.30) and (5.2.34) yield (5.2.3) and (5.2.5).

5.3 Discussion

Note that for $\Theta = 0$, the quasistatic TC model take the exact same form of the quasistatic BCF model, where we formally identify

$$\begin{aligned} M &\leftrightarrow D, \\ \digamma &\leftrightarrow F, \\ C_\pm &\leftrightarrow K_\pm, \\ \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} &\leftrightarrow \varrho_{\mathrm{eq}}, \text{ and} \\ \gamma &\leftrightarrow \Gamma. \end{aligned} \tag{5.3.1}$$

It is no surprise therefore, under the same formal identifications, that our continuum limit reduces to those found for the BCF model. In particular, E and Yip find the a^2 order continuum limit of an infinite train of steps to be:

$$h_t = Fa^3 + \left(\frac{F(K_+ - K_-)(K_+ + K_-)D^2}{2((K_+ + K_-)D|h_x| + K_+K_-a)^2} \right) a^4 h_{xx}. \tag{5.3.2}$$

where they take $\varrho^{\mathrm{b}} = a^{-2}$. Assuming, as we do, that h is monotone decreasing in x, this is equivalent to (5.2.3) taking $\Theta = 0$ and with the above formal identifications (5.3.1). This is seen by noting that for $\Theta = 0$, equation $(5.3.1)_2$ reduces to the requirement that $\tilde{\mu}^{\mathrm{s}} = \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}}$. Since $\frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}}$ is a constant, the term $\partial \tilde{\mu}^{\mathrm{s}}/\partial x = 0$, and our continuum limit reduces to

$$\begin{aligned} \varrho^{\mathrm{b}} h_t &= a\digamma + \frac{a^2 \digamma (l_- - l_+)}{2} \frac{\partial\left(\alpha(|h_x|)\right)}{\partial x} \\ &= a\digamma + \frac{a^2 \digamma (l_- - l_+)(l_+ + l_-)h_{xx}}{2(1 + (l_+ + l_-)|h_x|)^2}, \end{aligned} \tag{5.3.3}$$

and since $l_\pm = \frac{M}{aC_\pm}$, we have

$$\varrho^{\mathrm{b}} h_t = a\digamma + \frac{a^2 \digamma (C_+ - C_-)(C_+ + C_-)M^2}{2((C_+ + C_-)M|h_x| + C_+C_-)^2} h_{xx}. \tag{5.3.4}$$

Remark 5.3.1. *If we keep terms of (5.2.3) and (5.2.5) up to order a, this system reduces to:*

$$\left.\begin{aligned} \varrho^b h_t = & \quad aF + a\frac{\partial}{\partial x}\left(\frac{M}{1+(l_+ + l_-)|h_x|}\frac{\partial \tilde{\mu}^s}{\partial x}\right), \\ \frac{\Psi^b}{\varrho^b} = & \quad -\frac{a(l_+ + l_-)\Theta}{1+(l_+ + l_-)|h_x|}\frac{\partial \tilde{\mu}^s}{\partial x} + \tilde{\mu}^s. \end{aligned}\right\} \tag{5.3.5}$$

Moreover, if there is symmetric attachment ($l_+ = l_- = \frac{l}{2}$), then the continuum limit reduces to:

$$\left.\begin{aligned} \varrho^b h_t = & \quad aF + a\frac{\partial}{\partial x}\left(\frac{M}{1+l|h_x|}\frac{\partial \tilde{\mu}^s}{\partial x}\right), \\ \frac{\Psi^b}{\varrho^b} = & \quad \tilde{\mu}^s - \frac{al\Theta}{1+l|h_x|}\frac{\partial \tilde{\mu}^s}{\partial x}. \end{aligned}\right\} \tag{5.3.6}$$

In the standard continuum theory of epitaxial crystal growth, mass balance requires that

$$\varrho^b V_{\mathcal{S}} = \operatorname{div}_{\mathcal{S}}(M_{\boldsymbol{N}} \nabla_{\mathcal{S}} \tilde{\mu}^s) + \tilde{F}, \tag{5.3.7}$$

where $V_{\mathcal{S}}$ is the normal velocity of the crystal surface, $\operatorname{div}_{\mathcal{S}}$ is the surface divergence, $\nabla_{\mathcal{S}}$ is the surface gradient, $\boldsymbol{N}$ is the unit normal to the surface, $M_{\boldsymbol{N}}$ is the adatom mobility which may depend on the surface orientation normal, $\tilde{\mu}^s$ is the surface chemical potential, and $\tilde{F}$ is a deposition term. In the case of a one dimension surface given for each time t by the graph of $y = h(x,t)$: $\operatorname{div}_{\mathcal{S}} = \nabla_{\mathcal{S}} = \frac{\partial}{\partial s}$, the derivative with respect to arclength, and $V_{\mathcal{S}}$ is the normal velocity of the curve $\boldsymbol{\alpha} : (x,t) \mapsto (x, h(x,t))$. Hence, as differential operators

$$\frac{\partial}{\partial s} = \frac{1}{|(1,h_x)|}\frac{\partial}{\partial x}, \tag{5.3.8}$$

and since the unit normal $\boldsymbol{N}$ to the curve $\boldsymbol{\alpha}$ is given by

$$\boldsymbol{N} = \left(\frac{-h_x}{\sqrt{1+|h_x|^2}}, \frac{1}{\sqrt{1+|h_x|^2}}\right). \tag{5.3.9}$$

Note that there is a one to one correspondence between $\boldsymbol{N}$ and the value of the slope h_x. Hence, we have that for some function $\tilde{\alpha}$, $M_{\boldsymbol{N}} = \tilde{\alpha}(h_x)$.

$$V_{\mathcal{S}} = \frac{\partial \boldsymbol{\alpha}}{\partial t} \cdot \left(\frac{-h_x}{\sqrt{1+|h_x|^2}}, \frac{1}{\sqrt{1+|h_x|^2}}\right) = \frac{h_t}{\sqrt{1+|h_x|^2}}. \tag{5.3.10}$$

Hence, (5.3.7) requires that

$$\frac{\varrho^b}{a} h_t = \frac{\partial}{\partial x}\left(\frac{\tilde{\alpha}(h_x)}{\sqrt{1+|h_x|^2}}\frac{\partial \tilde{\mu}^s}{\partial x}\right) + \tilde{F}\sqrt{1+|h_x|^2}. \qquad (5.3.11)$$

We see that may identify F *with* $\tilde{F} \approx \tilde{F}\sqrt{1+|h_x|^2}$ *when* $|h_x| \approx 0$, *and* $\tilde{\alpha}(h_x)/\sqrt{1+|h_x|^2}$ *with* $M/(1+l|h_x|)$.

6 Thermodynamically consistent continuum limits of concentric circular wedding cake step profiles

6.1 Introduction

In this chapter, we focus on the wedding cake structure in which a crystal surface consists of descending concentric circular steps (see Fig. 6.1). Such nanostructures are observed during low-temperature molecular beam epitaxy on metallic surfaces (cf. [40]). Unlike in the previous chapter, the step line tension is an important ingredient in determining the motion of concentric steps and the resulting continuum-limit equations. To simplify the presentation, we first consider the relaxation problem, i.e., $\mathcal{F}, \breve{\sigma} = 0$. We then turn to the growth problem, in which $\mathcal{F} > 0$ and $\breve{\sigma} = 0$. Since $\mathcal{F}$ appears linearly in the continuum limit, the result of the first calculation is subsumed in the second. However, we use the results of the relaxation calculation in the growth calculation. Finally, we treat the desorption problem in which $\mathcal{F} = 0$ and $\breve{\sigma} > 0$.

6.2 Surface relaxation

For concentric circular steps forming a wedding cake structure undergoing surface relaxation (that is, $\mathcal{F}, \breve{\sigma} = 0$), the boundary value problem (4.6.6)-(4.6.7) and the velocity equation (4.6.8) take the form:

$$\left.\begin{aligned}
0 &= \frac{M}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \mu_j}{\partial r}\right) && \text{in } (r_j, r_{j+1}),\\
M\frac{\partial \mu_j}{\partial r} &= C_+\left(\mu_j - \mu_j^{\mathrm{s}}\right) && \text{at } r = r_j,\\
M\frac{\partial \mu_j}{\partial r} &= -C_-\left(\mu_j - \mu_{j+1}^{\mathrm{s}}\right) && \text{at } r = r_{j+1},\\
\varrho^{\mathrm{b}} V_j &= C_+\left(\mu_j - \mu_j^{\mathrm{s}}\right) + C_-\left(\mu_{j-1} - \mu_j^{\mathrm{s}}\right) && \text{at } r = r_j,
\end{aligned}\right\} \tag{6.2.1}$$

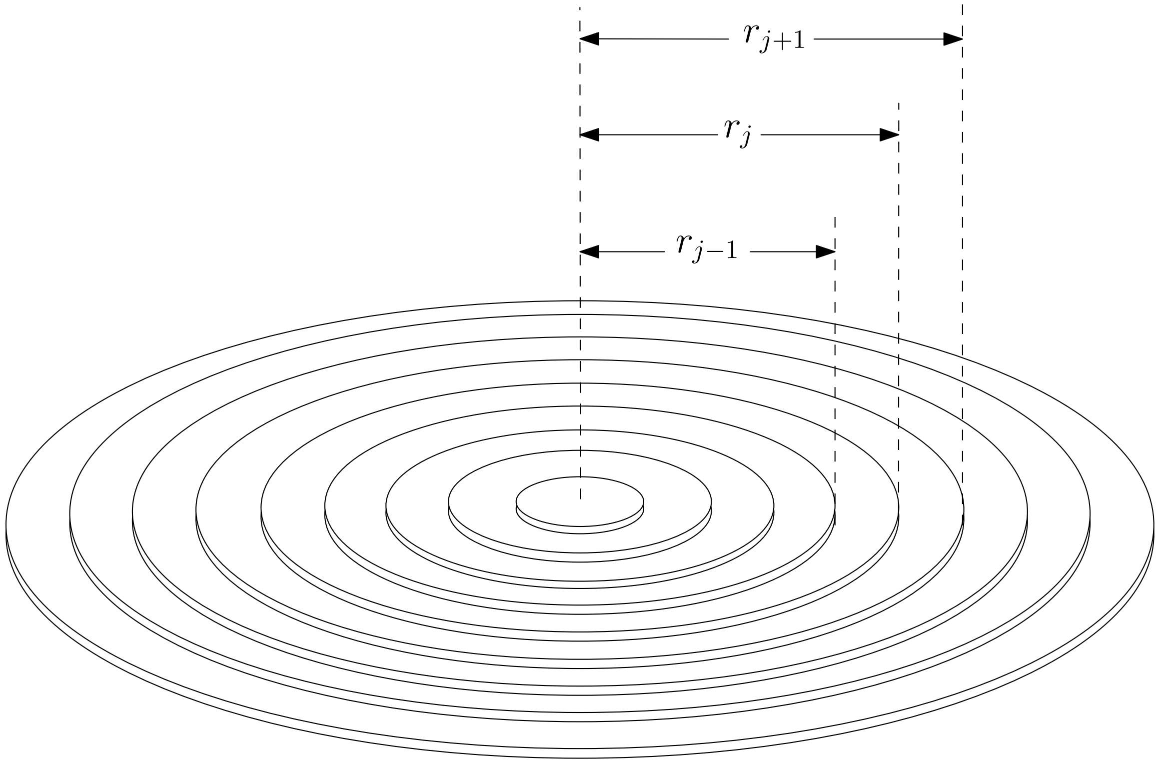

Figure 6.1: Schematic of a wedding cake structure.

where μ^{s} satisfies the modified Gibbs–Thomson relation

$$\mu^{\mathrm{s}}_j = \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} + \Theta(\mu_j - \mu_{j-1}) + \frac{\gamma}{r_j} \qquad \text{at } r = r_j. \tag{6.2.2}$$

The main results of this section are the following continuum limits of the velocity equation $(6.2.1)_4$ governing the height function h

$$\varrho^{\mathrm{b}} h_t = \frac{a}{r}\frac{\partial}{\partial r}\left\{ rM\alpha(|h_r|)\big[1 + a\widehat{\alpha}(|h_r|)\big]\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial r}\right\}, \tag{6.2.3}$$

and of the modified Gibbs–Thomson relation (6.2.2) governing the surface chemical potential $\tilde{\mu}^{\mathrm{s}}$:

$$\begin{aligned}\tilde{\mu}^{\mathrm{s}} = \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} + \frac{\gamma}{r} + a\Theta\alpha(|h_r|)\left[l_+ + l_- - \frac{a\widehat{\alpha}(|h_r|)}{|h_r|}\right]\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial r} \\ - \frac{a^2\Theta}{|h_r|}\frac{\partial}{\partial r}\left[r\widehat{\alpha}(|h_r|)\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial r}\right],\end{aligned} \tag{6.2.4}$$

where α is defined in (5.2.4) and $\widehat{\alpha}$ is defined by

$$\widehat{\alpha}(|h_r|) = \frac{(l_- - l_+)\,\alpha(|h_r|)}{2r}. \tag{6.2.5}$$

Approximating the diffusive flux J_j at the jth step

By $(6.2.1)_{1,2,3}$, we have

$$\mu_j(r) = A_j \ln r + B_j, \tag{6.2.6}$$

where A_j and B_j are prescribed in terms of μ^{s}_j and μ^{s}_{j+1} using $(6.2.1)_{2,3}$ and, in particular, A_j is given by

$$A_j = \frac{\mu^{\mathrm{s}}_{j+1} - \mu^{\mathrm{s}}_j}{\ln\left(\frac{r_{j+1}}{r_j}\right) + \left(\frac{M}{C_- r_{j+1}} + \frac{M}{C_+ r_j}\right)}. \tag{6.2.7}$$

Hence, for J_j defined on (r_j, r_{j+1}) as

$$J_j(r) = -M\frac{\partial \mu_j(r)}{\partial r} = -\frac{MA_j}{r}, \tag{6.2.8}$$

by (6.2.7), we have that

$$J_j(r_j) = -\frac{M(\mu^{\mathrm{s}}_{j+1} - \mu^{\mathrm{s}}_j)}{r_j\left[\ln\left(\frac{r_{j+1}}{r_j}\right) + \left(\frac{M}{C_- r_{j+1}} + \frac{M}{C_+ r_j}\right)\right]}. \tag{6.2.9}$$

Fixing r_j (i.e., $r_j = O(1)$),

$$r_j\left[\ln\left(\frac{r_{j+1}}{r_j}\right) + \left(\frac{M}{C_- r_{j+1}} + \frac{M}{C_+ r_j}\right)\right] \overset{3}{\approx} \delta r_j + L_+ + L_- - \frac{\delta r_j^2}{2r_j} - \frac{L_-\delta r_j}{r_j}, \tag{6.2.10}$$

where $\overset{n}{\approx}$ is defined as in (5.1.9) and by $(5.1.10)_1$ we have taken

$$\delta r_j = r_{j+1} - r_j \overset{3}{\approx} \frac{a}{|h_r|} + \frac{a}{|h_r|}\frac{\partial}{\partial r}\left(\frac{a}{|h_r|}\right), \tag{6.2.11}$$

and $L_\pm = al_\pm = M/C_\pm$ with $l_\pm$ independent of a. Applying (6.2.10) and (6.2.11) to (6.2.9) we find

$$\begin{aligned} J_j(r_j) &\overset{2}{\approx} -\frac{M\left[\delta r_j\frac{\partial\tilde{\mu}^{\mathrm{s}}(r_j)}{\partial r} + \frac{\delta r_j^2}{2}\frac{\partial^2\mu^{\mathrm{s}}(r_j)}{\partial r^2}\right]\left[1 + \frac{\frac{\delta r_j^2}{2r_j} + L_-\frac{\delta r_j}{r_j}}{\delta r_j + L_+ + L_-}\right]}{\delta r_j + L_+ + L_-} \\ &\overset{2}{\approx} -\tilde{M}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial r} - \frac{a}{2|h_r|}\frac{\partial}{\partial r}\left(\tilde{M}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial r}\right) - \frac{a\left(1 + 2l_-|h_r|\right)\tilde{M}^2}{2|h_r|Mr}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial r}\bigg|_{r=r_j}, \end{aligned} \tag{6.2.12}$$

where $\tilde{M}$ is defined by (cf. (5.2.17))

$$\tilde{M}(r) = \frac{M}{1 + (l_+ + l_-)|h_r(r)|} = M\alpha(|h_r(r)|). \tag{6.2.13}$$

We may modify the last term of (6.2.12) by noting

$$(1 + 2l_-|h_r|)\tilde{M}^2 = \frac{M\,(1 + 2l_-|h_r|)}{(1 + (l_- + l_+)|h_r|)^2} = \tilde{M} + (l_- - l_+)|h_r|\frac{\tilde{M}^2}{M}. \tag{6.2.14}$$

Then (6.2.12) and (6.2.14) yield

$$J_j(r_j) \overset{2}{\approx} -\tilde{M}\frac{\partial \tilde{\mu}^s}{\partial r} - \frac{a}{2|h_r|}\frac{1}{r}\frac{\partial}{\partial r}\left(r\tilde{M}\frac{\partial \tilde{\mu}^s}{\partial r}\right) - \frac{a(l_- - l_+)\tilde{M}^2}{2Mr}\frac{\partial \tilde{\mu}^s}{\partial r}\bigg|_{r=r_j}. \tag{6.2.15}$$

We define

$$\begin{aligned} \mathcal{J}_0 = &\; -\tilde{M}\frac{\partial \tilde{\mu}^s}{\partial r}, \\ \mathcal{J}_1 = &\; -\frac{a}{2|h_r|}\frac{1}{r}\frac{\partial}{\partial r}\left(r\tilde{M}\frac{\partial \tilde{\mu}^s}{\partial r}\right) - \frac{a(l_- - l_+)\tilde{M}^2}{2Mr}\frac{\partial \tilde{\mu}^s}{\partial r}, \end{aligned} \tag{6.2.16}$$

and $\mathcal{J}_2 = O(a^2)$ such that the function $\mathcal{J}$ defined by

$$\mathcal{J} = \mathcal{J}_0 + \mathcal{J}_1 + \mathcal{J}_2 \tag{6.2.17}$$

satisfies

$$J_j(r_j) \overset{3}{\approx} \mathcal{J}(r_j). \tag{6.2.18}$$

Approximating the diffusive flux J_{j-1} at the jth step

By (6.2.8), we have

$$J_j(r_{j+1}) = \frac{r_j J_j(r_j)}{r_{j+1}}. \tag{6.2.19}$$

Applying (6.2.18) to (6.2.19), it follows that

$$J_{j-1}(r_j) = \frac{r_{j-1}J_{j-1}(r_{j-1})}{r_j} \overset{3}{\approx} \frac{r_{j-1}\mathcal{J}(r_{j-1})}{r_j}. \tag{6.2.20}$$

Next, we expand $r_{j-1}\mathcal{J}(r_{j-1})$ at r_j to find

$$\begin{aligned} r_{j-1}\mathcal{J}(r_{j-1}) &\overset{3}{\approx} r_j\mathcal{J}(r_j) - \delta r_{j-1}\frac{\partial(r_j\mathcal{J}(r_j))}{\partial r} + \frac{\delta r_{j-1}^2}{2}\frac{\partial^2(r_j\mathcal{J}(r_j))}{\partial r^2} \\ &\overset{3}{\approx} r\mathcal{J} + \frac{a}{|h_r|}\frac{\partial}{\partial r}\left\{-r\left(\mathcal{J}_0+\mathcal{J}_1\right) + \frac{a}{2|h_r|}\frac{\partial(r\mathcal{J}_0)}{\partial r}\right\}\Bigg|_{r=r_j} \\ &= r\mathcal{J} + \frac{a}{|h_r|}\frac{\partial}{\partial r}\left[\left(r\tilde{M} + \frac{a\left(l_- - l_+\right)\tilde{M}^2}{2M}\right)\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial r}\right]\Bigg|_{r=r_j}. \end{aligned} \tag{6.2.21}$$

Hence, by (6.2.20) and (6.2.21) we have that

$$J_{j-1}(r_j) \overset{3}{\approx} \mathcal{J} + \frac{a}{|h_r|}\frac{1}{r}\frac{\partial}{\partial r}\left[\left(r\tilde{M} + \frac{a\left(l_- - l_+\right)\tilde{M}^2}{2M}\right)\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial r}\right]\Bigg|_{r=r_j}. \tag{6.2.22}$$

Continuum limit

By $(6.2.1)_4$,

$$\varrho^{\mathrm{b}}V_j = -J_j(r_j) + J_{j-1}(r_j), \tag{6.2.23}$$

and recalling (5.1.12) that in the continuum limit $V_j = \frac{h_t(r_j)}{|h_r(r_j)|}$, we have that the continuum limit of the velocity equation is found upon use of (6.2.18) and (6.2.22)

$$\varrho^{\mathrm{b}}h_t = \frac{a}{r}\frac{\partial}{\partial r}\left[\left(r\tilde{M} + \frac{a\left(l_- - l_+\right)\tilde{M}^2}{2M}\right)\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial r}\right]. \tag{6.2.24}$$

The boundary conditions $(6.2.1)_{2,3}$ imply that the modified Gibbs–Thomson relation (6.2.2) may be written as

$$\frac{\mu_j^{\mathrm{s}} - \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}}}{\Theta} = -\left(\frac{J_j(r_j)}{C_+} + \frac{J_{j-1}(r_j)}{C_-}\right). \tag{6.2.25}$$

Since $C_\pm = O(1/a)$, we find that (6.2.18) and (6.2.22) applied to (6.2.25) implies:

$$\frac{\mu_j^{\mathrm{s}} - \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} - \frac{\gamma}{r_j}}{\Theta} \overset{3}{\approx} -\frac{\mathcal{J}_0+\mathcal{J}_1}{C_+} - \frac{\mathcal{J}_0+\mathcal{J}_1+\frac{a}{|h_r|}\frac{1}{r}\frac{\partial}{\partial r}\left(r\tilde{M}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial r}\right)}{C_-}\Bigg|_{r=r_j}. \tag{6.2.26}$$

Hence, in the continuum limit

$$\begin{aligned} \frac{\tilde{\mu}^{\mathrm{s}} - \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} - \frac{\gamma}{r}}{\Theta} &= a\left(l_+ + l_-\right)\frac{\tilde{M}}{M}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial r} \\ &\quad - \frac{a^2(l_- - l_+)}{2|h_r|}\left[\frac{\tilde{M}^2}{M^2 r}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial r} + \frac{\partial}{\partial r}\left(\frac{\tilde{M}}{M}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial r}\right)\right]. \end{aligned} \tag{6.2.27}$$

In terms of $\alpha(|h_r|)$ and $\widehat{\alpha}(|h_r|)$, the continuum limits (6.2.27) and (6.2.24) yield (6.2.4) and (6.2.3).

