Verification of the influence of surface energies on the effective mobility

Research Thesis

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Abstract

The coupled motion of grain boundaries and exterior surfaces, which join along “groove roots,” is a common phenomenon which occurs to some degree in all finite poly-crystalline specimens and can be critical in determining the microstructure of the resultant material. A commonly used geometry in studying this coupled effect is the “half loop” geometry.

The “half loop” geometry consists of a U-shaped, half-loop grain extending entirely through the thickness of an otherwise single crystal. The two grains are of the same material and differ only in their relative crystalline orientation. The interface between the two grains, called grain boundary, contacts the exterior surface at a “groove root” where various balance laws hold.

This geometry, in which one grain grows at the expense of the other, contains two types of motion; one is motion by mean curvature of the grain boundary, and the other is motion by surface diffusion of the exterior surfaces. These motions can be modeled by a three-dimensional system of time-dependent, non-linear partial differential equations.

There is a parameter m, defined as the ratio of the free energy of the grain boundary to the free energy of the exterior surface, which is influential in the determining boundary conditions, and $m > 0$ causes the appearance of “thermal grooving” at the intersection of the grain boundary with the exterior surface. Although, theoretically the parameter m may vary between 0 and 2, typically, for example in metals, $0 < m < 1/3$, and hence m can be taken to be a small positive parameter.

Therefore, appealing to asymptotic analysis, one may seek asymptotic solutions to the non-linear problem described above, based on the parameter m or some power of m. It is known that when $m = 0$, the “thermal groove” vanishes and the grain boundary velocity is directly proportional to the grain boundary curvature. In this case the problem possess “traveling wave” solutions, namely the U-shaped grain moves parallel to itself (in the horizontal direction), with constant speed.

In this thesis we investigate the behavior of the first order perturbation terms of the solution to the problem with $m = 0$. Employing an arc-length parametrization of the “thermal groove” and asymptotic expansions in $m^{2/3}$ we obtain a system of three linear partial differential equations for the perturbation terms, for the non-linear problem described above. The equation obtained from moving by mean curvature, leads to the conclusion that the grain boundary profiles are parabolic. ...(TO ADD MORE RESULTS AND CONCLUSIONS...)

List of Symbols

Δ_s Laplace-Beltrami operator, known also as surface Laplacian

∇_s Surface gradient

$<,>$ Scalar product

X^j Surface j, $j = \mathrm{I}, \mathrm{II}, \mathrm{III}$

τ^j Tangential unit vector of the surface X^j, $j = \mathrm{I}, \mathrm{II}, \mathrm{III}$, pointing away from it

γ^j Surface free energy of the surface X^j, $j = \mathrm{I}, \mathrm{II}, \mathrm{III}$

m The ratio of the exterior surface energy to the surface energy of grain boundary

$\mathbf{V}$ The normal velocity

μ Chemical potential

Chapter 1 Introduction

In this chapter we shall discuss the following issues

1. To introduce the problem and to express it using some parametrization

2. To explain that m is a small parameter (or to add it in a separate section with the framework of basic assumptions, or to add the discussion about m in the first section)

3. To explain the physical background for the mean curvature equation, and to mention that $A > 0$

4. To explain the physical background for the surface diffusion equation

5. The physical background to BC

6. To obtain the formula for κ using differential geometry

7. To obtain Δ_s, using differential geometry

8. To obtain a traveling wave solution to 2D problem

9. To conclude from (7) that there is no difference how to re-scale our problem (using Q or R)

1.1 Physical Introduction

The “half loop geometry” was first introduced by Shvindlerman, et al. [10]

A **grain boundary** is the interface between two grains in a polycrystalline material. Grain boundaries disrupt the motion of dislocations through a material, so reducing crystallite size is a common way to improve strength, as described by the Hall-Petch relationship. Since grain boundaries are defects in the crystal structure they tend to decrease the electrical and thermal conductivity of the material. The high interfacial energy and relatively weak bonding in most grain boundaries often makes them preferred sites for the onset of corrosion and for the precipitation of new phases from the solid. They are also important to many of the mechanisms of creep.

Crystallinity refers to the degree of structural order in a solid. In a crystal, the atoms or molecules are arranged in a regular, periodic manner. The degree of crystallinity has a big influence on hardness, density, transparency and diffusion. In a gas, the relative positions of the atoms or molecules are completely random. Amorphous materials, such as liquids and glasses, represent an intermediate case, having order over short distances (a few atomic or molecular spacings) but not over longer distances.

Many materials (such as glass-ceramics and some polymers), can be prepared in such a way as to produce a mixture of crystalline and amorphous regions. In such cases, crystallinity is usually specified as a percentage of the volume of the material that is crystalline. Even within materials that are completely crystalline, however, the degree of structural perfection can vary. For instance, most metallic alloys are crystalline, but they usually comprise many independent crystalline regions (grains or crystallites) in various orientations separated by grain boundaries; furthermore, they contain other defects (notably dislocations) that reduce the degree of structural perfection. The most highly perfect crystals are silicon boules produced for semiconductor electronics; these are large single crystals (so they have no grain boundaries), are nearly free of dislocations, and have precisely controlled concentrations of defect atoms.

Crystallinity can be measured using x-ray diffraction, but calorimetric techniques are also commonly used.

Retrieved from ”http://en.wikipedia.org/wiki/Crystallinity”

Surface diffusion is a general process involving the motion of adatoms, molecules, and atomic clusters (adparticles) at solid material surfaces [5]. The process can generally be thought of in terms of particles jumping between adjacent adsorption sites on a surface.

1.2 The Problem

In this thesis, we analyze the coupled motion of a grain boundary which is attached at a "groove root," known also as a "thermal groove," to an exterior surface which evolves under the influence of surface diffusion in a "half loop" geometry, see fig. 1.1. In the "half loop" geometry, two crystalline grains evolve in shape which began initially as parallel components in a single block of material. The two grains comprising the bi-crystal are identical, except for their relative crystalline orientation. This discrepancy manifests itself as a grain boundary which moves in order to reduce the surface energy and to relieve the orientation mismatch. Since both grains are of the same material, no bulk energetic effects need to be taken into account. Neglecting possible effects of elasticity, anisotropy, and defects, the net driving force arises from minimization of the surface energies along the exterior and interior surface. For comparisons of experiments and simulations made in the geometry shown in fig. 1.1, see [1].

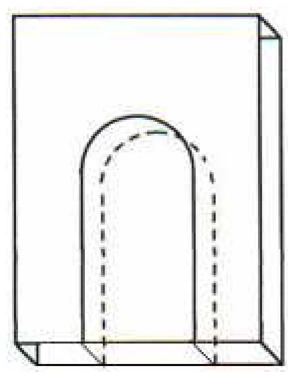

Figure 1.1: Capillarity driven grain boundary migration in a half loop geometry.

We assume that the grain boundary evolves according to motion by mean curvature,

$$\mathbf{V} = A\kappa, \tag{1.2.1}$$

where $\mathbf{V}$ denotes the normal velocity of the surface and κ denotes its mean curvature. Away from the "groove root," the exterior surface motion is given by surface diffusion

$$\mathbf{V} = -B\Delta_s\kappa, \tag{1.2.2}$$

where Δ_s is the Laplace-Beltrami operator. At the groove root the boundary conditions are given by the "persistence condition" which states that the grain boundary and the exterior surface remain attached, the Young's law, continuity of the surface chemical potentials, and the balance of mass flux. Young's law can be written as

$$\tau^{\mathrm{I}} + \tau^{\mathrm{II}} + m\tau^{\mathrm{III}} = 0, \tag{1.2.3}$$

where $m = \frac{\gamma_{\text{grain boundary}}}{\gamma_{\text{exterior surface}}}$ denotes the ratio between surface energies of grain boundary and exterior surface, $\tau^j, j = \mathrm{I}, \mathrm{II}, \mathrm{III}$ is the unit tangential vector of the surface $X^j,\ j = \mathrm{I}, \mathrm{II}, \mathrm{III}$, respectively, normal to the "groove root" and pointing away from it (see fig. 1.2). Continuity of the surface chemical potentials and the balance of mass flux can be written as

$$\kappa^{\mathrm{I}} = \kappa^{\mathrm{II}}, \tag{1.2.4}$$

and

$$< \tau^{\mathrm{I}}, \nabla_s \kappa^{\mathrm{I}} > + < \tau^{\mathrm{II}}, \nabla_s \kappa^{\mathrm{II}} >= 0, \tag{1.2.5}$$

where ∇_s denotes the surface gradient, $^{\mathrm{I}}$ and $^{\mathrm{II}}$ denote that we are on the surface to the right or to the left from the "groove root," respectively.

The purpose of this section is to introduce a parametric representation of all variables appearing in the equations (1.2.1) and (1.2.2), and in the boundary conditions (1.2.3)– (1.2.5). So, let $X(\alpha, \beta, t) = (x(\alpha, \beta, t), y(\alpha, \beta, t), z(\alpha, \beta, t))$ be a parametric representation of a 2D surface in 3D. Then its mean curvature can be expressed as

$$\kappa = \frac{< X_\alpha, X_\alpha > X_{\beta\beta} - 2 < X_\alpha, X_\beta > X_{\alpha\beta} + < X_\beta, X_\beta > X_{\alpha\alpha}}{2 < X_\alpha, X_\alpha >< X_\beta, X_\beta > -2 < X_\alpha, X_\beta >^2} \cdot \vec{n}, \tag{1.2.6}$$

where $\vec{n}$ denotes the unit normal which may be expressed as

$$\vec{n} = \frac{X_\alpha \times X_\beta}{\|X_\alpha \times X_\beta\|}. \tag{1.2.7}$$

Moreover, we shall make use of the following formula, which is easy to check (see ADD REF...),

$$||X_\alpha \times X_\beta|| = \sqrt{||X_\alpha||^2 ||X_\beta||^2 - < X_\alpha, X_\beta >^2}, \tag{1.2.8}$$

which holds for any smooth surface X parameterized by α, β.

Let us recall that the surface Laplacian operator may be defined as

$$\Delta_s = \nabla_s \cdot\ \nabla_s \quad \text{where } \nabla_s = \nabla - n\partial_n. \tag{1.2.9}$$

The tangential gradient ∇_s applied to the function κ defined on the parametric surface $X = (x(\alpha, \beta, t), y(\alpha, \beta, t), z(\alpha, \beta, t))$ can be expressed as

$$\nabla_s \kappa = \frac{< X_\beta, X_\beta > \kappa_\alpha X_\alpha - < X_\alpha, X_\beta > \kappa_\beta X_\alpha - < X_\alpha, X_\beta > \kappa_\alpha X_\beta + < X_\alpha, X_\alpha > \kappa_\beta X_\beta}{< X_\alpha, X_\alpha >< X_\beta, X_\beta > - < X_\alpha, X_\beta >^2}. \tag{1.2.10}$$

The surface Laplacian operator acting on κ is then given by

$$\Delta_s \kappa = \frac{1}{\sqrt{g}} \left[\frac{\partial}{\partial \alpha} \left(\frac{< X_\beta, X_\beta > \kappa_\alpha - < X_\alpha, X_\beta > \kappa_\beta}{\sqrt{g}} \right) + \frac{\partial}{\partial \beta} \left(\frac{< X_\alpha, X_\alpha > \kappa_\beta - < X_\alpha, X_\beta > \kappa_\alpha}{\sqrt{g}} \right) \right], \tag{1.2.11}$$

where g is defined by

$$g = < X_\alpha, X_\alpha >< X_\beta, X_\beta > - < X_\alpha, X_\beta >^2 .$$

Finally, the normal velocity $\mathbf{V}$ of the parametric surface X is

$$\mathbf{V} = X_t \vec{n}, \tag{1.2.12}$$

and the unit tangent τ to the surface X can be given by

$$\tau = . \tag{1.2.13}$$

1.2.1 An Explanation of how to get the formula (1.2.6) for mean curvature

Let $U = (\alpha, \beta) \subset \mathbb{R}^2$ be a bounded domain, $\mathbf{r} : U \to \mathbb{R}^3$ a smooth mapping, more precisely $x(\alpha,\beta), y(\alpha,\beta), z(\alpha,\beta) \in C^2$; such that $X = (x(\alpha,\beta), y(\alpha,\beta), z(\alpha,\beta))$ represents a *regular* surface in 3D (i.e., a surface such that at each point there exists a unique tangent plane to the surface). Suppose that $a = (\alpha, \beta) \in U$, and let the point A correspond to the image of a on the surface X. We define the *tangent plane* $T_a U$ as the set of all velocity vectors of curves on U passing through a, and similarly we define the *tangent plane* $T_A X$ as the set of all velocity vectors on the surface X passing through A.

The linear transformation

$$d\mathbf{r}_a : T_a U \to T_A X$$

is called a *differential* if for every velocity vector $\mathbf{P}$ corresponding to the curve $\gamma : (-\epsilon, \epsilon) \to U$ such that $\gamma(0) = a$,

$$\mathbf{P} = \frac{d\gamma}{d\sigma}\Big|_{\sigma=0} = (\frac{d\alpha}{d\sigma}, \frac{d\beta}{d\sigma})\Big|_{\sigma=0} = (v_1, v_2),$$
$$\mathbf{Q} = d\mathbf{r}_a(\mathbf{P}) = v_1 \frac{\partial X}{\partial \alpha} + v_2 \frac{\partial X}{\partial \beta}.$$

The *first fundamental form*

$$I_a : T_a U \times T_a U \to \mathbb{R}$$

is defined as the bilinear form

$$I_a(\mathbf{P}_1, \mathbf{P}_2) = < d\mathbf{r}_a(\mathbf{P}_1), d\mathbf{r}_a(\mathbf{P}_2) >, \quad \mathbf{P}_1, \mathbf{P}_2 \in T_a U. \tag{1.2.14}$$

If $\mathbf{P}_1 = (v_1, v_2)$ and $\mathbf{P}_2 = (w_1, w_2)$, then by the definition of the differential

$$d\mathbf{r}_a(\mathbf{P}_1) = v_1 \frac{\partial X}{\partial \alpha} + v_2 \frac{\partial X}{\partial \beta},$$
$$d\mathbf{r}_a(\mathbf{P}_2) = w_1 \frac{\partial X}{\partial \alpha} + w_2 \frac{\partial X}{\partial \beta}.$$

Hence,

$$I_a(\mathbf{P}_1,\mathbf{P}_2) =< v_1\frac{\partial X}{\partial\alpha} + v_2\frac{\partial X}{\partial\beta}, w_1\frac{\partial X}{\partial\alpha} + w_2\frac{\partial X}{\partial\beta} >= \sum_{i,j=1}^{2} v_i w_j < \mathbf{r}_i, \mathbf{r}_j >, \tag{1.2.15}$$

where

$$\mathbf{r}_1 = \frac{\partial X}{\partial\alpha}, \quad \mathbf{r}_2 = \frac{\partial X}{\partial\beta}. \tag{1.2.16}$$

Let

$$g_{ij} =< \mathbf{r}_i, \mathbf{r}_j >,$$

then we obtain from (1.2.15) that

$$I_a(\mathbf{P}_1,\mathbf{P}_2) = \sum_{i,j=1}^{2} v_i w_j g_{ij}, \quad \mathbf{P}_1,\mathbf{P}_2 \in T_aU. \tag{1.2.17}$$

Thus, we obtained that the first fundamental form I_a can be defined via the matrix of functions

$$\begin{pmatrix} g_{11} & g_{12} \\ g_{12} & g_{22} \end{pmatrix}, \tag{1.2.18}$$

which, as it is proved in [6], is symmetric and positive. It is known as the *Riemannian metric*.

Suppose now, that our surface is oriented, i.e., a continuously defined unit normal field has been defined on it. The *second fundamental form*

$$II_a : T_aU \times T_aU \to \mathbb{R}, \quad \mathbf{r}(a) = A$$

is defined as the bilinear form

$$II_a(\mathbf{P},\mathbf{Q}) = - < d\mathbf{r}_a(\mathbf{P}), d\mathbf{n}_a(\mathbf{Q}) >, \quad \mathbf{P},\mathbf{Q} \in T_aU, \tag{1.2.19}$$

where $\mathbf{n}(\alpha,\beta)$ denotes the unit normal which has been defined on the surface $X(\alpha,\beta)$. More precisely, if

$$\mathbf{P} = (v_1, v_2), \quad \mathbf{Q} = (w_1, w_2)$$

then

$$d\mathbf{r}_a(\mathbf{P}) = v_1\frac{\partial X}{\partial\alpha} + v_2\frac{\partial X}{\partial\beta},$$
$$d\mathbf{n}_a(\mathbf{Q}) = w_1\frac{\partial \mathbf{n}}{\partial\alpha} + w_2\frac{\partial \mathbf{n}}{\partial\beta}.$$

Hence, we get that the second fundamental form can be expressed as

$$II_a(\mathbf{P},\mathbf{Q}) = - \sum_{i,j=1}^{2} v_i w_j < \mathbf{r}_i, \mathbf{n}_j >, \tag{1.2.20}$$

where

$$\mathbf{n}_1 = \frac{\partial \mathbf{n}}{\partial \alpha}, \quad \mathbf{n}_2 = \frac{\partial \mathbf{n}}{\partial \beta},$$

and $\mathbf{r}_i$, $i = 1, 2$ are as defined in (1.2.16). Setting

$$b_{ij} := - < \mathbf{r}_i, \mathbf{n}_j >,$$

we can write the second fundamental form as

$$II_a(\mathbf{P}, \mathbf{Q}) = \sum_{i,j=1}^{2} v_i w_j b_{ij}. \tag{1.2.21}$$

By using the fact (see e.g., [6]) that

$$b_{ij} = - < \mathbf{r}_i, \mathbf{n}_j > = < \mathbf{r}_{ij}, \mathbf{n} >, \tag{1.2.22}$$

it is easy to prove that the second fundamental form is symmetric. Hence, the second fundamental form is defined by the symmetric matrix,

$$\begin{pmatrix} b_{11} & b_{12} \\ b_{12} & b_{22} \end{pmatrix}. \tag{1.2.23}$$

Let $\rho(s) = (\alpha(s), \beta(s))$ denote a smooth curve on the surface $X \subset \mathbb{R}^3$, and suppose that s is an arc-length parametrization. For any fixed point $s = s_0 \in U$, we shall now calculate the curvature of $\rho(s)$ at $s = s_0$ using the first and second fundamental forms.

In accordance with our previous discussion, $\mathbf{n}$ shall denote the unit normal vector to the surface X at the point $A = \rho(s_0)$, and, we shall denote by $\mathbf{n}_\theta$ the *principal normal* of the curve $\rho(s)$ at the point A. Here $\theta \in [0, \pi]$ is the angle between $\mathbf{n}$ and $\mathbf{n}_\theta$. It now follows from the Frénet formula (see ...) that

$$\rho'' = \kappa_\theta \mathbf{n}_\theta, \tag{1.2.24}$$

where $\kappa_\theta \geq 0$ is the curvature of the curve at the point A. Hence,

$$< \rho'', \mathbf{n} > = \kappa_\theta < \mathbf{n}_\theta, \mathbf{n} > = \kappa_\theta \cos\theta.$$

More explicitly,

$$\begin{aligned} \rho' &= \mathbf{r}_1 \alpha' + \mathbf{r}_2 \beta' \\ \rho'' &= \mathbf{r}_1 \alpha'' + \mathbf{r}_2 \beta'' + \mathbf{r}_{11} \alpha'^2 + 2\mathbf{r}_{12} \alpha' \beta' + \mathbf{r}_{22} \beta'^2, \end{aligned}$$

and $< \mathbf{r}_i, \mathbf{n} > = 0$. Hence, taking the scalar product of ρ'' with $\mathbf{n}$, and then using (1.2.22), we get that

$$\kappa_\theta \cos\theta = < \rho'', \mathbf{n} > = b_{11} \alpha'^2 + 2 b_{12} \alpha' \beta' + b_{22} \beta'^2.$$

Using the definition of the second fundamental form, we see that

$$\kappa_\theta \cos\theta = II_a(\mathbf{P}, \mathbf{P}), \tag{1.2.25}$$

where $\mathbf{P} = (\alpha', \beta')$, and $\rho'(s) = d\mathbf{r}_a(\mathbf{P})$ is the tangent vector to the curve $\rho(s)$ at the point $A = \rho(s_0)$. We emphasize that since s has been taken to denote an arc-length parametrization of the curve ρ,

$$I_a(\mathbf{P}, \mathbf{P}) = 1.$$

The formula (1.2.25) can be readily generalized. Let C denote an arbitrary smooth curve on the surface X passing through a given point A. Then the following formula holds

$$\kappa_\theta \cos\theta = \frac{II_a(\mathbf{Q}, \mathbf{Q})}{I_a(\mathbf{Q}, \mathbf{Q})}, \tag{1.2.26}$$

where $\mathbf{P} = d\mathbf{r}_a(\mathbf{Q})$, the differential of the vector $\mathbf{Q} \in T_aU$, is tangential to the curve C at A.

Now, let $\mathbf{P}$ be a unit tangent to the surface X at point A, and denote by $\mathbf{n}$ the normal to the surface at A. Let $\mathbf{n}_\theta$ be a vector orthogonal to $\mathbf{P}$, such that the planar angle, in the plane orthogonal to $\mathbf{P}$, between $\mathbf{n}_\theta$ and $\mathbf{n}$ is θ where $\theta \in (-\pi/2, \pi/2)$. Let P_θ denote the plane spanned by the vectors $\mathbf{P}$ and $\mathbf{n}_\theta$. The intersection $P_\theta \cap X$ is a planar curve, which is referred to as *transection* of the surface X. Its curvature κ_θ is a real (positive or negative) number, which satisfies the formula (1.2.26).