6.3 Growth

We now turn to the task of finding the continuum limit for concentric steps during growth (i.e., $F > 0$ and $\breve{\sigma} = 0$). For this choice of parameters, the boundary value problem (4.6.6)-(4.6.7) and the velocity equation (4.6.8) take the form:

$$\left.\begin{aligned} 0 &= \frac{M}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \mu_j}{\partial r}\right) + F && \text{in } (r_j, r_{j+1}),\\ M\frac{\partial \mu_j}{\partial r} &= C_+\left(\mu_j - \mu_j^{\mathrm{s}}\right) && \text{at } r = r_j,\\ M\frac{\partial \mu_j}{\partial r} &= -C_-\left(\mu_j - \mu_{j+1}^{\mathrm{s}}\right) && \text{at } r = r_{j+1},\\ \varrho^{\mathrm{b}} V_j &= C_+\left(\mu_j - \mu_j^{\mathrm{s}}\right) + C_-\left(\mu_{j-1} - \mu_j^{\mathrm{s}}\right) && \text{at } r = r_j, \end{aligned}\right\} \tag{6.3.1}$$

where μ_j^{s} satisfies the modified Gibbs–Thomson relation (4.6.5)

$$\mu_j^{\mathrm{s}} = \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} + \Theta(\mu_j - \mu_{j-1}) + \frac{\gamma}{r_j} \quad \text{at } r = r_j. \tag{6.3.2}$$

The main results of this section are the continuum limits of the velocity equation (6.3.1)

$$\varrho^{\mathrm{b}} h_t = \frac{a}{r}\frac{\partial}{\partial r}\left\{ rM\alpha(|h_r|)\left[1 + a\widehat{\alpha}(|h_r|)\right]\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial r}\right\} + aF\left[1 + \frac{a}{r}\frac{\partial(r^2\widehat{\alpha}(|h_r|))}{\partial r}\right], \tag{6.3.3}$$

and of the modified Gibbs–Thomson relation (6.3.2)

$$\begin{aligned} \tilde{\mu}^{\mathrm{s}} = \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} + \frac{\gamma}{r} + a\Theta\alpha(|h_r|)\left[l_+ + l_- - \frac{a\widehat{\alpha}(|h_r|)}{|h_r|}\right]\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial r} \\ - \frac{a^2\Theta}{|h_r|}\frac{\partial}{\partial r}\left[r\widehat{\alpha}(|h_r|)\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial r}\right] - \frac{a^2 F\Theta r\widehat{\alpha}(|h_r|)}{M|h_r|}, \end{aligned} \tag{6.3.4}$$

where α and $\widehat{\alpha}$ is defined in (5.2.4) and (6.2.5), respectively.

Approximating the diffusive flux J_j at the jth step

Solving the ODE $(6.3.1)_1$ for μ_j, we find

$$\mu_j(r) = -\frac{F}{4M}r^2 + A_j \ln r + B_j \text{ on } (r_j, r_{j+1}), \tag{6.3.5}$$

where

$$A_j = \frac{\mu^{\mathrm{s}}_{j+1} - \mu^{\mathrm{s}}_j + \frac{F}{4M}\left(2\left(\frac{Mr_j}{C_+} + \frac{Mr_{j+1}}{C_-}\right) + r_{j+1}^2 - r_j^2\right)}{\ln\left(\frac{r_{j+1}}{r_j}\right) + \left(\frac{M}{C_+ r_j} + \frac{M}{C_- r_{j+1}}\right)}. \tag{6.3.6}$$

The adatom flux $J_j(r) = -M\frac{\partial \mu_j(r)}{\partial r}$ satisfies

$$J_j(r_j) = -\frac{M\left(\mu^{\mathrm{s}}_{j+1} - \mu^{\mathrm{s}}_j\right) + \frac{F}{2}\left(\frac{r_{j+1}^2 - r_j^2}{2} + \left(\frac{Mr_j}{C_+} + \frac{Mr_{j+1}}{C_-}\right)\right)}{r_j\left(\ln\left(\frac{r_{j+1}}{r_j}\right) + \left(\frac{M}{C_+ r_j} + \frac{M}{C_- r_{j+1}}\right)\right)} + \frac{F r_j}{2}. \tag{6.3.7}$$

We found previously,

$$\begin{aligned} &-\frac{M(\mu^{\mathrm{s}}_{j+1} - \mu^{\mathrm{s}}_j)}{r_j\left[\ln\left(\frac{r_{j+1}}{r_j}\right) + \left(\frac{M}{C_- r_{j+1}} + \frac{M}{C_+ r_j}\right)\right]} \\ &\qquad \overset{2}{\approx} -\tilde{M}\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial r} - \frac{a}{2|h_r| r}\frac{\partial}{\partial r}\left(r\tilde{M}\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial r}\right) - \frac{a\left(l_- - l_+\right)\tilde{M}^2}{2Mr}\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial r}\bigg|_{r=r_j}, \end{aligned} \tag{6.3.8}$$

as seen in (6.2.9) and (6.2.9). In particular, it follow from (6.2.10) that

$$\frac{1}{r_j\left[\ln\left(\frac{r_{j+1}}{r_j}\right) + \left(\frac{M}{C_- r_{j+1}} + \frac{M}{C_+ r_j}\right)\right]} \overset{1}{\approx} \frac{1 + \frac{1}{2r_j}\frac{\delta r_j^2 + 2L_-\delta r_j}{\delta r_j + L_+ + L_-}}{\delta r_j + L_+ + L_-}. \tag{6.3.9}$$

Therefore,

$$\begin{aligned} \frac{\frac{r_{j+1}^2 - r_j^2}{2} + \left(\frac{Mr_j}{C_+} + \frac{Mr_{j+1}}{C_-}\right)}{r_j\left[\ln\left(\frac{r_{j+1}}{r_j}\right) + \left(\frac{M}{C_- r_{j+1}} + \frac{M}{C_+ r_j}\right)\right]} &\overset{2}{\approx} \frac{r_j\left(\delta r_j + L_+ + L_-\right) + \frac{\delta r_j}{2}\left(\delta r_j + 2L_-\right)}{\delta r_j + L_+ + L_-} \\ &= r_j + \frac{\delta r_j\left(\delta r_j + 2L_-\right)}{\delta r_j + L_+ + L_-} \\ &\overset{2}{\approx} r + \frac{a}{|h_r|} + a(l_- - l_+)\alpha(|h_r|)\bigg|_{r=r_j}. \end{aligned} \tag{6.3.10}$$

Substituting the approximations (6.3.10) and (6.3.8) into the formula for the flux $J_j(r_j)$, we find that

$$\begin{aligned} J_j(r_j) \overset{2}{\approx} &-\tilde{M}\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial r} - \frac{a}{2|h_r|}\left[F + \frac{1}{r}\frac{\partial}{\partial r}\left(r\tilde{M}\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial r}\right)\right] \\ &- \frac{a\left(l_- - l_+\right)}{2}\left[\frac{F\tilde{M}}{M} + \frac{\tilde{M}^2}{Mr}\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial r}\right]\bigg|_{r=r_j}. \end{aligned} \tag{6.3.11}$$

We define $\mathcal{J}_0, \mathcal{J}_1$ and $\mathcal{J}$ by

$$
\begin{aligned}
\mathcal{J}_0 =& -\tilde{M}\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial r}, \\
\mathcal{J}_1 =& -\frac{a}{2|h_r|}\left[\digamma + \frac{1}{r}\frac{\partial}{\partial r}\left(r\tilde{M}\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial r}\right)\right] - \frac{a(l_- - l_+)}{2}\left[\frac{\digamma \tilde{M}}{M} + \frac{\tilde{M}^2}{Mr}\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial r}\right], \\
\mathcal{J} =& \mathcal{J}_0 + \mathcal{J}_1 + \mathcal{J}_2,
\end{aligned}
\tag{6.3.12}
$$

such that

$$
J_j(r_j) \stackrel{3}{\approx} \mathcal{J}(r_j) \tag{6.3.13}
$$

and $\mathcal{J}_2(r) = O(a^2)$.

Approximating the diffusive flux J_{j-1} at the jth step

From (6.3.5) and the definition of $J_j = -M\frac{\partial \mu_j}{\partial r}$, it is easy to see that

$$
r_{j+1}J_j(r_{j+1}) = \frac{\digamma}{2}(r_{j+1}^2 - r_j^2) + r_j J(r_j), \tag{6.3.14}
$$

from which it follows that if $J_j(r_j) \stackrel{3}{\approx} \mathcal{J}(r_j)$, then

$$
\begin{aligned}
J_{j-1}(r_j) &= \digamma\left(\delta r_{j-1} - \frac{\delta r_{j-1}^2}{2r_j}\right) + \frac{r_{j-1}}{r_j}J_{j-1}(r_{j-1}) \\
&\stackrel{3}{\approx} \frac{a\digamma}{|h_r(r_j)|} - \frac{a\digamma}{2r_j|h_r(r_j)|}\frac{\partial}{\partial r}\left[\frac{ar_j}{|h_r(r_j)|}\right] + \frac{r_{j-1}\mathcal{J}(r_{j-1})}{r_j},
\end{aligned}
\tag{6.3.15}
$$

using the usual approximation (6.2.11) of δr_{j-1}. Next, we expand $r_{j-1}\mathcal{J}(r_{j-1})$ about r_j, and find

$$
\begin{aligned}
r_{j-1}\mathcal{J}(r_{j-1}) &\stackrel{3}{\approx} r_j\mathcal{J}(r_j) - \delta r_{j-1}\frac{\partial\left(r_j\mathcal{J}(r_j)\right)}{\partial r} + \frac{\delta r_{j-1}^2}{2}\frac{\partial^2\left(r_j\mathcal{J}(r_j)\right)}{\partial r^2} \\
&\stackrel{3}{\approx} r\mathcal{J} - \left[\frac{a}{|h_r|} - \frac{a}{2|h_r|}\frac{\partial\left(\frac{a}{|h_r|}\right)}{\partial r}\right]\frac{\partial\left(r\mathcal{J}\right)}{\partial r} + \frac{a^2}{2|h_r|^2}\frac{\partial^2\left(r\mathcal{J}\right)}{\partial r^2}\Bigg|_{r=r_j} \\
&= r\mathcal{J} - \frac{a}{|h_r|}\frac{\partial(r\mathcal{J})}{\partial r} + \frac{a}{2|h_r|}\frac{\partial}{\partial r}\left[\frac{a}{|h_r|}\frac{\partial\left(r\mathcal{J}\right)}{\partial r}\right]\Bigg|_{r=r_j}.
\end{aligned}
\tag{6.3.16}
$$

Hence, applying (6.3.16) to (6.3.15) we have the approximation

$$
\begin{aligned}
J_{j-1}(r_j) &\overset{3}{\approx} \mathcal{J} + \frac{aF}{|h_r|} - \frac{aF}{2|h_r|r}\frac{\partial\left(\frac{ar}{|h_r|}\right)}{\partial r} - \frac{a}{|h_r|r}\frac{\partial}{\partial r}\left[r\mathcal{J} - \frac{a}{2|h_r|}\frac{\partial(r\mathcal{J})}{\partial r}\right]\Bigg|_{r=r_j} \qquad (6.3.17)\\
&= \mathcal{J} + \frac{aF}{|h_r|} - \frac{a}{|h_r|r}\frac{\partial}{\partial r}\left[r\left(\mathcal{J} + \frac{aF}{2|h_r|} - \frac{a}{2|h_r|}\frac{1}{r}\frac{\partial}{\partial r}(r\mathcal{J})\right)\right]\Bigg|_{r=r_j}.
\end{aligned}
$$

Continuum limit

We may now find the continuum limit of the velocity equation $(6.3.1)_4$ and the modified Gibbs–Thomson relation (6.3.2). Since in the continuum limit $V_j = \frac{h_t(r_j)}{|h_r(r_j)|}$ and

$$
\varrho^{\mathrm{b}} V_j = -J_j(r_j) + J_{j-1}(r_j), \qquad (6.3.18)
$$

we find in the continuum limit, by (6.3.13) and (6.3.17)

$$
\varrho^{\mathrm{b}}\frac{h_t}{|h_r|} = \frac{aF}{|h_r|} + \frac{a}{|h_r|}\frac{1}{r}\frac{\partial}{\partial r}\left[r\tilde{M}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial r}\right] + \frac{a^2(l_- - l_+)}{2|h_r|}\frac{1}{r}\frac{\partial}{\partial r}\left[F r\frac{\tilde{M}}{M} + \frac{\tilde{M}^2}{M}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial r}\right], \qquad (6.3.19)
$$

which may be re-arranged as

$$
\varrho^{\mathrm{b}} h_t = aF + \frac{a}{r}\frac{\partial}{\partial r}\left[\frac{aF(l_- - l_+)r\tilde{M}}{2M} + \left(r\tilde{M} + \frac{a(l_- - l_+)}{2}\frac{\tilde{M}^2}{M}\right)\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial r}\right]. \qquad (6.3.20)
$$

Moreover, since

$$
\frac{\mu_j^{\mathrm{s}} - \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} - \frac{\gamma}{r_j}}{\Theta} = -\left(\frac{J_j(r_j)}{C_+} + \frac{J_{j-1}(r_j)}{C_-}\right), \qquad (6.3.21)
$$

we find in the continuum limit

$$
\begin{aligned}
\frac{\tilde{\mu}^{\mathrm{s}} - \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} - \frac{\gamma}{r}}{\Theta} &= -\left(\frac{\mathcal{J}_0 + \mathcal{J}_1}{C_+} + \frac{\mathcal{J}_0 + \mathcal{J}_1}{C_-} + \frac{a}{|h_r|}\frac{F + \frac{1}{r}\frac{\partial}{\partial r}(r\tilde{M}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial r})}{C_-}\right)\\
&= \frac{a(l_+ + l_-)\tilde{M}}{M}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial r} \qquad (6.3.22)\\
&\quad - \frac{a^2(l_- - l_+)}{2|h_r|}\left[\frac{F\tilde{M}}{M^2} + \frac{\partial}{\partial r}\left(\frac{\tilde{M}}{M}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial r}\right) + \frac{\tilde{M}^2}{rM^2}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial r}\right].
\end{aligned}
$$

Writing (6.3.20) and (6.3.22) in terms of $\alpha(|h_r|)$ and $\widehat{\alpha}(|h_r|)$, we arrive at the claimed continuum limit (6.3.3) and (6.3.4).

6.4 Growth with desorption

We now find the continuum limit for concentric steps for growth during desorption. The boundary value problem (4.6.6)-(4.6.7) and the velocity equation (4.6.8) take the form

$$\left.\begin{aligned} 0 &= \frac{M}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \mu_j}{\partial r}\right) - \breve{\sigma}\mu_j && \text{in } (r_j, r_{j+1}), \\ M\frac{\partial \mu_j}{\partial r} &= C_+\left(\mu_j - \mu_j^{\mathrm{s}}\right) && \text{at } r = r_j, \\ M\frac{\partial \mu_j}{\partial r} &= -C_-\left(\mu_j - \mu_{j+1}^{\mathrm{s}}\right) && \text{at } r = r_{j+1}, \\ \varrho^{\mathrm{b}} V_j &= C_+\left(\mu_j - \mu_j^{\mathrm{s}}\right) + C_-\left(\mu_{j-1} - \mu_j^{\mathrm{s}}\right) && \text{at } r = r_j, \end{aligned}\right\} \tag{6.4.1}$$

where the modified Gibbs–Thomson relation (4.6.5 requires that

$$\mu_j^{\mathrm{s}} = \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} + \Theta(\mu_j - \mu_{j-1}) + \frac{\gamma}{r_j} \qquad \text{at } r = r_j. \tag{6.4.2}$$

The main results of this section are the continuum limits of the velocity equation (6.4.1) governing the height function h

$$\varrho^{\mathrm{b}} h_t = \frac{a}{r}\frac{\partial}{\partial r}\left\{rM\alpha(|h_r|)\left[1 + a\widehat{\alpha}(|h_r|)\right]\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial r}\right\} - a\breve{\sigma}\left[1 + \frac{a}{r}\frac{\partial(r^2\widehat{\alpha}(|h_r|))}{\partial r}\right]\tilde{\mu}^{\mathrm{s}}, \tag{6.4.3}$$

and of the modified Gibbs–Thomson relation (6.4.2) governing the surface chemical potential $\tilde{\mu}^{\mathrm{s}}$

$$\begin{aligned} \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} = \left(1 - \frac{a^2\breve{\sigma}r\widehat{\alpha}(|h_r|)}{M|h_r|}\right)\tilde{\mu}^{\mathrm{s}} - \frac{\gamma}{r} - a\Theta\alpha(|h_r|)\left[l_+ + l_- - \frac{a\widehat{\alpha}(|h_r|)}{|h_r|}\right]\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial r} \\ + \frac{a^2\Theta}{|h_r|}\frac{\partial}{\partial r}\left[r\widehat{\alpha}(|h_r|)\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial r}\right], \end{aligned} \tag{6.4.4}$$

where α and $\widehat{\alpha}$ are defined in (5.2.4) and (6.2.5), respectively.

Let

$$\mathsf{r} = \sqrt{\frac{\breve{\sigma}}{M}}r, \; c_\pm = \frac{C_\pm}{\sqrt{\breve{\sigma}M}}, \text{ and } g = \sqrt{\frac{\breve{\sigma}}{M}}\gamma. \tag{6.4.5}$$

We assume that $l_\pm = M/(aC_\pm)$ and $\breve{\sigma}$ are independent of a. Hence, for $\lambda_\pm = 1/(ac_\pm)$, we have that

$$\lambda_\pm = \frac{1}{ac_\pm} = O(1). \tag{6.4.6}$$

Then $\mu_j = \mu_j(\mathsf{r})$ solves the problem

$$\left.\begin{aligned} 0 &= \frac{1}{\mathsf{r}}\frac{\partial}{\partial \mathsf{r}}(\mathsf{r}\frac{\partial \mu_j}{\partial \mathsf{r}}) - \mu_j && \text{in } (\mathsf{r}_j, \mathsf{r}_{j+1}), \\ \frac{\partial \mu_j}{\partial \mathsf{r}} &= c_+\left(\mu_j - \mu_j^{\mathrm{s}}\right) && \text{at } \mathsf{r} = \mathsf{r}_j, \\ \frac{\partial \mu_j}{\partial \mathsf{r}} &= -c_-\left(\mu_j - \mu_{j+1}^{\mathrm{s}}\right) && \text{at } \mathsf{r} = \mathsf{r}_{j+1}, \\ \frac{\varrho^{\mathrm{b}}}{\breve{\sigma}}V_j &= c_+\left(\mu_j^+ - \mu_j^{\mathrm{s}}\right) + c_-\left(\mu_j^- - \mu_j^{\mathrm{s}}\right) && \text{at } \mathsf{r} = \mathsf{r}_j, \end{aligned}\right\} \tag{6.4.7}$$

with μ_j satisfying

$$\mu_j^{\mathrm{s}} = \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} + \Theta(\mu_j - \mu_{j-1}) + \frac{g}{\mathsf{r}_j} \quad \text{at } \mathsf{r} = \mathsf{r}_j. \tag{6.4.8}$$

The solution of this system may be written solution in terms of the modified Bessel functions I_0, K_0 as follows

$$\mu_j(\mathsf{r}) = A_j I_0(\mathsf{r}) + B_j K_0(\mathsf{r}), \text{ on } (\mathsf{r}_j, \mathsf{r}_{j+1}), \tag{6.4.9}$$

where A_j and B_j are constants given by

$$A_j = \frac{c_+c_-\left\{\mu_{j+1}^{\mathrm{s}}K_0(\mathsf{r}_j) - \mu_j^{\mathrm{s}}K_0(\mathsf{r}_{j+1})\right\} + \left\{c_+\mu_j^{\mathrm{s}}K_1(\mathsf{r}_{j+1}) + c_-\mu_{j+1}^{\mathrm{s}}K_1(\mathsf{r}_j)\right\}}{\sigma_1(\mathsf{r}_j, \mathsf{r}_{j+1}) + c_+\sigma_2(\mathsf{r}_j, \mathsf{r}_{j+1}) + c_-\sigma_3(\mathsf{r}_j, \mathsf{r}_{j+1}) + c_+c_-\sigma_4(\mathsf{r}_j, \mathsf{r}_{j+1})} \tag{6.4.10}$$

and

$$B_j = \frac{c_+c_-\left\{\mu_j^{\mathrm{s}}I_0(\mathsf{r}_{j+1}) - \mu_{j+1}^{\mathrm{s}}I_0(\mathsf{r}_j)\right\} + \left\{c_+\mu_j^{\mathrm{s}}I_1(\mathsf{r}_{j+1}) + c_-\mu_{j+1}^{\mathrm{s}}I_1(\mathsf{r}_j)\right\}}{\sigma_1(\mathsf{r}_j, \mathsf{r}_{j+1}) + c_+\sigma_2(\mathsf{r}_j, \mathsf{r}_{j+1}) + c_-\sigma_3(\mathsf{r}_j, \mathsf{r}_{j+1}) + c_+c_-\sigma_4(\mathsf{r}_j, \mathsf{r}_{j+1})}, \tag{6.4.11}$$

where σ_k are defined as in Chapter 3, by

$$\left.\begin{aligned} \sigma_1(x,y) &= \quad K_1(x)I_1(y) - I_1(x)K_1(y), \\ \sigma_2(x,y) &= \quad I_0(x)K_1(y) + K_0(x)I_1(y), \\ \sigma_3(x,y) &= \quad I_1(x)K_0(y) + K_1(x)I_0(y), \\ \sigma_4(x,y) &= \quad K_0(x)I_0(y) - I_0(x)K_0(y). \end{aligned}\right\} \tag{6.4.12}$$

Approximating the diffusive flux J_j at the jth step

We find that

$$J_j(\mathsf{r}_j) = -A_j I_1(\mathsf{r}_j) + B_j K_1(\mathsf{r}_j) \\ = \frac{P_1(\mathsf{r}_j, \mathsf{r}_{j+1})}{Q(\mathsf{r}_j, \mathsf{r}_{j+1})}, \tag{6.4.13}$$

where

$$P_1(x, y) = \tilde{\mu}^{\mathrm{s}}(x) \left[\sigma_3(x, y) + a\lambda_- \sigma_1(x, y)\right] - \sigma_3(x, x)\tilde{\mu}^{\mathrm{s}}(y) \tag{6.4.14}$$

and

$$Q(x, y) = a^2 \lambda_- \lambda_+ \sigma_1(x, y) + a\lambda_- \sigma_2(x, y) + a\lambda_+ \sigma_3(x, y) + \sigma_4(x, y). \tag{6.4.15}$$

Hence, we have for $\delta\mathsf{r}_j = \mathsf{r}_{j+1} - \mathsf{r}_j = O(a)$

$$Q(\mathsf{r}_j, \mathsf{r}_j + \delta\mathsf{r}_j) \overset{3}{\approx} Q(\mathsf{r}_j, \mathsf{r}_j) + \delta\mathsf{r}_j \frac{\partial Q}{\partial y}(\mathsf{r}_j, \mathsf{r}_j) + \frac{\delta\mathsf{r}_j^2}{2}\frac{\partial^2 Q}{\partial y^2}(\mathsf{r}_j, \mathsf{r}_j) \\ \overset{3}{\approx} \sigma_2(\mathsf{r}_j, \mathsf{r}_j) \left\{ a(\lambda_+ + \lambda_-) + \delta\mathsf{r}_j - \frac{1}{\mathsf{r}_j}\left(a\lambda_- \delta\mathsf{r}_j + \frac{\delta\mathsf{r}_j^2}{2} \right) \right\}, \tag{6.4.16}$$

and, appealing to the property that $\sigma_2(x, x) = \sigma_3(x, x)$,

$$\begin{aligned} P_1(\mathsf{r}_j, \mathsf{r}_j + \delta\mathsf{r}_j) &\overset{3}{\approx} P_1(\mathsf{r}_j, \mathsf{r}_j) + \delta\mathsf{r}_j \frac{\partial P_1}{\partial y}(\mathsf{r}_j, \mathsf{r}_j) + \frac{\delta\mathsf{r}_j^2}{2}\frac{\partial^2 P_1}{\partial y^2}(\mathsf{r}_j, \mathsf{r}_j) \\ &\overset{3}{\approx} -\delta\mathsf{r}_j \sigma_3(\mathsf{r}_j, \mathsf{r}_j) \frac{\partial \tilde{\mu}^{\mathrm{s}}(\mathsf{r}_j)}{\partial \mathsf{r}} + a\lambda_- \delta\mathsf{r}_j \tilde{\mu}^{\mathrm{s}}(\mathsf{r}_j)\sigma_3(\mathsf{r}_j, \mathsf{r}_j) \\ &\quad + \frac{\delta\mathsf{r}_j^2 \sigma_3(\mathsf{r}_j, \mathsf{r}_j)}{2}\left(\tilde{\mu}^{\mathrm{s}}(\mathsf{r}_j) - \frac{\partial^2 \tilde{\mu}^{\mathrm{s}}(\mathsf{r}_j)}{\partial \mathsf{r}^2} \right) \\ &\overset{3}{\approx} \delta\mathsf{r}_j \sigma_2(\mathsf{r}_j, \mathsf{r}_j) \left\{ a\lambda_- \tilde{\mu}^{\mathrm{s}}(\mathsf{r}_j) - \frac{\partial \tilde{\mu}^{\mathrm{s}}(\mathsf{r}_j)}{\partial \mathsf{r}} \right. \\ &\quad \left. + \frac{\delta\mathsf{r}_j}{2}\left(\tilde{\mu}^{\mathrm{s}}(\mathsf{r}_j) - \frac{\partial^2 \tilde{\mu}^{\mathrm{s}}(\mathsf{r}_j)}{\partial \mathsf{r}^2} \right) \right\}. \end{aligned} \tag{6.4.17}$$

Recall that, by $(5.1.10)_1$,

$$\delta r_j \overset{3}{\approx} \frac{a}{|h_r|} + \frac{a}{2|h_r|}\frac{\partial}{\partial r}\left(\frac{a}{|h_r|} \right), \tag{6.4.18}$$

which implies that

$$\begin{aligned}\delta \mathsf{r}_j &\overset{3}{\approx} \sqrt{\frac{\breve{\sigma}}{M}}\left(\frac{a}{|h_r|}+\frac{a}{2|h_r|}\frac{\partial}{\partial r}\left(\frac{a}{|h_r|}\right)\right)\\ &= \frac{a}{|h_{\mathsf{r}}|}+\frac{a}{2|h_{\mathsf{r}}|}\frac{\partial}{\partial \mathsf{r}}\left(\frac{a}{|h_{\mathsf{r}}|}\right).\end{aligned} \tag{6.4.19}$$

Put

$$\mathcal{M} = \frac{1}{1+(\lambda_+ + \lambda_-)|h_r|}. \tag{6.4.20}$$

Then, by (6.4.16):

$$\begin{aligned}\frac{\delta \mathsf{r}_j \sigma_2(\mathsf{r}_j,\mathsf{r}_j)}{Q(\mathsf{r}_j,\mathsf{r}_j+\delta \mathsf{r}_j)} &= \frac{\delta \mathsf{r}_j}{\left\{\left(\frac{1}{c_+}+\frac{1}{c_-}\right)+\delta \mathsf{r}_j\right\}-\frac{1}{\mathsf{r}_j}\left(\frac{\delta \mathsf{r}_j}{c_-}+\frac{\delta \mathsf{r}_j^2}{2}\right)+O(a^3)}\\ &\overset{2}{\approx} \frac{\frac{a}{|h_{\mathsf{r}}|}}{\frac{a}{|h_{\mathsf{r}}|}+a(\lambda_+ + \lambda_-)}+\frac{a}{2|h_{\mathsf{r}}|}\frac{\partial}{\partial \mathsf{r}}\left[\frac{\frac{a}{|h_{\mathsf{r}}|}}{\frac{a}{|h_{\mathsf{r}}|}+a(\lambda_+ + \lambda_-)}\right]\\ &\quad +\frac{1}{\mathsf{r}}\frac{\frac{a}{|h_{\mathsf{r}}|}\left(\frac{a^2\lambda_-}{|h_{\mathsf{r}}|}+\frac{a^2}{2|h_{\mathsf{r}}|^2}\right)}{\left(\frac{a}{|h_{\mathsf{r}}|}+a(\lambda_+ + \lambda_-)\right)^2}\Bigg|_{\mathsf{r}=\mathsf{r}_j}\\ &= \mathcal{M}+\frac{a}{2|h_{\mathsf{r}}|}\frac{\partial(\mathcal{M})}{\partial \mathsf{r}}+\frac{a\mathcal{M}^2}{2\mathsf{r}|h_{\mathsf{r}}|}\left(2\lambda_-|h_{\mathsf{r}}|+1\right)\Big|_{\mathsf{r}=\mathsf{r}_j}\\ &= \mathcal{M}+\frac{a}{2|h_{\mathsf{r}}|}\frac{1}{\mathsf{r}}\frac{\partial(\mathsf{r}\mathcal{M})}{\partial \mathsf{r}}+\frac{a(\lambda_- - \lambda_+)\mathcal{M}^2}{2\mathsf{r}}\Big|_{\mathsf{r}=\mathsf{r}_j}.\end{aligned} \tag{6.4.21}$$

Therefore, by (6.4.13), (6.4.17), and (6.4.21)

$$\begin{aligned}J_j(\mathsf{r}_j) &\overset{2}{\approx} \left\{a\lambda_-\tilde{\mu}^{\mathrm{s}}-\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial \mathsf{r}}+\frac{a}{2|h_{\mathsf{r}}|}\left(\tilde{\mu}^{\mathrm{s}}-\frac{\partial^2\tilde{\mu}^{\mathrm{s}}}{\partial \mathsf{r}^2}\right)\right\}\\ &\quad\times\left\{\mathcal{M}+\frac{a}{2|h_{\mathsf{r}}|}\frac{1}{\mathsf{r}}\frac{\partial(\mathsf{r}\mathcal{M})}{\partial \mathsf{r}}+\frac{a(\lambda_- - \lambda_+)}{2\mathsf{r}}\mathcal{M}^2\right\}\Bigg|_{\mathsf{r}=\mathsf{r}_j}\\ &\overset{2}{\approx} -\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial \mathsf{r}}\mathcal{M}+a\tilde{\mu}^{\mathrm{s}}\left(\frac{1}{2|h_{\mathsf{r}}|}+\lambda_-\right)\mathcal{M}-a(\lambda_- - \lambda_+)\frac{\mathcal{M}^2}{2\mathsf{r}}\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial \mathsf{r}}\\ &\quad -\frac{a}{2|h_{\mathsf{r}}|}\frac{1}{\mathsf{r}}\left[\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial \mathsf{r}}\frac{\partial(\mathsf{r}\mathcal{M})}{\partial \mathsf{r}}+\mathsf{r}\mathcal{M}\frac{\partial^2\tilde{\mu}^{\mathrm{s}}}{\partial \mathsf{r}^2}\right]\Bigg|_{\mathsf{r}=\mathsf{r}_j}\\ &\overset{2}{\approx} -\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial \mathsf{r}}\mathcal{M}+\frac{a}{2|h_{\mathsf{r}}|}\left[\tilde{\mu}^{\mathrm{s}}-\frac{1}{\mathsf{r}}\frac{\partial}{\partial \mathsf{r}}\left(\mathsf{r}\mathcal{M}\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial \mathsf{r}}\right)\right]\\ &\quad +\frac{a(\lambda_- - \lambda_+)\mathcal{M}}{2}\left[\tilde{\mu}^{\mathrm{s}}-\frac{\mathcal{M}}{\mathsf{r}}\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial \mathsf{r}}\right]\Bigg|_{r=r_j}.\end{aligned} \tag{6.4.22}$$

We define

$$\mathcal{J}_0 = -\mathcal{M}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial \mathsf{r}}, \tag{6.4.23}$$

$$\mathcal{J}_1 = \frac{a}{2|h_{\mathsf{r}}|}\left[\tilde{\mu}^{\mathrm{s}} - \frac{1}{\mathsf{r}}\frac{\partial}{\partial \mathsf{r}}\left(\mathsf{r}\mathcal{M}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial \mathsf{r}}\right)\right] + \frac{a(\lambda_- - \lambda_+)\mathcal{M}}{2}\left[\tilde{\mu}^{\mathrm{s}} - \frac{\mathcal{M}}{\mathsf{r}}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial \mathsf{r}}\right], \tag{6.4.24}$$

and $\mathcal{J}_2$ such that

$$J_j(\mathsf{r}_j) \overset{3}{\approx} \mathcal{J}_0(\mathsf{r}_j) + \mathcal{J}_1(\mathsf{r}_j) + \mathcal{J}_2(\mathsf{r}_j) \tag{6.4.25}$$

and $\mathcal{J}_2(\mathsf{r}_j) = O(a^2)$.

Approximating the diffusive flux J_{j-1} at the jth step

We use the approximation

$$J_{j-1}(\mathsf{r}_j) \overset{3}{\approx} J_{j-1}(\mathsf{r}_{j-1}) + \delta\mathsf{r}_{j-1}\frac{\partial J_{j-1}(\mathsf{r}_{j-1})}{\partial \mathsf{r}} + \frac{\delta\mathsf{r}_{j-1}^2}{2}\frac{\partial^2 J_{j-1}(\mathsf{r}_{j-1})}{\partial \mathsf{r}^2}. \tag{6.4.26}$$

Computing from the definition of $J_{j-1}(\mathsf{r}) = -\frac{\partial\mu_{j-1}(\mathsf{r})}{\partial \mathsf{r}}$, we find

$$\left.\begin{aligned} \frac{\partial J_{j-1}(\mathsf{r}_{j-1})}{\partial \mathsf{r}} &= -\chi(\mathsf{r}_{j-1}, \mathsf{r}_j) - \frac{J_{j-1}(\mathsf{r}_{j-1})}{\mathsf{r}_{j-1}}, \\ \frac{\partial^2 J_{j-1}(\mathsf{r}_{j-1})}{\partial \mathsf{r}^2} &= \left(1 + \frac{2}{\mathsf{r}_{j-1}^2}\right) J_{j-1}(\mathsf{r}_{j-1}) + \frac{\chi(\mathsf{r}_{j-1}, \mathsf{r}_j)}{\mathsf{r}_{j-1}}, \end{aligned}\right\} \tag{6.4.27}$$

where

$$\chi(\mathsf{r}_{j-1}, \mathsf{r}_j) = \frac{P_2(\mathsf{r}_{j-1}, \mathsf{r}_j)}{Q(\mathsf{r}_{j-1}, \mathsf{r}_j)}, \tag{6.4.28}$$

and

$$P_2(\mathsf{r}_{j-1}, \mathsf{r}_j) = \tilde{\mu}^{\mathrm{s}}(\mathsf{r}_{j-1})\sigma_4(\mathsf{r}_{j-1}, \mathsf{r}_j) + \left[a\lambda_-\tilde{\mu}^{\mathrm{s}}(\mathsf{r}_{j-1}) + a\lambda_+\tilde{\mu}^{\mathrm{s}}(\mathsf{r}_j)\right]\sigma_2(\mathsf{r}_{j-1}, \mathsf{r}_{j-1}), \tag{6.4.29}$$

and Q is defined as in $(6.4.15)_2$

It suffices to find the expansion of $\chi(\mathsf{r}_{j-1}, \mathsf{r}_j)$ about $(\mathsf{r}_j, \mathsf{r}_j)$ up to order $O(\delta\mathsf{r}_{j-1}^2)$ since $\chi(\mathsf{r}_{j-1}, \mathsf{r}_j)$ is multiplied at least by a $\delta\mathsf{r}_{j-1}$ in (6.4.26). Hence, we find, in the same manner as our approximation of $J_j(\mathsf{r}_j)$,

$$\begin{aligned} P_2(\mathsf{r}_{j-1},\mathsf{r}_j) &\overset{3}{\approx} P_2(\mathsf{r}_j,\mathsf{r}_j) - \delta\mathsf{r}_{j-1}\frac{\partial P_2}{\partial x}(\mathsf{r}_j,\mathsf{r}_j) + \frac{\delta\mathsf{r}_{j-1}^2}{2}\frac{\partial^2 P_2}{\partial x^2}(\mathsf{r}_j,\mathsf{r}_j) \\ &\overset{3}{\approx} \sigma_2(\mathsf{r}_j,\mathsf{r}_j)\Big\{a(\lambda_+ + \lambda_-)\tilde{\mu}^{\mathrm{s}}(\mathsf{r}_j) \\ &\quad + \delta\mathsf{r}_{j-1}\left(\tilde{\mu}^{\mathrm{s}}(\mathsf{r}_j) + \frac{a\lambda_+\tilde{\mu}^{\mathrm{s}}(\mathsf{r}_j)}{\mathsf{r}_j} - a\lambda_-\frac{\partial\tilde{\mu}^{\mathrm{s}}(\mathsf{r}_j)}{\partial\mathsf{r}}\right) \\ &\quad + \frac{\delta\mathsf{r}_{j-1}^2}{2}\left(\frac{\tilde{\mu}^{\mathrm{s}}(\mathsf{r}_j)}{\mathsf{r}_j} - 2\frac{\partial\tilde{\mu}^{\mathrm{s}}(\mathsf{r}_j)}{\partial\mathsf{r}}\right)\Big\}. \end{aligned} \tag{6.4.30}$$

and

$$\begin{aligned} Q(\mathsf{r}_{j-1},\mathsf{r}_j) &\overset{3}{\approx} Q(\mathsf{r}_j,\mathsf{r}_j) - \delta\mathsf{r}_{j-1}\frac{\partial Q(\mathsf{r}_j,\mathsf{r}_j)}{\partial x} + \frac{\delta\mathsf{r}_{j-1}^2}{2}\frac{\partial^2 Q(\mathsf{r}_j,\mathsf{r}_j)}{\partial x^2} \\ &\overset{3}{\approx} \sigma_2(\mathsf{r}_j,\mathsf{r}_j)\left(a(\lambda_+ + \lambda_-) + \delta\mathsf{r}_{j-1}\left(1 + \frac{a\lambda_+}{\mathsf{r}_j}\right) + \frac{\delta\mathsf{r}_{j-1}^2}{2\mathsf{r}_j}\right). \end{aligned} \tag{6.4.31}$$

It follows that

$$\begin{aligned} \frac{\delta\mathsf{r}_{j-1}\sigma_2(\mathsf{r}_j,\mathsf{r}_j)}{Q(\mathsf{r}_{j-1},\mathsf{r}_j)} &\overset{3}{\approx} \frac{\frac{a}{|h_\mathsf{r}|}}{\frac{a}{|h_\mathsf{r}|} + a(\lambda_+ + \lambda_-)} - \frac{a}{2|h_\mathsf{r}|}\frac{\partial}{\partial\mathsf{r}}\left(\frac{\frac{a}{|h_\mathsf{r}|}}{\frac{a}{|h_\mathsf{r}|} + a(\lambda_+ + \lambda_-)}\right) \\ &\quad - \left.\frac{\frac{a^2}{\mathsf{r}|h_\mathsf{r}|^2}\left(a\lambda_+ + \frac{a}{2|h_\mathsf{r}|}\right)}{\left(\frac{a}{|h_\mathsf{r}|} + a(\lambda_+ + \lambda_-)\right)^2}\right|_{\mathsf{r}=\mathsf{r}_j} \\ &\overset{3}{\approx} \left.\mathcal{M} - \frac{a}{2|h_\mathsf{r}|}\frac{1}{\mathsf{r}}\frac{\partial}{\partial\mathsf{r}}(\mathsf{r}\mathcal{M}) + \frac{a(\lambda_- - \lambda_+)\mathcal{M}^2}{2\mathsf{r}}\right|_{\mathsf{r}=\mathsf{r}_j}. \end{aligned} \tag{6.4.32}$$

Hence, applying (6.4.30) and (6.4.32) to (6.4.28)

$$\begin{aligned} \delta\mathsf{r}_{j-1}\chi(\mathsf{r}_{j-1},\mathsf{r}_j) &\overset{3}{\approx} \left\{\mathcal{M} - \frac{a}{2|h_\mathsf{r}|}\frac{1}{\mathsf{r}}\frac{\partial(\mathsf{r}\mathcal{M})}{\partial\mathsf{r}} + \frac{a(\lambda_- - \lambda_+)\mathcal{M}^2}{2\mathsf{r}}\right\} \\ &\quad \times\left\{a(\lambda_+ + \lambda_-)\tilde{\mu}^{\mathrm{s}} + \delta\mathsf{r}_{j-1}\left(\tilde{\mu}^{\mathrm{s}} + \frac{a\lambda_+\tilde{\mu}^{\mathrm{s}}}{\mathsf{r}} - a\lambda_-\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial\mathsf{r}}\right)\right. \\ &\quad \left.\left. + \delta\mathsf{r}_{j-1}^2\left(\frac{\tilde{\mu}^{\mathrm{s}}}{2\mathsf{r}} - \frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial\mathsf{r}}\right)\right\}\right|_{\mathsf{r}=\mathsf{r}_j} \\ &= \left\{\mathcal{M} - \frac{a}{2|h_\mathsf{r}|}\frac{1}{\mathsf{r}}\frac{\partial(\mathsf{r}\mathcal{M})}{\partial\mathsf{r}} + \frac{a(\lambda_- - \lambda_+)\mathcal{M}^2}{2\mathsf{r}}\right\} \\ &\quad \times\left\{a(\lambda_+ + \lambda_-)\tilde{\mu}^{\mathrm{s}} + \frac{a\tilde{\mu}^{\mathrm{s}}}{|h_\mathsf{r}|}\left[1 + \frac{a\lambda_+}{\mathsf{r}} - \frac{\partial\left(\frac{a}{2|h_\mathsf{r}|}\right)}{\partial\mathsf{r}}\right]\right. \\ &\quad \left.\left. - \frac{a^2\lambda_-}{|h_\mathsf{r}|}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial\mathsf{r}} + \frac{a^2}{2|h_\mathsf{r}|^2}\left(\frac{\tilde{\mu}^{\mathrm{s}}}{\mathsf{r}} - 2\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial\mathsf{r}}\right)\right\}\right|_{\mathsf{r}=\mathsf{r}_j} \\ &\overset{3}{\approx} \chi_1(\mathsf{r}_j) + \chi_2(\mathsf{r}_j), \end{aligned} \tag{6.4.33}$$

where

$$\chi_1 = \tilde{\mu}^{\mathrm{s}} \mathcal{M} \left(a(\lambda_+ + \lambda_-) + \frac{a}{|h_{\mathsf{r}}|} \right), \tag{6.4.34}$$

and

$$\begin{aligned} \chi_2 = \frac{a\mathcal{M}}{|h_{\mathsf{r}}|} &\left[-a\lambda_- \frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial \mathsf{r}} + \frac{a\lambda_+ \tilde{\mu}^{\mathrm{s}}}{\mathsf{r}} - \frac{\tilde{\mu}^{\mathrm{s}}}{2} \frac{\partial}{\partial \mathsf{r}} \left(\frac{a}{|h_{\mathsf{r}}|} \right) + \frac{a}{2|h_{\mathsf{r}}|} \left(\frac{\tilde{\mu}^{\mathrm{s}}}{\mathsf{r}} - 2 \frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial \mathsf{r}} \right) \right] \\ &+ \frac{\tilde{\mu}^{\mathrm{s}}}{2} \left[a(\lambda_+ + \lambda_-) + \frac{a}{|h_{\mathsf{r}}|} \right] \left[a\left(\lambda_- - \lambda_+\right) \frac{\mathcal{M}^2}{\mathsf{r}} - \frac{a}{|h_{\mathsf{r}}|} \frac{1}{\mathsf{r}} \frac{\partial \left(\mathsf{r}\mathcal{M}\right)}{\partial \mathsf{r}} \right]. \end{aligned} \tag{6.4.35}$$

Moreover,

$$\delta \mathsf{r}_{j-1}^2 \chi(\mathsf{r}_{j-1}, \mathsf{r}_j) \overset{3}{\approx} \frac{a^2 \chi_1(\mathsf{r}_j)}{|h_{\mathsf{r}}(\mathsf{r}_j)|^2}. \tag{6.4.36}$$

We may simplify χ_1 and χ_2 further to

$$\chi_1 = \frac{a\tilde{\mu}^{\mathrm{s}}}{|h_{\mathsf{r}}|}, \tag{6.4.37}$$

and

$$\chi_2 = -\frac{a}{2|h_{\mathsf{r}}|} \frac{\partial \left(\frac{a}{|h_{\mathsf{r}}|} \right)}{\partial \mathsf{r}} \tilde{\mu}^{\mathrm{s}} - \frac{a\mathcal{M}}{|h_{\mathsf{r}}|} \frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial \mathsf{r}} \left(\frac{a}{|h_{\mathsf{r}}|} + a\lambda_- \right). \tag{6.4.38}$$

Putting the approximation (6.4.33) into (6.4.26) and using (6.4.27) and (6.4.33) with the simplifications (6.4.37) and (6.4.38),

$$
\begin{aligned}
J_{j-1}(\mathsf{r}_{j-1}) &\overset{3}{\approx} \mathcal{J}(\mathsf{r}_{j-1}) - (\chi_1(\mathsf{r}_j) + \chi_2(\mathsf{r}_j)) - \frac{\delta \mathsf{r}_{j-1}}{\mathsf{r}_{j-1}} \left(\mathcal{J}_0(\mathsf{r}_{j-1}) + \mathcal{J}_1(\mathsf{r}_{j-1})\right) \\
&\quad + \frac{\delta \mathsf{r}_{j-1}^2}{2} \left(1 + \frac{2}{\mathsf{r}_{j-1}^2}\right) \mathcal{J}_0(\mathsf{r}_{j-1}) + \frac{\delta \mathsf{r}_{j-1} \chi_1(\mathsf{r}_j)}{2\mathsf{r}_{j-1}} \\
&\overset{3}{\approx} \mathcal{J}(\mathsf{r}_j) - \delta \mathsf{r}_{j-1} \frac{\partial \left(\mathcal{J}_0(\mathsf{r}_j) + \mathcal{J}_1(\mathsf{r}_j)\right)}{\partial \mathsf{r}} + \frac{\delta \mathsf{r}_{j-1}^2}{2} \frac{\partial^2 \mathcal{J}_0(\mathsf{r}_j)}{\partial \mathsf{r}^2} - \chi_1(\mathsf{r}_j) \\
&\quad - \chi_2(\mathsf{r}_j) - \delta \mathsf{r}_{j-1} \left[\frac{\mathcal{J}_0(\mathsf{r}_j)}{\mathsf{r}_j} + \frac{\mathcal{J}_1(\mathsf{r}_j)}{\mathsf{r}_j} - \delta \mathsf{r}_{j-1} \frac{\partial \left(\frac{\mathcal{J}_0(\mathsf{r}_j)}{\mathsf{r}_j}\right)}{\partial \mathsf{r}}\right] \\
&\quad + \left(1 + \frac{2}{\mathsf{r}_j^2}\right) \frac{\delta \mathsf{r}_{j-1}^2 \mathcal{J}_0(\mathsf{r}_j)}{2} + \frac{\delta \mathsf{r}_{j-1} \chi_1(\mathsf{r}_j)}{2\mathsf{r}_j} \qquad (6.4.39) \\
&\overset{3}{\approx} \mathcal{J} - \frac{a}{|h_\mathsf{r}|} \frac{\partial \left(\mathcal{J}_0 + \mathcal{J}_1\right)}{\partial \mathsf{r}} + \frac{a}{2|h_\mathsf{r}|} \frac{\partial \left(\frac{a}{|h_\mathsf{r}|}\right)}{\partial \mathsf{r}} \frac{\partial \mathcal{J}_0}{\partial \mathsf{r}} + \frac{a^2}{2|h_\mathsf{r}|^2} \frac{\partial^2 \mathcal{J}_0}{\partial \mathsf{r}^2} \\
&\quad - \chi_1 - \chi_2 - \frac{a}{|h_\mathsf{r}|} \left[\frac{\mathcal{J}_0}{\mathsf{r}} - \frac{\mathcal{J}_0}{2\mathsf{r}} \frac{\partial \left(\frac{a}{|h_\mathsf{r}|}\right)}{\partial \mathsf{r}} + \frac{\mathcal{J}_1}{\mathsf{r}} - \frac{a}{|h_\mathsf{r}|} \frac{\partial \left(\frac{\mathcal{J}_0}{\mathsf{r}}\right)}{\partial \mathsf{r}}\right] \\
&\quad + \frac{a^2 \mathcal{J}_0}{2|h_\mathsf{r}|^2} \left(1 + \frac{2}{\mathsf{r}^2}\right) + \frac{a \chi_1}{2\mathsf{r}|h_\mathsf{r}|} \Bigg|_{\mathsf{r}=\mathsf{r}_j} \\
&= \mathcal{J}(\mathsf{r}_j) + R_1(\mathsf{r}_j) + R_2(\mathsf{r}_j),
\end{aligned}
$$

where

$$
\left.
\begin{aligned}
R_1 &= -\frac{a}{|h_\mathsf{r}|} \left(\frac{\partial \mathcal{J}_0}{\partial \mathsf{r}} + \frac{\mathcal{J}_0}{\mathsf{r}}\right) - \chi_1, \\
R_2 &= \frac{a}{2|h_\mathsf{r}|} \frac{\partial}{\partial \mathsf{r}} \left(\frac{a}{|h_\mathsf{r}|}\right) \frac{\mathcal{J}_0}{\mathsf{r}} + \frac{a}{2|h_\mathsf{r}|} \frac{\partial}{\partial \mathsf{r}} \left(\frac{a}{|h_\mathsf{r}|}\right) \frac{\partial \mathcal{J}_0}{\partial \mathsf{r}} \\
&\quad - \frac{a}{|h_\mathsf{r}|} \frac{\partial \mathcal{J}_1}{\partial \mathsf{r}} - \frac{a}{|h_\mathsf{r}|} \frac{\mathcal{J}_1}{\mathsf{r}} + \frac{a^2}{2|h_\mathsf{r}|^2} \frac{\partial^2 \mathcal{J}_0}{\partial \mathsf{r}^2} + \frac{a^2}{|h_\mathsf{r}|^2} \frac{\partial}{\partial \mathsf{r}} \left(\frac{\mathcal{J}_0}{\mathsf{r}}\right) \\
&\quad + \frac{a^2}{|h_\mathsf{r}|^2} \left(\frac{1}{2} + \frac{1}{\mathsf{r}^2}\right) \mathcal{J}_0 + \frac{a}{2|h_\mathsf{r}|} \frac{1}{\mathsf{r}} \chi_1 - \chi_2.
\end{aligned}
\right\} \qquad (6.4.40)
$$