When $\theta = 0$, the transection is called a *normal transection.* From (1.2.26) we can easily see that the curvature of the normal transection defined by $\mathbf{P} = d\mathbf{r}_a(\mathbf{Q})$, is given by

$$\kappa_{\mathbf{P}} = \frac{II_a(\mathbf{Q}, \mathbf{Q})}{I_a(\mathbf{Q}, \mathbf{Q})} = -\frac{< W_A(\mathbf{P}), \mathbf{P} >}{< \mathbf{P}, \mathbf{P} >}, \tag{1.2.27}$$

where $W_A(\mathbf{P})$ is the *Weingarten transformation*

$$W_A : T_AX \to T_AX$$

which for $\mathbf{P} = \mathbf{r}_1 v_1 + \mathbf{r}_2 v_2 \in T_AX$ satisfies

$$W_A(\mathbf{P}) = \mathbf{n}_1 v_1 + \mathbf{n}_2 v_2. \tag{1.2.28}$$

From the symmetry of the second fundamental form, we find that

$$< W_A(\mathbf{P}), \mathbf{Q} >=< \mathbf{P}, W_A(\mathbf{Q}) > .$$

Hence, it follows that the Weingarten transformation is self-adjacent. We shall now prove the following result:

Theorem 1.2.1. *There exist two orthogonal directions*

$$\mathbf{P}_1, \mathbf{P}_2 \in T_A X, \quad \mathbf{P}_1 \perp \mathbf{P}_2, \quad ||\mathbf{P}_1|| = ||\mathbf{P}_2|| = 1$$

known as the principal directions, such that the function $\kappa_{\mathbf{P}}$*, as a function of the unit vector* $\mathbf{P} \in T_A X$*, assumes its minimum at* $\mathbf{P} = \mathbf{P}_1$ *and its maximum at* $\mathbf{P} = \mathbf{P}_2$*. If* $\mathbf{P} \in T_A X$ *is any tangent vector which generates an angle* γ *with the principal direction* $\mathbf{P}_1$*, then*

$$\kappa_{\mathbf{P}} = \kappa_{\mathbf{P}_1} \cos^2 \gamma + \kappa_{\mathbf{P}_2} \sin^2 \gamma. \tag{1.2.29}$$

Proof. Since the Weingarten transformation W_A is linear and self-adjacent, there exists an orthonormal basis of eigenvectors for the operator W_A such that

$$W_A(\mathbf{P}_1) = \lambda_1 \mathbf{P}_1, \quad W_A(\mathbf{P}_2) = \lambda_2 \mathbf{P}_2, \quad < \mathbf{P}_i, \mathbf{P}_j >= \delta_{ij}.$$

Moreover, any unit vector $\mathbf{P}$ can be written as

$$\mathbf{P} = \mathbf{P}_1 \cos \gamma + \mathbf{P}_2 \sin \gamma,$$

where $\gamma \in [0, 2\pi]$. After acting W_A on $\mathbf{P}$, one obtains that

$$W_A(\mathbf{P}) = W_A(\mathbf{P}_1) \cos \gamma + W_A(\mathbf{P}_2) \sin \gamma = \lambda_1 \mathbf{P}_1 \cos \gamma + \lambda_2 \mathbf{P}_2 \sin \gamma,$$

and a simple calculation yields that

$$< W_A(\mathbf{P}), (\mathbf{P}) >= \lambda_1 \cos^2 \gamma + \lambda_2 \sin^2 \gamma,$$

which, using (1.2.27), implies that

$$\kappa_{\mathbf{P}} = -\lambda_1 \cos^2 \gamma - \lambda_2 \sin^2 \gamma.$$

Finally, we get that for $\gamma = 0$

$$\kappa_{\mathbf{P}_1} = -\lambda_1,$$

and for $\gamma = \pi/2$

$$\kappa_{\mathbf{P}_2} = -\lambda_2.$$

Thus,

$$\kappa_{\mathbf{P}} = \kappa_{\mathbf{P}_1} \cos^2 \gamma + \kappa_{\mathbf{P}_2} \sin^2 \gamma.$$

□

The curvatures of the normal transections, $\kappa_{\mathbf{P}_1}$ and $\kappa_{\mathbf{P}_2}$, are known as the *principal curvatures*. The *mean curvature* of surface X at the point A is defined as the arithmetic average of the principal curvatures, namely

$$K = \frac{1}{2}(\kappa_{\mathbf{P}_1} + \kappa_{\mathbf{P}_2}). \tag{1.2.30}$$

In order to obtain a formula for principal curvatures, we recall that the principal directions $\mathbf{P} \in T_A X$ are the eigenvectors of the Weingarten transformation, namely

$$W_A(\mathbf{P}) = -\kappa_{\mathbf{P}}\mathbf{P}, \quad \mathbf{P} \neq 0.$$

Setting $\mathbf{P} = \mathbf{r}_1 v_1 + \mathbf{r}_2 v_2$ and $W_A(\mathbf{P}) = \mathbf{n}_1 v_1 + \mathbf{n}_2 v_2$, we get that

$$\mathbf{n}_1 v_1 + \mathbf{n}_2 v_2 = -\kappa(\mathbf{r}_1 v_1 + \mathbf{r}_2 v_2), \quad \kappa = \kappa_{\mathbf{P}}.$$

After scalar multiplication of the last equality by $\mathbf{r}_1$ and $\mathbf{r}_2$ respectively, one obtains the system

$$\begin{cases} < \mathbf{n}_1, \mathbf{r}_1 > v_1 + < \mathbf{n}_2, \mathbf{r}_1 > v_2 = -\kappa < \mathbf{r}_1, \mathbf{r}_1 > v_1 - \kappa < \mathbf{r}_2, \mathbf{r}_1 > v_2, \\ < \mathbf{n}_1, \mathbf{r}_2 > v_1 + < \mathbf{n}_2, \mathbf{r}_2 > v_2 = -\kappa < \mathbf{r}_1, \mathbf{r}_2 > v_1 - \kappa < \mathbf{r}_2, \mathbf{r}_2 > v_2, \end{cases}$$

which may be expressed in terms of the coefficients of second fundamental form

$$\begin{cases} b_{11} v_1 + b_{12} v_2 = -\kappa g_{11} v_1 - \kappa g_{12} v_2, \\ b_{21} v_1 + b_{22} v_2 = -\kappa g_{21} v_1 - \kappa g_{22} v_2. \end{cases}$$

So, κ is a principal curvature, if and only if the linear system

$$\sum_{j=1}^{2} (b_{ij} - \kappa g_{ij}) v_j = 0, \quad i = 1, 2$$

has a nontrivial solution, or in other words if and only if

$$\det \begin{pmatrix} b_{11} - \kappa g_{11} & b_{12} - \kappa g_{12} \\ b_{12} - \kappa g_{12} & b_{22} - \kappa g_{22} \end{pmatrix} = 0.$$

This leads to a quadratic equation for κ

$$g\kappa^2 - (g_{11} b_{22} + g_{22} b_{11} - 2 b_{12} g_{12})\kappa + b = 0, \tag{1.2.31}$$

where g and b are the determinants of the first and second fundamental forms, respectively. The roots of (1.2.31) are the principal curvatures. Finally, according to Vietta's formula for the sum of the roots of a quadratic polynomial, and from the definition of mean curvature (1.2.30), we readily obtain that the mean curvature is given by

$$K = \frac{g_{11} b_{22} + g_{22} b_{11} - 2 b_{12} g_{12}}{2g},$$

which corresponds precisely to formula (1.2.6).

1.3 Traveling wave solutions

Suppose that $\Gamma = (x, r(x,t))$, is a smooth curve (at least in C^2) in the xy-plane, which normally intersects the x-axis at some $x = \hat{x}$, where $\hat{x}$ may depend on time, and which is symmetric with respect to the x-axis. Then, at $x = \hat{x}$

$$r(\hat{x}, t) = 0, \tag{1.3.1a}$$

and

$$r_x(\hat{x}, t) = \infty. \tag{1.3.1b}$$

If we impose, in addition, that as $x \to \infty$, Γ approaches some prescribed real positive value Q, AS ARCADY DID, then we obtain a third boundary condition, namely,

$$r(\infty, t) = Q. \tag{1.3.1c}$$

Now, let us denote by s the arc-length parametrization of Γ, $\Gamma(s) = (x(s), r(x(s), t))$, such that $s = 0$ at $x = \hat{x}$, and let us assume that $\Gamma(s)$ evolves according to motion by mean curvature, namely

$$\mathbf{V} = AK. \tag{1.3.2}$$

See Section 1.2 for a detailed explanation.

In order to solve the equation (1.3.2) together with the boundary conditions (1.3.1) (or, in other words, in order to find $\Gamma(s) = (x(s), r(x(s), t))$ which satisfies (1.3.1) and (1.3.2)), we shall write the equation (1.3.2) using our parametrization. First, let τ be the unit tangent vector to Γ,

$$\tau = \frac{(1, r_x)}{\sqrt{1 + r_x^2}},$$

then, the unit normal $\mathbf{n}$ to Γ can be expressed as

$$\mathbf{n} = \frac{(r_x, -1)}{\sqrt{1 + r_x^2}}. \tag{1.3.3}$$

Therefore, the normal velocity $\mathbf{V}$ which appears on the left hand side of (1.3.2), can be expressed as

$$\mathbf{V} = \frac{< (0, r_t), (r_x, -1) >}{\sqrt{1 + r_x^2}} = \frac{-r_t}{\sqrt{1 + r_x^2}}. \tag{1.3.4}$$

As to the right hand side of (1.3.2), the mean curvature of $\Gamma(s)$, where s is the arc-length parametrization of Γ, can be expressed by

$$K = \frac{< (x_{ss}, r_{xx} x_s^2 + r_x x_{ss}), (r_x, -1) >}{\sqrt{1 + r_x^2}} = \frac{r_x x_{ss} - r_{xx} x_s^2 - r_x x_{ss}}{\sqrt{1 + r_x^2}} = -\frac{r_{xx} x_s^2}{\sqrt{1 + r_x^2}}. \tag{1.3.5}$$

Now, since s is the arc-length parametrization of Γ, namely

$$s = \int_{\hat{x}}^{x} \sqrt{1 + r_x^2(\tilde{x}, t)} d\tilde{x},$$

we get that

$$s_x = \sqrt{1 + r_x^2(x,t)}.$$

Therefore

$$x_s = \frac{1}{\sqrt{1 + r_x^2}},$$

which substituted to (1.3.5) yields

$$K = -\frac{r_{xx}}{(1 + r_x^2)^{3/2}}. \tag{1.3.6}$$

Finally, substituting (1.3.4) and (1.3.6) into equation (1.3.2), we obtain that our curve Γ, satisfies the equation

$$r_t = A\frac{r_{xx}}{1 + r_x^2}. \tag{1.3.7}$$

In this section, we shall look for *traveling wave* solutions to the problem defined by equation (1.3.7) and the boundary conditions given in (1.3.1). We remark that there may exist many other types of solutions to this problem. Thus, we shall look for solutions which move with constant velocity in the direction parallel to the x-axis. These solutions can be expressed as

$$r(x,t) = g(x - Vt), \tag{1.3.8}$$

where g is any smooth function of one variable and V is defined as

$$V := \hat{x}_t.$$

Substituting (1.3.8) into equation (1.3.7) and into the boundary conditions (1.3.1), we obtain the following ordinary differential equation in g

$$Vg' = -A\frac{g''}{1 + g'^2}, \tag{1.3.9}$$

and the following boundary conditions

$$g(0) = 0, \tag{1.3.10a}$$

$$g_x|_{x=0} = \infty, \tag{1.3.10b}$$

and

$$g(\infty) = Q, \quad \Big(\text{and} \quad g(-\infty) = -Q\Big). \tag{1.3.10c}$$

Integration of (1.3.9) yields two families of solutions

$$Vg = -A\arctan{(g')} - Ak_1, \tag{1.3.11}$$

and

$$V g = A\text{arccot}(g') - Ak_2, \tag{1.3.12}$$

where k_1 and k_2 are arbitrary constants of integration. We shall show later in this section, that the two families of solutions (1.3.11) and (1.3.12) lead to equivalent solutions to the problem consisting of the equation (1.3.9) and the boundary condition (1.3.10a).

Equation (1.3.11) can be rewritten as

$$g' = -\tan \frac{Vg + Ak_1}{A} \tag{1.3.13}$$

which can be integrated to yield

$$g = -\frac{Ak_1}{V} + \frac{A}{V} \arcsin{(C_1 e^{-\frac{V}{A}x})}. \tag{1.3.14}$$

Similarly the solution of (1.3.12) is given by

$$g = -\frac{Ak_2}{V} + \frac{A}{V} \arccos{(C_2 e^{-\frac{V}{A}x})}. \tag{1.3.15}$$

In (1.3.14), (1.3.15), C_1 and C_2 are arbitrary constants of integration.

The solutions (1.3.14), (1.3.15) are meaningful if and only if the parameters C_1, and C_2 satisfy, respectively, the following conditions

$$-1 \leq C_1 e^{-\frac{V}{A}x} \leq 1, \quad -1 \leq C_2 e^{-\frac{V}{A}x} \leq 1, \quad \forall x \in (0, \infty). \tag{1.3.16}$$

Since, both of the above conditions imply that we want a solution which remains bounded as $x \to \infty$, and since by assumption...(I SHALL ADD THIS ASSUMPTION IN THE INTRODUCTION..) $A > 0$, we conclude that V must satisfy $V > 0$.

It is easy to see that, another way to write the family of solutions (1.3.14) to the equation (1.3.9) is as

$$\sin \frac{Vg + Ak_1}{A} = C_1 e^{-\frac{V}{A}x}, \tag{1.3.17}$$

or in other words

$$\sin{(k_1)} \cos \frac{Vg}{A} + \cos{(k_1)} \sin \frac{Vg}{A} = C_1 e^{-\frac{V}{A}x}. \tag{1.3.18}$$

Now, using the boundary condition (1.3.10a), we get for this family of solutions that

$$C_1 = \sin{(k_1)},$$

yielding solutions of the form

$$C_1 \cos \frac{Vg}{A} \pm \sqrt{1 - C_1^2} \sin \frac{Vg}{A} = C_1 e^{-\frac{V}{A}x}. \tag{1.3.19}$$

Similarly, we can write the second family of solutions (1.3.15), as

$$\cos \frac{Vg + Ak_2}{A} = C_2 e^{-\frac{V}{A}x},$$

or in other words

$$\cos (k_2) \cos \frac{Vg}{A} - \sin (k_2) \sin \frac{Vg}{A} = C_2 e^{-\frac{V}{A}x}.$$

The boundary condition (1.3.10a) gives us now that

$$C_2 = \cos (k_2),$$

hence,

$$C_2 \cos \frac{Vg}{A} \mp \sqrt{1 - C_2^2} \sin \frac{Vg}{A} = C_2 e^{-\frac{V}{A}x}. \tag{1.3.20}$$

Noting (1.3.16), it is easy to see that (1.3.19) coincides with (1.3.20). Thus, in fact we have obtained the same family of solutions twice. Hence, from now on, we shall refer only to the first family of solutions (1.3.14) to the equation (1.3.9).

The second boundary condition (1.3.10b) can be expressed as

$$x_g|_{x=0, g=0} = 0.$$

Therefore, calculating the derivative with respect to g using (1.3.17), we get that

$$V \cos \frac{Vg + Ak_1}{A} = C_1 V e^{-\frac{V}{A}x} x_g,$$

and thus,

$$\cos (k_1) = 0.$$

Hence, by (1.3.18) we obtain that if $g(x)$ satisfies both boundary conditions (1.3.10a) and (1.3.10b), then

$$C_1 = \sin (k_1) = \pm\sqrt{1 - \cos^2 (k_1)} = \pm 1,$$

and

$$g(x) = \pm \frac{A}{V} \arccos (e^{-\frac{V}{A}x}). \tag{1.3.21}$$

Equivalently, using (1.3.14), this solution may be rewritten as

$$g(x) = \mp \frac{A\pi}{2V} \pm \frac{A}{V} \arcsin (e^{-\frac{V}{A}x}). \tag{1.3.22}$$

Finally, imposing the third boundary condition (1.3.10c), we obtain from the expression for the solution given in (1.3.22), that

$$V = \frac{A\pi}{2Q},$$

hence implying that

$$g(x) = \mp Q \pm \frac{2Q}{\pi} \arcsin\left(e^{-\frac{\pi}{2Q}x}\right). \tag{1.3.23}$$

In practical calculations, we will assume, for simplicity that $Q = 1$, so $g(x)$ is given by

$$g(x) = \mp 1 \pm \frac{2}{\pi} \arcsin\left(e^{-\frac{\pi}{2}x}\right), \tag{1.3.24}$$

and V can be expressed as

$$V = \frac{A\pi}{2}. \tag{1.3.25}$$

1.3.1 Two Equivalent geometric normalizations

We propose two different geometric normalizations of the variable x, which both allow us to define a *small* dimensionless parameter. The first way is by introducing a small parameter

$$\lambda = \frac{L}{Q}, \tag{1.3.26}$$

where $Q = g(\infty)$ and g denotes the traveling wave solution which was discussed in Section 1.3, and L is the initial height of the film. The second way is by defining a small parameter

$$\widetilde{\lambda} = \frac{L}{R_0}, \tag{1.3.27}$$

where R_0 is the radius at "nose" of the traveling wave where $x = 0$, and L is the initial height of the film.

We obtain the equivalence by considering

$$\kappa = \frac{g_{xx}(x)}{(1 + g_x{}^2(x))^{3/2}}. \tag{1.3.28}$$

By (2.2.87), $g_x(x)$ is given by

$$g_x(x) = \frac{e^{-\frac{\pi}{2Q}x}}{\sqrt{1 - e^{-\frac{\pi}{Q}x}}}, \tag{1.3.29}$$

and $g_{xx}(x)$ is given by

$$g_{xx}(x) = -\frac{\pi(e^{-\frac{\pi}{2Q}x})}{2Q(1 - e^{-\frac{\pi}{Q}x})^{3/2}}.$$

Hence (1.3.28) yields that

$$\kappa = -\frac{\pi}{2Q}(e^{-\frac{\pi}{2Q}x}). \tag{1.3.30}$$

Thus, when $x = 0$

$$\kappa = -\frac{\pi}{2Q},$$

and therefore

$$R_0 = -\frac{1}{\kappa} = \frac{2Q}{\pi}.$$

In other words

$$\frac{R_0}{Q} = \frac{2}{\pi},$$

and, the ratio between λ and $\widetilde{\lambda}$ is $\mathcal{O}(1)$, so the two normalizations (1.3.26) and (1.3.27) can be concluded to be equivalent.

1.4 Physical Background

1.4.1 Obtaining the Surface Diffusion Equation in One Dimension

Many materials are poly-crystalline, meaning that they are composed of small crystals, called grains, each composed of atoms in a lattice or other regular arrangement. The interface between two grains is somewhat analogous to a film separating two bubbles of air in soap froth, because it has an excess free energy roughly proportional to the surface area of the film. As in soap froths, there are triple junctions where three grains come into contact.

The energy of grain boundaries is due to the presence of atoms having "broken bonds" as compared to their arrangement in the interior of the crystal. Even if there is atomic rearrangement at and near the surface which decrease this excess energy, as can happen quite dramatically, an excess energy still exists. Furthermore, the structure of a surface is usually anisotropic, i.e., different in different directions. Thus the *surface free energy* per unit area $\gamma(\mathbf{n})$, which underlies the driving force, namely the work at constant pressure and temperature which must be supplied to create a unit area of surface with orientation $\mathbf{n}$, is a function of the interface normal direction and the orientations of the crystals which meet along that interface.

(J. TAYLOR-SOME MATHEMATICAL CHALLENGES IN MATERIALS SCIENCE) and (**http://www.ctcms.nist.gov/ roosen**)

In order to obtain the surface diffusion equation (1.2.2), let us consider a curved element of a smoothly curved surface, which will be denoted by dS. Consider the surface of a portion of a crystal lying either above or below $z = 0$, which is described by the single valued function $z = \zeta(x, y)$ where x, y, z are Cartesian coordinates. The orientation of an element of surface is given via the partial derivatives ζ_x, ζ_y, namely $\mathbf{n} = \frac{(\zeta_x, \zeta_y, -1)}{\sqrt{1+\zeta_x^2+\zeta_y^2}}$, and hence, the surface free energy per unit area $\gamma(\mathbf{n})$, may be expressed as $\gamma(\zeta_x, \zeta_y)$. Noting that on the xy-plane $dS = \sqrt{1 + \zeta_x^2 + \zeta_y^2} dxdy$, we obtain that $\gamma dS = e dxdy$ where

$$e = \gamma(\zeta_x, \zeta_y)(1 + \zeta_x^2 + \zeta_y^2)^{1/2}. \tag{1.4.1}$$

Thus the *free energy of the surface* of the portion of the crystal lying, say, above $z = 0$, may be expressed as

$$E = \int e(\zeta_x, \zeta_y)dxdy, \tag{1.4.2}$$

where the integration is taken over a region in the xy-plane bounded by Γ, the intersection of the surface with $z = 0$.

Let us first consider a variation δE of E, such that $\delta\zeta$ vanishes on Γ but is otherwise arbitrary. Then, after formally interchanging the operations of variation and integration by parts, we obtain

$$\delta E = \int \delta e(\zeta_x, \zeta_y)dxdy = -\int \Big[\frac{\partial}{\partial x}\frac{\partial e}{\partial \zeta_x} + \frac{\partial}{\partial y}\frac{\partial e}{\partial \zeta_y}\Big]\delta\zeta dxdy. \tag{1.4.3}$$

If we equate equation (1.4.3) with

$$\delta E = \pm \int \mu\delta\zeta dxdy, \tag{1.4.4}$$

where the $\pm$ sign refers to a surface lying above or below $z = 0$, respectively, then μ is known as the *chemical potential*, which can be defined as free energy per unit volume of the added or subtracted material relative to the bulk phase. Thus we obtain for arbitrary $\delta\zeta$ that

$$\frac{\partial}{\partial x}\frac{\partial e}{\partial \zeta_x} + \frac{\partial}{\partial y}\frac{\partial e}{\partial \zeta_y} \pm \mu = 0, \tag{1.4.5}$$

which in turn implies that

$$\mu = \mp\Big[\frac{\partial^2 e}{\partial \zeta_x^2}\zeta_{xx} + 2\frac{\partial^2 e}{\partial \zeta_x \zeta_y}\zeta_{xy} + \frac{\partial^2 e}{\partial \zeta_y^2}\zeta_{yy}\Big], \tag{1.4.6}$$

where the $\pm$ sign refers to a surface lying above or below the plane $z = 0$, respectively. Equation (1.4.6) is equivalent to Herring formula [3] for the chemical potential at a point P of the surface,

$$\mu = \Big(\gamma + \frac{\partial^2\gamma}{\partial n_1^2}\Big)\frac{\kappa_1}{2} + \Big(\gamma + \frac{\partial^2\gamma}{\partial n_2^2}\Big)\frac{\kappa_2}{2}, \tag{1.4.7}$$

where, n_1 and n_2 are the normals of the principal curves through P and the derivatives are taken along these curves. To see this, we choose a local Cartesian frame with the z-axis along the local outward normal to P so that $\zeta_x = \zeta_y = 0$. Then, using equation (1.4.1), and choosing the xy-axes to coincide with the principal directions at P so that $\zeta_{xy} = 0$ and $\zeta_{xx} = -\frac{\kappa_1}{2}$ and $\zeta_{yy} = -\frac{\kappa_2}{2}$, where κ_1 and κ_2 are the principal curvatures with the conventional signs, we obtain (1.4.7). Equation (1.4.7) shows that μ is independent of Cartesian frame and depends only on the local geometry and the local value of γ and its derivatives.

In the *isotropic case*, which we shall be dealing here (I SHALL ADD THIS ASSUMPTION..), γ is independent of orientation, and equation (1.4.7) reduces to Gibbs-Thomson relation

$$\mu_P = \gamma\kappa, \tag{1.4.8}$$

where $\kappa = \frac{\kappa_1+\kappa_2}{2}$ is the mean curvature at P. An intuitive interpretation of equation (1.4.8) is that as the curvature of the surface increases, the average coordination of a surface atom decreases causing the chemical potential to increase.

We further assume that the value of μ at any point, in the presence of a surface flux of atoms, can be approximated by the equilibrium value corresponding to zero flux. This assumption is known as the assumption of local equilibrium.

Surface gradients of μ give rise to surface fluxes $\vec{J}_a$ (atoms per unit length per unit time), which are well defined and may be written as [7]

$$\vec{J}_a = \nu\vec{v}, \tag{1.4.9}$$

where ν is the number of drifting atoms per unit area (known as the *Debye frequency*) and $\vec{v}$ is the average velocity of the drifting atoms with respect to the underlying lattice.

Assuming local equilibrium, it is possible to write $\vec{v}$ using the Nernst-Einstein formula [8], as the product of a mobility and a driving force which may be expressed in terms of the gradient of the equilibrium chemical potential [8]. This yields that

$$\vec{v} = \left(\frac{\overline{D}}{kT}\right) \cdot \nabla_s(\Omega\mu), \tag{1.4.10}$$

where $\overline{D}$ is the surface diffusion tensor (which is a rank 2 tensor), Ω is the atomic volume, k is the Boltzmann constant, and $\nabla_s(\Omega\mu)$ is the surface gradient of the equilibrium chemical potential per atom in which μ is given by equations (1.4.6) or (1.4.7). Implicit in equation (1.4.10) is the assumption that all of the free energy gradient is used to drive surface diffusion and none of it drives the exchanges of ad-atoms with sources and sinks. Defining $\vec{J} = \Omega\vec{J}_a$ to be the volume flux (volume per unit time per unit length), we have from equations (1.4.9) and (1.4.10) that

$$\vec{J} = \nu\Omega^2\left(\frac{\overline{D}}{kT}\right) \cdot \nabla_s\mu. \tag{1.4.11}$$

Now, that we have obtained a formula for $\vec{J}$, shape change may be determined from the continuity equation [7]

$$\frac{\partial n}{\partial t} + \nabla_s \cdot \vec{J} = 0, \tag{1.4.12}$$

where $\frac{\partial n}{\partial t}$ is the rate of advance of the surface in the direction of the outward pointing normal (which corresponds in our previous notation to the normal velocity $\mathbf{V}$), and the second term is the surface divergence of $\vec{J}$. Equations (1.4.11) and (1.4.12) determine the capillarity-induced shape change of a body evolving by surface diffusion, under the assumption of local equilibrium; they conform to the general framework outlined by Herring [3].

Finally, as was mentioned earlier, since we are dealing in this thesis with the isotropic case only, combining equations (1.4.8), (1.4.11) and (1.4.12) yields

$$\mathbf{V} = -\gamma\nu\Omega^2\Big(\frac{\overline{D}}{kT}\Big)\Delta_s\kappa, \tag{1.4.13}$$

where $\mathbf{V} \equiv \frac{\partial n}{\partial t}$ is the normal velocity, $\Delta_s = \nabla_s \cdot \nabla_s$ is the Laplace-Beltrami operator, and κ is the mean curvature. It is easy to see that the equation (1.4.13) coincides with equation (1.2.2) with $B = \gamma\nu\Omega^2\Big(\frac{\overline{D}}{kT}\Big)$.

(MULLINS-CAPILLARITY-INDUCED SURFACE MORPHOLOGIES)

In a given material, grain boundary mobilities depend on grain boundary crystallography, temperature, local composition and defect concentration in the material. Two types of interface migration may be distinguished. In one case, the rate at which an interface moves is controlled by the diffusional flux of chemical species along the interface (in our context this motion is governed by the surface diffusion equation (1.2.2)). In the second (which will be referred in this thesis as motion by mean curvature), there is no net flux across the boundary, and the composition on both sides of the boundary is unmodified by the motion of the boundary. This latter type of motion is referred to as conservative interface migration and the interface mobility associated with it is an intrinsic property of the material and structural properties of the interface.

Intrinsic grain boundary migration depends upon the grain boundary structure, the driving force and temperature. The atomic structure of grain boundaries determines the grain boundary thermodynamics and the mechanism of grain boundary migration. Driving forces for interface migration include interface curvature and differences in the free energy of the phases. The driving force in our case is the *chemical potential* μ, which is given by

$$\mu = -\frac{\delta E}{\delta r}, \tag{1.4.14}$$

where δE is the change in free energy of the system when a unit area of interface moves distance δr normal to itself (this definition is equivalent to the definition given in (1.4.4)).

Assuming that grain boundary motion is thermally activated, we can use absolute reaction rate theory to predict the relationship between grain boundary velocity $\mathbf{V}$ and the driving force μ. If the grain boundary moves by single atoms hopping across the boundary, the boundary will move with a migration rate $\mathbf{V}$ given by [11]

$$\mathbf{V} = \mu\frac{b\nu\Omega}{kT}e^{-\frac{\Delta E}{kT}}, \tag{1.4.15}$$

where b is the boundary displacement associated with the hopping event, ν is Debye frequency, ΔE is the difference in free energies between the atom in the two grains, T is the temperature, k is Boltzmann constant, and Ω is the volume associated with the hopping atom. Equation (1.4.15) suggests that the velocity is directly proportional to the driving force. The proportionality constant, $M = \frac{b\nu\Omega}{kT}e^{-\frac{\Delta E}{kT}}$, is only a function of material properties, physical constants and temperature and is known as the grain boundary mobility, and we may write (1.4.15) as

$$\mathbf{V} = M\mu. \tag{1.4.16}$$

The change in the free energy of the system associated with the reduction in grain boundary area provides the driving force for normal grain growth. This driving force leads the grain boundaries to migrate toward their center of curvature. The relationship between this type of curvature driven growth and the grain boundary energy is provided by Gibbs-Thomson relation (1.4.8). In this case, the grain boundary velocity is proportional to the curvature:

$$\mathbf{V} = M\gamma\kappa, \tag{1.4.17}$$

which coincides with the equation (1.2.1), referred in this thesis as “motion by mean curvature”, with $A \equiv M\gamma > 0$.

Two different methods have been widely used to experimentally determine grain boundary mobility: direct observation of the migration of individual boundaries and measurement of the rate of change of the mean grain size in grain growth experiments [2].

1.4.2 Boundary Conditions

We begin this section by explaining the physical background of **Young's law**. First, we assume that local equilibrium holds along the triple line. We recall that the condition for local equilibrium that relates the geometry of thermal groove (the dihedral angles at the triple line) and its crystallography (the crystalline orientation) to the energies of the three surfaces was originally described by Herring [4]:

$$\sum_{j=\mathrm{I}}^{\mathrm{III}} \Big(\gamma^j \tau^j + \frac{\partial \gamma^j}{\partial \mathbf{n}_j} \Big) = 0. \tag{1.4.18}$$

In (1.4.18), γ^j is the excess free energy per unit area of the three surfaces X^j, $j = \mathrm{I}, \mathrm{II}, \mathrm{III}$, (see fig. 1.2), τ^j is the tangential unit vector of X^j, $j = \mathrm{I}, \mathrm{II}, \mathrm{III}$ normal to the triple line $\mathbf{l}$ and pointing away from it, and $\mathbf{n}_j$ is the unit vector normal to the line of intersection such that $\mathbf{n}_j = \mathbf{l} \times \tau^j$.

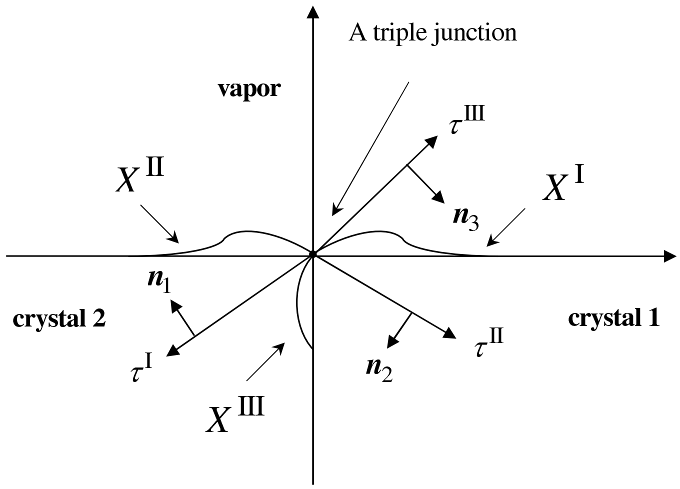

Figure 1.2: Schematic cross-sectional view of a triple junction, where the "groove root" line $\mathbf{l}$ points into the plane of the page.

In the isotropic case, as discussed earlier, γ is independent of orientation. Hence $\frac{\partial \gamma^j}{\partial \mathbf{n}_j} = 0$, so from (1.4.18) we readily obtain Young's law

$$\gamma^{\text{I}}\tau^{\text{I}} + \gamma^{\text{II}}\tau^{\text{II}} + \gamma^{\text{III}}\tau^{\text{III}} = 0. \tag{1.4.19}$$

Finally, since in our case the two grains comprising the bi-crystal are identical, except for their relative crystalline orientation, we have that $\gamma^{\text{I}} = \gamma^{\text{II}}$. Hence, if we set $m := \frac{\gamma_{\text{grain boundary}}}{\gamma_{\text{exterior surface}}} = \frac{\gamma^{\text{III}}}{\gamma^{\text{I}}}$, and divide equation (1.4.19) by γ^{I}, we obtain

$$\tau^{\text{I}} + \tau^{\text{II}} + m\tau^{\text{III}} = 0, \tag{1.4.20}$$

namely, Young's law as it was written in (1.2.3). Although, theoretically the parameter m may vary between 0 and 2, typically, for example in metals, $0 < m < 1/3$, and can be taken to be a small parameter [REF].

(Experimental Method for Determining Surface Energy Anisotropy and Its Application to Magnesia David M. Saylor, Darren E. Maso, and Gregory S. Rohrer.....)

Next, with regard to the **continuity of the surface chemical potentials**, we see that this can be expressed as

$$\mu^{\text{I}} = \mu^{\text{II}}, \tag{1.4.21}$$

where μ^{I} and μ^{II} denote the chemical potentials of the surfaces X^{I} and X^{II}, which lie to the right and to the left of the "groove root" line, respectively. Now, since we dealing with the isotropic case, using (1.4.8) and recalling that $\gamma^{\text{I}} = \gamma^{\text{II}}$, we readily obtain from (1.4.21) that the continuity of surface chemical potentials may be written as

$$\kappa^{\text{I}} = \kappa^{\text{II}}, \tag{1.4.22}$$

which is exactly (1.2.4).

Finally, as to the **balance of the mass flux**, it is reasonable to require that instantaneous matter fluxes into and out of a triple junction should be equal. So, if we denote by τ^j, $j = \mathrm{I}, \mathrm{II}$, the unit tangent vectors at the triple junction of the surfaces X^{I} and X^{II}, respectively, pointing away from the surfaces (see fig. 1.2), we see that the balance of mass flux may be written as

$$< \tau^{\mathrm{I}}, \vec{J}^{\,\mathrm{I}} > + < \tau^{\mathrm{II}}, \vec{J}^{\,\mathrm{II}} >= 0. \tag{1.4.23}$$

Using (1.4.11), which gives us that $\vec{J} \propto \nabla_s \kappa$, we readily get from (1.4.23) that

$$< \tau^{\mathrm{I}}, \nabla_s \kappa^{\mathrm{I}} > + < \tau^{\mathrm{II}}, \nabla_s \kappa^{\mathrm{II}} >= 0, \tag{1.4.24}$$

which is similar to (1.2.5).

Chapter 2 Obtaining the problem in our geometry

We shall now express the problem (1.2.2)–(1.2.5), described in the Section 1.2, in terms which shall facilitate our analysis of the motion. First, we shall write our problem, in accordance with..., in dimensional formulation, and afterwards, we shall re-scale it to obtain an appropriate dimensionless formulation.

2.1 Parametrization of the surfaces and relations between the variables

Suppose the grain groove boundary is defined by the function $\xi(x,t)$ in the xy-plane. We denote by s the arc-length of the function $\xi(x,t)$, by d the distance of any point from the curve $(x,\xi(x,t))$ (see fig. 2.1) and by z the "height" of the point.

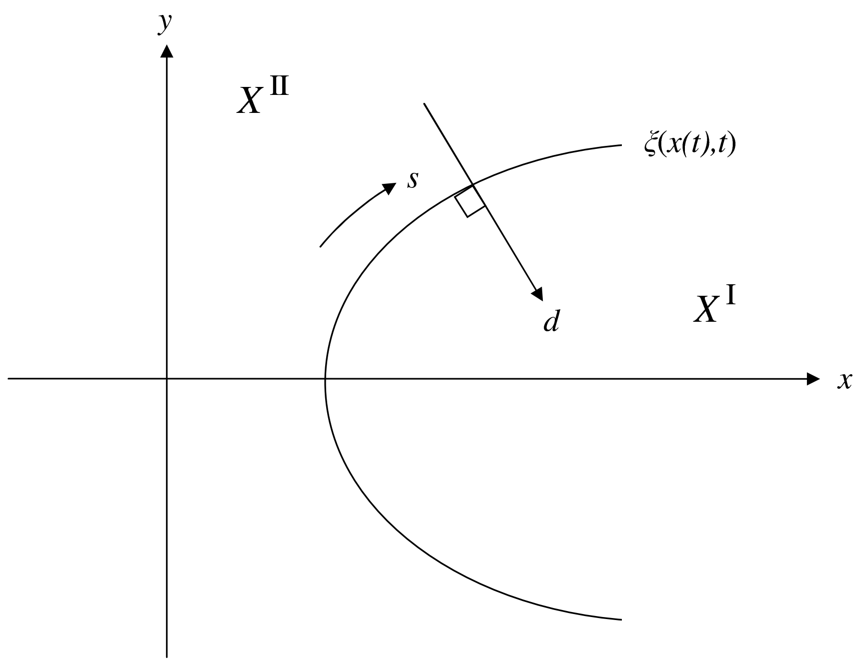

Figure 2.1: View from above-coordinates (d,s).

Then the parametrization of our three surfaces, as shown in fig. 2.2–2.4, is given by

$$
\begin{aligned}
X^{\mathrm{I}}(d,s,t) &= (\varphi^{\mathrm{I}}(d,s,t), \psi^{\mathrm{I}}(d,s,t), h^{\mathrm{I}}(d,s,t)),\\
X^{\mathrm{II}}(d,s,t) &= (\varphi^{\mathrm{II}}(d,s,t), \psi^{\mathrm{II}}(d,s,t), h^{\mathrm{II}}(d,s,t)),\\
X^{\mathrm{III}}(s,z,t) &= (\varphi^{\mathrm{III}}(s,z,t), \psi^{\mathrm{III}}(s,z,t), u(s,z,t)),
\end{aligned} \tag{2.1.1}
$$

where

$$u(s,z,t) = \frac{z}{\bar{u}(s,t)}L, \quad \text{and } \bar{u}(s,t) = L + h(0,s,t),$$

(L is the unperturbed thickness of the thin nano-film, far from the embedded grain, $h^j, j = \mathrm{I}, \mathrm{II}$ are the perturbations in thickness of the surfaces $X^j, j = \mathrm{I}, \mathrm{II}$, respectively, with regard to the initial state). Note that the purpose of this choice is that $0 \le u \le 1$, $0 \le z \le \bar{u}(s,t)$. The functions $\varphi^j, \psi^j,\ j = \mathrm{I}, \mathrm{II}, \mathrm{III}$ are defined as follows

$$
\begin{aligned}
\varphi^{\mathrm{I}}(d,s,t) &= x(s,t) + \tilde{x}(t) + d\sin\beta,\\
\psi^{\mathrm{I}}(d,s,t) &= \xi(x(s,t),t) - d\cos\beta,\\
\varphi^{\mathrm{II}}(d,s,t) &= x(s,t) + \tilde{x}(t) + d\sin\beta,\\
\psi^{\mathrm{II}}(d,s,t) &= \xi(x(s,t),t) - d\cos\beta,\\
\varphi^{\mathrm{III}}(s,z,t) &= x(s,t) + \tilde{x}(t) + D(s,u(s,z,t),t)\sin\beta,\\
\psi^{\mathrm{III}}(s,z,t) &= \xi(x(s,t),t) - D(s,u(s,z,t),t)\cos\beta.
\end{aligned}
\tag{2.1.2}
$$

Here $x(s,t)$ is given implicitly by the integral

$$
s = \int_{\tilde{x}(t)}^{x} \sqrt{1 + {\xi_x}^2(\check{x},t)}\, d\check{x},
\tag{2.1.3}
$$

and in the sequel we shall see that

$$
\tilde{x}'(t) = V,
$$

where V is the velocity along the x-axis in the xy-plane of the point $(\tilde{x}(t), 0, \bar{u}(0,t))$, which corresponds to the "nose" of the groove root; and β,

$$
\beta = \arctan \xi_x(x(s,t),t),
\tag{2.1.4}
$$

is the angle between the tangent of the function $\xi(x,t)$ and the x-axis (positive direction). The unknown functions are $h^{\mathrm{I}}(d,s,t), h^{\mathrm{II}}(d,s,t), \xi(x(s,t),t), V(t)$, and $D(s,u(s,z,t),t)$.

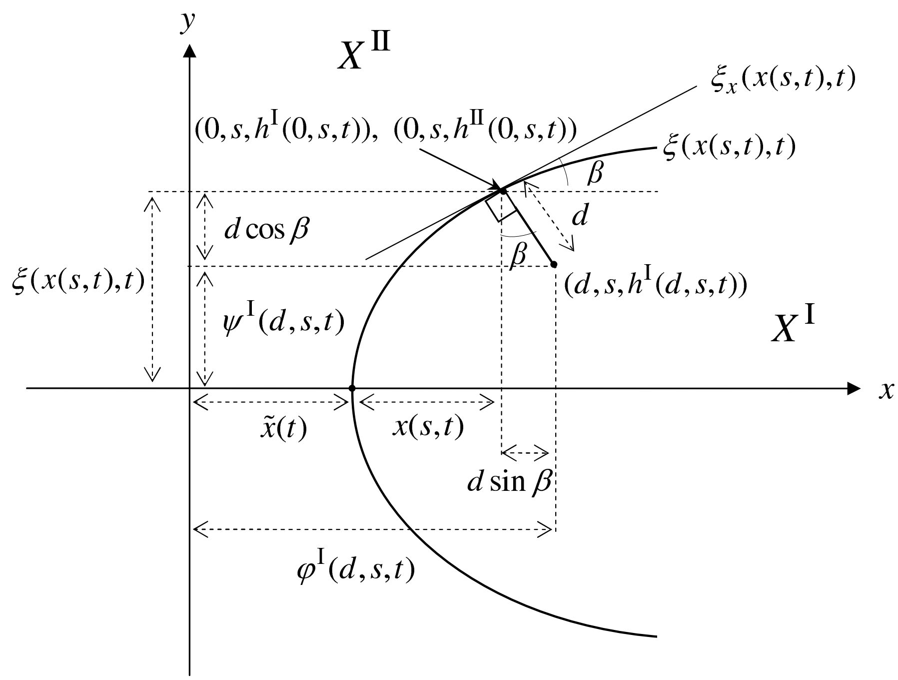

Figure 2.2: View from above on the surfaces X^{I} and X^{II}, obtaining the functions φ^{I} and ψ^{I}.

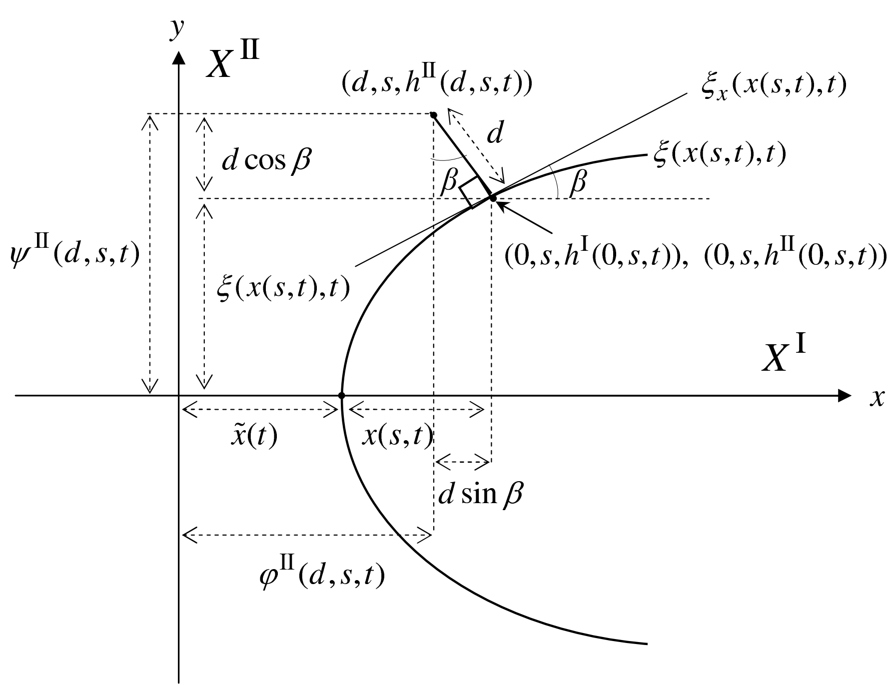

Figure 2.3: View from above on the surfaces X^{I} and X^{II}, obtaining the functions φ^{II} and ψ^{II}.

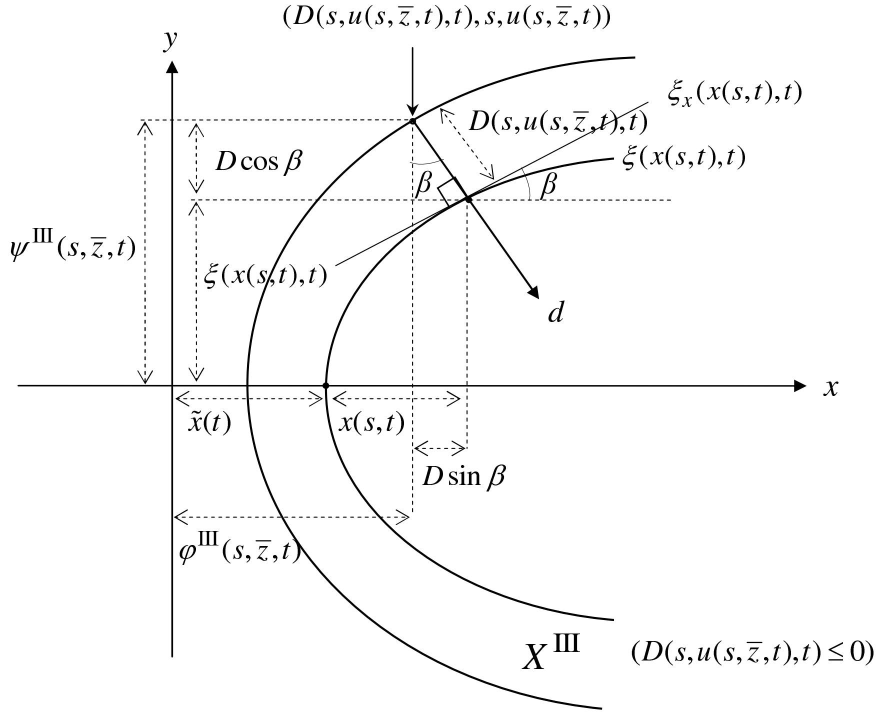

Figure 2.4: Projection of the "groove root" $(x(s,t)+\tilde{x}(t), \xi(x(s,t),t))$ on the xy-plane at some fixed height $0 \leq z = \bar{z} \leq \bar{u}$, and obtaining the functions φ^{III} and ψ^{III}.

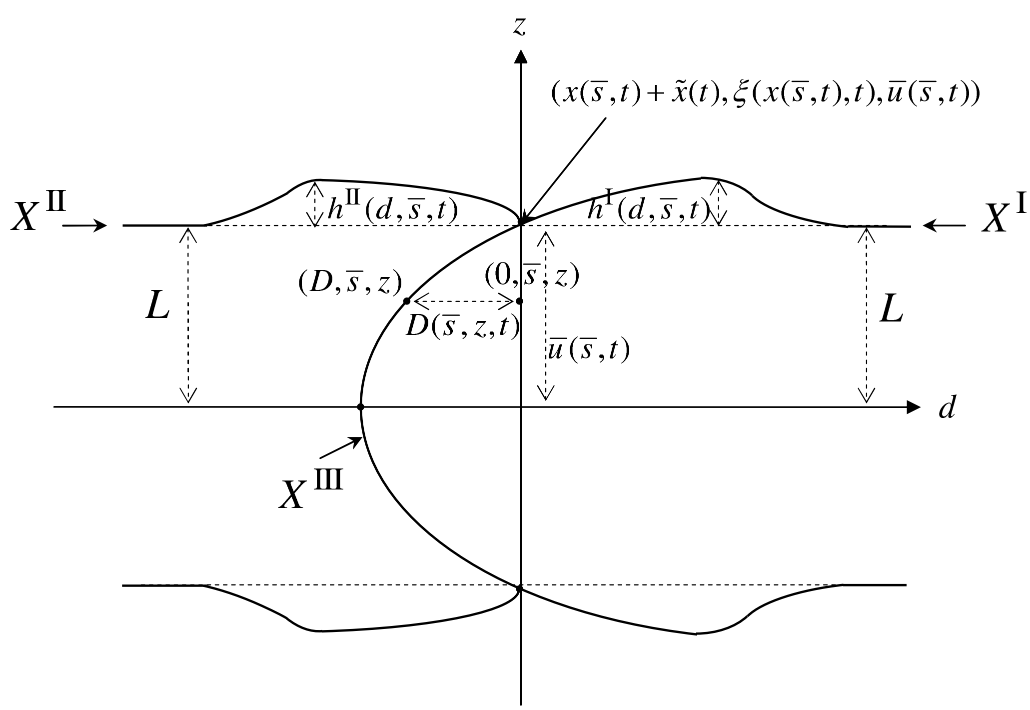

Figure 2.5: The cross-sectional view at the fixed $s=\bar{s}$, $(x(\bar{s},t)+\tilde{x}(t), \xi(x(\bar{s},t),t), \bar{u}(\bar{s},t))$.