We may simplify R_1 using the definitions (6.2.16) and (6.4.38):

$$
R_1 = \frac{a}{|h_\mathsf{r}|} \left(\frac{1}{\mathsf{r}} \frac{\partial}{\partial \mathsf{r}} \left(\mathsf{r} \mathcal{M} \frac{\partial \tilde{\mu}^\mathrm{s}}{\partial \mathsf{r}}\right) - \tilde{\mu}^\mathrm{s}\right). \qquad (6.4.41)
$$

To simplify R_2, we define R_2^*

$$\begin{aligned} R_2^* &= R_2 + \frac{a}{|h_{\mathsf{r}}|}\frac{1}{\mathsf{r}}\frac{\partial}{\partial \mathsf{r}}\left[\mathcal{J}_1 - \frac{a}{2|h_{\mathsf{r}}|}\tilde{\mu}^{\mathrm{s}} + \frac{a}{2|h_{\mathsf{r}}|}\frac{1}{\mathsf{r}}\frac{\partial\left(\mathsf{r}\mathcal{M}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial \mathsf{r}}\right)}{\partial \mathsf{r}}\right] \\ &= R_2 + \frac{a^2(\lambda_- - \lambda_+)}{2|h_{\mathsf{r}}|\mathsf{r}}\frac{\partial}{\partial \mathsf{r}}\left[\mathsf{r}\mathcal{M}\tilde{\mu}^{\mathrm{s}} - \mathcal{M}^2\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial \mathsf{r}}\right]. \end{aligned} \tag{6.4.42}$$

Then by (6.4.23)-(6.4.24), (6.4.37), (6.4.38), and (6.4.40) we have

$$\begin{aligned} R_2^* + \chi_2 =& -\frac{a\mathcal{M}}{2|h_{\mathsf{r}}|\mathsf{r}}\frac{\partial\left(\frac{a}{|h_{\mathsf{r}}|}\right)}{\partial \mathsf{r}}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial \mathsf{r}} + \frac{a}{|h_{\mathsf{r}}|}\frac{1}{\mathsf{r}}\frac{\partial}{\partial \mathsf{r}}\left[\mathsf{r}\left(-\frac{a\tilde{\mu}^{\mathrm{s}}}{2|h_{\mathsf{r}}|} + \frac{a}{2|h_{\mathsf{r}}|\mathsf{r}}\frac{\partial\left(\mathsf{r}\mathcal{M}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial \mathsf{r}}\right)}{\partial \mathsf{r}}\right)\right] \\ &+ \frac{a}{2|h_{\mathsf{r}}|}\frac{\partial\left(\frac{a}{|h_{\mathsf{r}}|}\frac{\partial\mathcal{J}_0}{\partial \mathsf{r}}\right)}{\partial \mathsf{r}} + \frac{a^2}{|h_{\mathsf{r}}|^2}\left(\frac{1}{\mathsf{r}}\frac{\partial\mathcal{J}_0}{\partial \mathsf{r}} + \frac{\mathcal{J}_0}{2}\right) + \frac{a\chi_1}{2|h_{\mathsf{r}}|\mathsf{r}} \\ =& \frac{a}{|h_{\mathsf{r}}|}\left\{\frac{1}{\mathsf{r}}\left[-\frac{\mathcal{M}}{2}\frac{\partial\left(\frac{a}{|h_{\mathsf{r}}|}\right)}{\partial \mathsf{r}}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial \mathsf{r}} + \frac{a\tilde{\mu}^{\mathrm{s}}}{2|h_{\mathsf{r}}|} + \frac{a}{2|h_{\mathsf{r}}|\mathsf{r}}\frac{\partial\left(\mathsf{r}\mathcal{M}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial \mathsf{r}}\right)}{\partial \mathsf{r}}\right]\right. \\ &+ \frac{\partial}{\partial \mathsf{r}}\left[-\frac{a\tilde{\mu}^{\mathrm{s}}}{2|h_{\mathsf{r}}|} + \frac{a}{2\mathsf{r}|h_{\mathsf{r}}|}\frac{\partial\left(\mathsf{r}\mathcal{M}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial \mathsf{r}}\right)}{\partial \mathsf{r}} - \frac{a}{2|h_{\mathsf{r}}|}\frac{\partial\left(\mathcal{M}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial \mathsf{r}}\right)}{\partial \mathsf{r}}\right] \\ &\left.-\frac{a}{|h_{\mathsf{r}}|}\left[\frac{1}{\mathsf{r}}\frac{\partial\left(\mathcal{M}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial \mathsf{r}}\right)}{\partial \mathsf{r}} + \frac{\mathcal{M}}{2}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial \mathsf{r}} - \frac{\tilde{\mu}^{\mathrm{s}}}{2\mathsf{r}}\right]\right\} \\ =& -\frac{a}{2|h_{\mathsf{r}}|}\left[\frac{a\mathcal{M}}{|h_{\mathsf{r}}|}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial \mathsf{r}} + \frac{\partial\left(\frac{a\tilde{\mu}^{\mathrm{s}}}{|h_{\mathsf{r}}|}\right)}{\partial \mathsf{r}}\right]. \end{aligned} \tag{6.4.43}$$

Therefore, by (6.4.38)

$$R_2^* = \frac{a^2(\lambda_- - \lambda_+)\mathcal{M}}{2|h_{\mathsf{r}}|}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial \mathsf{r}}. \tag{6.4.44}$$

Appealing to (6.4.39), (6.4.41), (6.4.42), and (6.4.44), we have

$$
\begin{aligned}
J_{j-1}(\mathsf{r}_j) &\overset{3}{\approx} \mathcal{J}(\mathsf{r}_j) + R_1(\mathsf{r}_j) + R_2(\mathsf{r}_j) \\
&= \mathcal{J} + \frac{a}{|h_\mathsf{r}|}\left\{\frac{1}{\mathsf{r}}\frac{\partial\left(\mathsf{r}\mathcal{M}\frac{\partial\tilde{\mu}^\mathrm{s}}{\partial\mathsf{r}}\right)}{\partial\mathsf{r}} - \tilde{\mu}^\mathrm{s}\right. \\
&\qquad \left.\left. - \frac{a(\lambda_- - \lambda_+)}{2}\left[\frac{1}{\mathsf{r}}\frac{\partial}{\partial\mathsf{r}}\left[\mathsf{r}\mathcal{M}\tilde{\mu}^\mathrm{s} - \mathcal{M}^2\frac{\partial\tilde{\mu}^\mathrm{s}}{\partial\mathsf{r}}\right] - \mathcal{M}\frac{\partial\tilde{\mu}^\mathrm{s}}{\partial\mathsf{r}}\right]\right\}\right|_{\mathsf{r}=\mathsf{r}_j} \\
&= \mathcal{J} + \frac{a}{|h_\mathsf{r}|}\left\{\frac{1}{\mathsf{r}}\frac{\partial\left(\mathsf{r}\mathcal{M}\frac{\partial\tilde{\mu}^\mathrm{s}}{\partial\mathsf{r}}\right)}{\partial\mathsf{r}} - \tilde{\mu}^\mathrm{s}\right. \\
&\qquad \left.\left. + \frac{a(\lambda_- - \lambda_+)}{2\mathsf{r}}\left[-\tilde{\mu}^\mathrm{s}\frac{\partial(\mathsf{r}\mathcal{M})}{\partial\mathsf{r}} + \frac{\partial\left(\mathcal{M}^2\frac{\partial\tilde{\mu}^\mathrm{s}}{\partial\mathsf{r}}\right)}{\partial\mathsf{r}}\right]\right\}\right|_{\mathsf{r}=\mathsf{r}_j}.
\end{aligned}
\tag{6.4.45}
$$

Continuum limit

Since

$$
\frac{\varrho^\mathrm{b}}{\breve{\sigma}}\frac{\mathrm{d}\mathsf{r}_j}{\mathrm{d}t} = -J_j(\mathsf{r}_j) + J_{j-1}(\mathsf{r}_j),
\tag{6.4.46}
$$

in the continuum limit, by (6.4.25) and (6.4.45) we have

$$
\begin{aligned}
\frac{\varrho^\mathrm{b}}{\breve{\sigma}}\frac{h_t}{|h_\mathsf{r}|} = -\mathcal{J} + \mathcal{J} + \frac{a}{|h_\mathsf{r}|}&\left\{\frac{1}{\mathsf{r}}\frac{\partial\left(\mathsf{r}\mathcal{M}\frac{\partial\tilde{\mu}^\mathrm{s}}{\partial\mathsf{r}}\right)}{\partial\mathsf{r}} - \tilde{\mu}^\mathrm{s}\right. \\
&\left. + \frac{a(\lambda_- - \lambda_+)}{2}\left[-\frac{\tilde{\mu}^\mathrm{s}}{\mathsf{r}}\frac{\partial(\mathsf{r}\mathcal{M})}{\partial\mathsf{r}} + \frac{1}{\mathsf{r}}\frac{\partial\left(\mathcal{M}^2\frac{\partial\tilde{\mu}^\mathrm{s}}{\partial\mathsf{r}}\right)}{\partial\mathsf{r}}\right]\right\},
\end{aligned}
\tag{6.4.47}
$$

or

$$
\frac{\varrho^\mathrm{b}}{\breve{\sigma}}h_t = -a\tilde{\mu}^\mathrm{s}\left[1 + \frac{a(\lambda_- - \lambda_+)}{2\mathsf{r}}\frac{\partial(\mathsf{r}\mathcal{M})}{\partial\mathsf{r}}\right] + \frac{a}{\mathsf{r}}\frac{\partial\left[\mathsf{r}\mathcal{M}\frac{\partial\tilde{\mu}^\mathrm{s}}{\partial\mathsf{r}}\left(1 + \frac{a(\lambda_- - \lambda_+)\mathcal{M}}{2\mathsf{r}}\right)\right]}{\partial\mathsf{r}},
\tag{6.4.48}
$$

where $\mathcal{M}$ is defined in (6.4.20) By (6.4.25) and (6.4.45) and the fact that

$$
\frac{\mu^\mathrm{s}_j - \frac{\Psi^\mathrm{b}}{\varrho^\mathrm{b}} - \frac{g}{\mathsf{r}_j}}{\Theta} = -a(\lambda_+ J_j(\mathsf{r}_j) + \lambda_- J_{j-1}(\mathsf{r}_j)),
\tag{6.4.49}
$$

the continuum limit of the modified Gibbs–Thomson relation is

$$
\begin{aligned}
\tilde{\mu}^\mathrm{s} = \frac{\Psi^\mathrm{b}}{\varrho^\mathrm{b}} + \frac{g}{\mathsf{r}} + \Theta&\left\{a(\lambda_+ + \lambda_-)\mathcal{M}\frac{\partial\tilde{\mu}^\mathrm{s}}{\partial\mathsf{r}}\right. \\
&\left. - \frac{a^2(\lambda_- - \lambda_+)}{2|h_\mathsf{r}|}\left[-\tilde{\mu}^\mathrm{s}\mathcal{M} + \frac{\mathcal{M}^2}{\mathsf{r}}\frac{\partial\tilde{\mu}^\mathrm{s}}{\partial\mathsf{r}} + \frac{\partial\left(\mathcal{M}\frac{\partial\tilde{\mu}^\mathrm{s}}{\partial\mathsf{r}}\right)}{\partial\mathsf{r}}\right]\right\}.
\end{aligned}
\tag{6.4.50}
$$

In the original coordinates, we have that in the continuum limit

$$\varrho^{\mathrm{b}} h_t = \frac{a}{r}\frac{\partial}{\partial r}\left[\left(r\tilde{M} + \frac{a\,(l_- - l_+)\,\tilde{M}^2}{2M}\right)\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial r}\right] - a\breve{\sigma}\tilde{\mu}^{\mathrm{s}}\left[1 + \frac{a(l_- - l_+)}{2r}\frac{\partial}{\partial r}\left(\frac{r\tilde{M}}{M}\right)\right] \tag{6.4.51}$$

and

$$\begin{aligned}\tilde{\mu}^{\mathrm{s}} = \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} + \frac{\gamma}{r} + \Theta\Bigg\{&\left(\frac{1}{C_+} + \frac{1}{C_-}\right)\tilde{M}\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial r} \\ &- \frac{a}{2|h_r|}\left(\frac{1}{C_-} - \frac{1}{C_+}\right)\left(-\frac{\tilde{\mu}^{\mathrm{s}}\breve{\sigma}\tilde{M}}{M} + \frac{\tilde{M}^2}{Mr}\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial r} + \frac{\partial}{\partial r}\left(\tilde{M}\frac{\partial \tilde{\mu}^{\mathrm{s}}}{\partial r}\right)\right)\Bigg\},\end{aligned} \tag{6.4.52}$$

where

$$\tilde{M}(r) = \frac{M}{1 + \frac{M}{a}\left(\frac{1}{C_+} + \frac{1}{C_-}\right)|h_r(r)|}, \tag{6.4.53}$$

which in terms of $\alpha(|h_r|)$ and $\widehat{\alpha}(|h_r|)$ is equivalent to (6.4.7).

7 Continuum limits for steps with slowly varying curvature

7.1 Introduction

In a recent paper [14], Margetis and Kohn derive the continuum limit of the quasistatic BCF model for steps with slowly varying curvature undergoing surface relaxation. In order to account for step-step interactions, they introduce an ad hoc term in the Gibbs–Thomson relation that accounts for elastic interactions. Their continuum limit takes the form of a fourth-order parabolic PDE for the surface height h. Although adatom diffusion on terraces is assumed to be isotropic, the surface mobility that appears in the continuum limit is of a tensorial nature, i.e., surface diffusion in the coarse-grained model is anisotropic.

In contrast, we consider both surface relaxation and growth. Furthermore, our starting point is the quasistatic version of the thermodynamically consistent model (4.6.6)-(4.6.8) derived in Chapter 4. The TC model accounts for step-step interactions via the jump in the adatom grand canonical potential, resulting in boundary conditions that couple adjacent terraces. These step-step interactions are diffusive in nature, and occur even in the absence of elastic effects.

We consider two modes of step-flow: surface relaxation (i.e., $F = 0$) and growth (i.e., $F > 0$), for simplicity in both cases we take $\breve{\sigma} = 0$. Consistent with [14] and [41], in the continuum limit the mobility is of a tensorial character, i.e., surface diffusion in the continuum limit is anisotropic. Whereas Margetis and Kohn arrive at a single PDE for the surface profile, our continuum limit takes the form of a system of coupled PDE for the surface height h and the surface chemical potential $\tilde{\mu}^{s}$, thereby generalizing the results of Chapters 5 and 6.

7.2 Generalized coordinates

We consider height functions h for which the level sets are boundary curves (i.e., closed and simple or unbounded and simple), and choose a parameterization $\mathbf{x} : \mathtt{N} \times \mathbb{R} \to \mathbb{R}^2$ of the domain of h such that (*i.*) $\mathfrak{s} \mapsto h(\mathfrak{n}_0, \mathfrak{s})$ parameterizes the level sets of h for each $\mathfrak{n}_0 \in \mathtt{N}$ and (*ii.*) h is a decreasing function of $\mathfrak{n}$. We assume further that the map $\mathbf{x}$ is chosen such that $\frac{\partial \mathbf{x}}{\partial \mathfrak{n}} \cdot \frac{\partial \mathbf{x}}{\partial \mathfrak{s}} = 0$. Let $\xi_{\mathfrak{n}}$ and $\xi_{\mathfrak{s}}$ denote the metric coefficients,

$$\xi_{\mathfrak{n}} = \left| \frac{\partial \mathbf{x}}{\partial \mathfrak{n}} \right| \qquad \text{and} \qquad \xi_{\mathfrak{s}} = \left| \frac{\partial \mathbf{x}}{\partial \mathfrak{n}} \right|, \tag{7.2.1}$$

and write $\mathbf{e}_{\mathfrak{n}}$ and $\mathbf{e}_{\mathfrak{s}}$, for the unit normal and tangential vectors to the level sets of h, i.e., the unit vectors in the direction $\mathfrak{n}$ and $\mathfrak{s}$, which may be computed using

$$\mathbf{e}_{\mathfrak{n}} = \frac{1}{\xi_{\mathfrak{n}}} \frac{\partial \mathbf{x}}{\partial \mathfrak{n}} \qquad \text{and} \qquad \mathbf{e}_{\mathfrak{s}} = \frac{1}{\xi_{\mathfrak{s}}} \frac{\partial \mathbf{x}}{\partial \mathfrak{n}}. \tag{7.2.2}$$

For the sake of brevity, we write $\partial_\perp$ and $\partial_\|$ for the normal and tangential differential operators:

$$\partial_\perp = \frac{1}{\xi_{\mathfrak{n}}} \frac{\partial}{\partial \mathfrak{n}} \qquad \text{and} \qquad \partial_\| = \frac{1}{\xi_{\mathfrak{s}}} \frac{\partial}{\partial \mathfrak{s}}. \tag{7.2.3}$$

Since $\nabla h(\mathfrak{n}_0, \mathfrak{s}_0)$ is orthogonal to the level set $h = h(\mathfrak{n}_0, \mathfrak{s}_0)$, we have that

$$|\nabla h| = \frac{1}{\xi_{\mathfrak{n}}} \left| \frac{\partial h}{\partial \mathfrak{n}} \right|. \tag{7.2.4}$$

It is a useful fact that, on the one hand, Frenet's theorem implies

$$\kappa = -\frac{1}{\xi_{\mathfrak{s}} \xi_{\mathfrak{n}}} \frac{\partial \xi_{\mathfrak{s}}}{\partial \mathfrak{n}}, \tag{7.2.5}$$

and, on the other hand, the curvature of a level set of h is the divergence of $\nabla h / |\nabla h|$. Hence,

$$\frac{1}{\xi_{\mathfrak{s}} \xi_{\mathfrak{n}}} \frac{\partial \xi_{\mathfrak{s}}}{\partial \mathfrak{n}} = -\operatorname{div} \frac{\nabla h}{|\nabla h|}. \tag{7.2.6}$$

Moreover, for any scalar field u,

$$\partial_\perp u = -\frac{\nabla u \cdot \nabla h}{|\nabla h|}. \tag{7.2.7}$$

Recall that the divergence of a vector field $\mathbf{u} = u_\perp \mathbf{e}_\mathfrak{n} + u_\parallel \mathbf{e}_\mathfrak{s}$ may be calculated using

$$\operatorname{div} \mathbf{u} = \frac{1}{\xi_\mathfrak{n}\xi_\mathfrak{s}} \left[\frac{\partial\left(\xi_\mathfrak{s} u_\perp\right)}{\partial \mathfrak{n}} + \frac{\partial\left(\xi_\mathfrak{n} u_\parallel\right)}{\partial \mathfrak{s}} \right]. \qquad (7.2.8)$$

A step $\mathcal{S}_j$ which forms a level set of h is identitified by the value $\mathfrak{n}_j$ such that $\mathcal{S}_j = \{\mathbf{x}(\mathfrak{n}_j, \mathfrak{s}) \in \mathbb{R}^2 \colon \mathfrak{s} \in \mathbb{R}\}$.

Consistent with (5.1.10), in the continuum limit procedure, we approximate the terrace widths $\delta\mathfrak{n}_j = \mathfrak{n}_{j+1} - \mathfrak{n}_j$ and $\delta\mathfrak{n}_{j-1} = \mathfrak{n}_j - \mathfrak{n}_{j-1}$ as follows

$$\left.\begin{aligned} \delta\mathfrak{n}_j &\overset{3}{\approx} \quad \frac{a}{\left|\frac{\partial h}{\partial \mathfrak{n}}\right|} + \frac{a}{2\left|\frac{\partial h}{\partial \mathfrak{n}}\right|}\frac{\partial}{\partial \mathfrak{n}}\left(\frac{a}{\left|\frac{\partial h}{\partial \mathfrak{n}}\right|}\right)\Bigg|_{\mathfrak{n}=\mathfrak{n}_j}, \\ \delta\mathfrak{n}_{j-1} &\overset{3}{\approx} \quad \frac{a}{\left|\frac{\partial h}{\partial \mathfrak{n}}\right|} - \frac{a}{2\left|\frac{\partial h}{\partial \mathfrak{n}}\right|}\frac{\partial}{\partial \mathfrak{n}}\left(\frac{a}{\left|\frac{\partial h}{\partial \mathfrak{n}}\right|}\right)\Bigg|_{\mathfrak{n}=\mathfrak{n}_j}, \end{aligned}\right\} \qquad (7.2.9)$$

where $\overset{n}{\approx}$ is defined in (5.1.9). In contrast to the previous cases, $\mathfrak{n}$ is not assumed to be an arclength parameterization, and in general $|\nabla h| = \frac{1}{\xi_\mathfrak{n}}\left|\frac{\partial h}{\partial \mathfrak{n}}\right|$.

7.3 Surface relaxation

In this section, we study the relaxation problem for the TC model governing the motion of steps with slowly varying curvature. We base our approach on the work of Margetis and Kohn [14] and Quah and Margetis [41]. The curvature of the level sets of h is assumed to vary on a length scale of order ε^{-1} where $\varepsilon^2 = O(a)$.