In the following calculations we may use several obvious relations:

$$\sin\beta - \xi_x \cos\beta = 0, \tag{2.1.5a}$$

$$\cos\beta + \xi_x \sin\beta = \frac{1}{\cos\beta}, \tag{2.1.5b}$$

$$1 + \xi_x^2 = \left(\frac{1}{\cos\beta}\right)^2, \tag{2.1.5c}$$

and

$$\beta_s = \xi_{xx} x_s \cos^2\beta. \tag{2.1.5d}$$

Moreover, since $s_x = \sqrt{1+\xi_x^2}$, from the Inverse Function Theorem we obtain two more equalities:

$$x_s = \frac{1}{\sqrt{1+\xi_x^2}} = \cos\beta \tag{2.1.5e}$$

and

$$x_s^2(1+\xi_x^2) = \left(\frac{1}{\sqrt{1+\xi_x^2}}\right)^2 (1+\xi_x^2) = 1. \tag{2.1.5f}$$

Next, we observe that

$$\beta_s = \xi_{xx} x_s \cos^2\beta = \frac{\xi_{xx} x_s}{1+\xi_x^2},$$

and thus,

$$x_{ss} = -\frac{\xi_x \xi_{xx} x_s}{(1+\xi_x^2)^{3/2}} = -\frac{\xi_x}{\sqrt{1+\xi_x^2}}\beta_s = -\xi_x x_s \beta_s,$$

and

$$\xi_{xx} x_s^2 \sin\beta = x_s \beta_s \frac{\sin\beta}{\cos^2\beta} = \xi_x x_s \beta_s \frac{1}{\cos\beta}$$

lead to the relation

$$\xi_{xx} x_s^2 \sin\beta + x_{ss}\frac{1}{\cos\beta} = 0. \tag{2.1.5g}$$

2.2 Asymptotic Analysis

In this section, **as discussed in the introduction**, we shall assume that m is a small parameter.

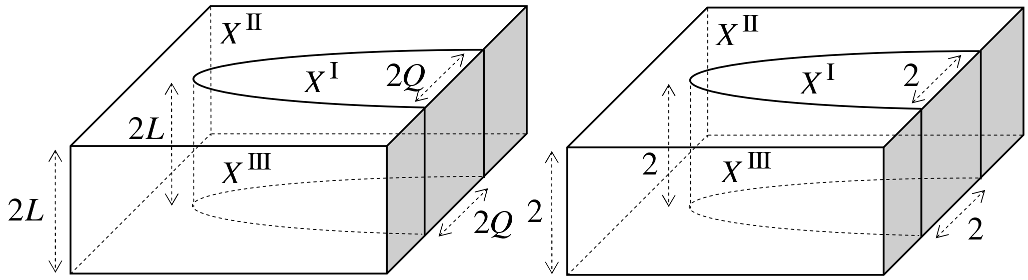

Figure 2.6: The structure with dimensional length scales marked and the same structure after the introduction of dimensionless variables.

2.2.1 Obtaining a dimensionless formulation

We denote by s^*, d^*, etc., dimensional parameters and functions and by s, d, etc., dimensionless parameters and functions.

To obtain a dimensionless formulation, L and Q are used to define typical length scales in z-direction and in xy-plane, respectively, and $\frac{Q^2}{A}$ is used as a typical time scale (see fig. 2.6).

Namely, we adopt the dimensionless parameters

$$
\begin{aligned}
s &:= s^*/Q, \\
d &:= d^*/Q, \\
z &:= z^*/L, \qquad (2.2.1)\\
t &:= \frac{A}{Q^2}t^*, \\
m &= \frac{\gamma_{\text{grain boundary}}}{\gamma_{\text{exterior surface}}},
\end{aligned}
$$

and dimensionless functions

$$
\begin{aligned}
x &:= x^*/Q, \\
\tilde{x} &:= \tilde{x}^*/Q, \\
\xi &:= \xi^*/Q, \\
D &:= D^*/Q, \\
h^j &:= h^{*j}/L, \quad j = \mathrm{I}, \mathrm{II}, \qquad (2.2.2)\\
\bar{u} &:= \bar{u}^*/L, \\
u &:= u^*/L, \\
K &:= QK^*, \\
\mathbf{V} &:= \frac{Q}{A}\mathbf{V}^*,
\end{aligned}
$$

where $\mathbf{V}$ is the normal velocity. Hence, the dimensionless partial derivatives can be obtained using the following formulae

$$
\begin{aligned}
x^*_{s^*} &= x_s,\\
x^*_{t^*} &= \frac{A}{Q}x_t,\\
\tilde{x}^*_{t^*} &= \frac{A}{Q}\tilde{x}_t,\\
\xi^*_{x^*} &= \xi_x,\\
\xi^*_{t^*} &= \frac{A}{Q}\xi_t,\\
D^*_{s^*} &= D_s,\\
D^*_{z^*} &= \frac{Q}{L}D_z,\\
D^*_{t^*} &= \frac{A}{Q}D_t,\\
{h^*}^j_{s^*} &= \frac{L}{Q}h^j_s, \quad j = \mathrm{I}, \mathrm{II},\\
{h^*}^j_{d^*} &= \frac{L}{Q}h^j_d, \quad j = \mathrm{I}, \mathrm{II},\\
{h^*}^j_{t^*} &= \frac{AL}{Q^2}h^j_t, \quad j = \mathrm{I}, \mathrm{II},\\
\bar{u}^*_{s^*} &= \frac{L}{Q}\bar{u}_s,\\
\bar{u}^*_{t^*} &= \frac{AL}{Q^2}\bar{u}_t,\\
K^*_{s^*} &= \frac{1}{Q^2}K_s,\\
K^*_{d^*} &= \frac{1}{Q^2}K_d,\\
\Delta_{s^*}K^* &= \frac{1}{Q^3}\Delta_s K.
\end{aligned}
\tag{2.2.3}
$$

All of the fig. 2.2–2.4, except fig. 2.5, remain valid after introducing the dimensionless variables, and fig. 2.5 will change in the following way:

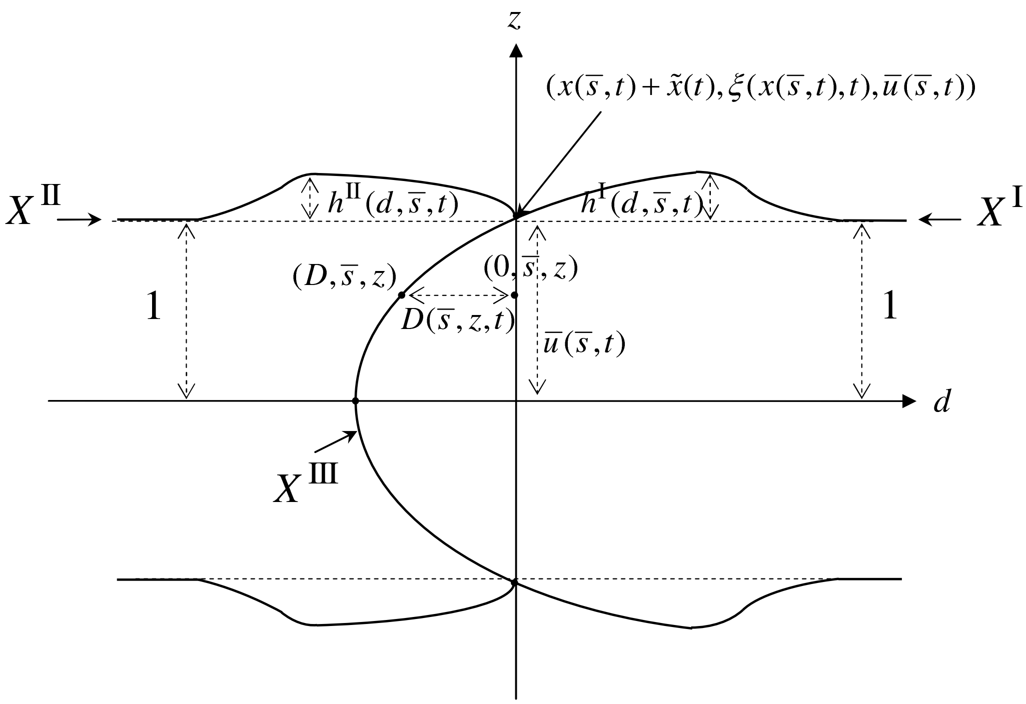

Figure 2.7: The dimensionless cross-sectional view at the fixed $s = \bar{s}$, $(x(\bar{s},t) + \tilde{x}(t), \xi(x(\bar{s},t),t), \bar{u}(\bar{s},t))$.

Next we summarize the dimensional first spatial derivatives of the functions ${\varphi^*}^{\mathrm{I}}(d^*, s^*, t^*)$, ${\psi^*}^{\mathrm{I}}(d^*, s^*, t^*)$, ${\varphi^*}^{\mathrm{III}}(s^*, z^*, t^*)$, ${\psi^*}^{\mathrm{III}}(s^*, z^*, t^*)$ and $u^*(s^*, z^*, t^*)$, and note, as follows from the definition (2.1.2), that the first spatial derivatives for ${\varphi^*}^{\mathrm{II}}(d^*, s^*, t^*), {\psi^*}^{\mathrm{II}}(d^*, s^*, t^*)$ may be calculated in a similar fashion as ${\varphi^*}^{\mathrm{I}}(d^*, s^*, t^*), {\psi^*}^{\mathrm{I}}(d^*, s^*, t^*)$, respectively.

(2.2.4)

$$
\begin{aligned}
{\varphi^*}^{\mathrm{I}}_{s^*} &= x^*_{s^*} + d^* \beta_{s^*} \cos\beta & {\varphi^*}^{\mathrm{I}}_{d^*} &= \sin\beta, \\
&= x_s + d\beta_s \cos\beta, & & \\
{\psi^*}^{\mathrm{I}}_{s^*} &= \xi^*_{x^*} x^*_{s^*} + d^* \beta_{s^*} \sin\beta & {\psi^*}^{\mathrm{I}}_{d^*} &= -\cos\beta, \\
&= \xi_x x_s + d\beta_s \sin\beta, & & \\
{\varphi^*}^{\mathrm{III}}_{s^*} &= x^*_{s^*} + (D^*_{s^*} + D^*_{u^*} u^*_{s^*}) \sin\beta + D^* \beta_{s^*} \cos\beta & {\varphi^*}^{\mathrm{III}}_{z^*} &= D^*_{u^*} u^*_{z^*} \sin\beta = \frac{Q}{L} D_u u_z \sin\beta, \\
&= x_s + (D_s + D_u u_s) \sin\beta + D\beta_s \cos\beta, & & \\
{\psi^*}^{\mathrm{III}}_{s^*} &= \xi^*_{x^*} x^*_{s^*} - (D^*_{s^*} + D^*_{u^*} u^*_{s^*}) \cos\beta + D^* \beta_{s^*} \sin\beta & {\psi^*}^{\mathrm{III}}_{z^*} &= -D^*_{u^*} u^*_{z^*} \cos\beta = -\frac{Q}{L} D_u u_z \cos\beta, \\
&= \xi_x x_s - (D_s + D_u u_s) \cos\beta + D\beta_s \sin\beta, & & \\
u^*_{s^*} &= -L z^* \frac{\bar{u}^*_{s^*}}{\bar{u}^{*2}} = -\frac{L}{Q} z \frac{\bar{u}_s}{\bar{u}^2}, & u^*_{z^*} &= \frac{L}{\bar{u}^*} = \frac{1}{\bar{u}},
\end{aligned}
$$

and the dimensional second spatial derivatives are given by

(2.2.5)

$$
\begin{aligned}
{\varphi^*}^{\mathrm{I}}_{s^*s^*} &= x^*_{s^*s^*} + d^*\beta_{s^*s^*}\cos\beta - d^*\beta^2_{s^*}\sin\beta \\
&= \frac{1}{Q}(x_{ss} + d\beta_{ss}\cos\beta - d\beta_s^2\sin\beta), \\
{\psi^*}^{\mathrm{I}}_{s^*s^*} &= \xi^*_{x^*x^*}{x^*_{s^*}}^2 + \xi^*_{x^*}x^*_{s^*s^*} + d^*\beta_{s^*s^*}\sin\beta + d^*\beta^2_{s^*}\cos\beta) \\
&= \frac{1}{Q}(\xi_{xx}x_s^2 + \xi_x x_{ss} + d\beta_{ss}\sin\beta + d\beta_s^2\cos\beta), \\
{\varphi^*}^{\mathrm{III}}_{s^*s^*} &= x^*_{s^*s^*} + (D^*_{s^*s^*} + D^*_{u^*u^*}{u^*_{s^*}}^2 + D^*_{u^*}u^*_{s^*s^*})\sin\beta + 2(D^*_{s^*} + D^*_{u^*}u^*_{s^*})\beta_{s^*}\cos\beta \\
&\quad + D^*\beta_{s^*s^*}\cos\beta - D^*\beta^2_{s^*}\sin\beta \\
&= \frac{1}{Q}\big[x_{ss} + (D_{ss} + D_{uu}u_s^2 + D_u u_{ss})\sin\beta + 2(D_s + D_u u_s)\beta_s\cos\beta + D\beta_{ss}\cos\beta - D\beta_s^2\sin\beta\big], \\
{\psi^*}^{\mathrm{III}}_{s^*s^*} &= \xi^*_{x^*x^*}x_s^{*2} + \xi^*_{x^*}x^*_{s^*s^*} - (D^*_{s^*s^*} + D^*_{u^*u^*}{u^*_{s^*}}^2 + D^*_{u^*}u^*_{s^*s^*})\cos\beta + 2(D^*_{s^*} + D^*_{u^*}u^*_{s^*})\beta_{s^*}\sin\beta \\
&\quad + D^*\beta_{s^*s^*}\sin\beta + D^*\beta^2_{s^*}\cos\beta \\
&= \frac{1}{Q}\big[\xi_{xx}x_s^2 + \xi_x x_{ss} - (D_{ss} + D_{uu}u_s^2 + D_u u_{ss})\cos\beta + 2(D_s + D_u u_s)\beta_s\sin\beta \\
&\quad + D\beta_{ss}\sin\beta + D\beta_s^2\cos\beta\big], \\
u^*_{s^*s^*} &= Lz^*\frac{2\bar{u}^{*2}_{s^*} - \bar{u}^*\bar{u}^*_{s^*s^*}}{\bar{u}^{*3}} = \frac{L}{Q^2}z\frac{2\bar{u}_s^2 - \bar{u}\bar{u}_{ss}}{\bar{u}^3}, \\
{\varphi^*}^{\mathrm{I}}_{d^*d^*} &= 0, \\
{\psi^*}^{\mathrm{I}}_{d^*d^*} &= 0, \\
{\varphi^*}^{\mathrm{III}}_{z^*z^*} &= (D^*_{u^*u^*}{u^*_{z^*}}^2 + D^*_{u^*}u^*_{z^*z^*})\sin\beta = \frac{Q}{L^2}D_{uu}u_z^2\sin\beta, \\
{\psi^*}^{\mathrm{III}}_{z^*z^*} &= -(D^*_{u^*u^*}{u^*_{z^*}}^2 + D^*_{u^*}u^*_{z^*z^*})\cos\beta = -\frac{Q}{L^2}D_{uu}u_z^2\cos\beta, \\
u^*_{z^*z^*} &= 0, \\
{\varphi^*}^{\mathrm{I}}_{s^*d^*} &= \beta_{s^*}\cos\beta = \frac{1}{Q}\beta_s\cos\beta, \\
{\psi^*}^{\mathrm{I}}_{s^*d^*} &= \beta_{s^*}\sin\beta = \frac{1}{Q}\beta_s\sin\beta, \\
{\varphi^*}^{\mathrm{III}}_{s^*z^*} &= (D^*_{u^*s^*}u^*_{z^*} + D^*_{u^*u^*}u^*_{s^*}u^*_{z^*} + D^*_{u^*}u^*_{s^*z^*})\sin\beta + D^*_{u^*}u^*_{z^*}\beta_{s^*}\cos\beta \\
&= \frac{1}{L}\big[(D_{us}u_z + D_{uu}u_s u_z + D_u u_{sz})\sin\beta + D_u u_z\beta_s\cos\beta\big], \\
{\psi^*}^{\mathrm{III}}_{s^*z^*} &= -(D^*_{u^*s^*}u^*_{z^*} + D^*_{u^*u^*}u^*_{s^*}u^*_{z^*} + D^*_{u^*}u^*_{s^*z^*})\cos\beta + D^*_{u^*}u^*_{z^*}\beta_{s^*}\sin\beta \\
&= \frac{1}{L}\big[-(D_{us}u_z + D_{uu}u_s u_z + D_u u_{sz})\cos\beta + D_u u_z\beta_s\sin\beta\big], \\
u^*_{s^*z^*} &= -L\frac{\bar{u}^*_{s^*}}{\bar{u}^{*2}} = -\frac{1}{Q}\frac{\bar{u}_s}{\bar{u}^2}.
\end{aligned}
$$

As to the dimensionless first time derivatives, they are given by

$$
\begin{aligned}
\varphi^{*\mathrm{I}}_{t^*} &= x^*_{t^*} + \tilde{x}^*_{t^*} + d^*\beta_{t^*}\cos\beta = \frac{A}{Q}(x_t + V + d\beta_t\cos\beta),\\
\psi^{*\mathrm{I}}_{t^*} &= \xi^*_{x^*}x^*_{t^*} + \xi^*_{t^*} + d^*\beta_{t^*}\sin\beta = \frac{A}{Q}(\xi_x x_t + \xi_t + d\beta_t\sin\beta),\\
\varphi^{*\mathrm{III}}_{t^*} &= x^*_{t^*} + \tilde{x}^*_{t^*} + (D^*_{t^*} + D^*_{u^*}u^*_{t^*})\sin\beta + D^*\beta_{t^*}\cos\beta\\
&= \frac{A}{Q}\big[x_t + V + (D_t + D_u u_t)\sin\beta + D\beta_t\cos\beta\big],\\
\psi^{*\mathrm{III}}_{t^*} &= \xi^*_{x^*}x^*_{t^*} + \xi^*_{t^*} - (D^*_{t^*} + D^*_{u^*}u^*_{t^*})\cos\beta + D^*\beta_{t^*}\sin\beta\\
&= \frac{A}{Q}\big[\xi_x x_t + \xi_t - (D_t + D_u u_t)\cos\beta + D\beta_t\sin\beta\big],\\
u^*_{t^*} &= -Lz^*\frac{\bar{u}^*_{t^*}}{\bar{u}^{*2}} = -\frac{AL}{Q^2}z\frac{\bar{u}_t}{\bar{u}^2}.
\end{aligned}
\tag{2.2.6}
$$

To facilitate the asymptotic analysis we assume that Q is large so that

$$
\frac{L}{Q} = m^{1/3}. \tag{2.2.7}
$$

We want now to expand Taylor series of all unknown dimensionless functions in $m^{2/3}$, around $m = 0$, namely

$$
\begin{aligned}
\xi &= \xi_0 + m^{2/3}\xi_1 + m^{4/3}\xi_2 + \mathcal{O}(m^2),\\
D &= D_0 + m^{2/3}D_1 + m^{4/3}D_2 + \mathcal{O}(m^2),\\
\bar{u} &= \bar{u}_0 + m^{2/3}\bar{u}_1 + m^{4/3}\bar{u}_2 + \mathcal{O}(m^2),\\
h^j &= h^j_0 + m^{2/3}h^j_1 + m^{4/3}h^j_2 + \mathcal{O}(m^2), \quad j = \mathrm{I}, \mathrm{II}.
\end{aligned}
\tag{2.2.8}
$$

The rationale for (2.2.7) and for expanding of all series in (2.2.8) in $m^{2/3}$ shall be explained in Section 2.2.2.

It should be emphasized, that if the function ξ has a Taylor expansion as in (2.2.8), then also $\beta = \arctan \xi_x(x(s,t),t)$ can be expanded in the series

$$
\beta = \beta_0 + m^{2/3}\beta_1 + m^{4/3}\beta_2 + \mathcal{O}(m^2),
$$

where, from Taylor's theorem it follows that

$$
\beta_0 = \arctan \xi_{0x}(x(s,t),t). \tag{2.2.9}
$$

Moreover, we know from the case $m = 0$ (see assumption (2.2.13) in Section 2.2.2), that in the expansions (2.2.8), the following equalities hold

$$
\xi_0(x,t) = \mp 1 \pm \frac{2}{\pi}\arcsin(e^{-\frac{\pi}{2}x}), \quad D_0 = 0, \quad \bar{u}_0 = 1, \quad \text{and} \quad h^j_0 = 0,\ j = \mathrm{I}, \mathrm{II}. \tag{2.2.10}
$$

2.2.2 Rationale for the framework of the asymptotic assumptions

Let

$$a = \frac{L}{Q}, \tag{2.2.11}$$

and let us assume that it is possible to expand all of the unknown functions, $\xi, D, \bar{u}$ and $h^j, j = \mathrm{I}, \mathrm{II}$ in terms of the same asymptotic series, namely

$$\begin{aligned} \xi &= \xi_0 + b\xi_1 + b^2\xi_2 + \mathcal{O}(b^3), \\ D &= D_0 + bD_1 + b^2 D_2 + \mathcal{O}(b^3), \\ \bar{u} &= \bar{u}_0 + b\bar{u}_1 + b^2\bar{u}_2 + \mathcal{O}(b^3), \\ h^j &= h_0^j + bh_1^j + b^2 h_2^j + \mathcal{O}(b^3), \quad j = \mathrm{I}, \mathrm{II}, \end{aligned} \tag{2.2.12}$$

where a and b are assumed to be small parameters, $a, b = o(1)$ in m.

We shall make two more assumptions which we shall use in the remainder of this section. The first is that when $b = 0$, there is no "thermal groove," or in other words, that $\xi = \xi_0$ coincides with the traveling wave solution which was discussed in Section 1.3, while $D, \bar{u}$ and $h^j, j = \mathrm{I}, \mathrm{II}$ satisfy

$$D_0 = 0, \quad \bar{u}_0 = 1, \quad \text{and} \quad h_0^j = 0, \quad j = \mathrm{I}, \mathrm{II}. \tag{2.2.13}$$

The second assumption is that

$$h_1^j \neq 0, \quad j = \mathrm{I}, \mathrm{II}. \tag{2.2.14}$$

Substituting the series (2.2.12) and the assumption (2.2.11) into the Young's law, and using the relations (2.1.5) we obtain that the third coordinate, expanded up through order $\mathcal{O}(b^2)$, should satisfy

$$\frac{-ah^{\mathrm{I}}_{0d} - abh^{\mathrm{I}}_{1d} + \mathcal{O}(b^2)}{\sqrt{1 + (ah^{\mathrm{I}}_{0d} + abh^{\mathrm{I}}_{1d})^2 + \mathcal{O}(b^4)}} + \frac{ah^{\mathrm{II}}_{0\,d} + abh^{\mathrm{II}}_{1\,d} + \mathcal{O}(b^2)}{\sqrt{1 + (ah^{\mathrm{II}}_{0\,d} + abh^{\mathrm{II}}_{1\,d})^2 + \mathcal{O}(b^4)}} = -m \tag{2.2.15}$$

(for a detailed explanation, see Section 2.2.5).

Now, using assumption (2.2.13), we expand the left hand side of (2.2.15) in a Taylor series in b up through $\mathcal{O}(b^2)$ to obtain

$$-abh^{\mathrm{I}}_{1d} + abh^{\mathrm{II}}_{1\,d} + \mathcal{O}(b^2) = -m, \tag{2.2.16}$$

and, due to (2.2.14), we readily get that it is reasonable to assume that a, b satisfy the condition

$$ab = m. \tag{2.2.17}$$

In analogy with the discussion concerning the third coordinate of Young's law, let us now consider the first coordinate of Young's law. Again, substituting the series (2.2.12), and using assumptions (2.2.11) and (2.2.13), and identities (2.1.5), we obtain that the first coordinate of Young's law, expanded to order $\mathcal{O}(b^3)$, should satisfy

$$\begin{aligned}\frac{-\sin\beta + a^2b^2 h^{\mathrm{I}}_{1s} h^{\mathrm{I}}_{1d} x_s + \mathcal{O}(b^3)}{\sqrt{1 + a^2b^2 {h^{\mathrm{I}}_{1d}}^2 + \mathcal{O}(b^4)}} + \frac{\sin\beta - a^2b^2 h^{\mathrm{II}}_{1\,s} h^{\mathrm{II}}_{1\,d} x_s + \mathcal{O}(b^3)}{\sqrt{1 + a^2b^2 {h^{\mathrm{II}}_{1\,d}}^2 + \mathcal{O}(b^4)}} \\ + m\frac{(\frac{b}{a}D_{1u} - \frac{b^2}{a}\bar{u}_1 D_{1u} + \frac{b^2}{a}D_{2u})\sin\beta - x_s(\frac{b^2}{a}D_{1s}D_{1u} - abz\bar{u}_{1s}) + \mathcal{O}(b^2)}{\sqrt{1 + \mathcal{O}(b)}} = 0,\end{aligned} \tag{2.2.18}$$

(for a detailed explanation, see Section 2.2.5).

After expanding the two first terms in (2.2.18) in a Taylor series up through $\mathcal{O}(b^3)$, we obtain

$$\begin{aligned}-\sin\beta + \frac{a^2b^2}{2}(2h^{\mathrm{I}}_{1s} h^{\mathrm{I}}_{1d} x_s + {h^{\mathrm{I}}_{1d}}^2 \sin\beta) + \sin\beta + \frac{a^2b^2}{2}(-2h^{\mathrm{II}}_{1\,s} h^{\mathrm{II}}_{1\,d} x_s - {h^{\mathrm{II}}_{1\,d}}^2 \sin\beta) + \mathcal{O}(b^3) \\ + m\frac{(\frac{b}{a}D_{1u} - \frac{b^2}{a}\bar{u}_1 D_{1u} + \frac{b^2}{a}D_{2u})\sin\beta - x_s(\frac{b^2}{a}D_{1s}D_{1u} - abz\bar{u}_{1s}) + \mathcal{O}(b^2)}{\sqrt{1 + \mathcal{O}(b)}} = 0.\end{aligned} \tag{2.2.19}$$

Dividing (2.2.19) by b and letting $b \downarrow 0$, we get

$$m(\frac{1}{a}D_{1u}\sin\beta + az\bar{u}_{1s}x_s) = 0,$$

which contradicts the assumption that $a = o(1)$, unless $D_{1u} = 0$. Thus, in order to avoid a contradiction to the framework which we have been developing, D_{1u} must satisfy

$$D_{1u} = 0, \tag{2.2.20}$$

and in order to maintain the dominant balance in (2.2.19), we shall require that

$$a^2b^2 = m\frac{b^2}{a},$$

yielding

$$a^3 = m. \tag{2.2.21}$$

Finally, from (2.2.17) and (2.2.21) we conclude that in order to enable the asymptotic analysis within the framework of all of the assumptions obtained in this section, a and b should satisfy

$$a = m^{1/3}, \quad b = m^{2/3}, \tag{2.2.22}$$

thus yielding that $\frac{L}{Q} = m^{1/3}$ and that all unknown functions are to be expanded in $m^{2/3}$.

2.2.3 Continuity Boundary Conditions

The first boundary condition, which imposes the continuity of the profile, can be stated in vector form as

$$X^{\mathrm{I}}(0,s,t) = X^{\mathrm{II}}(0,s,t) = X^{\mathrm{III}}(s,\bar{u}(s,t),t). \tag{2.2.23}$$

Since u normalizes the z-axis by $\bar{u}(s,t)$, from (2.2.23) we cannot straight forwardly deduce the equalities in terms of coordinates, but first we shall consider the surface X^{III} in the same coordinate system as the surfaces X^{I} and X^{II}, namely we shall attend to X^{III} as

$$X^{\mathrm{III}}(s,z,t) = (x(s,t) + \tilde{x}(t) + D(s,z,t)\sin\beta, \xi(x(s,t),t) - D(s,z,t)\cos\beta, z),$$

see fig. 2.5.

Hence, for $z = \bar{u}(s,t)$ in terms of coordinates introduced in (2.1.1) the equality (2.2.23) may be written as

$$\begin{aligned}&(x(s,t)+\tilde{x}(t), \xi(x(s,t),t), h^{\mathrm{I}}(0,s,t)) = (x(s,t)+\tilde{x}(t), \xi(x(s,t),t), h^{\mathrm{II}}(0,s,t))\\ &= (x(s,t)+\tilde{x}(t)+D(s,\bar{u}(s,t),t)\sin\beta, \xi(x(s,t),t) - D(s,\bar{u}(s,t),t)\cos\beta, \bar{u}(s,t)).\end{aligned} \tag{2.2.24}$$

Thus, we get

$$\begin{aligned}&h^{\mathrm{I}}(0,s,t) = h^{\mathrm{II}}(0,s,t) = \bar{u}(s,t) - 1,\\ &D(s,\bar{u}(s,t),t) = 0,\end{aligned}$$

which is identical for the dimensionless and the dimensional variables. Finally, using our assumption (2.2.13), we obtain for the leading orders of u, h^j, $j = \mathrm{I}, \mathrm{II}$, and D, that

$$\begin{aligned}&\bar{u}_0(s,t) = 1,\\ &h_1^{\mathrm{I}}(0,s,t) = h_1^{\mathrm{II}}(0,s,t) = \bar{u}_1(s,t),\\ &D_1(s,\bar{u}(s,t),t) = D_2(s,\bar{u}(s,t),t) = 0.\end{aligned} \tag{2.2.25}$$

The second continuity condition is continuity of the curvature, namely $K^{\mathrm{I}} = K^{\mathrm{II}}$ along the “groove root”. Using (1.2.6) we know that

(2.2.26)

$$K^{*\mathrm{I}} = \frac{< ||X^{*\mathrm{I}}_{s^*}||^2 X^{*\mathrm{I}}_{d^*d^*} - 2 < X^{*\mathrm{I}}_{s^*}, X^{*\mathrm{I}}_{d^*} > X^{*\mathrm{I}}_{s^*d^*} + ||X^{*\mathrm{I}}_{d^*}||^2 X^{*\mathrm{I}}_{s^*s^*}, X^{*\mathrm{I}}_{s^*} \times X^{*\mathrm{I}}_{d^*} >}{2(||X^{*\mathrm{I}}_{s^*}||^2 ||X^{*\mathrm{I}}_{d^*}||^2 - < X^{*\mathrm{I}}_{s^*}, X^{*\mathrm{I}}_{d^*} >^2)^{3/2}}.$$

Along the “groove root,” i.e., for $(d^*, s^*) = (0, s^*)$, using the expressions for derivatives (2.2.4) and (2.2.5), the identities (2.1.5), the dimensionless formulation, the Taylor expansions and the assumption (2.2.7), we obtain

$$\begin{aligned}< X^{*\mathrm{I}}_{s^*}, X^{*\mathrm{I}}_{d^*} > &= \varphi^{*\mathrm{I}}_{s^*}\varphi^{*\mathrm{I}}_{d^*} + \psi^{*\mathrm{I}}_{s^*}\psi^{*\mathrm{I}}_{d^*} + h^{*\mathrm{I}}_{s^*}h^{*\mathrm{I}}_{d^*}\\ &= x_s(\sin\beta - \xi_x\cos\beta) + \frac{L^2}{Q^2}m^{4/3}h^{\mathrm{I}}_{1s}h^{\mathrm{I}}_{1d} + \mathcal{O}(m^{8/3}) = \mathcal{O}(m^2),\end{aligned} \tag{2.2.27a}$$

(2.2.27b) $$||X^{*\mathrm{I}}_{s^*}||^2 = {\varphi^{*\mathrm{I}}_{s^*}}^2 + {\psi^{*\mathrm{I}}_{s^*}}^2 + {h^{*\mathrm{I}}_{s^*}}^2 = x_s^2(1+\xi_x^2) + \frac{L^2}{Q^2}m^{4/3}{h^{\mathrm{I}}_{1s}}^2 = 1 + \mathcal{O}(m^2),$$

(2.2.27c) $$||X^{*\mathrm{I}}_{d^*}||^2 = {\varphi^{*\mathrm{I}}_{d^*}}^2 + {\psi^{*\mathrm{I}}_{d^*}}^2 + {h^{*\mathrm{I}}_{d^*}}^2 = \sin^2\beta + \cos^2\beta + \frac{L^2}{Q^2}m^{4/3}{h^{\mathrm{I}}_{1d}}^2 = 1 + \mathcal{O}(m^2).$$

Hence, substituting (2.2.27) into (2.2.26) we get that the dimensionless curvature of the surface X^{I} is given by

(2.2.28)
$$\begin{aligned}
K^{\mathrm{I}} &= QK^{*\mathrm{I}} \\
&= Q\frac{< (1+\mathcal{O}(m^2))(0,0,\frac{m}{Q}h^{\mathrm{I}}_{1dd}) + \mathcal{O}(m^2) + \frac{1}{Q}(1+\mathcal{O}(m^2))(x_{ss}, \xi_{xx}x_s^2 + \xi_x x_{ss}, mh^{\mathrm{I}}_{1ss}), X^{*\mathrm{I}}_{s^*} \times X^{*\mathrm{I}}_{d^*} >}{2((1+\mathcal{O}(m^2))^2 - \mathcal{O}(m^4))^{3/2}} \\
&= \frac{1}{2} < (0,0,mh^{\mathrm{I}}_{1dd}) + (x_{ss}, \xi_{xx}x_s^2 + \xi_x x_{ss}, mh^{\mathrm{I}}_{1ss}), X^{*\mathrm{I}}_{s^*} \times X^{*\mathrm{I}}_{d^*} > + \mathcal{O}(m^2),
\end{aligned}$$

where

(2.2.29)
$$\begin{aligned}
X^{*\mathrm{I}}_{s^*} \times X^{*\mathrm{I}}_{d^*} &= (h^{*\mathrm{I}}_{d^*}\psi^{*\mathrm{I}}_{s^*} - \psi^{*\mathrm{I}}_{d^*}h^{*\mathrm{I}}_{s^*}, -h^{*\mathrm{I}}_{d^*}\varphi^{*\mathrm{I}}_{s^*} + \varphi^{*\mathrm{I}}_{d^*}h^{*\mathrm{I}}_{s^*}, \varphi^{*\mathrm{I}}_{s^*}\psi^{*\mathrm{I}}_{d^*} - \psi^{*\mathrm{I}}_{s^*}\varphi^{*\mathrm{I}}_{d^*}) \\
&= (m(h^{\mathrm{I}}_{1d}\xi_x x_s + h^{\mathrm{I}}_{1s}\cos\beta), m(-h^{\mathrm{I}}_{1d}x_s + h^{\mathrm{I}}_{1s}\sin\beta), -x_s\underbrace{(\cos\beta + \xi_x\sin\beta)}_{=\frac{1}{\cos\beta}}) + \mathcal{O}(m^2) \\
&= (0,0,-1) + m(h^{\mathrm{I}}_{1d}\xi_x x_s + h^{\mathrm{I}}_{1s}\cos\beta, -h^{\mathrm{I}}_{1d}x_s + h^{\mathrm{I}}_{1s}\sin\beta, 0) + \mathcal{O}(m^2);
\end{aligned}$$

and we readily obtain

(2.2.30)
$$\begin{aligned}
K^{\mathrm{I}} &= \frac{m}{2}(-h^{\mathrm{I}}_{1dd} - h^{\mathrm{I}}_{1ss} + h^{\mathrm{I}}_{1d}\xi_x x_s x_{ss} + h^{\mathrm{I}}_{1s}x_{ss}\cos\beta - h^{\mathrm{I}}_{1d}\xi_{xx}x_s^3 + h^{\mathrm{I}}_{1s}\xi_{xx}x_s^2\sin\beta \\
&\quad - h^{\mathrm{I}}_{1d}\xi_x x_s x_{ss} + h^{\mathrm{I}}_{1s}\xi_x x_{ss}\sin\beta) + \mathcal{O}(m^2) \\
&= \frac{m}{2}(-h^{\mathrm{I}}_{1dd} - h^{\mathrm{I}}_{1ss} - h^{\mathrm{I}}_{1d}\xi_{xx}x_s^3 + \underbrace{h^{\mathrm{I}}_{1s}x_{ss}\frac{1}{\cos\beta} + h^{\mathrm{I}}_{1s}\xi_{xx}x_s^2\sin\beta}_{=0}) + \mathcal{O}(m^2) \\
&= \frac{m}{2}(-h^{\mathrm{I}}_{1dd} - h^{\mathrm{I}}_{1ss} - h^{\mathrm{I}}_{1d}\xi_{xx}x_s^3) + \mathcal{O}(m^2).
\end{aligned}$$

Similar calculation shows that

(2.2.31) $$K^{\mathrm{II}} = \frac{m}{2}(-h^{\mathrm{II}}_{1\,dd} - h^{\mathrm{II}}_{1\,ss} - h^{\mathrm{II}}_{1\,d}\xi_{xx}x_s^3) + \mathcal{O}(m^2).$$

Using the Taylor series for $\xi(x,t)$, the identities (2.1.5), as well as (2.2.30) and (2.2.31), we obtain from the curvature continuity condition that

(2.2.32) $$h^{\mathrm{I}}_{1dd} + h^{\mathrm{I}}_{1ss} + h^{\mathrm{I}}_{1d}\frac{\xi_{0xx}}{(1+\xi_{0x}^2)^{3/2}} = h^{\mathrm{II}}_{1\,dd} + h^{\mathrm{II}}_{1\,ss} + h^{\mathrm{II}}_{1\,d}\frac{\xi_{0xx}}{(1+\xi_{0x}^2)^{3/2}}.$$

Finally, since (2.2.25) holds along the grain groove, all derivatives of h^{I}_1 and h^{II}_1 with respect to s are equal, in particular

$$h^{\mathrm{I}}_{1ss}(0,s,t) = h^{\mathrm{II}}_{1\,ss}(0,s,t),$$

so these two terms cancel each other in equation (2.2.32). Moreover, using

$$h^{\mathrm{I}}_{1d}(0,s,t) - h^{\mathrm{II}}_{1\,d}(0,s,t) = 1,$$

which will be demonstrated shortly and which follows from Young's law (2.2.54), we get that

$$h^{\mathrm{I}}_{1dd}(0,s,t) - h^{\mathrm{II}}_{1\,dd}(0,s,t) = -\frac{\xi_{0xx}}{(1+\xi_{0x}^2)^{3/2}}(x(s,t),t). \tag{2.2.33}$$

(GEOMETRIC INTERPRETATION??? The interpretation should be with respect to the principal directions of the curvature)

2.2.4 Mass Flux

We shall denote by $\tau^{\mathrm{I}}, \tau^{\mathrm{II}}$ and τ^{III}, three unit tangents to the surfaces $X^{\mathrm{I}}, X^{\mathrm{II}}$ and X^{III}, respectively, which belong to the plane perpendicular to s at the groove root. See fig. 2.8 and 2.9.

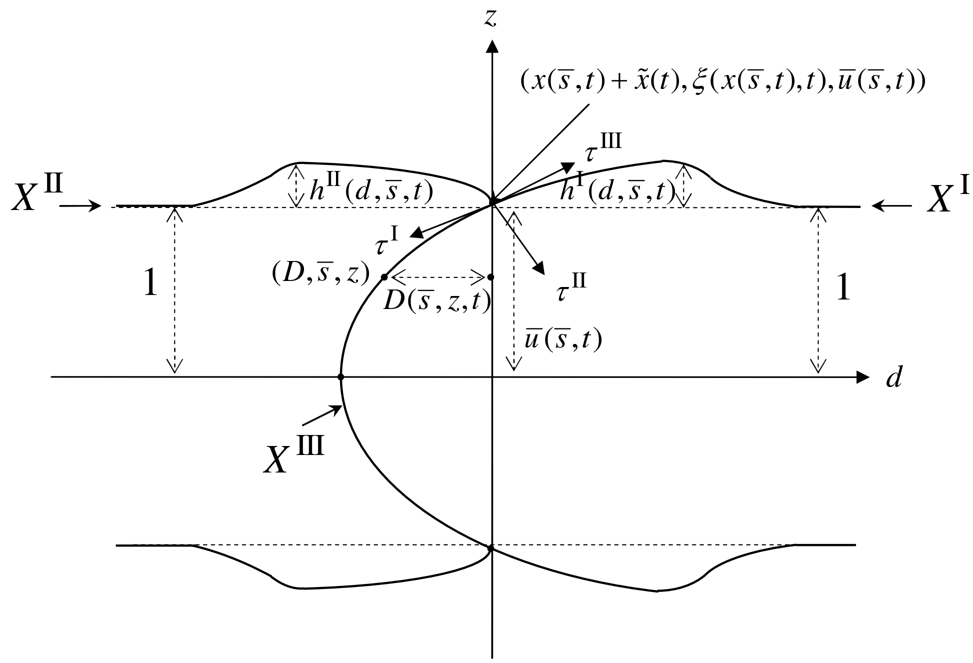

Figure 2.8: The unit tangent vectors τ^{I}, τ^{II}, and τ^{III} to the surfaces X^{I}, X^{II}, and X^{III}, respectively, at some fixed $s = \bar{s}$.

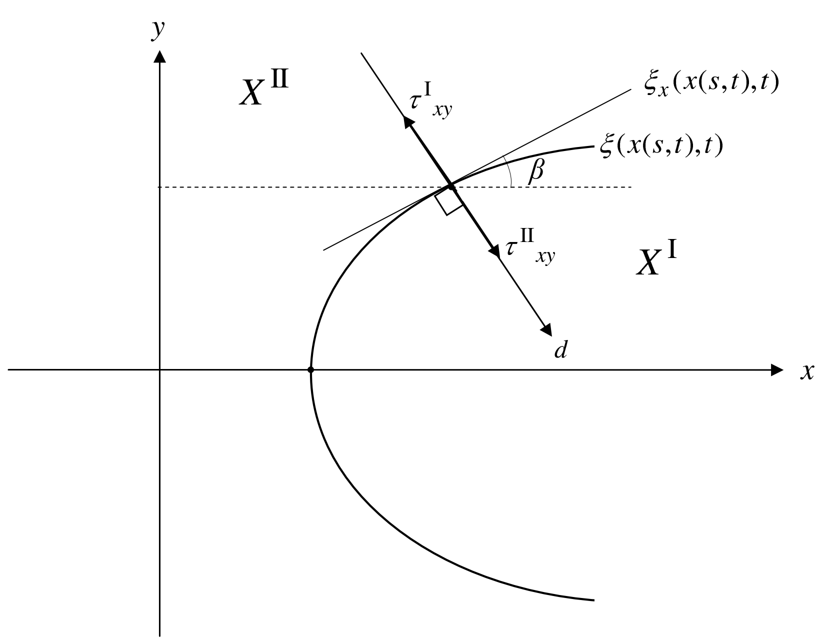

Figure 2.9: The projection on the xy-plane of the unit tangent vectors τ^{I} and τ^{II} to the surfaces X^{I} and X^{II}, respectively.

It is easily verified that

$$\tau^{*\mathrm{I}} = \frac{-X^{*\mathrm{I}}_{d^*} + < X^{*\mathrm{I}}_{s^*}, X^{*\mathrm{I}}_{d^*} > X^{*\mathrm{I}}_{s^*}}{||X^{*\mathrm{I}}_{d^*} - < X^{*\mathrm{I}}_{s^*}, X^{*\mathrm{I}}_{d^*} > X^{*\mathrm{I}}_{s^*}||}, \tag{2.2.34}$$

$$\tau^{*\mathrm{II}} = \frac{X^{*\mathrm{II}}_{d^*} - < X^{*\mathrm{II}}_{s^*}, X^{*\mathrm{II}}_{d^*} > X^{*\mathrm{II}}_{s^*}}{||X^{*\mathrm{II}}_{d^*} - < X^{*\mathrm{II}}_{s^*}, X^{*\mathrm{II}}_{d^*} > X^{*\mathrm{II}}_{s^*}||}, \tag{2.2.35}$$

and

$$\tau^{*\mathrm{III}} = \frac{X^{*\mathrm{III}}_{z^*} - < X^{*\mathrm{III}}_{s^*}, X^{*\mathrm{III}}_{z^*} > X^{*\mathrm{III}}_{s^*}}{||X^{*\mathrm{III}}_{z^*} - < X^{*\mathrm{III}}_{s^*}, X^{*\mathrm{III}}_{z^*} > X^{*\mathrm{III}}_{s^*}||}, \tag{2.2.36}$$

τ^{III} to be used later in Section 2.2.5. Since,

$$\tau^j \perp X^j_s, \quad j = \mathrm{I}, \mathrm{II},$$

we get that

$$< \tau^{*j}, \nabla_s K^{*j} >= \frac{- < X^{*j}_{s^*}, X^{*j}_{d^*} > K^{*j}_{s^*} + ||X^{*j}_{s^*}||^2 K^{*j}_{d^*}}{||X^{*j}_{s^*}||^2 ||X^{*j}_{d^*}||^2 - < X^{*j}_{s^*}, X^{*j}_{d^*} >^2} < \tau^{*j}, X^{*j}_{d^*} >, \quad j = \mathrm{I}, \mathrm{II}. \tag{2.2.37}$$

Now, from (2.2.34) we get

$$< \tau^{*\mathrm{I}}, X^{*\mathrm{I}}_{d^*} >= \frac{-||X^{*\mathrm{I}}_{d^*}||^2 + < X^{*\mathrm{I}}_{s^*}, X^{*\mathrm{I}}_{d^*} >^2}{||X^{*\mathrm{I}}_{d^*} - < X^{*\mathrm{I}}_{s^*}, X^{*\mathrm{I}}_{d^*} > X^{*\mathrm{I}}_{s^*}||}, \tag{2.2.38}$$

and from (2.2.35) we obtain

$$< \tau^{*\mathrm{II}}, X^{*\mathrm{II}}_{d^*} >= \frac{||X^{*\mathrm{II}}_{d^*}||^2 - < X^{*\mathrm{II}}_{s^*}, X^{*\mathrm{II}}_{d^*} >^2}{||X^{*\mathrm{II}}_{d^*} - < X^{*\mathrm{II}}_{s^*}, X^{*\mathrm{II}}_{d^*} > X^{*\mathrm{II}}_{s^*}||}. \tag{2.2.39}$$