Separation of Variables

The purpose of this section is to provide the formal multiscale argument for the separation of variables when we assume slowly varying curvature. Suppose that $\xi_\mathfrak{n}, \xi_\mathfrak{s}$ vary slowly with $\mathfrak{s}$, so that for a small $\varepsilon > 0$, and $\bar{\mathfrak{s}} = \varepsilon\mathfrak{s}$,

$$\left.\begin{aligned} \xi_\mathfrak{n}(\mathfrak{n}, \mathfrak{s}, \bar{\mathfrak{s}}) &= \quad \xi_\mathfrak{n}(\mathfrak{n}, \bar{\mathfrak{s}}), \\ \xi_\mathfrak{s}(\mathfrak{n}, \mathfrak{s}, \bar{\mathfrak{s}}) &= \quad \xi_\mathfrak{s}(\mathfrak{n}, \bar{\mathfrak{s}}). \end{aligned}\right\} \qquad (7.3.1)$$

Let μ_j denote the adatom chemical potential on the terrace defined on the terrace bounded by steps located at $\mathfrak{n} = \mathfrak{n}_j$ and $\mathfrak{n} = \mathfrak{n}_{j+1}$. Then the requirement, in the case of relaxation, that $\Delta\mu_j = 0$, may be recast as

$$\frac{\partial}{\partial\mathfrak{n}}\left(\frac{\xi_\mathfrak{s}}{\xi_\mathfrak{n}}\frac{\partial\mu_j}{\partial\mathfrak{n}}\right) + \frac{\partial}{\partial\mathfrak{s}}\left(\frac{\xi_\mathfrak{n}}{\xi_\mathfrak{s}}\frac{\partial\mu_j}{\partial\mathfrak{s}}\right) + \varepsilon\left[\frac{\partial}{\partial\bar{\mathfrak{s}}}\left(\frac{\xi_\mathfrak{n}}{\xi_\mathfrak{s}}\frac{\partial\mu_j}{\partial\mathfrak{s}}\right) + \frac{\partial}{\partial\mathfrak{s}}\left(\frac{\xi_\mathfrak{n}}{\xi_\mathfrak{s}}\frac{\partial\mu_j}{\partial\bar{\mathfrak{s}}}\right)\right] + \varepsilon^2\frac{\partial}{\partial\bar{\mathfrak{s}}}\left(\frac{\xi_\mathfrak{n}}{\xi_\mathfrak{s}}\frac{\partial\mu_j}{\partial\bar{\mathfrak{s}}}\right) = 0, \quad (7.3.2)$$

and the boundary conditions are

$$\left.\begin{aligned} \frac{M}{\xi_\mathfrak{n}}\frac{\partial\mu_j}{\partial\mathfrak{n}} &= C_+\left(\mu_j - \mu_j^{\mathrm{s}}\right) && \text{on } \mathfrak{n} = \mathfrak{n}_j, \\ \frac{M}{\xi_\mathfrak{n}}\frac{\partial\mu_j}{\partial\mathfrak{n}} &= -C_-\left(\mu_j - \mu_{j+1}^{\mathrm{s}}\right) && \text{on } \mathfrak{n} = \mathfrak{n}_{j+1}, \end{aligned}\right\} \quad (7.3.3)$$

where the step chemical potential μ_j^{s} satisfies the modified Gibbs–Thomson relation, which in these coordinates, takes the form

$$\mu_j^{\mathrm{s}} = \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} + \Theta(\mu|_{\mathfrak{n}=\mathfrak{n}_j}^{+} - \mu|_{\mathfrak{n}=\mathfrak{n}_j}^{-}) + \frac{\gamma}{\xi_\mathfrak{n}\xi_\mathfrak{s}}\frac{\partial\xi_\mathfrak{s}}{\partial\mathfrak{n}}\bigg|_{\mathfrak{n}=\mathfrak{n}_j}. \quad (7.3.4)$$

Assuming that $\xi_\mathfrak{n} = \xi_\mathfrak{n}(\mathfrak{n}, \bar{\mathfrak{s}})$ and $\kappa = \kappa(\mathfrak{n}, \bar{\mathfrak{s}})$, we have that for the expansion

$$\mu_j(\mathfrak{n}, \mathfrak{s}, \bar{\mathfrak{s}}) = \mu_j^{(0)}(\mathfrak{n}, \mathfrak{s}, \bar{\mathfrak{s}}) + \varepsilon\mu_j^{(1)}(\mathfrak{n}, \mathfrak{s}, \bar{\mathfrak{s}}) + \varepsilon^2\mu_j^{(2)}(\mathfrak{n}, \mathfrak{s}, \bar{\mathfrak{s}}) + \cdots, \quad (7.3.5)$$

matching orders of ε, on the domain $\{(\mathfrak{n}, \mathfrak{s}) \in (\mathfrak{n}_j, \mathfrak{n}_{j+1}) \times \mathbb{R}\}$ the functions $\mu_j^{(k)}$ satisfy

$$\begin{aligned}
0 &= \frac{\partial}{\partial\mathfrak{n}}\left[\frac{\xi_\mathfrak{s}}{\xi_\mathfrak{n}}\frac{\partial\mu_j^{(0)}}{\partial\mathfrak{n}}\right] + \frac{\partial}{\partial\mathfrak{s}}\left[\frac{\xi_\mathfrak{n}}{\xi_\mathfrak{s}}\frac{\partial\mu_j^{(0)}}{\partial\mathfrak{s}}\right], \\
0 &= \frac{\partial}{\partial\mathfrak{n}}\left[\frac{\xi_\mathfrak{s}}{\xi_\mathfrak{n}}\frac{\partial\mu_j^{(1)}}{\partial\mathfrak{n}}\right] + \frac{\partial}{\partial\mathfrak{s}}\left[\frac{\xi_\mathfrak{n}}{\xi_\mathfrak{s}}\frac{\partial\mu_j^{(1)}}{\partial\mathfrak{s}} + \frac{\xi_\mathfrak{n}}{\xi_\mathfrak{s}}\frac{\partial\mu_j^{(0)}}{\partial\bar{\mathfrak{s}}}\right] + \frac{\partial}{\partial\bar{\mathfrak{s}}}\left[\frac{\xi_\mathfrak{n}}{\xi_\mathfrak{s}}\frac{\partial\mu_j^{(0)}}{\partial\mathfrak{s}}\right], \\
0 &= \frac{\partial}{\partial\mathfrak{n}}\left[\frac{\xi_\mathfrak{s}}{\xi_\mathfrak{n}}\frac{\partial\mu_j^{(2)}}{\partial\mathfrak{n}}\right] + \frac{\partial}{\partial\mathfrak{s}}\left[\frac{\xi_\mathfrak{n}}{\xi_\mathfrak{s}}\frac{\partial\mu_j^{(2)}}{\partial\mathfrak{s}} + \frac{\xi_\mathfrak{n}}{\xi_\mathfrak{s}}\frac{\partial\mu_j^{(1)}}{\partial\bar{\mathfrak{s}}}\right] + \frac{\partial}{\partial\bar{\mathfrak{s}}}\left[\frac{\xi_\mathfrak{n}}{\xi_\mathfrak{s}}\frac{\partial\mu_j^{(1)}}{\partial\mathfrak{s}} + \frac{\xi_\mathfrak{n}}{\xi_\mathfrak{s}}\frac{\partial\mu_j^{(0)}}{\partial\bar{\mathfrak{s}}}\right], \\
0 &= \frac{\partial}{\partial\mathfrak{n}}\left[\frac{\xi_\mathfrak{s}}{\xi_\mathfrak{n}}\frac{\partial\mu_j^{(3)}}{\partial\mathfrak{n}}\right] + \frac{\partial}{\partial\mathfrak{s}}\left[\frac{\xi_\mathfrak{n}}{\xi_\mathfrak{s}}\frac{\partial\mu_j^{(3)}}{\partial\bar{\mathfrak{s}}} + \frac{\xi_\mathfrak{n}}{\xi_\mathfrak{s}}\frac{\partial\mu_j^{(2)}}{\partial\bar{\mathfrak{s}}}\right] + \frac{\partial}{\partial\bar{\mathfrak{s}}}\left[\frac{\xi_\mathfrak{n}}{\xi_\mathfrak{s}}\frac{\partial\mu_j^{(2)}}{\partial\mathfrak{s}} + \frac{\xi_\mathfrak{n}}{\xi_\mathfrak{s}}\frac{\partial\mu_j^{(1)}}{\partial\bar{\mathfrak{s}}}\right],
\end{aligned} \quad (7.3.6)$$

with boundary conditions:

$$\begin{aligned} \frac{M}{\xi_\mathfrak{n}}\frac{\partial\mu_j^{(k)}}{\partial\mathfrak{n}} &= C_+\left(\mu_j^{(k)} - \mu_j^{\mathrm{s},(k)}\right) \text{ on } \mathcal{S}_j, \\ \frac{M}{\xi_\mathfrak{n}}\frac{\partial\mu_j^{(k)}}{\partial\mathfrak{n}} &= -C_-\left(\mu_j^{(k)} - \mu_{j+1}^{\mathrm{s},(k)}\right) \text{ on } \mathcal{S}_{j+1}, \end{aligned} \quad (7.3.7)$$

for $k = 1, 2, 3, \ldots$, where

$$\mu_j^{\mathrm{s},(0)} = \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} + \Theta(\mu_j^{(0)} - \mu_{j-1}^{(0)}) + \frac{\gamma}{\xi_{\mathfrak{n}}\xi_{\mathfrak{s}}}\frac{\partial \xi_{\mathfrak{s}}}{\partial \mathfrak{n}}\bigg|_{\mathfrak{n}=\mathfrak{n}_j}, \qquad \mu_j^{\mathrm{s},(k)} = \Theta(\mu_j^{(k)} - \mu_{j-1}^{(k)})|_{\mathfrak{n}=\mathfrak{n}_j} \text{ for } k > 0. \tag{7.3.8}$$

With this definition of $\mu_j^{\mathrm{s},(k)}$, we have formally that

$$\mu_j^{\mathrm{s}} = \mu_j^{\mathrm{s},(0)} + \varepsilon \mu_j^{\mathrm{s},(1)} + \varepsilon^2 \mu_j^{\mathrm{s},(2)} + \cdots . \tag{7.3.9}$$

The problem $(7.3.6)_1$ subject to the boundary conditions (7.3.7) with $k = 0$ has solution

$$\mu_j^{(0)}(\mathfrak{n}, \bar{\mathfrak{s}}) = A_j(\bar{\mathfrak{s}}) \int_{\mathfrak{n}_j}^{\mathfrak{n}} \frac{\xi_{\mathfrak{n}}}{\xi_{\mathfrak{s}}} \mathrm{d}\mathfrak{n}' + B_j(\bar{\mathfrak{s}}) \text{ for } \mathfrak{n} \in (\mathfrak{n}_j, \mathfrak{n}_{j+1}), \tag{7.3.10}$$

where

$$A_j = \frac{\mu_{j+1}^{\mathrm{s},(0)} - \mu_j^{\mathrm{s},(0)}}{\left(\frac{M}{C_+ \xi_{\mathfrak{s}}|_{\mathfrak{n}=\mathfrak{n}_j}} + \frac{M}{C_- \xi_{\mathfrak{s}}|_{\mathfrak{n}_{j+1}}}\right) + \int_{\mathfrak{n}_j}^{\mathfrak{n}_{j+1}} \frac{\xi_{\mathfrak{n}}}{\xi_{\mathfrak{s}}} \mathrm{d}\mathfrak{n}} \tag{7.3.11}$$

and

$$B_j = \mu_j^{\mathrm{s},(0)} + \frac{M A_j}{C_+ \xi_{\mathfrak{s}}|_{\mathfrak{n}=\mathfrak{n}_j}}. \tag{7.3.12}$$

Since $\mu_j^{(0)}, \xi_{\mathfrak{n}}$, and $\xi_{\mathfrak{s}}$ are $\mathfrak{s}$ independent (i.e., depend on $(\mathfrak{n}, \bar{\mathfrak{s}})$ alone), the function $\mu_j^{(1)}$ is a solution to the PDE:

$$0 = \frac{\partial}{\partial \mathfrak{n}}\left(\frac{\xi_{\mathfrak{s}}}{\xi_{\mathfrak{n}}}\frac{\partial \mu_j^{(1)}}{\partial \mathfrak{n}}\right) + \frac{\partial}{\partial \mathfrak{s}}\left(\frac{\xi_{\mathfrak{n}}}{\xi_{\mathfrak{s}}}\frac{\partial \mu_j^{(1)}}{\partial \mathfrak{s}}\right) \tag{7.3.13}$$

on the domain $(\mathfrak{n}_j, \mathfrak{n}_{j+1}) \times \mathcal{R}$ subject to boundary conditions $(7.3.7)_2$, and $\mu_j^{(1)} \equiv 0$ is a solution of the problem[1]. Hence, the function $\mu_j^{(2)}$ satisfies on the domain $(\mathfrak{n}_j, \mathfrak{n}_{j+1}) \times \mathbb{R}$

$$\frac{\partial}{\partial \mathfrak{n}}\left(\frac{\xi_{\mathfrak{s}}}{\xi_{\mathfrak{n}}}\frac{\partial \mu_j^{(2)}}{\partial \mathfrak{n}}\right) + \frac{\partial}{\partial \mathfrak{s}}\left(\frac{\xi_{\mathfrak{n}}}{\xi_{\mathfrak{s}}}\frac{\partial \mu_j^{(2)}}{\partial \mathfrak{s}}\right) + \frac{\partial}{\partial \bar{\mathfrak{s}}}\left(\frac{\xi_{\mathfrak{n}}}{\xi_{\mathfrak{s}}}\frac{\partial \mu_j^{(0)}}{\partial \bar{\mathfrak{s}}}\right) = 0, \tag{7.3.14}$$

[1] We conjecture that it is the unique solution. The uniqueness question in this context is complicated by the coupling in the boundary conditions.

with boundary conditions

$$\left.\begin{aligned} \frac{M}{\xi_{\mathfrak{n}}}\frac{\partial \mu_j^{(2)}}{\partial \mathfrak{n}} &= C_+(\mu_j^{(2)} - \mu^{s,(2)}) \qquad \text{on } \mathfrak{n} = \mathfrak{n}_j, \\ \frac{M}{\xi_{\mathfrak{n}}}\frac{\partial \mu_j^{(2)}}{\partial \mathfrak{n}} &= -C_-(\mu_j^{(2)} - \mu^{s,(2)}) \quad \text{on } \mathfrak{n} = \mathfrak{n}_{j+1}. \end{aligned}\right\} \tag{7.3.15}$$

As such, $\mu_j^{(2)}$ also depends only on $(\mathfrak{n}, \bar{\mathfrak{s}})$, and we have

$$\frac{\partial}{\partial \mathfrak{n}}\left(\frac{\xi_{\mathfrak{s}}}{\xi_{\mathfrak{n}}}\frac{\partial \mu_j^{(2)}}{\partial \mathfrak{n}}\right) = -\frac{\partial}{\partial \bar{\mathfrak{s}}}\left(\frac{\xi_{\mathfrak{n}}}{\xi_{\mathfrak{s}}}\frac{\partial \mu_j^{(0)}}{\partial \bar{\mathfrak{s}}}\right). \tag{7.3.16}$$

If $\mu_j^{(1)} \equiv 0$ is the unique solution to the $\mu_j^{(1)}$ problem, then $\mu_j^{(3)} \equiv 0$, since $\mu_j^{(3)}$ solves the same boundary value problem. Let $J_{j,\perp}$ be defined by

$$J_{j,\perp} = -\frac{M}{\xi_{\mathfrak{n}}}\frac{\partial \mu_j}{\partial \mathfrak{n}} = -M\partial_{\perp}\mu_j. \tag{7.3.17}$$

It follows from (7.3.5) that $J_{j,\perp}$ satisfies

$$J_{j,\perp} = -\frac{M}{\xi_{\mathfrak{n}}}\frac{\partial \mu_j^{(0)}}{\partial \mathfrak{n}} - \frac{M\varepsilon^2}{\xi_{\mathfrak{n}}}\frac{\partial \mu_j^{(2)}}{\partial \mathfrak{n}} + O(\varepsilon^4), \tag{7.3.18}$$

recalling that $\mu_j^{(1)} \equiv 0$. Moreover, by (7.3.16),

$$\frac{\partial\left(\xi_{\mathfrak{s}} J_{j,\perp}\right)}{\partial \mathfrak{n}} = -M\varepsilon^2\frac{\partial}{\partial \mathfrak{n}}\left(\frac{\xi_{\mathfrak{s}}}{\xi_{\mathfrak{n}}}\frac{\partial \mu_j^{(2)}}{\partial \mathfrak{n}}\right) + O(\varepsilon^4) = M\varepsilon^2\frac{\partial}{\partial \bar{\mathfrak{s}}}\left(\frac{\xi_{\mathfrak{n}}}{\xi_{\mathfrak{s}}}\frac{\partial \mu_j^{(0)}}{\partial \bar{\mathfrak{s}}}\right) + O(\varepsilon^4). \tag{7.3.19}$$

To find the continuum limit, we find approximations to the diffusive fluxes $J_{j,\perp}$, $J_{j,\parallel}$, and $J_{j-1,\perp}$ at the jth step.

Approximating the diffusive flux $J_{j,\parallel}$ at the jth step

As in the previous chapters, we take $M, \xi_{\mathfrak{s}}, \xi_{\mathfrak{n}}, \mu_j^{(0)}, l_{\pm}$ to be fixed as $a \to 0$, and we neglect terms of order ε^3 or higher. We also assume that

$$\mu_j^{s,(0)}, \xi_{\mathfrak{s}}|_{\mathfrak{n}=\mathfrak{n}_j}, \xi_{\mathfrak{n}}|_{\mathfrak{n}=\mathfrak{n}_j} = O(1), \tag{7.3.20}$$

with $\mu_j^{s,(0)} \overset{3}{\approx} \tilde{\mu}^s(\mathfrak{n}_j)$ and $\frac{\partial \mu_j^{s,(0)}}{\partial \mathfrak{s}} \overset{3}{\approx} \frac{\partial \tilde{\mu}^s(\mathfrak{n}_j)}{\partial \mathfrak{s}}$ in the continuum limit, where $\tilde{\mu}^s$ is a smooth function of $(\mathfrak{n}, \bar{\mathfrak{s}})$. This latter supposition is reasonable, since we assume that the continuum functions are in some sense interpolant along the level sets of h.

By our assumption that $\varepsilon = O(a^{1/2})$ and since $\mu^{(1)} \equiv 0$, we have

$$J_{j,\parallel} = -M \frac{1}{\xi_{\mathfrak{s}}} \frac{\partial \mu_j}{\partial \mathfrak{s}} \overset{1}{\approx} -\frac{M\varepsilon}{\xi_{\mathfrak{s}}} \frac{\partial \mu_j^{(0)}}{\partial \bar{\mathfrak{s}}}. \tag{7.3.21}$$

At the jth step, by (7.3.10) and (7.3.11), it follows that

$$J_{j,\parallel}\big|_{\mathfrak{n}=\mathfrak{n}_j} \overset{1}{\approx} -\frac{M\varepsilon}{\xi_{\mathfrak{s}}} \frac{\partial \mu^{s,(0)}}{\partial \bar{\mathfrak{s}}}\bigg|_{\mathfrak{n}=\mathfrak{n}_j} \overset{1}{\approx} \frac{M}{\xi_{\mathfrak{s}}} \frac{\partial \tilde{\mu}^s}{\partial \mathfrak{s}}\bigg|_{\mathfrak{n}=\mathfrak{n}_j}. \tag{7.3.22}$$

Approximating the diffusive flux $J_{j,\perp}$ at the jth step

The first-order Taylor approximation of the difference of $\mu_{j+1}^{s,(0)}$ and $\mu_j^{s,(0)}$ gives us that:

$$\frac{\mu_{j+1}^{s,(0)} - \mu_j^{s,(0)}}{\delta\mathfrak{n}_j \xi_{\mathfrak{n}}|_{\mathfrak{n}=\mathfrak{n}_j}} \overset{2}{\approx} \partial_\perp \tilde{\mu}^s + \frac{\delta\mathfrak{n}_j}{2\xi_{\mathfrak{n}}} \frac{\partial^2 \tilde{\mu}^s}{\partial \mathfrak{n}^2}\bigg|_{\mathfrak{n}=\mathfrak{n}_j}. \tag{7.3.23}$$

Similarly, the denominator of A_j $(7.3.11)_1$ is approximated by

$$\begin{aligned}
&\frac{\xi_{\mathfrak{s}}}{\delta\mathfrak{n}_j \xi_{\mathfrak{n}}} \left\{ \frac{M}{C_+ \xi_{\mathfrak{s}}} + \frac{M}{C_- \xi_{\mathfrak{s}}} + \int_{\mathfrak{n}_j}^{\mathfrak{n}_{j+1}} \frac{\xi_{\mathfrak{n}}}{\xi_{\mathfrak{s}}} \, d\mathfrak{n} \right\}\bigg|_{\mathfrak{n}=\mathfrak{n}_j} \\
&\overset{2}{\approx} \frac{L_+ + L_-}{\delta\mathfrak{n}_j \xi_{\mathfrak{n}}} + 1 - \frac{L_- \frac{\partial \xi_{\mathfrak{s}}}{\partial \mathfrak{n}}}{\xi_{\mathfrak{n}} \xi_{\mathfrak{s}}} + \frac{\xi_{\mathfrak{s}} \delta\mathfrak{n}_j}{2\xi_{\mathfrak{n}}} \left[L_- \frac{\partial^2}{\partial \mathfrak{n}^2} \left(\frac{1}{\xi_{\mathfrak{s}}} \right) + \frac{\partial}{\partial \mathfrak{n}} \left(\frac{\xi_{\mathfrak{n}}}{\xi_{\mathfrak{s}}} \right) \right]\bigg|_{\mathfrak{n}=\mathfrak{n}_j} \\
&\overset{2}{\approx} \frac{L_+ + L_-}{\delta\mathfrak{n}_j \xi_{\mathfrak{n}}} + 1 - \frac{L_- \frac{\partial \xi_{\mathfrak{s}}}{\partial \mathfrak{n}}}{\xi_{\mathfrak{n}} \xi_{\mathfrak{s}}} + \frac{\xi_{\mathfrak{s}} \delta\mathfrak{n}_j}{2\xi_{\mathfrak{n}}} \frac{\partial}{\partial \mathfrak{n}} \left(\frac{\xi_{\mathfrak{n}}}{\xi_{\mathfrak{s}}} \right)\bigg|_{\mathfrak{n}=\mathfrak{n}_j}.
\end{aligned} \tag{7.3.24}$$

Hence, in the continuum limit

$$J_{j,\perp}\big|_{\mathfrak{n}=\mathfrak{n}_j} \overset{2}{\approx} -\frac{M\left(\partial_\perp \tilde{\mu}^s + \frac{\delta\mathfrak{n}_j}{2\xi_{\mathfrak{n}}} \frac{\partial^2 \tilde{\mu}^s}{\partial \mathfrak{n}^2}\right)}{1 + \frac{a(l_+ + l_-)}{\delta\mathfrak{n}_j \xi_{\mathfrak{n}}}} - \frac{M \partial_\perp \tilde{\mu}^s \left(\frac{M}{C_-} \frac{\frac{\partial \xi_{\mathfrak{s}}}{\partial \mathfrak{n}}}{\xi_{\mathfrak{n}} \xi_{\mathfrak{s}}} - \frac{\xi_{\mathfrak{s}} \delta\mathfrak{n}_j}{2\xi_{\mathfrak{n}}} \frac{\partial}{\partial \mathfrak{n}} \left(\frac{\xi_{\mathfrak{n}}}{\xi_{\mathfrak{s}}} \right) \right)}{\left(1 + \frac{a(l_+ + l_-)}{\delta\mathfrak{n}_j \xi_{\mathfrak{n}}}\right)^2}\Bigg|_{\mathfrak{n}=\mathfrak{n}_j}. \tag{7.3.25}$$

We use the following notation (cf. (5.2.17))

$$\tilde{M} = \frac{M}{1 + (l_+ + l_-)|\nabla h|} = M\alpha(|\nabla h|). \tag{7.3.26}$$

Next, we approximate

$$\frac{1}{1+\frac{a(l_++l_-)}{\delta\mathfrak{n}_j\xi_\mathfrak{n}|_{\mathfrak{n}=\mathfrak{n}_j}}} = \frac{\delta\mathfrak{n}_j\xi_\mathfrak{n}|_{\mathfrak{n}=\mathfrak{n}_j}}{\delta\mathfrak{n}_j\xi_\mathfrak{n}|_{\mathfrak{n}=\mathfrak{n}_j}+a(l_++l_-)} \tag{7.3.27}$$

by substitution of $(7.2.9)_1$ to find

$$\frac{1}{1+\frac{a(l_++l_-)}{\delta\mathfrak{n}_j\xi_\mathfrak{n}|_{\mathfrak{n}=\mathfrak{n}_j}}} \overset{2}{\approx} p\left(\frac{a}{2|\nabla h|}\frac{\partial}{\partial\mathfrak{n}}\left(\frac{a}{\left|\frac{\partial h}{\partial\mathfrak{n}}\right|}\right)\right)\Bigg|_{\mathfrak{n}=\mathfrak{n}_j}, \tag{7.3.28}$$

where $p(t)$ is defined by

$$p(t) = \frac{\frac{a}{|\nabla h|}+t}{\frac{a}{|\nabla h|}+t+a(l_++l_-)} = \frac{\frac{a}{|\nabla h|}}{\frac{a}{|\nabla h|}+a(l_++l_-)} + \frac{a(l_++l_-)t}{\left(\frac{a}{|\nabla h|}+a(l_++l_-)\right)^2}+O(t^2). \tag{7.3.29}$$