Hence, substituting the derivatives (2.2.27) into (2.2.37), we get that for surface X^{I}

$$< \tau^{*\mathrm{I}}, \nabla_s K^{*\mathrm{I}} >= \frac{-\mathcal{O}(m^2) + (1 + \mathcal{O}(m^2)) K^{*\mathrm{I}}_{d^*}}{(1 + \mathcal{O}(m^2))^2 - \mathcal{O}(m^4)} < \tau^{*\mathrm{I}}, X^{*\mathrm{I}}_{d^*} >=< \tau^{*\mathrm{I}}, X^{*\mathrm{I}}_{d^*} > K^{*\mathrm{I}}_{d^*} + \mathcal{O}(m^2), \tag{2.2.40}$$

and similarly substituting the derivatives into (2.2.38) we get that

$$< \tau^{*\mathrm{I}}, X^{*\mathrm{I}}_{d^*} >= \frac{-(1 + \mathcal{O}(m^2)) + \mathcal{O}(m^4)}{||X^{*\mathrm{I}}_{d^*} - \underbrace{< X^{*\mathrm{I}}_{s^*}, X^{*\mathrm{I}}_{d^*} >}_{\mathcal{O}(m^2)} X^{*\mathrm{I}}_{s^*}||} = \frac{-1 + \mathcal{O}(m^2)}{1 + \mathcal{O}(m^2)} = -1 + \mathcal{O}(m^2). \tag{2.2.41}$$

So, (2.2.40), (2.2.41) yield that

$$< \tau^{*\mathrm{I}}, \nabla_s K^{*\mathrm{I}} >= -K^{*\mathrm{I}}_{d^*} + \mathcal{O}(m^2). \tag{2.2.42}$$

A similar calculation yields that

$$< \tau^{*\mathrm{II}}, \nabla_s K^{*\mathrm{II}} >= K^{*\mathrm{II}}_{d^*} + \mathcal{O}(m^2), \tag{2.2.43}$$

so the Mass Flux equality... implies here that

$$K^{*\mathrm{I}}_{d^*} = K^{*\mathrm{II}}_{d^*},$$

which leads that

$$K_d^{\mathrm{I}} = K_d^{\mathrm{II}}. \tag{2.2.44}$$

From (2.2.30), we have that

$$K_d^{\mathrm{I}} = \frac{m}{2}(-h^{\mathrm{I}}_{1ddd} - h^{\mathrm{I}}_{1ssd} - h^{\mathrm{I}}_{1dd}\xi_{xx}x_s^3) + \mathcal{O}(m^2), \tag{2.2.45}$$

and by (2.2.31),

$$K_d^{\mathrm{II}} = \frac{m}{2}(-h^{\mathrm{II}}_{1\,ddd} - h^{\mathrm{II}}_{1\,ssd} - h^{\mathrm{II}}_{1\,dd}\xi_{xx}x_s^3) + \mathcal{O}(m^2). \tag{2.2.46}$$

Substituting (2.2.45) and (2.2.46) into (2.2.44), we get

$$h^{\mathrm{I}}_{1ddd} + h^{\mathrm{I}}_{1ssd} + h^{\mathrm{I}}_{1dd}\xi_{xx}x_s^3 = h^{\mathrm{II}}_{1\,ddd} + h^{\mathrm{II}}_{1\,ssd} + h^{\mathrm{II}}_{1\,dd}\xi_{xx}x_s^3. \tag{2.2.47}$$

Now, using (2.2.54), which says that $h^{\mathrm{I}}_{1d}(0,s,t) - h^{\mathrm{II}}_{1\,d}(0,s,t) = 1$, and which follows from Young's law as shall be proved shortly, we conclude that

$$h^{\mathrm{I}}_{1ssd}(0,s,t) = h^{\mathrm{II}}_{1\,ssd}(0,s,t).$$

Hence, these terms cancel each other out in (2.2.47). Moreover, using (2.2.33), which follows from continuity of the curvature, in (2.2.47), we conclude that continuity of the mass flux implies here that

$$h^{\mathrm{I}}_{1ddd}(0,s,t) - h^{\mathrm{II}}_{1\,ddd}(0,s,t) = \frac{\xi_{0xx}^{\,2}}{(1+\xi_{0x}^{\,2})^3}. \tag{2.2.48}$$

2.2.5 Young's Law

Using (2.2.34), (2.2.35) and (2.2.36), we see that the Young's law (**??**) may be written as

(2.2.49)

$$\frac{-X^{*\mathrm{I}}_{d^*}(s^*,0) + < X^{*\mathrm{I}}_{s^*}(s^*,0), X^{*\mathrm{I}}_{d^*}(s^*,0) > X^{*\mathrm{I}}_{s^*}(s^*,0)}{||X^{*\mathrm{I}}_{d^*}(s^*,0) - < X^{*\mathrm{I}}_{s^*}(s^*,0), X^{*\mathrm{I}}_{d^*}(s^*,0) > X^{*\mathrm{I}}_{s^*}(s^*,0)||}$$
$$+\frac{X^{*\mathrm{II}}_{d^*}(s^*,0) - < X^{*\mathrm{II}}_{s^*}(s^*,0), X^{*\mathrm{II}}_{d^*}(s^*,0) > X^{*\mathrm{II}}_{s^*}(s^*,0)}{||X^{*\mathrm{II}}_{d^*}(s^*,0) - < X^{*\mathrm{II}}_{s^*}(s^*,0), X^{*\mathrm{II}}_{d^*}(s^*,0) > X^{*\mathrm{II}}_{s^*}(s^*,0)||}$$
$$+m\frac{X^{*\mathrm{III}}_{z^*}(s^*,\bar{u}^*) - < X^{*\mathrm{III}}_{s^*}(s^*,\bar{u}^*), X^{*\mathrm{III}}_{z^*}(s^*,\bar{u}^*) > X^{*\mathrm{III}}_{s^*}(s^*,\bar{u}^*)}{||X^{*\mathrm{III}}_{z^*}(s^*,\bar{u}^*) - < X^{*\mathrm{III}}_{s^*}(s^*,\bar{u}^*), X^{*\mathrm{III}}_{z^*}(s^*,\bar{u}^*) > X^{*\mathrm{III}}_{s^*}(s^*,\bar{u}^*)||} = 0, \quad \text{where } m = \frac{\gamma_{\text{gr. boundary}}}{\gamma_{\text{ext. surface}}}.$$

So, in terms of dimensional coordinates, (2.1.1), Young's law may be written as

$$
\begin{aligned}
(2.2.50)\qquad &\frac{-({\varphi^*}^{\rm I}_{d^*},{\psi^*}^{\rm I}_{d^*},{h^*}^{\rm I}_{d^*})+({\varphi^*}^{\rm I}_{s^*}{\varphi^*}^{\rm I}_{d^*}+{\psi^*}^{\rm I}_{s^*}{\psi^*}^{\rm I}_{d^*}+{h^*}^{\rm I}_{s^*}{h^*}^{\rm I}_{d^*})({\varphi^*}^{\rm I}_{s^*},{\psi^*}^{\rm I}_{s^*},{h^*}^{\rm I}_{s^*})}{||({\varphi^*}^{\rm I}_{d^*},{\psi^*}^{\rm I}_{d^*},{h^*}^{\rm I}_{d^*})-({\varphi^*}^{\rm I}_{s^*}{\varphi^*}^{\rm I}_{d^*}+{\psi^*}^{\rm I}_{s^*}{\psi^*}^{\rm I}_{d^*}+{h^*}^{\rm I}_{s^*}{h^*}^{\rm I}_{d^*})({\varphi^*}^{\rm I}_{s^*},{\psi^*}^{\rm I}_{s^*},{h^*}^{\rm I}_{s^*})||}\\
&+\frac{({\varphi^*}^{\rm II}_{d^*},{\psi^*}^{\rm II}_{d^*},{h^*}^{\rm II}_{d^*})-({\varphi^*}^{\rm II}_{s^*}{\varphi^*}^{\rm II}_{d^*}+{\psi^*}^{\rm II}_{s^*}{\psi^*}^{\rm II}_{d^*}+{h^*}^{\rm II}_{s^*}{h^*}^{\rm II}_{d^*})({\varphi^*}^{\rm II}_{s^*},{\psi^*}^{\rm II}_{s^*},{h^*}^{\rm II}_{s^*})}{||({\varphi^*}^{\rm II}_{d^*},{\psi^*}^{\rm II}_{d^*},{h^*}^{\rm II}_{d^*})-({\varphi^*}^{\rm II}_{s^*}{\varphi^*}^{\rm II}_{d^*}+{\psi^*}^{\rm II}_{s^*}{\psi^*}^{\rm II}_{d^*}+{h^*}^{\rm II}_{s^*}{h^*}^{\rm II}_{d^*})({\varphi^*}^{\rm II}_{s^*},{\psi^*}^{\rm II}_{s^*},{h^*}^{\rm II}_{s^*})||}\\
&+m\frac{({\varphi^*}^{\rm III}_{z^*},{\psi^*}^{\rm III}_{z^*},{u^*}_{z^*})-({\varphi^*}^{\rm III}_{s^*}{\varphi^*}^{\rm III}_{z^*}+{\psi^*}^{\rm III}_{s^*}{\psi^*}^{\rm III}_{z^*}+{u^*}_{s^*}{u^*}_{z^*})({\varphi^*}^{\rm III}_{s^*},{\psi^*}^{\rm III}_{s^*},{u^*}_{s^*})}{||({\varphi^*}^{\rm III}_{z^*},{\psi^*}^{\rm III}_{z^*},{u^*}_{z^*})-({\varphi^*}^{\rm III}_{s^*}{\varphi^*}^{\rm III}_{z^*}+{\psi^*}^{\rm III}_{s^*}{\psi^*}^{\rm III}_{z^*}+{u^*}_{s^*}{u^*}_{z^*})({\varphi^*}^{\rm III}_{s^*},{\psi^*}^{\rm III}_{s^*},{u^*}_{s^*})||}=0.
\end{aligned}
$$

Substituting the expressions for the dimensionless derivatives, (2.2.4), and the Taylor expansions, (2.2.8) and then using (2.1.5a), we obtain that at $(s, 0, \bar{u})$,

(2.2.51a)

$$
\begin{aligned}
&-({\varphi^*}^{\rm I}_{d^*},{\psi^*}^{\rm I}_{d^*},{h^*}^{\rm I}_{d^*})+({\varphi^*}^{\rm I}_{s^*}{\varphi^*}^{\rm I}_{d^*}+{\psi^*}^{\rm I}_{s^*}{\psi^*}^{\rm I}_{d^*}+{h^*}^{\rm I}_{s^*}{h^*}^{\rm I}_{d^*})({\varphi^*}^{\rm I}_{s^*},{\psi^*}^{\rm I}_{s^*},{h^*}^{\rm I}_{s^*})\\
&=-(\sin\beta,-\cos\beta,\frac{L}{Q}(m^{2/3}h^{\rm I}_{1d}+\mathcal{O}(m^{4/3})))+\Big(x_s\sin\beta-\xi_x x_s\cos\beta+\frac{L^2}{Q^2}(m^{4/3}h^{\rm I}_{1s}h^{\rm I}_{1d}+\mathcal{O}(m^2))\Big)\\
&\quad(x_s,\xi_x x_s,\frac{L}{Q}(m^{2/3}h^{\rm I}_{1s}+\mathcal{O}(m^{4/3})))\\
&=-(\sin\beta,-\cos\beta,mh^{\rm I}_{1d}+\mathcal{O}(m^{5/3}))+(m^2h^{\rm I}_{1s}h^{\rm I}_{1d}+\mathcal{O}(m^{8/3}))(x_s,\xi_x x_s,\mathcal{O}(m)),
\end{aligned}
$$

(2.2.51b)

$$
\begin{aligned}
&({\varphi^*}^{\rm II}_{d^*},{\psi^*}^{\rm II}_{d^*},{h^*}^{\rm II}_{d^*})-({\varphi^*}^{\rm II}_{s^*}{\varphi^*}^{\rm II}_{d^*}+{\psi^*}^{\rm II}_{s^*}{\psi^*}^{\rm II}_{d^*}+{h^*}^{\rm II}_{s^*}{h^*}^{\rm II}_{d^*})({\varphi^*}^{\rm II}_{s^*},{\psi^*}^{\rm II}_{s^*},{h^*}^{\rm II}_{s^*})\\
&=(\sin\beta,-\cos\beta,\frac{L}{Q}(m^{2/3}h^{\rm II}_{1\,d}+\mathcal{O}(m^{4/3})))-\Big(x_s\sin\beta-\xi_x x_s\cos\beta+\frac{L^2}{Q^2}(m^{4/3}h^{\rm II}_{1\,s}h^{\rm II}_{1\,d}+\mathcal{O}(m^2)))\Big)\\
&\quad(x_s,\xi_x x_s,\frac{L}{Q}(m^{2/3}h^{\rm II}_{1\,s}+\mathcal{O}(m^{4/3})))\\
&=(\sin\beta,-\cos\beta,mh^{\rm II}_{1\,d}+\mathcal{O}(m^{5/3}))-(m^2h^{\rm II}_{1\,s}h^{\rm II}_{1\,d}+\mathcal{O}(m^{8/3}))(x_s,\xi_x x_s,\mathcal{O}(m)),
\end{aligned}
$$

(2.2.51c)

$$
\begin{aligned}
&({\varphi^*}^{\rm III}_{z^*},{\psi^*}^{\rm III}_{z^*},{u^*}_{z^*})-({\varphi^*}^{\rm III}_{s^*}{\varphi^*}^{\rm III}_{z^*}+{\psi^*}^{\rm III}_{s^*}{\psi^*}^{\rm III}_{z^*}+{u^*}_{s^*}{u^*}_{z^*})({\varphi^*}^{\rm III}_{s^*},{\psi^*}^{\rm III}_{s^*},{u^*}_{s^*})\\
&=\Big(\frac{Q}{L}(m^{2/3}D_{1u}u_z+m^{4/3}D_{2u}u_z+\mathcal{O}(m^2))\sin\beta,-\frac{Q}{L}(m^{2/3}D_{1u}u_z+m^{4/3}D_{2u}u_z+\mathcal{O}(m^2))\cos\beta,u_z\Big)\\
&-\eta\mathbf{b}\\
&=\frac{1}{1+m^{2/3}\bar{u}_1+\mathcal{O}(m^{4/3})}\Big((m^{1/3}D_{1u}+mD_{2u})\sin\beta+\mathcal{O}(m^{5/3}),\\
&\qquad\qquad-(m^{1/3}D_{1u}+mD_{2u})\cos\beta+\mathcal{O}(m^{5/3}),1\Big)-\eta\mathbf{b}\\
&=\Big((m^{1/3}D_{1u}-m\bar{u}_1D_{1u}+mD_{2u})\sin\beta+\mathcal{O}(m^{5/3}),-(m^{1/3}D_{1u}-m\bar{u}_1D_{1u}+mD_{2u})\cos\beta+\mathcal{O}(m^{5/3}),\\
&1-m^{2/3}\bar{u}_1+\mathcal{O}(m^{4/3})\Big)-\eta\mathbf{b},
\end{aligned}
$$

where

$$
\begin{aligned}
\eta =& {\varphi^*}^{\mathrm{III}}_{s^*}{\varphi^*}^{\mathrm{III}}_{z^*} + {\psi^*}^{\mathrm{III}}_{s^*}{\psi^*}^{\mathrm{III}}_{z^*} + {u^*}_{s^*}{u^*}_{z^*} \\
=& \frac{Q}{L}\big[x_s + m^{2/3}(D_{1s} + \frac{L}{Q}D_{1u}u_s)\sin\beta + m^{2/3}D_1\beta_s\cos\beta + \mathcal{O}(m^{4/3})\big]\big[m^{2/3}D_{1u}u_z + m^{4/3}D_{2u}u_z \\
&+ \mathcal{O}(m^2)\big]\sin\beta \\
&- \frac{Q}{L}\big[\xi_x x_s - m^{2/3}(D_{1s} + \frac{L}{Q}D_{1u}u_s)\cos\beta + m^{2/3}D_1\beta_s\sin\beta + \mathcal{O}(m^{4/3})\big]\big[m^{2/3}D_{1u}u_z + m^{4/3}D_{2u}u_z \\
&+ \mathcal{O}(m^2)\big]\cos\beta + \frac{L}{Q}u_s u_z \\
=& u_z\Big\{\big[x_s + m^{2/3}(D_{1s} - \frac{L}{Q}z\frac{m^{2/3}\bar{u}_{1s} + \mathcal{O}(m^{4/3})}{(1 + m^{2/3}\bar{u}_1 + \mathcal{O}(m^{4/3}))^2}D_{1u})\sin\beta + m^{2/3}D_1\beta_s\cos\beta + \mathcal{O}(m^{4/3})\big] \\
&\quad \big[m^{1/3}D_{1u} + mD_{2u} + \mathcal{O}(m^{5/3})\big]\sin\beta \\
&\quad - \big[\xi_x x_s - m^{2/3}(D_{1s} - \frac{L}{Q}z\frac{m^{2/3}\bar{u}_{1s} + \mathcal{O}(m^{4/3})}{(1 + m^{2/3}\bar{u}_1 + \mathcal{O}(m^{4/3}))^2}D_{1u})\cos\beta + m^{2/3}D_1\beta_s\sin\beta + \mathcal{O}(m^{4/3})\big] \\
&\quad \big[m^{1/3}D_{1u} + mD_{2u} + \mathcal{O}(m^{5/3})\big]\cos\beta - \frac{L}{Q}z\frac{m^{2/3}\bar{u}_{1s} + \mathcal{O}(m^{4/3})}{(1 + m^{2/3}\bar{u}_1 + \mathcal{O}(m^{4/3}))^2}\Big\} \\
=& u_z\big[(m^{1/3}D_{1u} + mD_{2u})(x_s\sin\beta - \xi_x x_s\cos\beta) + mD_{1s}D_{1u}(\sin^2\beta + \cos^2\beta) \\
&+ mD_1D_{1u}\beta_s(\cos\beta\sin\beta - \sin\beta\cos\beta) - mz\bar{u}_{1s} + \mathcal{O}(m^{4/3})\big] \\
=& \frac{1}{1 + m^{2/3}\bar{u}_1 + \mathcal{O}(m^{4/3})}\big[mD_{1s}D_{1u} - mz\bar{u}_{1s} + \mathcal{O}(m^{4/3})\big] \\
=& mD_{1s}D_{1u} - mz\bar{u}_{1s} + \mathcal{O}(m^{4/3}),
\end{aligned}
$$

and

$$
\begin{aligned}
\mathbf{b} =& ({\varphi^*}^{\mathrm{III}}_{s^*}, {\psi^*}^{\mathrm{III}}_{s^*}, {u^*}_{s^*}) \\
=& \Big(x_s + m^{2/3}(D_{1s} + \underbrace{\frac{L}{Q}D_{1u}u_s}_{\mathcal{O}(m)})\sin\beta + m^{2/3}D_1\beta_s\cos\beta + \mathcal{O}(m^{4/3}), \\
&\xi_x x_s - m^{2/3}(D_{1s} + \underbrace{\frac{L}{Q}D_{1u}u_s}_{\mathcal{O}(m)})\cos\beta + m^{2/3}D_1\beta_s\sin\beta + \mathcal{O}(m^{4/3}), -\frac{L}{Q}z\frac{m^{2/3}\bar{u}_{1s} + \mathcal{O}(m^{4/3})}{(1 + m^{2/3}\bar{u}_1 + \mathcal{O}(m^{4/3}))^2}\Big) \\
=& \Big(x_s + m^{2/3}D_{1s}\sin\beta + m^{2/3}D_1\beta_s\cos\beta + \mathcal{O}(m^{4/3}), \\
&\xi_x x_s - m^{2/3}D_{1s}\cos\beta + m^{2/3}D_1\beta_s\sin\beta + \mathcal{O}(m^{4/3}), -mz\bar{u}_{1s} + \mathcal{O}(m^{5/3})\Big).
\end{aligned}
$$

Substituting (2.2.51) into (2.2.50) we obtain

$$\begin{aligned}
&\frac{-(\sin\beta, -\cos\beta, mh^{\mathrm{I}}_{1d} + \mathcal{O}(m^{5/3})) + (m^2 h^{\mathrm{I}}_{1s} h^{\mathrm{I}}_{1d} + \mathcal{O}(m^{8/3}))(x_s, \xi_x x_s, \mathcal{O}(m))}{||(\sin\beta, -\cos\beta, mh^{\mathrm{I}}_{1d} + \mathcal{O}(m^{5/3})) - (m^2 h^{\mathrm{I}}_{1s} h^{\mathrm{I}}_{1d} + \mathcal{O}(m^{8/3}))(x_s, \xi_x x_s, \mathcal{O}(m))||} \\
&+\frac{(\sin\beta, -\cos\beta, mh^{\mathrm{II}}_{1\,d} + \mathcal{O}(m^{5/3})) - (m^2 h^{\mathrm{II}}_{1\,s} h^{\mathrm{II}}_{1\,d} + \mathcal{O}(m^{8/3}))(x_s, \xi_x x_s, \mathcal{O}(m))}{||(\sin\beta, -\cos\beta, mh^{\mathrm{II}}_{1\,d} + \mathcal{O}(m^{5/3})) - (m^2 h^{\mathrm{II}}_{1\,s} h^{\mathrm{II}}_{1\,d} + \mathcal{O}(m^{8/3}))(x_s, \xi_x x_s, \mathcal{O}(m))||} \\
&+m\frac{(a_1, a_2, a_3)}{||(a_1, a_2, a_3)||} = 0,
\end{aligned} \tag{2.2.52}$$

where

$$\begin{aligned}
a_1 &= (m^{1/3} D_{1u} - m\bar{u}_1 D_{1u} + mD_{2u})\sin\beta \\
&\quad - \left[mD_{1s}D_{1u} - mz\bar{u}_{1s}\right]\left[x_s + m^{2/3}D_{1s}\sin\beta + m^{2/3}D_1\beta_s\cos\beta\right] + \mathcal{O}(m^{4/3}) \\
&= (m^{1/3} D_{1u} - m\bar{u}_1 D_{1u} + mD_{2u})\sin\beta - x_s(mD_{1s}D_{1u} - mz\bar{u}_{1s}) + \mathcal{O}(m^{4/3}) \\
a_2 &= -(m^{1/3} D_{1u} - m\bar{u}_1 D_{1u} + mD_{2u})\cos\beta \\
&\quad - \left[mD_{1s}D_{1u} - mz\bar{u}_{1s}\right]\left[\xi_x x_s - m^{2/3}D_{1s}\cos\beta + m^{2/3}D_1\beta_s\sin\beta\right] + \mathcal{O}(m^{4/3}) \\
&= -(m^{1/3} D_{1u} - m\bar{u}_1 D_{1u} + mD_{2u})\cos\beta - \xi_x x_s(mD_{1s}D_{1u} - mz\bar{u}_{1s}) + \mathcal{O}(m^{4/3}) \\
a_3 &= 1 - m^{2/3}\bar{u}_1 + (mD_{1s}D_{1u} - mz\bar{u}_{1s})mz\bar{u}_{1s} + \mathcal{O}(m^{4/3}) \\
&= 1 - m^{2/3}\bar{u}_1 + \mathcal{O}(m^{4/3}).
\end{aligned}$$