Hence,

$$\frac{1}{1+\frac{a(l_++l_-)}{\delta\mathfrak{n}_j\xi_\mathfrak{n}|_{\mathfrak{n}=\mathfrak{n}_j}}} \overset{2}{\approx} \frac{1}{1+(l_++l_-)|\nabla h|} + \frac{a}{2}\frac{(l_++l_-)|\nabla h|}{(1+(l_++l_-)|\nabla h|)^2}\frac{\partial}{\partial\mathfrak{n}}\left(\frac{1}{\left|\frac{\partial h}{\partial\mathfrak{n}}\right|}\right)\Bigg|_{\mathfrak{n}=\mathfrak{n}_j}. \tag{7.3.30}$$

The second term of (7.3.25) can be simplified as follows

$$\begin{aligned}\frac{\frac{M}{C_-}\frac{\frac{\partial\xi_\mathfrak{s}}{\partial\mathfrak{n}}}{\xi_\mathfrak{n}\xi_\mathfrak{s}}-\frac{\xi_\mathfrak{s}\delta\mathfrak{n}_j}{2\xi_\mathfrak{n}}\frac{\partial\left(\frac{\xi_\mathfrak{n}}{\xi_\mathfrak{s}}\right)}{\partial\mathfrak{n}}}{\left(1+\frac{a(l_++l_-)}{\delta\mathfrak{n}_j\xi_\mathfrak{n}}\right)^2}\Bigg|_{\mathfrak{n}=\mathfrak{n}_j} &= \left.\frac{\frac{\xi_\mathfrak{n}\delta\mathfrak{n}_j}{2\xi_\mathfrak{n}\xi_\mathfrak{s}}\frac{\partial\xi_\mathfrak{s}}{\partial\mathfrak{n}}}{1+\frac{a(l_++l_-)}{\xi_\mathfrak{n}\delta\mathfrak{n}_j}}+\frac{\frac{a(l_--l_+)}{2\xi_\mathfrak{n}\xi_\mathfrak{s}}\frac{\partial\xi_\mathfrak{s}}{\partial\mathfrak{n}}-\frac{\delta\mathfrak{n}_j}{2\xi_\mathfrak{n}}\frac{\partial\xi_\mathfrak{n}}{\partial\mathfrak{n}}}{\left(1+\frac{a(l_++l_-)}{\xi_\mathfrak{n}\delta\mathfrak{n}_j}\right)^2}\right|_{\mathfrak{n}=\mathfrak{n}_j} \\ &\overset{2}{\approx} \left.\frac{\frac{a}{2|\nabla h|\xi_\mathfrak{n}\xi_\mathfrak{s}}\frac{\partial\xi_\mathfrak{s}}{\partial\mathfrak{n}}+\frac{\frac{a(l_--l_+)}{2\xi_\mathfrak{n}\xi_\mathfrak{s}}\frac{\partial\xi_\mathfrak{s}}{\partial\mathfrak{n}}-\frac{a}{2|\nabla h|\xi_\mathfrak{n}^2}\frac{\partial\xi_\mathfrak{n}}{\partial\mathfrak{n}}}{(1+(l_++l_-)|\nabla h|)}}{1+(l_++l_-)|\nabla h|}\right|_{\mathfrak{n}=\mathfrak{n}_j}.\end{aligned} \tag{7.3.31}$$

Therefore, substituting (7.3.30) and (7.3.31) into (7.3.25), we find

$$\begin{aligned}J_{j,\perp}|_{\mathfrak{n}=\mathfrak{n}_j} \overset{2}{\approx}= &-\tilde{M}\partial_\perp\tilde{\mu}^{\mathrm{s}}-\frac{a(l_--l_+)\tilde{M}^2\partial_\perp\tilde{\mu}^{\mathrm{s}}}{2M}\frac{\frac{\partial\xi_\mathfrak{s}}{\partial\mathfrak{n}}}{\xi_\mathfrak{s}\xi_\mathfrak{n}} \\ &-\frac{a}{2|\nabla h|}\left[\partial_\perp\left(\tilde{M}\partial_\perp\tilde{\mu}^{\mathrm{s}}\right)+\frac{\frac{\partial\xi_\mathfrak{s}}{\partial\mathfrak{n}}}{\xi_\mathfrak{n}\xi_\mathfrak{s}}\tilde{M}\partial_\perp\tilde{\mu}^{\mathrm{s}}\right]\Bigg|_{\mathfrak{n}=\mathfrak{n}_j}.\end{aligned} \tag{7.3.32}$$

Hence,

$$J_{j,\perp}|_{\mathfrak{n}=\mathfrak{n}_j} \overset{2}{\approx} -\frac{\tilde{M}}{\xi_\mathfrak{n}}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial\mathfrak{n}} - \frac{a}{2|\nabla h|}\frac{1}{\xi_\mathfrak{s}\xi_\mathfrak{n}}\frac{\partial}{\partial\mathfrak{n}}\left(\frac{M\frac{\xi_\mathfrak{s}}{\xi_\mathfrak{n}}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial\mathfrak{n}}}{1+(l_+ + l_-)|\nabla h|}\right) \\ \left. - \frac{a(l_- - l_+)M\partial_\perp\tilde{\mu}^{\mathrm{s}}}{(1+(l_+ + l_-)|\nabla h|)^2}\frac{\frac{\partial\xi_\mathfrak{s}}{\partial\mathfrak{n}}}{2\xi_\mathfrak{s}\xi_\mathfrak{n}}\right|_{\mathfrak{n}=\mathfrak{n}_j}. \quad (7.3.33)$$

Approximating the diffusive flux $J_{j-1,\perp}$ at the jth step

We now find the appropriate approximation of $J_{j-1,\perp}|_{\mathfrak{n}=\mathfrak{n}_j}$. As in the previous chapters, we define

$$\mathcal{J}_{0,\perp} = -\tilde{M}\partial_\perp\tilde{\mu}^{\mathrm{s}}, \quad (7.3.34)$$

$$\mathcal{J}_{1,\perp} = -\frac{a}{2|\nabla h|}\frac{1}{\xi_\mathfrak{s}\xi_\mathfrak{n}}\frac{\partial}{\partial\mathfrak{n}}\left(\frac{M\frac{\xi_\mathfrak{s}}{\xi_\mathfrak{n}}\frac{\partial\tilde{\mu}^{\mathrm{s}}}{\partial\mathfrak{n}}}{1+(l_+ + l_-)|\nabla h|}\right) - \frac{a(l_- - l_+)M\partial_\perp\tilde{\mu}^{\mathrm{s}}}{(1+(l_+ + l_-)|\nabla h|)^2}\frac{\frac{\partial\xi_\mathfrak{s}}{\partial\mathfrak{n}}}{2\xi_\mathfrak{s}\xi_\mathfrak{n}}, \quad (7.3.35)$$

and $\mathcal{J}_{2,\perp} = O(a^2)$ such that

$$\mathcal{J}_\perp = \mathcal{J}_{0,\perp} + \mathcal{J}_{1,\perp} + \mathcal{J}_{2,\perp} \quad (7.3.36)$$

satisfies

$$J_{j,\perp}|_{\mathfrak{n}=\mathfrak{n}_j} \overset{3}{\approx} \mathcal{J}_\perp(\mathfrak{n}_j). \quad (7.3.37)$$

To use $\mathcal{J}_\perp$ in approximating the diffusive flux $J_{j-1,\perp}|_{\mathfrak{n}=\mathfrak{n}_j}$, we first approximate this flux in terms of $J_{j-1,\perp}|_{\mathfrak{n}=\mathfrak{n}_{j-1}}$ using Taylor polynomials. We then apply our approximation (7.3.37) and invoke (7.3.19). Finally, we use the basic approximation for the terrace width (7.2.9). Explicitly,

$$\begin{aligned}
\xi_{\mathfrak{s}} J_{j-1,\perp}|_{\mathfrak{n}=\mathfrak{n}_j} &\overset{3}{\approx} \xi_{\mathfrak{s}} J_{j-1,\perp} + \delta\mathfrak{n}_{j-1}\frac{\partial\left(\xi_{\mathfrak{s}} J_{j-1,\perp}\right)}{\partial\mathfrak{n}} + \frac{(\delta\mathfrak{n}_{j-1})^2}{2}\frac{\partial^2\left(\xi_{\mathfrak{s}} J_{j-1,\perp}\right)}{\partial\mathfrak{n}^2}\Bigg|_{\mathfrak{n}=\mathfrak{n}_{j-1}} \\
&\overset{3}{\approx} \xi_{\mathfrak{s}}\mathcal{J}_\perp - \varepsilon^2\delta\mathfrak{n}_{j-1}\frac{\partial\left(\frac{\xi_{\mathfrak{n}}}{\xi_{\mathfrak{s}}}\frac{\partial\mu^{(0)}}{\partial\bar{\mathfrak{s}}}\right)}{\partial\bar{\mathfrak{s}}} + \frac{\varepsilon^2(\delta\mathfrak{n}_{j-1})^2}{2}\frac{\partial^2\left(\frac{\xi_{\mathfrak{s}}}{\xi_{\mathfrak{n}}}\frac{\partial\mu^{(2)}}{\partial\mathfrak{n}}\right)}{\partial\mathfrak{n}^2}\Bigg|_{\mathfrak{n}=\mathfrak{n}_{j-1}} \\
&\overset{3}{\approx} \xi_{\mathfrak{s}}\mathcal{J}_\perp - \varepsilon^2\delta\mathfrak{n}_{j-1}\frac{\partial}{\partial\bar{\mathfrak{s}}}\left(\frac{\xi_{\mathfrak{n}}}{\xi_{\mathfrak{s}}}\frac{\partial\mu^{(0)}}{\partial\bar{\mathfrak{s}}}\right)\Bigg|_{\mathfrak{n}=\mathfrak{n}_{j-1}} \\
&\overset{3}{\approx} \xi_{\mathfrak{s}}\mathcal{J}_\perp - \delta\mathfrak{n}_{j-1}\frac{\partial(\xi_{\mathfrak{s}}\mathcal{J}_\perp)}{\partial\mathfrak{n}} + \frac{\delta\mathfrak{n}_{j-1}^2}{2}\frac{\partial^2\left(\xi_{\mathfrak{s}}\mathcal{J}_\perp\right)}{\partial\mathfrak{n}^2} \\
&\qquad -\varepsilon^2\delta\mathfrak{n}_{j-1}\frac{\partial}{\partial\bar{\mathfrak{s}}}\left[\frac{\xi_{\mathfrak{n}}}{\xi_{\mathfrak{s}}}\frac{\partial\mu^{(0)}}{\partial\bar{\mathfrak{s}}}\right]\Bigg|_{\mathfrak{n}=\mathfrak{n}_j} \\
&\overset{3}{\approx} \xi_{\mathfrak{s}}\mathcal{J}_\perp - \frac{a}{|\nabla h|}\frac{1}{\xi_{\mathfrak{n}}}\frac{\partial(\xi_{\mathfrak{s}}\mathcal{J}_\perp)}{\partial\mathfrak{n}} + \frac{a}{2|\nabla h|}\frac{1}{\xi_{\mathfrak{n}}^2}\frac{\partial\left(\frac{a}{|\nabla h|}\right)}{\partial\mathfrak{n}}\frac{\partial\left(\xi_{\mathfrak{s}}\mathcal{J}_{0,\perp}\right)}{\partial\mathfrak{n}} \\
&\qquad + \frac{a^2}{2|\nabla h|^2\xi_{\mathfrak{n}}^2}\frac{\partial^2(\xi_{\mathfrak{s}}\mathcal{J}_{0,\perp})}{\partial\mathfrak{n}^2} - \varepsilon^2\frac{a}{|\nabla h|\xi_{\mathfrak{n}}}\frac{\partial}{\partial\bar{\mathfrak{s}}}\left(\frac{\xi_{\mathfrak{n}}}{\xi_{\mathfrak{s}}}\frac{\partial\mu^{(0)}}{\partial\bar{\mathfrak{s}}}\right)\Bigg|_{\mathfrak{n}=\mathfrak{n}_j}.
\end{aligned} \tag{7.3.38}$$

Upon simplification, we find that the appropriate approximation for $J_{j-1,\perp}|_{\mathfrak{n}=\mathfrak{n}_j}$ is given in terms of the continuum functions as

$$\begin{aligned}
J_{j-1,\perp}|_{\mathfrak{n}=\mathfrak{n}_j} &\overset{3}{\approx} \mathcal{J}_\perp - \frac{a}{|\nabla h|}\operatorname{div}\left(\mathcal{J}_{0,\perp}\mathbf{e}_{\mathfrak{n}} + \mathcal{J}_\parallel\mathbf{e}_{\mathfrak{s}}\right) \\
&\qquad + \frac{a(l_- - l_+)}{2|\nabla h|}\frac{1}{\xi_{\mathfrak{n}}\xi_{\mathfrak{s}}}\frac{\partial}{\partial\mathfrak{n}}\left(\frac{\frac{\partial\xi_{\mathfrak{s}}}{\partial\mathfrak{n}}}{\xi_{\mathfrak{n}}\xi_{\mathfrak{s}}}\xi_{\mathfrak{s}}\frac{M\partial_\perp\tilde{\mu}^{s}}{(1+(l_+ + l_-)|\nabla h|)^2}\right)\Bigg|_{\mathfrak{n}=\mathfrak{n}_j},
\end{aligned} \tag{7.3.39}$$

where $\mathcal{J}_\perp(\mathfrak{n})$ is the approximation to $J_{j,\perp}|_{\mathfrak{n}=\mathfrak{n}_j} \overset{3}{\approx} \mathcal{J}_\perp(\mathfrak{n}_j)$. We have used the fact that $\mu^{(3)} \equiv 0$.

Let the continuum mobility $\mathbf{M}$ denote the matrix

$$\mathbf{M} = \tilde{M}\mathbf{e}_{\mathfrak{n}} \otimes \mathbf{e}_{\mathfrak{n}} + M\mathbf{e}_{\mathfrak{s}} \otimes \mathbf{e}_{\mathfrak{s}}, \tag{7.3.40}$$

and let the mobility correction $\widehat{\mathbf{M}}$ denote the matrix

$$\widehat{\mathbf{M}} = \frac{M(l_- - l_+)}{2(1+(l_+ + l_-)|\nabla h|)^2}\operatorname{div}\left(\frac{\nabla h}{|\nabla h|}\right)\mathbf{e}_{\mathfrak{n}} \otimes \mathbf{e}_{\mathfrak{n}}. \tag{7.3.41}$$

Recall that $\frac{1}{\xi_{\mathfrak{n}}\xi_{\mathfrak{s}}}\frac{\partial\xi_{\mathfrak{s}}}{\partial\mathfrak{n}} = -\operatorname{div}\left(\frac{\nabla h}{|\nabla h|}\right)$, then we have

$$J_{j-1,\perp}|_{\mathfrak{n}=\mathfrak{n}_j} \overset{3}{\approx} \mathcal{J}_\perp + \frac{a}{|\nabla h|}\operatorname{div}\left[\left(\mathbf{M} - a\widehat{\mathbf{M}}\right)\nabla\tilde{\mu}^{s}\right]\Bigg|_{\mathfrak{n}=\mathfrak{n}_j} \tag{7.3.42}$$

Continuum limits

We are now ready to write the continuum limits of the velocity equation and the modified Gibbs–Thomson relation. Since the velocity equation can be written as

$$\varrho^{\mathrm{b}} V_j = J_{j-1,\perp}|_{\mathfrak{n}=\mathfrak{n}_j} - J_{j,\perp}|_{\mathfrak{n}=\mathfrak{n}_j} \tag{7.3.43}$$

and the modified Gibbs–Thomson relation (7.3.4) can be written as

$$\frac{\mu_j^{\mathrm{s}} - \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} + \gamma\kappa_j}{\Theta} = -\left(\frac{J_{j-1,\perp}}{C_-} + \frac{J_{j,\perp}}{C_+}\right)\Bigg|_{\mathfrak{n}=\mathfrak{n}_j}, \tag{7.3.44}$$

what remains is to use (7.3.37) and (7.3.39) neglecting terms of order a^3 or higher.

As in the previous chapters, we approximate the normal velocity of the step as the normal velocity of the level set of h. In particular, we use $V_j \approx h_t(\mathfrak{s}, \mathfrak{n}_j, t)/|\nabla h(\mathfrak{s}, \mathfrak{n}_j, t)|$. Thus, the continuum limit of the velocity equation is given by

$$\varrho^{\mathrm{b}} h_t = a \,\mathrm{div}\left[\left(\mathbf{M} - a\widehat{\mathbf{M}}\right)\nabla\tilde{\mu}^{\mathrm{s}}\right], \tag{7.3.45}$$

where $\widehat{\mathbf{M}}$ is defined in (7.3.41), and $\mathbf{M}$ is defined in (7.3.40).

Therefore, appealing to (7.3.39), (7.3.34), and (7.3.35) in the continuum limit we find

$$\begin{aligned}\frac{\tilde{\mu}^{\mathrm{s}} - \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} + \gamma\kappa}{\Theta} = {}& \frac{a(l_+ + l_-)\tilde{M}\partial_\perp\tilde{\mu}^{\mathrm{s}}}{M} \\ & - \frac{a^2\,(l_- - l_+)}{2|\nabla h|}\left(\frac{\tilde{M}^2\partial_\perp\tilde{\mu}^{\mathrm{s}}}{M^2}\frac{\frac{\partial\xi_{\mathfrak{s}}}{\partial\mathfrak{n}}}{\xi_{\mathfrak{n}}\xi_{\mathfrak{s}}} + \partial_\perp\left(\frac{\tilde{M}}{M}\partial_\perp\tilde{\mu}^{\mathrm{s}}\right)\right).\end{aligned} \tag{7.3.46}$$

By (7.2.6) and (7.2.7), we may write the continuum limit of the modified Gibbs–Thomson relation (7.3.46) as follows:

$$\begin{aligned}\tilde{\mu}^{\mathrm{s}} = {}& \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} - \gamma\,\mathrm{div}\left(\frac{\nabla h}{|\nabla h|}\right) - \frac{a\Theta}{|\nabla h|}\Bigg\{(l_+ + l_-)\alpha(|\nabla h|)\nabla\tilde{\mu}^{\mathrm{s}}\cdot\nabla h + \frac{a(l_- - l_+)}{2|\nabla h|} \\ & \times\left[\alpha(|\nabla h|)^2\nabla\tilde{\mu}^{\mathrm{s}}\cdot\nabla h\,\mathrm{div}\left(\frac{\nabla h}{|\nabla h|}\right) + \nabla h\cdot\nabla\left(\frac{\alpha(|\nabla h|)\nabla\tilde{\mu}^{\mathrm{s}}\cdot\nabla h}{|\nabla h|}\right)\right]\Bigg\}.\end{aligned} \tag{7.3.47}$$

7.4 Growth

Under the same geometric assumptions as in the relaxation case, we consider the quasistatic TC model of step motion during growth ($F > 0$ and $\breve{\sigma} = 0$). Using the same variables as in the previous section, the adatom chemical potential satisfies the following boundary value problem

$$\left.\begin{array}{rcll} 0 & = & M\Delta\mu_j + F & \text{in } (\mathfrak{n}_j, \mathfrak{n}_{j+1}), \\ \dfrac{M}{\xi_\mathfrak{n}}\dfrac{\partial\mu_j}{\partial\mathfrak{n}} & = & C_+\left(\mu_j - \mu_j^{\mathrm{s},(0)}\right) & \text{at } \mathfrak{n} = \mathfrak{n}_j, \\ \dfrac{M}{\xi_\mathfrak{n}}\dfrac{\partial\mu_j}{\partial\mathfrak{n}} & = & -C_-\left(\mu_j - \mu_{j+1}^{\mathrm{s},(0)}\right) & \text{at } \mathfrak{n} = \mathfrak{n}_{j+1}, \end{array}\right\} \tag{7.4.1}$$

where the step chemical potential couples the diffusion processes on adjacent terraces since it satisfies

$$\mu_j^{\mathrm{s}} = \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} + \Theta(\mu_j - \mu_{j-1}) - \gamma\kappa_j \qquad \text{at } \mathfrak{n} = \mathfrak{n}_j, \tag{7.4.2}$$

and the normal velocity of the step is given by

$$\varrho^{\mathrm{b}} V_j = C_+(\mu_j^{(0)} - \mu_j^{\mathrm{s},(0)}) + C_-(\mu_{j-1}^{(0)} - \mu_j^{\mathrm{s},(0)}) \qquad \text{at } \mathfrak{n} = \mathfrak{n}_j. \tag{7.4.3}$$

As we saw in the previous section, it suffices to consider only the zeroth-order (in ε) sub-problem for steps with slowly varying curvature:

$$\left.\begin{array}{rcll} 0 & = & M\dfrac{1}{\xi_\mathfrak{s}\xi_\mathfrak{n}}\dfrac{\partial}{\partial\mathfrak{n}}\left(\dfrac{\xi_\mathfrak{s}}{\xi_\mathfrak{n}}\dfrac{\partial\mu_j^{(0)}}{\partial\mathfrak{n}}\right) + F & \text{in } (\mathfrak{n}_j, \mathfrak{n}_{j+1}), \\ \dfrac{M}{\xi_\mathfrak{n}}\dfrac{\partial\mu_j^{(0)}}{\partial\mathfrak{n}} & = & C_+\left(\mu_j^{(0)} - \mu_j^{\mathrm{s},(0)}\right) & \text{at } \mathfrak{n} = \mathfrak{n}_j, \\ \dfrac{M}{\xi_\mathfrak{n}}\dfrac{\partial\mu_j^{(0)}}{\partial\mathfrak{n}} & = & -C_-\left(\mu_j^{(0)} - \mu_{j+1}^{\mathrm{s},(0)}\right) & \text{at } \mathfrak{n} = \mathfrak{n}_{j+1}, \\ \mu_j^{\mathrm{s},(0)} & = & \dfrac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} + \Theta[\![\mu^{(0)}]\!] - \gamma\kappa_j & \text{at } \mathfrak{n} = \mathfrak{n}_j, \\ \varrho^{\mathrm{b}} V_j & = & C_+(\mu_j^{(0)} - \mu_j^{\mathrm{s}}) + C_-(\mu_{j-1}^{(0)} - \mu_j^{\mathrm{s}}) & \text{at } \mathfrak{n} = \mathfrak{n}_j, \end{array}\right\} \tag{7.4.4}$$

The main result of this section is to establish that this problem has a continuum limit taking the form of a coupled system of PDE for the surface height h:

$$\varrho^{\mathrm{b}} h_t = aF\left(1 - \frac{a(l_- - l_+)}{2}\operatorname{div}\left(\frac{1}{|\nabla h|}\mathbf{M}\nabla h\right)\right) + a\operatorname{div}\left[\left(\mathbf{M}\nabla\tilde{\mu}^{\mathrm{s}} - a\widehat{\mathbf{M}}\right)\nabla\tilde{\mu}^{\mathrm{s}}\right], \tag{7.4.5}$$

and the surface chemical potential $\tilde{\mu}^{\mathrm{s}}$

$$\begin{aligned}\tilde{\mu}^{\mathrm{s}} = {} & \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} - \gamma\operatorname{div}\left(\frac{\nabla h}{|\nabla h|}\right) - \frac{a\Theta}{|\nabla h|}\left\{\frac{(l_+ + l_-)\nabla\tilde{\mu}^{\mathrm{s}}\cdot\nabla h}{1 + (l_+ + l_-)|\nabla h|} + \frac{(l_- - l_+)}{2}\right.\\ & \times\left[\frac{F}{M}\frac{1}{1 + (l_+ + l_-)|\nabla h|} + \frac{(\nabla\tilde{\mu}^{\mathrm{s}}\cdot\nabla h)}{|\nabla h|\left(1 + (l_+ + l_-)|\nabla h|\right)^2}\operatorname{div}\left(\frac{\nabla h}{|\nabla h|}\right)\right.\\ & \left.\left. + \nabla\left(\frac{\nabla\tilde{\mu}^{\mathrm{s}}\cdot\nabla h}{|\nabla h|\left(1 + (l_+ + l_-)|\nabla h|\right)}\right)\cdot\frac{\nabla h}{|\nabla h|}\right]\right\}.\end{aligned} \tag{7.4.6}$$

where

$$\widehat{\mathbf{M}} = \frac{(l_- - l_+)}{2}\frac{\tilde{M}^2}{M}\operatorname{div}\left(\frac{\nabla h}{|\nabla h|}\right)\mathbf{e}_{\mathfrak{n}}\otimes\mathbf{e}_{\mathfrak{n}}, \tag{7.4.7}$$

and

$$\mathbf{M} = \tilde{M}\mathbf{e}_{\mathfrak{n}}\otimes\mathbf{e}_{\mathfrak{n}} + M\mathbf{e}_{\mathfrak{s}}\otimes\mathbf{e}_{\mathfrak{s}}. \tag{7.4.8}$$

Recall that $\tilde{M}$ is defined by

$$\tilde{M} = \frac{M}{1 + (l_+ + l_-)|\nabla h|}. \tag{7.4.9}$$

Approximating the diffusive flux $J_{j,\perp}$ at the jth step

The equation $(7.4.4)_1$ has solution

$$\mu_j^{(0)}(\mathfrak{n}) = \varphi_j(\mathfrak{n}) + A_j\psi_j(\mathfrak{n}) + B_j, \tag{7.4.10}$$

where φ_j is defined by

$$\varphi_j(\mathfrak{n}) = -\frac{F}{M}\int_{\mathfrak{n}_j}^{\mathfrak{n}}\frac{\xi_{\mathfrak{n}}(\mathfrak{n}')}{\xi_{\mathfrak{s}}(\mathfrak{n}')}\int_{\mathfrak{n}_j}^{\mathfrak{n}'}\xi_{\mathfrak{n}}(\mathfrak{n}'')\xi_{\mathfrak{s}}(\mathfrak{n}'')\,d\mathfrak{n}''\,d\mathfrak{n}', \tag{7.4.11}$$

(7.4.12)

and ψ_j is defined by

$$\psi_j(\mathfrak{n}) = \int_{\mathfrak{n}_j}^{\mathfrak{n}} \frac{\xi_{\mathfrak{n}}(\mathfrak{n}')}{\xi_{\mathfrak{s}}(\mathfrak{n}')} \,\mathrm{d}\mathfrak{n}'. \tag{7.4.13}$$

The boundary conditions $(7.4.4)_{2,3}$ require

$$\left.\begin{aligned} A_j = & \quad \frac{\mu_{j+1}^{\mathrm{s},(0)} - \mu_j^{\mathrm{s},(0)} - \left(\varphi_j|_{\mathfrak{n}_{j+1}} + \frac{M}{C_-\xi_{\mathfrak{n}}|_{\mathfrak{n}_{j+1}}} \frac{\partial \varphi_j}{\partial \mathfrak{n}}|_{\mathfrak{n}_{j+1}}\right)}{M\left(\frac{1}{C_+\xi_{\mathfrak{s}}|_{\mathfrak{n}=\mathfrak{n}_j}} + \frac{1}{C_-\xi_{\mathfrak{s}}|_{\mathfrak{n}_{j+1}}}\right) + \int_{\mathfrak{n}_j}^{\mathfrak{n}_{j+1}} \frac{\xi_{\mathfrak{n}}}{\xi_{\mathfrak{s}}} \,\mathrm{d}\mathfrak{n}}, \\ B_j = & \quad \mu_j^{\mathrm{s},(0)} + \frac{MA_j}{C_+\xi_{\mathfrak{s}}|_{\mathfrak{n}=\mathfrak{n}_j}}. \end{aligned}\right\} \tag{7.4.14}$$

We now find the appropriate continuum limit, $\mathcal{J}_\perp(\mathfrak{n}_j)$, of $J_{j,\perp}|_{\mathfrak{n}=\mathfrak{n}_j}$. As before,

$$J_{j,\perp}|_{\mathfrak{n}=\mathfrak{n}_j} = -\frac{M}{\xi_{\mathfrak{n}}|_{\mathfrak{n}=\mathfrak{n}_j}} \left.\frac{\partial \mu_j}{\partial \mathfrak{n}}\right|_{\mathfrak{n}=\mathfrak{n}_j} \overset{2}{\approx} -\frac{MA_j}{\xi_{\mathfrak{s}}|_{\mathfrak{n}=\mathfrak{n}_j}}, \tag{7.4.15}$$

where A_j is defined in $(7.4.14)_1$. Moreover, from the previous calculation leading to (7.3.33), we have

$$\begin{aligned} -\frac{M(\mu_{j+1}^{\mathrm{s},(0)} - \mu_j^{\mathrm{s},(0)})}{\xi_{\mathfrak{s}}|_{\mathfrak{n}=\mathfrak{n}_j}\left(M\left(\frac{1}{C_+\xi_{\mathfrak{s}}|_{\mathfrak{n}=\mathfrak{n}_j}} + \frac{1}{C_-\xi_{\mathfrak{s}}|_{\mathfrak{n}_{j+1}}}\right) + \int_{\mathfrak{n}_j}^{\mathfrak{n}_{j+1}} \frac{\xi_{\mathfrak{n}}}{\xi_{\mathfrak{s}}}\,\mathrm{d}\mathfrak{n}\right)} &\overset{2}{\approx} -\tilde{M}\partial_\perp\tilde{\mu}^{\mathrm{s}} - \frac{a}{2|\nabla h|}\partial_\perp\left(\tilde{M}\partial_\perp\tilde{\mu}^{\mathrm{s}}\right) \\ &- \frac{a}{2|\nabla h|}\frac{\tilde{M}\partial_\perp\tilde{\mu}^{\mathrm{s}}}{\xi_{\mathfrak{n}}\xi_{\mathfrak{s}}}\frac{\partial \xi_{\mathfrak{s}}}{\partial \mathfrak{n}} \quad \left. -\frac{1}{2}\left(\frac{1}{C_-} - \frac{1}{C_+}\right)\frac{\tilde{M}^2\partial_\perp\tilde{\mu}^{\mathrm{s}}}{\xi_{\mathfrak{s}}\xi_{\mathfrak{n}}}\frac{\partial \xi_{\mathfrak{s}}}{\partial \mathfrak{n}}\right|_{\mathfrak{n}=\mathfrak{n}_j}. \end{aligned} \tag{7.4.16}$$

It remains for us to approximate

$$-\frac{M\hat{A}_j}{\xi_{\mathfrak{s}}|_{\mathfrak{n}=\mathfrak{n}_j}} := \frac{M\left(\varphi_j|_{\mathfrak{n}_{j+1}} + \frac{M}{C_-\xi_{\mathfrak{n}}|_{\mathfrak{n}_{j+1}}}\frac{\partial \varphi_j}{\partial \mathfrak{n}}|_{\mathfrak{n}_{j+1}}\right)}{\xi_{\mathfrak{s}}|_{\mathfrak{n}=\mathfrak{n}_j}\left(M\left(\frac{1}{C_+\xi_{\mathfrak{s}}|_{\mathfrak{n}=\mathfrak{n}_j}} + \frac{1}{C_-\xi_{\mathfrak{s}}|_{\mathfrak{n}_{j+1}}}\right) + \int_{\mathfrak{n}_j}^{\mathfrak{n}_{j+1}} \frac{\xi_{\mathfrak{n}}}{\xi_{\mathfrak{s}}}\,\mathrm{d}\mathfrak{n}\right)}. \tag{7.4.17}$$

Note that

$$\varphi_j(\mathfrak{n}_{j+1}) = -\frac{F}{M}\int_{\mathfrak{n}_j}^{\mathfrak{n}_{j+1}} \frac{\xi_{\mathfrak{n}}(\mathfrak{n}')}{\xi_{\mathfrak{s}}(\mathfrak{n}')}\int_{\mathfrak{n}_j}^{\mathfrak{n}'} \xi_{\mathfrak{n}}(\mathfrak{n}'')\xi_{\mathfrak{s}}(\mathfrak{n}'')\,\mathrm{d}\mathfrak{n}''\,\mathrm{d}\mathfrak{n}' \overset{3}{\approx} -\frac{F\xi_{\mathfrak{n}}^2|_{\mathfrak{n}=\mathfrak{n}_j}\delta\mathfrak{n}_j^2}{2M}, \tag{7.4.18}$$

and

$$\frac{M}{C_-\xi_{\mathfrak{n}}}\left.\frac{\partial \varphi_j}{\partial \mathfrak{n}}\right|_{\mathfrak{n}_{j+1}} = -\frac{F}{C_-\xi_{\mathfrak{s}}|_{\mathfrak{n}_{j+1}}}\int_{\mathfrak{n}_j}^{\mathfrak{n}_{j+1}} \xi_{\mathfrak{n}}(\mathfrak{n}')\xi_{\mathfrak{s}}(\mathfrak{n}')\,\mathrm{d}\mathfrak{n}' \overset{3}{\approx} -\frac{al_-F\delta\mathfrak{n}_j\xi_{\mathfrak{n}}|_{\mathfrak{n}=\mathfrak{n}_j}}{M}. \tag{7.4.19}$$

Hence, we have

$$
\begin{aligned}
-\frac{M\hat{A}_j}{\xi_{\mathfrak{s}}|_{\mathfrak{n}=\mathfrak{n}_j}} &\overset{2}{\approx} \frac{\frac{-\mathsf{F}\xi_{\mathfrak{n}}|_{\mathfrak{n}_j}\delta\mathfrak{n}_j}{2} - \frac{M\mathsf{F}}{C_-}}{1+\frac{a(l_++l_-)}{\delta\mathfrak{n}_j\xi_{\mathfrak{n}}|_{\mathfrak{n}=\mathfrak{n}_j}}} \\
&\overset{2}{\approx} -\frac{\mathsf{F}\left(\frac{a}{2|\nabla h|}+al_-\right)}{1+(l_++l_-)|\nabla h|}\Bigg|_{\mathfrak{n}=\mathfrak{n}_j} \\
&\overset{2}{\approx} -\mathsf{F}\left(\frac{a}{2|\nabla h|}+\frac{a(l_--l_+)\tilde{M}}{2M}\right)\Bigg|_{\mathfrak{n}=\mathfrak{n}_j}.
\end{aligned}
\tag{7.4.20}
$$

Approximating the diffusive flux $J_{j-1,\perp}$ at the jth step

Taking (7.4.16) and (7.4.20) together, we see that for

$$
\begin{aligned}
\mathcal{J}_{0,\perp} =& -\tilde{M}\partial_\perp\tilde{\mu}^{\mathrm{s}}, \\
\mathcal{J}_{1,\perp} =& -\frac{a}{2|\nabla h|}\frac{1}{\xi_{\mathfrak{n}}\xi_{\mathfrak{s}}}\frac{\partial}{\partial\mathfrak{n}}\left(\xi_{\mathfrak{s}}\tilde{M}\partial_\perp\tilde{\mu}^{\mathrm{s}}\right) - \frac{1}{2}\left(\frac{1}{C_-}-\frac{1}{C_+}\right)\frac{\frac{\partial\xi_{\mathfrak{s}}}{\partial\mathfrak{n}}}{\xi_{\mathfrak{s}}\xi_{\mathfrak{n}}}\tilde{M}^2\partial_\perp\tilde{\mu}^{\mathrm{s}}, \\
\mathcal{J}_{\mathsf{F},\perp} =& -\mathsf{F}\left(\frac{a}{2|\nabla h|}+\frac{a(l_--l_+)\tilde{M}}{2M}\right),
\end{aligned}
\tag{7.4.21}
$$

we may choose $\mathcal{J}_{2,\perp} = O(a^2)$ such that

$$
J_{j,\perp}|_{\mathfrak{n}=\mathfrak{n}_j} \overset{3}{\approx} \mathcal{J}_\perp(\mathfrak{n}_j) \tag{7.4.22}
$$

where $\mathcal{J}_\perp$ is defined to be

$$
\mathcal{J}_\perp = \mathcal{J}_{0,\perp} + \mathcal{J}_{1,\perp} + \mathcal{J}_{\mathsf{F},\perp} + \mathcal{J}_{2,\perp}. \tag{7.4.23}
$$

Recall that the divergence of $\boldsymbol{J}_j = -M\nabla\mu^{(0)}$ satisfies

$$
\operatorname{div}\boldsymbol{J}_j = \mathsf{F}, \tag{7.4.24}
$$

by (7.4.4). Hence, we have that

$$
\frac{\partial(\xi_{\mathfrak{s}}J_{j,\perp})}{\partial\mathfrak{n}} = \mathsf{F}\xi_{\mathfrak{s}}\xi_{\mathfrak{n}} - \frac{\partial}{\partial\mathfrak{s}}(\xi_{\mathfrak{n}}J_{j,\|}). \tag{7.4.25}
$$

Therefore, we approximate $J_{j-1,\perp}$ at the jth step using

$$\begin{aligned}\xi_{\mathfrak{s}} J_{j-1,\perp}|_{\mathfrak{n}=\mathfrak{n}_j} &\overset{3}{\approx} J_{j-1,\perp}\xi_{\mathfrak{s}} - \delta\mathfrak{n}_{j-1}\frac{\partial(\xi_{\mathfrak{n}} J_{j,\parallel})}{\partial\mathfrak{s}} \\ &\quad + F\left(\delta\mathfrak{n}_{j-1}(\xi_{\mathfrak{s}}\xi_{\mathfrak{n}}) + \frac{\delta\mathfrak{n}_{j-1}^2}{2}\frac{\partial\left(\xi_{\mathfrak{s}}\xi_{\mathfrak{n}}\right)}{\partial\mathfrak{n}}\right)\Bigg|_{\mathfrak{n}=\mathfrak{n}_{j-1}} \\ &\overset{3}{\approx} \mathcal{J}_{\perp}\xi_{\mathfrak{s}} - \delta\mathfrak{n}_{j-1}\frac{\partial(\xi_{\mathfrak{n}} J_{j,\parallel})}{\partial\mathfrak{s}} \\ &\quad + F\left(\delta\mathfrak{n}_{j-1}\xi_{\mathfrak{s}}\xi_{\mathfrak{n}} + \frac{\delta\mathfrak{n}_{j-1}^2}{2}\frac{\partial(\xi_{\mathfrak{s}}\xi_{\mathfrak{n}})}{\partial\mathfrak{n}}\right)\Bigg|_{\mathfrak{n}=\mathfrak{n}_{j-1}}.\end{aligned} \tag{7.4.26}$$

The first term is Taylor expanded about $\mathfrak{n}_j$ to order $\delta\mathfrak{n}_j^2$, the second term is of order $\delta\mathfrak{n}_j$ and is thereby expanded about $\mathfrak{n}_j$ to order $\delta\mathfrak{n}_j$, and the third and final is of order a^3 and therefore is not expanded further than order 1. The first term in (7.4.26) is approximated as

$$\begin{aligned}\mathcal{J}_{\perp}\xi_{\mathfrak{s}}|_{\mathfrak{n}=\mathfrak{n}_{j-1}} &\overset{3}{\approx} \mathcal{J}_{\perp}\xi_{\mathfrak{s}} - \delta\mathfrak{n}_{j-1}\frac{\partial\left(\mathcal{J}_{\perp}\xi_{\mathfrak{s}}\right)}{\partial\mathfrak{n}} + \frac{\delta\mathfrak{n}_{j-1}^2}{2}\frac{\partial^2\left(\mathcal{J}_{\perp}\xi_{\mathfrak{s}}\right)}{\partial\mathfrak{n}^2}\Bigg|_{\mathfrak{n}=\mathfrak{n}_j} \\ &\overset{3}{\approx} \mathcal{J}_{\perp}\xi_{\mathfrak{s}} + \frac{a^2}{2|\frac{\partial h}{\partial\mathfrak{n}}|^2}\frac{\partial^2\left(\mathcal{J}_{0,\perp}\xi_{\mathfrak{s}}\right)}{\partial\mathfrak{n}^2} \\ &\quad - \left(\frac{a}{|\frac{\partial h}{\partial\mathfrak{n}}|} - \frac{a}{|\frac{\partial h}{\partial\mathfrak{n}}|}\frac{\partial\left(\frac{a}{2|\frac{\partial h}{\partial\mathfrak{n}}|}\right)}{\partial\mathfrak{n}}\right)\frac{\partial\left(\xi_{\mathfrak{s}}\left(\mathcal{J}_{0,\perp}+\mathcal{J}_{1,\perp}+\mathcal{J}_{F,\perp}\right)\right)}{\partial\mathfrak{n}}\Bigg|_{\mathfrak{n}=\mathfrak{n}_j} \\ &\overset{3}{\approx} \mathcal{J}_{\perp}\xi_{\mathfrak{s}} - \frac{a}{|\nabla h|}\frac{1}{\xi_{\mathfrak{n}}}\frac{\partial}{\partial\mathfrak{n}}\left(\mathcal{J}_{0,\perp}\xi_{\mathfrak{s}} + \mathcal{J}_{1,\perp}\xi_{\mathfrak{s}} + \mathcal{J}_{F,\perp}\xi_{\mathfrak{s}}\right) \\ &\quad + \frac{a}{2|\nabla h|}\frac{1}{\xi_{\mathfrak{n}}}\frac{\partial}{\partial\mathfrak{n}}\left(\frac{a}{|\frac{\partial h}{\partial\mathfrak{n}}|}\frac{\partial\left(\mathcal{J}_{0,\perp}\xi_{\mathfrak{s}}\right)}{\partial\mathfrak{n}}\right)\Bigg|_{\mathfrak{n}=\mathfrak{n}_j}.\end{aligned} \tag{7.4.27}$$

The second term in (7.4.26) is approximated as

$$-\delta\mathfrak{n}_{j-1}\frac{\partial(\xi_{\mathfrak{n}} J_{j,\parallel})}{\partial\mathfrak{s}}\Bigg|_{\mathfrak{n}=\mathfrak{n}_{j-1}} \overset{3}{\approx} -\frac{a}{|\frac{\partial h}{\partial\mathfrak{n}}|}\frac{\partial\left(\xi_{\mathfrak{n}}\mathcal{J}_{\parallel}\right)}{\partial\mathfrak{s}}\Bigg|_{\mathfrak{n}=\mathfrak{n}_j}, \tag{7.4.28}$$

where

$$\mathcal{J}_{\parallel}(\mathfrak{n}_j) = -M\partial_{\parallel}\tilde{\mu}^{\mathrm{s}}|_{\mathfrak{n}=\mathfrak{n}_j} = O(a). \tag{7.4.29}$$

Finally, the third term in (7.4.26) is approximated as

$$
\begin{aligned}
&\digamma\,\delta\mathfrak{n}_{j-1}(\xi_{\mathfrak{s}}\xi_{\mathfrak{n}}) + \digamma\frac{\delta\mathfrak{n}_{j-1}^2}{2}\frac{\partial\left(\xi_{\mathfrak{s}}\xi_{\mathfrak{n}}\right)}{\partial\mathfrak{n}}\bigg|_{\mathfrak{n}=\mathfrak{n}_{j-1}} \\
&\qquad \overset{3}{\approx} \digamma\,\delta\mathfrak{n}_{j-1}(\xi_{\mathfrak{s}}\xi_{\mathfrak{n}}) - \digamma\,\delta\mathfrak{n}_{j-1}^2\frac{\partial(\xi_{\mathfrak{s}}\xi_{\mathfrak{n}})}{\partial\mathfrak{n}} + \digamma\frac{\delta\mathfrak{n}_{j-1}^2}{2}\frac{\partial(\xi_{\mathfrak{s}}\xi_{\mathfrak{n}})}{\partial\mathfrak{n}}\bigg|_{\mathfrak{n}=\mathfrak{n}_j} \\
&\qquad \overset{3}{\approx} \xi_{\mathfrak{s}}\xi_{\mathfrak{n}}\left\{\frac{a\digamma}{|\frac{\partial h}{\partial\mathfrak{n}}|} - \frac{a\digamma}{2|\frac{\partial h}{\partial\mathfrak{n}}|}\frac{\partial}{\partial\mathfrak{n}}\left(\frac{a}{|\frac{\partial h}{\partial\mathfrak{n}}|}\right)\right\} - \frac{a^2\digamma}{2|\frac{\partial h}{\partial\mathfrak{n}}|^2}\frac{\partial\left(\xi_{\mathfrak{s}}\xi_{\mathfrak{n}}\right)}{\partial\mathfrak{n}}\bigg|_{\mathfrak{n}=\mathfrak{n}_j} \\
&\qquad \overset{3}{\approx} \frac{a\digamma\xi_{\mathfrak{s}}}{|\nabla h|} - \frac{a\digamma}{2|\nabla h|}\frac{1}{\xi_{\mathfrak{n}}}\frac{\partial}{\partial\mathfrak{n}}\left(\frac{a\xi_{\mathfrak{s}}}{|\nabla h|}\right)\bigg|_{\mathfrak{n}=\mathfrak{n}_j}.
\end{aligned}
\tag{7.4.30}
$$

Combining the approximations (7.4.27), 7.4.28), and (7.4.30), we find that $J_{j-1,\perp}|_{\mathfrak{n}=\mathfrak{n}_j}$ is approximated by

$$
\begin{aligned}
J_{j-1,\perp}|_{\mathfrak{n}=\mathfrak{n}_j} \overset{3}{\approx}\ & \mathcal{J}_{\perp} - \frac{a}{|\nabla h|}\frac{1}{\xi_{\mathfrak{s}}\xi_{\mathfrak{n}}}\frac{\partial}{\partial\mathfrak{n}}\left(\mathcal{J}_{0,\perp}\xi_{\mathfrak{s}} + \mathcal{J}_{1,\perp}\xi_{\mathfrak{s}}\right) \\
& + \frac{a}{2|\nabla h|}\frac{1}{\xi_{\mathfrak{s}}\xi_{\mathfrak{n}}}\frac{\partial}{\partial\mathfrak{n}}\left(\frac{a}{|\nabla h|}\frac{1}{\xi_{\mathfrak{n}}}\frac{\partial}{\partial\mathfrak{n}}(\mathcal{J}_{0,\perp}\xi_{\mathfrak{s}})\right) \\
& - \frac{a}{|\nabla h|}\frac{1}{\xi_{\mathfrak{n}}\xi_{\mathfrak{s}}}\frac{\partial}{\partial\mathfrak{s}}\left(\xi_{\mathfrak{n}}\mathcal{J}_{\parallel}\right) \\
& + \frac{a\digamma}{|\nabla h|}\left\{1 + \frac{1}{2}\left(\frac{1}{C_-} - \frac{1}{C_+}\right)\frac{1}{\xi_{\mathfrak{n}}\xi_{\mathfrak{s}}}\frac{\partial}{\partial\mathfrak{n}}\left(\xi_{\mathfrak{s}}\tilde{M}\right)\right\}\bigg|_{\mathfrak{n}=\mathfrak{n}_j},
\end{aligned}
\tag{7.4.31}
$$

where $\mathcal{J}_{0,\perp}, \mathcal{J}_{1,\perp}$ are defined in (7.4.21).