Hence, if we consider the third coordinate in equation (2.2.52) to $\mathcal{O}(m^{5/3})$ accuracy, we obtain

$$\frac{-mh^{\mathrm{I}}_{1d} + \mathcal{O}(m^{5/3})}{\sqrt{1+\mathcal{O}(m^2)}} + \frac{mh^{\mathrm{II}}_{1\,d} + \mathcal{O}(m^{5/3})}{\sqrt{1+\mathcal{O}(m^2)}} + m\frac{1+\mathcal{O}(m^{2/3})}{\sqrt{1+\mathcal{O}(m^{2/3})}} = 0, \tag{2.2.53}$$

which after division by m and tending m to zero, $m \downarrow 0$ leads to

$$-h^{\mathrm{I}}_{1d} + h^{\mathrm{II}}_{1\,d} + 1 = 0;$$

namely,

$$h^{\mathrm{I}}_{1d}(0,s,t) - h^{\mathrm{II}}_{1\,d}(0,s,t) = 1. \tag{2.2.54}$$

If we now consider the first coordinate of equation (2.2.52) to $\mathcal{O}(m^{7/3})$ accuracy, we obtain

$$\begin{aligned}
&\frac{-\sin\beta + m^2 h^{\mathrm{I}}_{1s} h^{\mathrm{I}}_{1d} x_s + \mathcal{O}(m^{8/3})}{\sqrt{1 + m^2 {h^{\mathrm{I}}_{1d}}^2 + \mathcal{O}(m^4)}} + \frac{\sin\beta - m^2 h^{\mathrm{II}}_{1\,s} h^{\mathrm{II}}_{1\,d} x_s + \mathcal{O}(m^{8/3})}{\sqrt{1 + m^2 {h^{\mathrm{II}}_{1\,d}}^2 + \mathcal{O}(m^4)}} \\
&+m\frac{(m^{1/3} D_{1u} - m\bar{u}_1 D_{1u} + mD_{2u})\sin\beta - x_s(mD_{1s}D_{1u} - mz\bar{u}_{1s}) + \mathcal{O}(m^{4/3})}{\sqrt{1+\mathcal{O}(m^{2/3})}} = 0.
\end{aligned} \tag{2.2.55}$$

By considering the Taylor expansion for expressions of the general form

$$\frac{a + bm^2}{\sqrt{1+cm^2}} \sim a + \frac{m^2}{2}(2b - ac) + \mathcal{O}(m^4), \tag{2.2.56}$$

we get from equation (2.2.55)

$$-\sin\beta+\frac{m^2}{2}(2h^{\mathrm{I}}_{1s}h^{\mathrm{I}}_{1d}x_s+h^{\mathrm{I}\,2}_{1d}\sin\beta)+\sin\beta+\frac{m^2}{2}(-2h^{\mathrm{II}}_{1\ s}h^{\mathrm{II}}_{1\ d}x_s-h^{\mathrm{II}2}_{1\ d}\sin\beta)+\mathcal{O}(m^{8/3})$$
$$+\frac{(m^{4/3}D_{1u}-m^2\bar{u}_1D_{1u}+m^2D_{2u})\sin\beta-x_s(m^2D_{1s}D_{1u}-m^2z\bar{u}_{1s})+\mathcal{O}(m^{7/3})}{\sqrt{1+\mathcal{O}(m^{2/3})}}=0.$$

Dividing this expression by $m^{4/3}$ and letting $m\downarrow 0$, we get

$$D_{1u}(s,\bar{u},t)=0, \tag{2.2.57}$$

which implies that $D_1\equiv 0$ (I SHALL ADD AN EXPLANATION...). And, if we now divide the same expression by m^2 and let $m\downarrow 0$, we obtain

$$(h^{\mathrm{I}}_{1s}h^{\mathrm{I}}_{1d}x_s-h^{\mathrm{II}}_{1\ s}h^{\mathrm{II}}_{1\ d}x_s)+\frac{1}{2}(h^{\mathrm{I}\,2}_{1d}-h^{\mathrm{II}2}_{1\ d})\sin\beta_0+D_{2u}\sin\beta_0+z\bar{u}_{1s}x_s=0. \tag{2.2.58}$$

Using (2.2.25), we deduce that

$$h^{\mathrm{I}}_{1s}(0,s,t)=h^{\mathrm{II}}_{1\ s}(0,s,t)=\bar{u}_{1s}(s,t),$$

and, by assumption $z=\bar{u}=1+\mathcal{O}(m^{2/3})$ along the groove root. So, from (2.2.58), using the identity (2.1.5e), we obtain

$$h^{\mathrm{I}}_{1s}(h^{\mathrm{I}}_{1d}-h^{\mathrm{II}}_{1\ d})\cos\beta_0+\frac{1}{2}(h^{\mathrm{I}}_{1d}-h^{\mathrm{II}}_{1\ d})(h^{\mathrm{I}}_{1d}+h^{\mathrm{II}}_{1\ d})\sin\beta_0+D_{2u}\sin\beta_0+h^{\mathrm{I}}_{1s}\cos\beta_0=0. \tag{2.2.59}$$

Finally, we using (2.2.54), we obtain

$$D_{2u}(s,\bar{u},t)=-\frac{1}{2}\left[h^{\mathrm{I}}_{1d}(0,s,t)+h^{\mathrm{II}}_{1\ d}(0,s,t)\right]-2h^{\mathrm{I}}_{1s}(0,s,t)\cot\beta_0. \tag{2.2.60}$$

2.2.6 Mean Curvature equation

The purpose of this section is to obtain the mean curvature equation, which governs the motion of the surface X^{III}, in terms of dimensionless unknown function $\xi(x(s,t),t)$, $V(t)$, $D(s,u(s,z,t),t)$, and $h^j(s,d,t),\ j=\mathrm{I},\mathrm{II}$, which were introduced in Section 2.1.

We begin by recalling that the original equation of the mean curvature (with dimensions) is given by

$$\mathbf{V}^{*\mathrm{III}}=AK^{*\mathrm{III}},$$

which after substituting dimensionless $\mathbf{V}^{\mathrm{III}},K^{\mathrm{III}}$, given in (2.2.2), leads to

$$\frac{A}{Q}\mathbf{V}^{\mathrm{III}}=\frac{A}{Q}K^{\mathrm{III}}.$$

Hence, the dimensionless equation of mean curvature is given by

$$\mathbf{V}^{\mathrm{III}}=K^{\mathrm{III}}, \tag{2.2.61}$$

where by (2.2.2), the dimensionless mean curvature of the surface $X^{\mathrm{III}} = X^{\mathrm{III}}(s,z,t)$ may be expressed as

(2.2.62)

$$K^{\mathrm{III}} = QK^{*\mathrm{III}}$$
$$= Q\frac{< ||X^{*\mathrm{III}}_{s^*}||^2 X^{*\mathrm{III}}_{z^*z^*} - 2 < X^{*\mathrm{III}}_{s^*}, X^{*\mathrm{III}}_{z^*} > X^{*\mathrm{III}}_{s^*z^*} + ||X^{*\mathrm{III}}_{z^*}||^2 X^{*\mathrm{III}}_{s^*s^*}, X^{*\mathrm{III}}_{s^*} \times X^{*\mathrm{III}}_{z^*} >}{2\left(||X^{*\mathrm{III}}_{s^*}||^2 ||X^{*\mathrm{III}}_{z^*}||^2 - < X^{*\mathrm{III}}_{s^*}, X^{*\mathrm{III}}_{z^*} >^2\right)^{3/2}}.$$

We wish now to obtain an explicit expression for K^{III} in terms of coordinates introduced in (2.1.1). We note that

$$(2.2.63)\quad X^{\mathrm{III}}_s \times X^{\mathrm{III}}_z = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \varphi^{\mathrm{III}}_s & \psi^{\mathrm{III}}_s & u_s \\ \varphi^{\mathrm{III}}_z & \psi^{\mathrm{III}}_z & u_z \end{vmatrix} = (\psi^{\mathrm{III}}_s u_z - u_s \psi^{\mathrm{III}}_z, -\varphi^{\mathrm{III}}_s u_z + u_s \varphi^{\mathrm{III}}_z, \varphi^{\mathrm{III}}_s \psi^{\mathrm{III}}_z - \psi^{\mathrm{III}}_s \varphi^{\mathrm{III}}_z).$$

For simplicity, throughout this section we shall adopt the notation, φ for φ^{III} and ψ for ψ^{III}.

Using the expressions for the derivatives (2.2.4) and (2.2.5), the Taylor expansions (2.2.8), the identities (2.1.5), and that Young's Law implies that $D_1 = 0$, we obtain

(2.2.64a)

$$||X^*{}_{s^*}||^2 X^*{}_{z^*z^*} = (\varphi^{*2}_{s^*} + \psi^{*2}_{s^*} + u^{*2}_{s^*})(\varphi^*{}_{z^*z^*}, \psi^*{}_{z^*z^*}, u^*{}_{z^*z^*})$$
$$= \frac{Q}{L^2}(\underbrace{x_s^2 + \xi_x^2 x_s^2}_{=1} + \mathcal{O}(m^{4/3}))(m^{4/3} D_{2uu} u_z^2 \sin\beta + \mathcal{O}(m^2), -m^{4/3} D_{2uu} u_z^2 \cos\beta + \mathcal{O}(m^2), 0)$$
$$= \frac{m}{L} \underbrace{u_z^2}_{=1+\mathcal{O}(m^{2/3})} (D_{2uu}\sin\beta, -D_{2uu}\cos\beta, 0) + \mathcal{O}(m^{5/3}),$$
$$= \frac{m}{L}(D_{2uu}\sin\beta, -D_{2uu}\cos\beta, 0) + \mathcal{O}(m^{5/3}),$$

(2.2.64b)

$$< X^*_{s^*}, X^*_{z^*} > X^*_{s^*z^*} = (\varphi^*{}_{s^*}\varphi^*{}_{z^*} + \psi^*{}_{s^*}\psi^*{}_{z^*} + u^*{}_{s^*}u^*{}_{z^*})(\varphi^*{}_{s^*z^*}, \psi^*{}_{s^*z^*}, u^*{}_{s^*z^*})$$
$$= (\frac{Q}{L} m^{4/3} x_s D_{2u} u_z \underbrace{(\sin\beta - \xi_x \cos\beta)}_{=0} - \frac{L}{Q} z m^{2/3} \frac{\bar{u}_{1s} + \mathcal{O}(m^{2/3})}{(1 + m^{2/3}\bar{u}_1 + \mathcal{O}(m^{4/3}))^3} + \mathcal{O}(m^2))$$
$$(\mathcal{O}(m^{4/3}), \mathcal{O}(m^{4/3}), -\frac{1}{Q} m^{2/3} \frac{\bar{u}_{1s} + \mathcal{O}(m^{2/3})}{(1 + m^{2/3}\bar{u}_1 + \mathcal{O}(m^{4/3}))^2}) = \mathcal{O}(m^{5/3}),$$

(2.2.64c)

$$||X^*{}_{z^*}||^2 X^*{}_{s^*s^*} = (\varphi^{*2}_{z^*} + \psi^{*2}_{z^*} + u^{*2}_{z^*})(\varphi^*{}_{s^*s^*}, \psi^*{}_{s^*s^*}, u^*{}_{s^*s^*})$$
$$= \frac{1}{Q}(\underbrace{\frac{Q^2}{L^2} m^{8/3}}_{=\mathcal{O}(m^2)} D_{2u}{}^2 u_z^2 (\sin^2\beta + \cos^2\beta) + \frac{1}{(1 + m^{2/3}\bar{u}_1 + \mathcal{O}(m^{4/3}))^2})$$

$$(x_{ss}+\mathcal{O}(m^{4/3}), \xi_{xx}x_s^2+\xi_x x_{ss}+\mathcal{O}(m^{4/3}), -mz\frac{\bar{u}_{1ss}}{(1+m^{2/3}\bar{u}_1+\mathcal{O}(m^{4/3}))^3}+\mathcal{O}(m^{4/3}))$$
$$= \frac{1}{Q}(x_{ss}, \xi_{xx}x_s^2+\xi_x x_{ss}, 0) - 2\frac{m^{2/3}}{Q}\bar{u}_1(x_{ss}, \xi_{xx}x_s^2+\xi_x x_{ss}, 0)$$
$$-\frac{m}{Q}(0,0,z\bar{u}_{1ss})+\mathcal{O}(m^{4/3}),$$

(2.2.64d)

$$X^*_{s^*}\times X^*_{z^*} = (\psi^*{}_{s^*}u^*{}_{z^*} - u^*{}_{s^*}\psi^*{}_{z^*}, -\varphi^*{}_{s^*}u^*{}_{z^*}+u^*{}_{s^*}\varphi^*{}_{z^*}, \varphi^*{}_{s^*}\psi^*{}_{z^*}-\psi^*{}_{s^*}\varphi^*{}_{z^*})$$
$$= ((\xi_x x_s+\mathcal{O}(m^{4/3}))\frac{1}{1+m^{2/3}\bar{u}_1+\mathcal{O}(m^{4/3})} - z\underbrace{\frac{m^{2/3}\bar{u}_{1s}+\mathcal{O}(m^{4/3})}{(1+m^{2/3}\bar{u}_1+\mathcal{O}(m^{4/3}))^2}m}_{=\mathcal{O}(m^{5/3})} D_{2u}u_z\cos\beta,$$
$$-(x_s+\mathcal{O}(m^{4/3}))\frac{1}{1+m^{2/3}\bar{u}_1+\mathcal{O}(m^{4/3})} - z\underbrace{\frac{m^{2/3}\bar{u}_{1s}+\mathcal{O}(m^{4/3})}{(1+m^{2/3}\bar{u}_1+\mathcal{O}(m^{4/3}))^2}m}_{=\mathcal{O}(m^{5/3})} D_{2u}u_z\sin\beta,$$
$$-\frac{Q}{L}x_s m^{4/3}D_{2u}u_z(\cos\beta+\xi_x\sin\beta)+\mathcal{O}(m^{5/3}))$$
$$= (\xi_x x_s, -x_s, 0) - m^{2/3}\bar{u}_1(\xi_x x_s, -x_s, 0) - m\underbrace{u_z}_{=1+\mathcal{O}(m^{2/3})}(0,0,D_{2u}\underbrace{x_s\frac{1}{\cos\beta}}_{=1}) + \mathcal{O}(m^{4/3})$$
$$= (\xi_x x_s, -x_s, 0) - m^{2/3}\bar{u}_1(\xi_x x_s, -x_s, 0) - m(0,0,D_{2u}) + \mathcal{O}(m^{4/3}).$$

Hence, scalar multiplication of (2.2.64a)–(2.2.64c) by (2.2.64d) yields that the numerator of K^{III} is given by

(2.2.65)

$$\begin{aligned}
\text{Numerator of } K^{\text{III}} =& Q\Bigg[\frac{1}{Q}(\xi_x x_s x_{ss} - \xi_{xx}x_s^3 - \xi_x x_s x_{ss}) \\
&-\frac{m^{2/3}}{Q}\bar{u}_1(\xi_x x_s x_{ss} - \xi_{xx}x_s^3 - \xi_x x_s x_{ss} + 2\xi_x x_s x_{ss} - 2\xi_{xx}x_s^3 - 2\xi_x x_s x_{ss}) \\
&+\frac{m}{L}D_{2uu}x_s(\xi_x\sin\beta+\cos\beta)\Bigg] + \mathcal{O}(m^{4/3}) \\
=& Q\left[-\frac{1}{Q}\xi_{xx}x_s^3 + 3\frac{m^{2/3}}{Q}\bar{u}_1\xi_{xx}x_s^3 + \frac{m}{L}D_{2uu}x_s\frac{1}{\cos\beta}\right] + \mathcal{O}(m^{4/3}) \\
=& -\xi_{xx}x_s^3 + m^{2/3}(3\bar{u}_1\xi_{xx}x_s^3 + D_{2uu}) + \mathcal{O}(m^{4/3}).
\end{aligned}$$

The denominator of K^{III} is given by

(2.2.66)

$$\begin{aligned}\text{Denominator of } K^{\text{III}} =&2\big[({\varphi^*}^2_{s^*}+{\psi^*}^2_{s^*}+{u^*}^2_{s^*})({\varphi^*}^2_{z^*}+{\psi^*}^2_{z^*}+{u^*}^2_{z^*})\\ &-({\varphi^*}_{s^*}{\varphi^*}_{z^*}+{\psi^*}_{s^*}{\psi^*}_{z^*}+{u^*}_{s^*}{u^*}_{z^*})^2\big]^{3/2}\\ =&2\big[(\underbrace{x_s^2+\xi_x^2x_s^2}_{=1}+\mathcal{O}(m^{4/3}))(1-2m^{2/3}\bar{u}_1+\mathcal{O}(m^{4/3}))-\mathcal{O}(m^2)\big]^{3/2}\\ =&2\big[(1-2m^{2/3}\bar{u}_1)+\mathcal{O}(m^{4/3})\big]^{3/2},\end{aligned}$$

so,

$$K^{\text{III}}=\frac{-\xi_{xx}x_s^3+m^{2/3}(D_{2uu}+3\bar{u}_1\xi_{xx}x_s^3)+\mathcal{O}(m^{4/3})}{2\left[(1-2m^{2/3}\bar{u}_1)+\mathcal{O}(m^{4/3})\right]^{3/2}}. \tag{2.2.67}$$

On the other hand, using the expressions for the time derivatives (2.2.6), we get that the normal velocity is given by

$$\begin{aligned}\mathbf{V}^{*\text{III}}||n^*|| =&< {X^*}^{\text{III}}_{t^*},{X^*}^{\text{III}}_{s^*}\times {X^*}^{\text{III}}_{z^*}>\\ =&<(\varphi^*_{t^*},\psi^*_{t^*},u^*_{t^*}),(\psi^*_{s^*}u^*_{z^*}-u^*_{s^*}\psi^*_{z^*},-\varphi^*_{s^*}u^*_{z^*}+u^*_{s^*}\varphi^*_{z^*},\varphi^*_{s^*}\psi^*_{z^*}-\psi^*_{s^*}\varphi^*_{z^*})>,\end{aligned}$$

so, recalling that $n^*=X^*_{s^*}\times X^*_{z^*}$, we obtain that the dimensionless normal velocity is given by

(2.2.68)

$$\begin{aligned}\mathbf{V}^{\text{III}}||n|| =& \frac{Q}{A}\mathbf{V}^*||n^*||\\ =& \frac{Q}{A}<\frac{A}{Q}\big((x_t+V+\mathcal{O}(m^{4/3}),\xi_xx_t+\xi_t+\mathcal{O}(m^{4/3}),-\frac{L}{Q}z\frac{m^{2/3}\bar{u}_{1t}+\mathcal{O}(m^{4/3})}{(1+m^{2/3}\bar{u}_1+\mathcal{O}(m^{4/3}))^2}\big)\big),\\ &(\xi_xx_s,-x_s,0)-m^{2/3}\bar{u}_1(\xi_xx_s,-x_s,0)-m(0,0,D_{2u})+\mathcal{O}(m^{4/3})>\\ =&<(x_t+V,\xi_xx_t+\xi_t,0)-m(0,0,z\bar{u}_{1t})+\mathcal{O}(m^{4/3}),\\ &(\xi_xx_s,-x_s,0)-m^{2/3}\bar{u}_1(\xi_xx_s,-x_s,0)-m(0,0,D_{2u})+\mathcal{O}(m^{4/3})>\\ =& (\xi_xx_sx_t+V\xi_xx_s-\xi_xx_sx_t-\xi_tx_s)-m^{2/3}\bar{u}_1(\xi_xx_sx_t+V\xi_xx_s-\xi_xx_sx_t-\xi_tx_s)+\mathcal{O}(m^{4/3})\\ =& V\xi_xx_s-\xi_tx_s+m^{2/3}\bar{u}_1(\xi_tx_s-V\xi_xx_s)+\mathcal{O}(m^{4/3}).\end{aligned}$$

Now substituting (2.2.67) and (2.2.68) into (2.2.61), we deduce that the governing dimensionless equation of surface X^{III} is

(2.2.69)

$$V\xi_xx_s-\xi_tx_s+m^{2/3}\bar{u}_1(\xi_tx_s-V\xi_xx_s)+\mathcal{O}(m^{4/3})=\frac{-\xi_{xx}x_s^3+m^{2/3}(D_{2uu}+3\bar{u}_1\xi_{xx}x_s^3)+\mathcal{O}(m^{4/3})}{2(1-2m^{2/3}\bar{u}_1)+\mathcal{O}(m^{4/3})}.$$

Using the Taylor expansion in $m^{2/3}$

$$\frac{a+bm^{2/3}}{c+dm^{2/3}}\sim\frac{a}{c}+m^{2/3}\frac{bc-ad}{c^2}+\mathcal{O}(m^{4/3}), \tag{2.2.70}$$

we obtain

$$
\begin{aligned}
&V\xi_x x_s - \xi_t x_s + m^{2/3}\bar{u}_1(\xi_t x_s - V\xi_x x_s) + \mathcal{O}(m^{4/3}) \\
&\quad = \frac{-\xi_{xx}x_s^3}{2} + m^{2/3}\frac{D_{2uu} + 3\bar{u}_1\xi_{xx}x_s^3 - 2\bar{u}_1\xi_{xx}x_s^3}{2} + \mathcal{O}(m^{4/3}) \\
&\quad = \frac{-\xi_{xx}x_s^3}{2} + m^{2/3}\frac{D_{2uu} + \bar{u}_1\xi_{xx}x_s^3}{2} + \mathcal{O}(m^{4/3}).
\end{aligned}
\tag{2.2.71}
$$

Now, if we divide (2.2.71) by x_s and use the identities (2.1.5e) and (2.1.5f), we get

(2.2.72)

$$V\xi_x - \xi_t + m^{2/3}\bar{u}_1(\xi_t - V\xi_x) + \mathcal{O}(m^{4/3}) = \frac{-\xi_{xx}}{2(1+\xi_x^2)} + m^{2/3}\left(\frac{1}{2\cos\beta}D_{2uu} + \frac{\bar{u}_1\xi_{xx}}{2(1+\xi_x^2)}\right) + \mathcal{O}(m^{4/3}).$$

Taylor expansion in $m^{2/3}$ of expressions of general form

$$\frac{a + bm^{2/3}}{1 + (c + dm^{2/3})^2} \sim \frac{a}{1+c^2} + m^{2/3}\frac{b(1+c^2) - 2acd}{(1+c^2)^2} + \mathcal{O}(m^{4/3}), \tag{2.2.73}$$

leads that the Taylor expansion of $\xi(x,t)$ in $m^{2/3}$ up to order $\mathcal{O}(m^{4/3})$, is given by

(2.2.74)

$$\frac{\xi_{xx}}{(1+\xi_x^2)} = \frac{\xi_{0xx} + m^{2/3}\xi_{1xx}}{1 + (\xi_{0x} + m^{2/3}\xi_{1x})^2} \sim \frac{\xi_{0xx}}{1 + {\xi_{0x}}^2} + m^{2/3}\frac{\xi_{1xx}(1+\xi_{0x}^2) - 2\xi_{0xx}\xi_{0x}\xi_{1x}}{(1+{\xi_{0x}}^2)^2} + \mathcal{O}(m^{4/3}).$$

Hence, using (2.2.74), we obtain that Taylor expanding of the various terms in (2.2.72) yields that

(2.2.75)

$$
\begin{aligned}
&V_0\xi_{0x} - \xi_{0t} + m^{2/3}\bar{u}_1(\xi_{0t} - V_0\xi_{0x} + V_0\xi_{1x} + V_1\xi_{0x} - \xi_{1t}) + \mathcal{O}(m^{4/3}) \\
&= \frac{-\xi_{0xx}}{2(1+\xi_{0x}^2)} + m^{2/3}\Big(\frac{1}{2\cos\beta_0}D_{2uu} + \frac{\bar{u}_1\xi_{0xx}}{2(1+\xi_{0x}^2)} - \frac{\xi_{1xx}(1+\xi_{0x}^2) - 2\xi_{0xx}\xi_{0x}\xi_{1x}}{2(1+{\xi_{0x}}^2)^2}\Big) + \mathcal{O}(m^{4/3}).
\end{aligned}
$$

As we have seen in Section 2.2.7, since $\xi_0(x,t)$ corresponds to a traveling wave solution, $\xi_{0t} = 0$, so (2.2.75) can be written as

(2.2.76)

$$
\begin{aligned}
&V_0\xi_{0x} + m^{2/3}\bar{u}_1(-V_0\xi_{0x} + V_0\xi_{1x} + V_1\xi_{0x} - \xi_{1t}) + \mathcal{O}(m^{4/3}) \\
&= \frac{-\xi_{0xx}}{2(1+\xi_{0x}^2)} + m^{2/3}\Big(\frac{1}{2\cos\beta_0}D_{2uu} + \frac{\bar{u}_1\xi_{0xx}}{2(1+\xi_{0x}^2)} - \frac{\xi_{1xx}(1+\xi_{0x}^2) - 2\xi_{0xx}\xi_{0x}\xi_{1x}}{2(1+{\xi_{0x}}^2)^2}\Big) + \mathcal{O}(m^{4/3}).
\end{aligned}
$$

Thus, to the leading order we obtain

$$V_0\xi_{0x} = -\frac{\xi_{0xx}}{2(1+\xi_{0x}^2)}, \tag{2.2.77}$$

which, as we know, holds identically for the case $m = 0$.