Continuum limits

The velocity equation has continuum limit

$$
\varrho^{\mathrm{b}} h_t = a\digamma + a\,\mathrm{div}\left(\mathbf{M}\left\{\nabla\tilde{\mu}^{\mathrm{s}} - \frac{\digamma}{2|\nabla h|}\left(\frac{1}{C_-} - \frac{1}{C_+}\right)\nabla h\right\} + \widehat{\mathbf{M}}\nabla\tilde{\mu}^{\mathrm{s}}\right), \tag{7.4.32}
$$

where

$$
\widehat{\mathbf{M}} = -\frac{1}{2}\left(\frac{1}{C_-} - \frac{1}{C_+}\right)\tilde{M}^2\,\mathrm{div}\left(\frac{\nabla h}{|\nabla h|}\right)\mathbf{e}_{\mathfrak{n}}\otimes\mathbf{e}_{\mathfrak{n}}, \tag{7.4.33}
$$

and

$$
\mathbf{M} = \tilde{M}\mathbf{e}_{\mathfrak{n}}\otimes\mathbf{e}_{\mathfrak{n}} + M\mathbf{e}_{\mathfrak{s}}\otimes\mathbf{e}_{\mathfrak{s}}. \tag{7.4.34}
$$

The modified Gibbs–Thomson relation $(7.4.4)_4$ has continuum limit

$$\begin{aligned}
\frac{\tilde{\mu}^{\mathrm{s}} - \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} + \gamma\kappa}{\Theta} &= -\left(\frac{1}{C_+} + \frac{1}{C_-}\right)\mathcal{J}_{0,\perp} - \left(\frac{1}{C_+} + \frac{1}{C_-}\right)\mathcal{J}_{1,\perp} \\
&\quad + \frac{a}{C_-|\nabla h|}\frac{1}{\xi_{\mathfrak{s}}\xi_{\mathfrak{n}}}\frac{\partial\left(\xi_{\mathfrak{s}}\mathcal{J}_{0,\perp}\right)}{\partial\mathfrak{n}} - \left(\frac{1}{C_+} + \frac{1}{C_-}\right)\mathcal{J}_{F,\perp} - \frac{aF}{C_-|\nabla h|} \\
&= \left(\frac{1}{C_+} + \frac{1}{C_-}\right)\tilde{M}\partial_\perp\tilde{\mu}^{\mathrm{s}} - \frac{1}{2}\left(\frac{1}{C_-} - \frac{1}{C_+}\right)\frac{a}{|\nabla h|} \\
&\quad \times \left\{\frac{F\tilde{M}}{M} + \frac{\tilde{M}^2\partial_\perp\tilde{\mu}^{\mathrm{s}}}{M\xi_{\mathfrak{n}}\xi_{\mathfrak{s}}}\frac{\partial\xi_{\mathfrak{s}}}{\partial\mathfrak{n}} + \partial_\perp\left(\tilde{M}\partial_\perp\tilde{\mu}^{\mathrm{s}}\right)\right\},
\end{aligned} \tag{7.4.35}$$

or, since κ and $-\frac{\frac{\partial\xi_{\mathfrak{s}}}{\partial\mathfrak{n}}}{\xi_{\mathfrak{n}}\xi_{\mathfrak{s}}}$ are the curvature of the level set of h, and the curvature of the level of h is given by $\operatorname{div}\left(\frac{\nabla h}{|\nabla h|}\right)$ and since $\partial_\perp u = \nabla u\cdot\mathbf{e}_{\mathfrak{n}} = -\nabla u\cdot\frac{\nabla h}{|\nabla h|}$, we have

$$\begin{aligned}
\tilde{\mu}^{\mathrm{s}} = \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} - \gamma\operatorname{div}\left(\frac{\nabla h}{|\nabla h|}\right) - \frac{a\Theta}{|\nabla h|}&\left\{\frac{(l_+ + l_-)\nabla\tilde{\mu}^{\mathrm{s}}\cdot\nabla h}{1 + (l_+ + l_-)|\nabla h|} + \frac{1}{2}\left(\frac{1}{C_-} - \frac{1}{C_+}\right)\right. \\
\times\left[\frac{F\tilde{M}}{M} + \frac{\tilde{M}^2\left(\nabla\tilde{\mu}^{\mathrm{s}}\cdot\nabla h\right)}{M|\nabla h|}\operatorname{div}\left(\frac{\nabla h}{|\nabla h|}\right)\right. &+ \left.\left.\nabla\left(\frac{\tilde{M}\nabla\tilde{\mu}^{\mathrm{s}}\cdot\nabla h}{|\nabla h|}\right)\cdot\frac{\nabla h}{|\nabla h|}\right]\right\}.
\end{aligned} \tag{7.4.36}$$

8 Epilogue

8.1 Summary of the work

In the first part of the thesis, Chapters 1, 2, and 3, we investigate conditions under which steps collide during step-flow epitaxial growth. The starting point is the quasistatic approximation of the BCF model:

$$\left.\begin{array}{rcll} D\Delta\varrho - \tau^{-1}\varrho + F &=& 0 & \text{in } \Omega_+ \cup \Omega_-, \\ D\nabla\varrho^+ \cdot \mathbf{n} &=& K_+\left(\varrho^+ - \varrho_{\rm eq} + \Gamma\kappa\right) & \text{along } \mathcal{S}, \\ -D\nabla\varrho^- \cdot \mathbf{n} &=& K_-\left(\varrho^- - \varrho_{\rm eq} + \Gamma\kappa\right) & \text{along } \mathcal{S}, \\ \varrho^{\rm b} V &=& D[\![\nabla\varrho]\!] \cdot \mathbf{n} & \text{along } \mathcal{S}. \end{array}\right\} \tag{8.1.1}$$

We consider rectilinear and concentric step trains. These geometries have the advantage of reducing (8.1.1) to a one-dimensional boundary value problem and that for such an initial profile, solutions of (8.1.1) preserve shape. This reduces the BCF model (8.1.1) to a system of differential equations.

In Chapter 2, we consider the motion of an infinite train of rectilinear, parallel steps in the absence of desorption. We show that, for N-terrace periodic step trains, uniform step spacing of the steps is asymptotically stable. We do so by proving that the standard deviation of the terrace widths is a Lyapunov function for the resulting dynamical system. Moreover, we establish that for $K_- > 0$ and $N > 2$, step motions exist for which collisions occur. Further, for $l^2(\mathbb{Z};\mathbb{R})$ perturbed terraces, we consider solutions to the BCF model for the three cases $K_- = 0$ (no adatom attachment from the upper terraces), $K_+ = K_-$ (symmetric attachment/detachment kinetics), and $K_+ = 0$ (no adatom from the lower terraces). In each case, we perturb a single terrace problem, and analyze the resulting dynamical system. When $K_- = 0$, steps never collide, irrespective of the initial terrace width. For symmetric attachment, outward perturbations that exceed a critical terrace width will invariably lead to step collisions, independently of the value of $K_+ = K_-$. Finally, when $K_+ = 0$, for any perturbations away from uniform spacing step collisions occur in finite, positive time.

In Chapter 3, we consider two configurations. The first consists of two rectilinear parallel step bounded by two reflecting walls. The second configuration, consists of a pair of concentric steps bounded by a reflecting wall. In both cases, under growth conditions, we establish that the normal Ehrlich–Schwoebel barrier is destabilizing with respect to step collisions. Specifically, both in the presence and absence of line tension, decreasing the kinetic coefficient for attachment from the upper terrace K_- results in more initial configurations that lead to step collisions. This is achieved using tools from the theory of non-linear ODE. In the presence of evaporation, we show that there is exists a unique step-motion trajectory that divides the triangle of allowable step positions into a stable region and an unstable one. Fixing the position of one the two steps there exists a critical width of the intermediate terrace corresponding to this unique step motion below which a step collision will inevitably occur. This analysis paves the way for the rigorous characterization of step bunching during nanowire growth.

The BCF model (8.1.1) does not ensure consistency with the first and second laws of thermodynamics. In Chapter 5, we generalize the BCF model such that the constitutive theory is compatible with the dissipation inequality. Importantly, we show that the step chemical potential obeys the modified Gibbs–Thomson relation:

$$\mu^{\mathrm{s}} = \frac{\Psi^{\mathrm{b}}}{\varrho^{\mathrm{b}}} - \frac{\tilde{\psi}^{\mathrm{s}}\kappa}{\varrho^{\mathrm{b}}} - \frac{[\![\omega]\!]}{\varrho^{\mathrm{b}}}, \tag{8.1.2}$$

where, in contrast to BCF, the jump in the grand canonical chemical potential couples the adjacent terraces, resulting in effective step-step interactions that are of a diffusive character. For small departures from local equilibrium, the TC is given by:

$$\left.\begin{aligned} 0 &= \operatorname{div}(M\nabla\mu) + F - \breve{\sigma}\mu && \text{in } \Omega_+ \cup \Omega_-, \\ M\nabla\mu^+ \cdot \mathbf{n} &= C_+(\mu^+ - \mu^{\mathrm{s}}) && \text{along } \mathcal{S}, \\ -M\nabla\mu^- \cdot \mathbf{n} &= C_-(\mu^- - \mu^{\mathrm{s}}) && \text{along } \mathcal{S}, \\ \varrho^{\mathrm{b}} V &= C_+(\mu^+ - \mu^{\mathrm{s}}) + C_-(\mu^- - \mu^{\mathrm{s}}) && \text{along } \mathcal{S}, \end{aligned}\right\} \tag{8.1.3}$$

with

$$\mu^{\mathrm{s}} = \mu^{\mathrm{b}} - \gamma\kappa + \Theta[\![\mu]\!], \tag{8.1.4}$$

where Θ is the adatom equilibrium coverage.

For a given step train, solving the dynamical system that allows the tracking of the motions of individual steps can be computationally exorbitant. Alternatively, the steps can be viewed as level sets of a smoothly evolving surface. In Chapters 5, 6 and 7, we derive continuum limits of the TC model under both surface relaxation and growth conditions. Existing continuum limits derived from the BCF model (8.1.1) typically take the form of a fourth order parabolic PDE for the surface height h. In contrast to these existing continuum limits, the ones we derive from (8.1.3) take the form of a pair of coupled PDE: one for the surface height h, the other for the surface chemical potential. To first-order in a the former PDE can be identified with the standard coarse-grained mass balance that governs the evolution of the surface, in which the dependence of the surface mobility on the underlying microscopic parameters is explicitly derived. The latter PDE generalizes the macroscopic Gibbs–Thomson relation by allowing for non-local terms that result from the coupling of adjacent terraces in the microscopic model. Throughout the final chapters, we retained higher order terms (in the step height a), and interestingly, we found that the terms that appear multiplying a measure of the ES barrier (viz. $\frac{1}{C_-} - \frac{1}{C_+}$). Hence, these higher-order terms serve as small correctors which account for effects of asymmetry in the attachment kinetics.

8.2 Open Problems

A number of mathematical problems pertaining to step-flow epitaxial crystal growth remain open. In what follows, we briefly describe what will be pursued in the immediate future.

Boundary Conditions

The boundary conditions for the continuum limits derived in Chapters 5, 6 and 7 remain to be specified. During relaxation, one must account for the development of facets due to the lack of nucleation. In the literature, this has been studied as a free-boundary problem in the context of the BCF model [42].

During growth one treats the peak as a free boundary, as well. Peaks provide a particular challenge, since one must account for nucleation of steps, which amounts to specifying the velocity of the peak as in [43].

Nanowire growth

With regards to nanowire growth, we plan to extend our analysis to more physically relevant boundary conditions. Specifically, rather than assuming that the outer boundary behaves like a reflecting wall, one may introduce boundary conditions that couple the diffusion of adatoms on the lateral side of the nanowire with the diffusion of adatoms on the upper circular side of the nanowire.

We will also consider TC version of the nanowire growth problem. This will pave the way for further comparison of the predictions for the two models, and the dependence of stability on the equilibrium adatom coverage Θ.

A Facts about Bessel functions

Here we state and prove various properties of the functions σ_k defined in (3.5.6).

A.1 The derivatives of the σ_k's

It is easy to verify the following relations of the derivatives of σ_k using standard formulae for the derivatives of I_0, I_1, K_0, and K_1:

$$\left.\begin{aligned}
\frac{\partial\sigma_1(x,y)}{\partial x} &= -\sigma_2(x,y) - \frac{\sigma_1(x,y)}{x}\\
\frac{\partial\sigma_1(x,y)}{\partial y} &= \sigma_3(x,y) - \frac{\sigma_1(x,y)}{y}\\
\frac{\partial\sigma_2(x,y)}{\partial x} &= -\sigma_1(x,y)\\
\frac{\partial\sigma_2(x,y)}{\partial y} &= \sigma_4(x,y) - \frac{\sigma_2(x,y)}{y}\\
\frac{\partial\sigma_3(x,y)}{\partial x} &= -\sigma_4(x,y) - \frac{\sigma_3(x,y)}{x}\\
\frac{\partial\sigma_3(x,y)}{\partial y} &= \sigma_1(x,y)\\
\frac{\partial\sigma_4(x,y)}{\partial x} &= -\sigma_3(x,y)\\
\frac{\partial\sigma_4(x,y)}{\partial y} &= \sigma_2(x,y).
\end{aligned}\right\} \tag{A.1.1}$$

A.2 Monotonicity and positivity of the σ_k

Recall that $\mathsf{T}(R) = \{(x,y) \in \mathbb{R} \colon 0 < x < y < R\}$

Theorem A.2.1. *For each $k = 1,2,3,4$, $\sigma_k(x,y) > 0$ for all $(x,y) \in \mathsf{T}(R)$. Moreover, for (x,y) in this triangle, $\sigma_1(x,y)$ is strictly decreasing in x and strictly increasing in y, $\sigma_2(x,y)$ is strictly decreasing in x, $\sigma_3(x,y)$ is strictly decreasing in x and increasing in y, and $\sigma_4(x,y)$ is strictly decreasing in x and strictly increasing in y.*

Proof. Since I_n and K_n are strictly positive functions on $(0, \infty)$ for any $n \geq 0$, it is clear that σ_2 and σ_3 are strictly positive on $(0, \infty) \times (0, \infty)$, let alone in $\mathsf{T}(R)$. Also, since $\sigma_1(x, x) = \sigma_4(x, x) = 0$, it suffices to show the claimed monotonicity in order to show σ_1 and σ_4 are strictly positive in $\mathsf{T}(R)$. Recall the following fact, which may be found in [44], about the Bessel functions I_n and K_n:

$$I_n'(x) = \frac{I_{n-1}(x) + I_{n+1}(x)}{2} \text{ and } K_n'(x) = (-1)^{n+1} \frac{K_{n-1}(x) + K_{n+1}(x)}{2}.$$

It follows that

$$\frac{\partial \sigma_1(x, y)}{\partial x} = -\frac{(K_0(x) + K_2(x))I_1(y) + (I_0(x) + I_2(x))K_1(y)}{2} < 0,$$
$$\frac{\partial \sigma_1(x, y)}{\partial y} = \frac{K_1(x)(I_0(y) + I_2(y)) + I_1(x)(K_0(y) + K_2(y))}{2} > 0,$$

In the previous section, we found that $\frac{\partial \sigma_4}{\partial x} = -\sigma_3$ and $\frac{\partial \sigma_4}{\partial y} = \sigma_2$, each of which are of the claimed sign in $\mathsf{T}(R)$. Thus, we have that $\sigma_k(x, y) > 0$ for all $(x, y) \in \mathsf{T}(R)$ for each $k = 1, 2, 3, 4$.

Since $\frac{\partial \sigma_2(x,y)}{\partial x} = -\sigma_1(x, y)$; $\frac{\partial \sigma_3(x,y)}{\partial x} = -\sigma_4(x, y) - \frac{\sigma_3(x,y)}{x}$; and $\frac{\partial \sigma_3(x,y)}{\partial y} = \sigma_1(x, y)$, we have that $\sigma_2(x, y)$ is strictly decreasing in x and $\sigma_3(x, y)$ is strictly decreasing in x and strictly increasing in y. □

B Facts about ordinary differential equations

Here we state and prove the existence and uniqueness theorems required for the various cases studied in the preceding. We also state and prove a theorem on the dependence of parameters.

B.1 Uniqueness and monotonicity

Theorem B.1.1 (Peano's uniqueness theorem for integral equations)**.** *Suppose $f : \mathbb{R}^2 \to \mathbb{R}$ is non-increasing in its second argument. Then the integral equation*

$$y(x) = \int_0^x f(t, y(t))\ dt$$

has at most one solution.

Corollary B.1.2. *If, for $i = 1$ and 2, $f_i\colon (0,a) \times (0,b) \to \mathbb{R}$ are two functions such that $f_i(t,y)$ are decreasing in y and such that there exists a solution, y_i, of the problems*

$$\left.\begin{array}{rcl} y' &=& f_i(t,y), \\ y(0) &=& 0, \end{array}\right\}$$

and $f_1(t,y) \leq f_2(t,y)$, then $y_1(t) \leq y_2(t)$ for all $0 < t < a$.

Proof. Suppose there exists an $\varepsilon > 0$ such that $y_1(t) > y_2(t)$ for all $0 < t < \varepsilon$. Then we may define a function $h\colon (0,\varepsilon) \times (0,b) \to \mathbb{R}$

$$h(t,y) = \begin{cases} f_1(t,y) & \text{if } y \geq y_1(t), \\ f_2(t,y) & \text{if } y < y_1(t). \end{cases}$$

For each $0 < t < \varepsilon$ and any $y < z$ either

1. $y > y_1(t)$:
$$h(t,y) = f_1(t,y) \geq f_1(t,z) = h(t,z),$$

2. $y \leq y_1(t)$ and $z \geq y_1(t)$:
$$h(t,y) = f_2(t,y) \geq f_2(t,y_1(t)) \geq f_1(t,y_1(t)) \geq f_1(t,z) = h(t,z), \text{ or}$$

3. $z < y_1(t)$:
$$h(t,y) = f_2(t,y) \geq f_2(t,z) = h(t,z).$$

Hence $h(t,y)$ is also decreasing in y. This implies that the problem

$$\left.\begin{aligned} y' &= h(t,y), \\ y(0) &= 0, \end{aligned}\right\}$$

has at most one solution. However, y_1 and y_2 are solutions. Thus, it cannot be the case that there exists an $\varepsilon > 0$ such that $y_1(t) > y_2(t)$ for all $t \in (0,\varepsilon)$.

Hence, for every $\varepsilon > 0$ there exists a time $0 < T < \varepsilon$ such that $y_1(T) \leq y_2(T)$. It suffices to show that if $y_1(T) \leq y_2(T)$, then $y_1(t) \leq y_2(t)$ for all $t \geq T$. Suppose not, then, by the continuity of y_1 and y_2, there exists a time $S \geq T$ such that $y_1(t) \leq y_2(t)$ for all $T \leq t \leq S$, and such that $y_1(t) > y_2(t)$ for $S < t < S + \varepsilon$. In particular, $y_1(S) = y_2(S)$. We may apply the previous argument to the IVP $y' = h(t,y)$ and $y(S) = y_1(S)$ to derive our contradiction. Therefore, $y_1(t) \leq y_2(t)$ for all $t \in (\varepsilon, a)$ for any $\varepsilon > 0$. Thus $y_1(t) \leq y_2(t)$ for all $t \in (0,a)$. □

B.2 Existence and terminal value problems

Consider the problems

$$\left.\begin{aligned} \dot{x} &= f(x), \\ x(0) &= x_0, \end{aligned}\right\} \tag{B.2.1}$$

where $f \in C^1(\mathsf{T})$ and T is an open, simply connected subset of $\mathbb{R}^2$, and $f(x) \neq 0$ for all $x \in \mathsf{T}$. We show that for such systems, solutions $x(t)$ with maximal interval of existence (α, β) have the property that for any compact subset F of T there exists a time $t > 0$ such that $x(t) \in \mathsf{T} - F$.

As such we state two theorems relevant to our situation as found in Perko's book on differential equations [45].

Theorem B.2.1 (The Poincaré-Bendixson Theorem)**.** *Suppose that $f \in C^1(\mathsf{T})$ where T is an open subset of $\mathbb{R}^2$ and that (B.2.1) has a trajectory Γ with Γ^+ contained in a compact subset K of T. Then if $\omega(\Gamma)$ contains no critical point of (B.2.1), $\omega(\Gamma)$ is a periodic orbit of (B.2.1).*

Since our system has no critical points, the Poincaré-Bendixson Theorem implies that if a trajectory Γ has the property that its future Γ^+ is contained in a compact subset K of T, then $\omega(\Gamma)$ is a periodic orbit. If Γ^+ is a subset of a compact set K, then the ω-limit set $\omega(\Gamma)$ is also a subset of K.

The theorem that disallows the existence of a periodic orbit follows from index theory.

Theorem B.2.2. *Suppose that $f \in C^1(\mathsf{T})$ where T is an open subset of $\mathbb{R}^2$ which contains a periodic orbit Γ of (B.2.1) as well as its interior U. Then U contains at least one critical point of (B.2.1).*

Since our set T is simply connected, it follows immediately from these theorems B.2.1 and B.2.2 that for any compact subset K of T and any solution $x(t)$ to (B.2.1) there exists a time $t > 0$ such that $x(t) \in \mathsf{T} - F$.

Corollary B.2.3 (Non-vanishing RHS lead to solutions exiting compact sets)**.** *Suppose that $f \in C^1(\mathsf{T})$ where T is an open, simply connected subset of $\mathbb{R}^2$ and that $f(x) \neq 0$ for any $x \in \mathsf{T}$. Then any trajectory Γ of the IVP (B.2.1) has the property* *that for any compact subset K of T the intersection $\Gamma^+ \cap (\mathsf{T} - K)$ is non-empty. In particular, given any compact subset K of T and a solution $x(t)$ to (B.2.1) with maximal interval of existence (α, β), there exists a sequence $\{t_n\}$ such that $t_n \to \beta$ and $x(t_n) \in \mathsf{T} - K$ as $n \to \infty$.*

An immediate consequence to this result is that if we assume further that T is bounded, then for a solution $x(t)$ to (B.2.1) with maximal interval of existence (α, β), there exists at least one point X on the boundary of T and a sequence of times $\{t_n\}$ such that $t_n \to \beta$ and $x(t_n) \to X$ as $n \to \infty$. If we further assume that $f \cdot \mathbf{e}_i \leq 0$ for all $i = 1, 2, \ldots, n$, then solutions exit the domain T at the final time β.

Theorem B.2.4 (Functions that exit compact sets of a bounded domain and are monotone in their coordinates exit the domain)**.** *Let T be a bounded open subset of $\mathbb{R}^n$. Suppose $x\colon (\alpha, \beta) \to \mathsf{T}$ is a differentiable function, $x(t) = (x_1(t), x_2(t), \ldots, x_n(t))$, with the properties that*

- *for any compact subset K of T and $\varepsilon > 0$, there exists a sequence t_k such that $t_k \to \beta$ and $x(t_k) \in \mathsf{T} - K$ as $k \to \infty$,*
- *x_i is monotone for each $i = 1, 2, \ldots, n$.*

Then the limit $\lim_{t \to \beta} x(t) = X$ exists with X an element of the boundary of T.

Proof. We prove this assuming $\beta < \infty$, since the case $\beta = \infty$ is similar. Define the compact subsets K_m of T as

$$K_m = \left\{ x \in \mathsf{T}\colon \inf_{y \in \partial \mathsf{T}} \{|x - y|\} \geq \frac{1}{m} \right\}.$$

Then choose recursively t_m by the following rules:

1. Choose $t_1 \in (\alpha, \beta)$ such that $x(t_1) \in \mathsf{T} - K_1$, and
2. for $m > 1$, choose $t_m \in \left(\beta - \frac{1}{m}, \beta\right) \cap (\alpha, \beta)$ such that $x(t_m) \in \mathsf{T} - K_m$.

Since $\{x(t_m)\}$ is an infinite set of points contained in the closure of T, denoted by $\overline{\mathsf{T}}$, and $\overline{\mathsf{T}}$ is compact, there exists a limit point $X \in \overline{\mathsf{T}}$ such that for a subsequence $\{t_{m_k}\}$, we have that $x(t_{m_k}) \to X$ as $k \to \infty$. It suffices then to show that $X \in \partial\mathsf{T}$, but this is obvious since there does not exist an $\varepsilon > 0$ such that $\inf_{y\in\partial\mathsf{T}}\{|X - y|\} > \varepsilon$, and so $X \notin \mathsf{T}$. Since each x_i is a monotone function, it follows easily that $x_i(t) \to X_i$ as $t \to \beta$, where $X = (X_1, X_2, \ldots, X_n)$. □

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