Moreover, since (2.2.77) is satisfied, the term $-m^{2/3}\bar{u}_1V_0\xi_{0x}$ on the left hand side of the equation (2.2.76) cancels with the term $m^{2/3}\frac{\bar{u}_1\xi_{0xx}}{2(1+\xi_{0x}^2)}$ on the right hand side of equation (2.2.76).

So at order $\mathcal{O}(m^{2/3})$, we obtain

$$V_0\xi_{1x} + V_1\xi_{0x} - \xi_{1t} = \frac{1}{2\cos\beta_0} D_{2uu} - \frac{\xi_{1xx}(1+\xi_{0x}^2) - 2\xi_{0xx}\xi_{0x}\xi_{1x}}{2(1+{\xi_{0x}}^2)^2}. \tag{2.2.78}$$

Since none of the functions appearing in equation (2.2.78), except D_{2uu}, depend on u, integration of (2.2.78) with respect to u, $0 \le u \le 1$, yields

$$V_0\xi_{1x} + V_1\xi_{0x} - \xi_{1t} = \frac{1}{2\cos\beta_0} D_{2u}\Big|_0^1 - \frac{\xi_{1xx}(1+\xi_{0x}^2) - 2\xi_{0xx}\xi_{0x}\xi_{1x}}{2(1+{\xi_{0x}}^2)^2}. \tag{2.2.79}$$

Using Young's law (2.2.60) and the boundary condition (2.2.25) at $z = \bar{u}$ which corresponds to $u = 1$, we readily obtain

$$\begin{aligned} V_0\xi_{1x} + V_1\xi_{0x} - \xi_{1t} = &- \frac{1}{4\cos\beta_0}\left[h^{\mathrm{I}}_{1d}(0,s,t) + h^{\mathrm{II}}_{1\,d}(0,s,t)\right] - \frac{1}{\sin\beta_0} h^{\mathrm{I}}_{1s}(0,s,t) \\ &- \frac{\xi_{1xx}(1+\xi_{0x}^2) - 2\xi_{0xx}\xi_{0x}\xi_{1x}}{2(1+{\xi_{0x}}^2)^2}. \end{aligned} \tag{2.2.80}$$

Finally, subtracting of (2.2.80) from (2.2.78) yields

$$0 = \frac{1}{2\cos\beta_0} D_{2uu} + \frac{1}{4\cos\beta_0}\left[h^{\mathrm{I}}_{1d}(0,s,t) + h^{\mathrm{II}}_{1\,d}(0,s,t)\right] + \frac{1}{\sin\beta_0} h^{\mathrm{I}}_{1s}(0,s,t),$$

namely

$$D_{2uu} = -\frac{1}{2}\left[h^{\mathrm{I}}_{1d}(0,s,t) + h^{\mathrm{II}}_{1\,d}(0,s,t)\right] - 2h^{\mathrm{I}}_{1s}(0,s,t)\cot\beta_0. \tag{2.2.81}$$

Since, the right hand side of (2.2.81) does not depend on z, equation (2.2.81) tells us that the function D_2 has a parabolic profile.

As for the function $\xi_1(x,t)$, it follows from (2.2.80), using the identity (2.1.5c) with respect to ξ_0, β_0, that $\xi_1(x,t)$ satisfies the one dimensional diffusion equation

(2.2.82)

$$\begin{aligned} V_0\xi_{1x} + V_1\xi_{0x} - \xi_{1t} = &- \frac{\xi_{1xx}}{2(1+{\xi_{0x}}^2)} + \frac{\xi_{0xx}\xi_{0x}\xi_{1x}}{(1+{\xi_{0x}}^2)^2} - \frac{1}{4}\left[h^{\mathrm{I}}_{1d}(0,s,t) + h^{\mathrm{II}}_{1\,d}(0,s,t)\right]\sqrt{1+\xi_{0x}^2} \\ &- h^{\mathrm{I}}_{1s}(0,s,t)\frac{\xi_{0x}}{\sqrt{1+\xi_{0x}^2}}. \end{aligned}$$

2.2.7 The solution in the case $m = 0$

When $m = 0$, there is no "groove root," so we can see our problem as a 2D problem. Suppose now that $\Gamma(x) = (\tilde{x}(t) + x, \xi(x,t))$ is a smooth curve in the xy-plane. The discussion here will parallel the discussion in Section 1.3, except for a difference in parametrization. The second coordinate of Γ, namely the function ξ, will depend now only on x and t as previously, while the first coordinate of Γ will depend on $\tilde{x}(t), x$ and t. This change of parametrization will effect only the normal velocity $\mathbf{V}$ of Γ, but not its mean curvature. Using the same notations as in the Section 1.3, we obtain that now the normal velocity is given by

$$\mathbf{V} = \frac{<(\tilde{x}_t, \xi_t), (\xi_x, -1)>}{\sqrt{1+\xi_x^2}} = \frac{\xi_x \tilde{x}_t - \xi_t}{\sqrt{1+\xi_x^2}}. \tag{2.2.83}$$

And the mean curvature may be expressed as

$$K = -\frac{\xi_{xx}}{2(1+\xi_x^2)^{3/2}}. \tag{2.2.84}$$

Here, K is half of the curvature, K, appearing in (1.3.5) (see Section 1.3), since, $K_{3D} = \frac{K_{2D}}{2}$, where K_{3D} is the mean curvature of Γ calculated by the $3D$ formula, and K_{2D} is calculated by means of $2D$ formula. So, in the case $m = 0$ we have obtained that our curve, which evolves by mean curvature, satisfies

$$\xi_x \tilde{x}_t - \xi_t = -\frac{\xi_{xx}}{2(1+\xi_x^2)}. \tag{2.2.85}$$

As in Section 1.3, we are interested in *traveling wave* solutions. As has already been mentioned, a traveling wave solution is a solution which "moves" with constant horizontal velocity (namely, parallel to the x-axis) V without changing its shape. In other words, the shape of $\xi(x - Vt_0, t_0)$ for some $t = t_0$ is identical to the shape of $\xi(x, 0)$ which was displaced Vt_0 units in the positive direction along the x-axis. Hence, the dependence of ξ on time t is only in the first coordinate of ξ, and we can conclude that in the case of current parametrization, $\xi_t = 0$ in the sense of partial derivative (of the second coordinate), and, from (2.2.85) we see that ξ satisfies the following equation

$$V\xi_x = -\frac{\xi_{xx}}{2(1+\xi_x^2)}, \tag{2.2.86}$$

where

$$V := \tilde{x}_t,$$

which is identical to (1.3.9) in Section 1.3, with $A = \frac{1}{2}$ and ξ instead of g. So we have seen that the function ξ appearing in the context of this section can be associated with the function g in Section 1.3. Thus the traveling wave solution of (2.2.86) can be written as

$$\xi(x) = \mp Q \pm \frac{2Q}{\pi} \arcsin\left(e^{-\frac{\pi}{2Q}x}\right), \tag{2.2.87}$$

where x does not depend on t.

As already has been mentioned, for practical calculations which will be done in the next chapter, we shall assume that $Q = 1$, so

$$\xi(x) = \mp 1 \pm \frac{2}{\pi} \arcsin\left(e^{-\frac{\pi}{2}x}\right), \tag{2.2.88}$$

and from (1.3.25) follows that when $A = \frac{1}{2}$ and $Q = 1$,

(2.2.89) $$V = \frac{\pi}{4}.$$

2.2.8 Surface diffusion

As explained in (2.2.26), the curvature of the surface X^{I} is given by

$$K^{*\mathrm{I}} = \frac{< ||X^{*\mathrm{I}}_{s^*}||^2 X^{*\mathrm{I}}_{d^*d^*} - 2 < X^{*\mathrm{I}}_{s^*}, X^{*\mathrm{I}}_{d^*} > X^{*\mathrm{I}}_{s^*d^*} + ||X^{*\mathrm{I}}_{d^*}||^2 X^{*\mathrm{I}}_{s^*s^*}, X^{*\mathrm{I}}_{s^*} \times X^{*\mathrm{I}}_{d^*} >}{2\left(||X^{*\mathrm{I}}_{s^*}||^2 ||X^{*\mathrm{I}}_{d^*}||^2 - < X^{*\mathrm{I}}_{s^*}, X^{*\mathrm{I}}_{d^*} >^2\right)^{3/2}}.$$

Hence, the dimensionless curvature of the surface X^{I} satisfies

(2.2.90) $$K^{\mathrm{I}} = QK^{*\mathrm{I}}.$$

Using the expressions for the partial derivatives given in (2.2.4) and (2.2.5), the Taylor expansions given in (2.2.8), and the identities given in (2.1.5), we obtain

(2.2.91a)

$$||X^{*\mathrm{I}}_{s^*}||^2 X^{*\mathrm{I}}_{d^*d^*} = ({\varphi^{*\mathrm{I}}_{s^*}}^2 + {\psi^{*\mathrm{I}}_{s^*}}^2 + {h^{*\mathrm{I}}_{s^*}}^2)(\varphi^{*\mathrm{I}}_{d^*d^*}, \psi^{*\mathrm{I}}_{d^*d^*}, h^{*\mathrm{I}}_{d^*d^*})$$
$$= \left[(x_s + d\beta_s \cos\beta)^2 + (\xi_x x_s + d\beta_s \sin\beta)^2 + \frac{L^2}{Q^2} m^{4/3} {h^{\mathrm{I}}_{1s}}^2 + \mathcal{O}(m^2)\right] (0, 0, \frac{L}{Q^2} m^{2/3} h^{\mathrm{I}}_{1dd} + \mathcal{O}(m^{5/3}))$$
$$= [x_s^2 + 2dx_s\beta_s\cos\beta + d^2\beta_s^2\cos^2\beta + \xi_x^2 x_s^2 + 2d\xi_x x_s \beta_s \sin\beta + d^2\beta_s^2 \sin^2\beta + \mathcal{O}(m^2)]$$
$$(0, 0, \frac{m}{Q} h^{\mathrm{I}}_{1dd} + \mathcal{O}(m^{5/3}))$$
$$= [1 + 2d\beta_s \underbrace{x_s \frac{1}{\cos\beta}}_{=1} + d^2\beta_s^2 + \mathcal{O}(m^2)](0, 0, \frac{m}{Q} h^{\mathrm{I}}_{1dd} + \mathcal{O}(m^{5/3}))$$
$$= [1 + 2d\beta_s + d^2\beta_s^2](0, 0, \frac{m}{Q} h^{\mathrm{I}}_{1dd}) + \mathcal{O}(m^{5/3})$$
$$= (1 + d\beta_s)^2 (0, 0, \frac{m}{Q} h^{\mathrm{I}}_{1dd}) + \mathcal{O}(m^{5/3}),$$

(2.2.91b)

$$< X^{*\mathrm{I}}_{s^*}, X^{*\mathrm{I}}_{d^*} > X^{*\mathrm{I}}_{s^*d^*} = (\varphi^{*\mathrm{I}}_{s^*}\varphi^{*\mathrm{I}}_{d^*} + \psi^{*\mathrm{I}}_{s^*}\psi^{*\mathrm{I}}_{d^*} + h^{*\mathrm{I}}_{s^*}h^{*\mathrm{I}}_{d^*})(\varphi^{*\mathrm{I}}_{s^*d^*}, \psi^{*\mathrm{I}}_{s^*d^*}, h^{*\mathrm{I}}_{s^*d^*})$$
$$= \frac{1}{Q}\Big[(x_s + d\beta_s\cos\beta)\sin\beta + (\xi_x x_s + d\beta_s \sin\beta)(-\cos\beta) + \frac{L^2}{Q^2} m^{4/3} h^{\mathrm{I}}_{1s} h^{\mathrm{I}}_{1d} + \mathcal{O}(m^2)\Big]$$
$$(\beta_s\cos\beta, \beta_s\sin\beta, mh^{\mathrm{I}}_{1sd})$$
$$= \frac{1}{Q}\Big[x_s\sin\beta + d\beta_s\cos\beta\sin\beta - \xi_x x_s\cos\beta - d\beta_s\sin\beta\cos\beta + \mathcal{O}(m^2)\Big](\beta_s\cos\beta, \beta_s\sin\beta, mh^{\mathrm{I}}_{1sd})$$
$$= \mathcal{O}(m^2),$$

(2.2.91c)

$$||X^{*\mathrm{I}}_{d^*}||^2 X^{*\mathrm{I}}_{s^*s^*} = ({\varphi^{*\mathrm{I}}_{d^*}}^2 + {\psi^{*\mathrm{I}}_{d^*}}^2 + {h^{*\mathrm{I}}_{d^*}}^2)(\varphi^{*\mathrm{I}}_{s^*s^*}, \psi^{*\mathrm{I}}_{s^*s^*}, h^{*\mathrm{I}}_{s^*s^*})$$

$$= \frac{1}{Q}\left[\sin^2\beta + \cos^2\beta + \frac{L^2}{Q^2}m^{4/3}{h^{\mathrm{I}}_{1d}}^2 + \mathcal{O}(m^2)\right]$$

$$(x_{ss} + d\beta_{ss}\cos\beta - d\beta_s^2\sin\beta, \xi_{xx}x_s^2 + \xi_x x_{ss} + d\beta_{ss}\sin\beta + d\beta_s^2\cos\beta, mh^{\mathrm{I}}_{1ss} + \mathcal{O}(m^{5/3}))$$

$$= \frac{1}{Q}(x_{ss} + d\beta_{ss}\cos\beta - d\beta_s^2\sin\beta, \xi_{xx}x_s^2 + \xi_x x_{ss} + d\beta_{ss}\sin\beta + d\beta_s^2\cos\beta, mh^{\mathrm{I}}_{1ss}) + \mathcal{O}(m^{5/3}),$$

(2.2.91d)

$$X^{*\mathrm{I}}_{s^*} \times X^{*\mathrm{I}}_{d^*} = (h^{*\mathrm{I}}_{d^*}\psi^{*\mathrm{I}}_{s^*} - \psi^{*\mathrm{I}}_{d^*}h^{*\mathrm{I}}_{s^*}, -h^{*\mathrm{I}}_{d^*}\varphi^{*\mathrm{I}}_{s^*} + \varphi^{*\mathrm{I}}_{d^*}h^{*\mathrm{I}}_{s^*}, \varphi^{*\mathrm{I}}_{s^*}\psi^{*\mathrm{I}}_{d^*} - \psi^{*\mathrm{I}}_{s^*}\varphi^{*\mathrm{I}}_{d^*})$$

$$= \Big(\frac{L}{Q}m^{2/3}h^{\mathrm{I}}_{1d}(\xi_x x_s + d\beta_s\sin\beta) + \frac{L}{Q}m^{2/3}h^{\mathrm{I}}_{1s}\cos\beta + \mathcal{O}(m^{5/3}),$$

$$- \frac{L}{Q}m^{2/3}h^{\mathrm{I}}_{1d}(x_s + d\beta_s\cos\beta) + \frac{L}{Q}m^{2/3}h^{\mathrm{I}}_{1s}\sin\beta + \mathcal{O}(m^{5/3}),$$

$$- (x_s + d\beta_s\cos\beta)\cos\beta - (\xi_x x_s + d\beta_s\sin\beta)\sin\beta\Big)$$

$$= (0, 0, -x_s\cos\beta - d\beta_s\cos^2\beta - \xi_x x_s\sin\beta - d\beta_s\sin^2\beta)$$

$$+ m\Big(h^{\mathrm{I}}_{1d}(\xi_x x_s + d\beta_s\sin\beta) + h^{\mathrm{I}}_{1s}\cos\beta, -h^{\mathrm{I}}_{1d}(x_s + d\beta_s\cos\beta) + h^{\mathrm{I}}_{1s}\sin\beta, 0\Big) + \mathcal{O}(m^{5/3})$$

$$= (0, 0, -x_s\frac{1}{\cos\beta} - d\beta_s) + m\Big(h^{\mathrm{I}}_{1d}(\xi_x x_s + d\beta_s\sin\beta) + h^{\mathrm{I}}_{1s}\cos\beta, -h^{\mathrm{I}}_{1d}(x_s + d\beta_s\cos\beta) + h^{\mathrm{I}}_{1s}\sin\beta, 0\Big)$$

$$+ \mathcal{O}(m^{5/3})$$

$$= (0, 0, -1 - d\beta_s) + m\Big(h^{\mathrm{I}}_{1d}(\xi_x x_s + d\beta_s\sin\beta) + h^{\mathrm{I}}_{1s}\cos\beta, -h^{\mathrm{I}}_{1d}(x_s + d\beta_s\cos\beta) + h^{\mathrm{I}}_{1s}\sin\beta, 0\Big)$$

$$+ \mathcal{O}(m^{5/3}).$$

Hence, using the identities in (2.1.5), we obtain that the dimensionless inner product of (2.2.91a)–

(2.2.91c) with (2.2.91d) is

(2.2.92)

$$
\begin{aligned}
\text{Numerator of } K^{\mathrm{I}} = {} & Q\Big\{\frac{m}{Q}\Big\{(-1-d\beta_s)\Big[(1+d\beta_s)^2 h^{\mathrm{I}}_{1dd} + h^{\mathrm{I}}_{1ss}\Big] \\
& + \Big[h^{\mathrm{I}}_{1d}(\xi_x x_s + d\beta_s \sin\beta) + h^{\mathrm{I}}_{1s}\cos\beta\Big](x_{ss} + d\beta_{ss}\cos\beta - d\beta_s^2\sin\beta) \\
& + \Big[-h^{\mathrm{I}}_{1d}(x_s + d\beta_s\cos\beta) + h^{\mathrm{I}}_{1s}\sin\beta\Big](\xi_{xx}x_s^2 + \xi_x x_{ss} + d\beta_{ss}\sin\beta + d\beta_s^2\cos\beta)\Big\} \\
& + \mathcal{O}(m^{5/3}) \\
= {} & m\Big\{-(1+d\beta_s)^3 h^{\mathrm{I}}_{1dd} - (1+d\beta_s)h^{\mathrm{I}}_{1ss} \\
& + h^{\mathrm{I}}_{1d}\Big[\xi_x x_s x_{ss} + d x_{ss}\beta_s\sin\beta + d\xi_x x_s\beta_{ss}\cos\beta + d^2\beta_s\beta_{ss}\sin\beta\cos\beta \\
& - d\xi_x x_s\beta_s^2\sin\beta - d^2\beta_s^3\sin^2\beta - \xi_{xx}x_s^3 - d\xi_{xx}x_s^2\beta_s\cos\beta \\
& - \xi_x x_{ss}x_s - d\xi_x x_{ss}\beta_s\cos\beta - d x_s\beta_{ss}\sin\beta - d^2\beta_s\beta_{ss}\cos\beta\sin\beta \\
& - d x_s\beta_s^2\cos\beta - d^2\beta_s^3\cos^2\beta\Big] \\
& + h^{\mathrm{I}}_{1s}\Big[x_{ss}\cos\beta + d\beta_{ss}\cos^2\beta - d\beta_s^2\sin\beta\cos\beta \\
& + \xi_{xx}x_s^2\sin\beta + \xi_x x_{ss}\sin\beta + d\beta_{ss}\sin^2\beta + d\beta_s^2\cos\beta\sin\beta\Big]\Big\} + \mathcal{O}(m^{5/3})\Big\} \\
= {} & m\Big\{-(1+d\beta_s)^3 h^{\mathrm{I}}_{1dd} - (1+d\beta_s)h^{\mathrm{I}}_{1ss} \\
& + h^{\mathrm{I}}_{1d}\Big[-d\xi_x x_s\beta_s^2\sin\beta - d^2\beta_s^3 - \xi_{xx}x_s^3 - d\xi_{xx}x_s^2\beta_s\cos\beta - d x_s\beta_s^2\cos\beta\Big] \\
& + h^{\mathrm{I}}_{1s}\Big[x_{ss}\frac{1}{\cos\beta} + d\beta_{ss} + \xi_{xx}x_s^2\sin\beta\Big]\Big\} + \mathcal{O}(m^{5/3}) \\
= {} & m\Big\{-(1+d\beta_s)^3 h^{\mathrm{I}}_{1dd} - (1+d\beta_s)h^{\mathrm{I}}_{1ss} \\
& + h^{\mathrm{I}}_{1d}\Big[-d\beta_s^2\underbrace{x_s\frac{1}{\cos\beta}}_{=1} - d^2\beta_s^3 - \underbrace{\xi_{xx}x_s^3}_{=\beta_s x_s^2\frac{1}{\cos^2\beta}} - d\underbrace{\xi_{xx}x_s^2}_{\beta_s x_s\frac{1}{\cos^2\beta}}\beta_s\cos\beta\Big] \\
& + h^{\mathrm{I}}_{1s}\Big[d\beta_{ss} + \underbrace{x_{ss}\frac{1}{\cos\beta} + \xi_{xx}x_s^2\sin\beta}_{=0}\Big]\Big\} + \mathcal{O}(m^{5/3}) \\
= {} & m\Big\{-(1+d\beta_s)^3 h^{\mathrm{I}}_{1dd} - (1+d\beta_s)h^{\mathrm{I}}_{1ss} + h^{\mathrm{I}}_{1d}\beta_s(-2d\beta_s - d^2\beta_s^2 - 1) + d\beta_{ss}h^{\mathrm{I}}_{1s}\Big\} \\
& + \mathcal{O}(m^{5/3}) \\
= {} & -m\Big\{(1+d\beta_s)^3 h^{\mathrm{I}}_{1dd} + (1+d\beta_s)h^{\mathrm{I}}_{1ss} + \beta_s(1+d\beta_s)^2 h^{\mathrm{I}}_{1d} - d\beta_{ss}h^{\mathrm{I}}_{1s}\Big\} + \mathcal{O}(m^{5/3}).
\end{aligned}
$$

The denominator of K^{I} is given by

$$
\begin{aligned}
\text{Denominator of } K^{\mathrm{I}} &= 2\Big(||X^{*\mathrm{I}}_{s^*}||^2||X^{*\mathrm{I}}_{d^*}||^2 - <X^{*\mathrm{I}}_{s^*}, X^{*\mathrm{I}}_{d^*}>^2\Big)^{3/2} \\
&= 2\Big[({\varphi^{*\mathrm{I}}_{s^*}}^2 + {\psi^{*\mathrm{I}}_{s^*}}^2 + {h^{*\mathrm{I}}_{s^*}}^2)({\varphi^{*\mathrm{I}}_{d^*}}^2 + {\psi^{*\mathrm{I}}_{d^*}}^2 + {h^{*\mathrm{I}}_{d^*}}^2) \\
&\qquad - (\varphi^{*\mathrm{I}}_{s^*}\varphi^{*\mathrm{I}}_{d^*} + \psi^{*\mathrm{I}}_{s^*}\psi^{*\mathrm{I}}_{d^*} + h^{*\mathrm{I}}_{s^*}h^{*\mathrm{I}}_{d^*})^2\Big]^{3/2} \\
&= 2\Big[((1+d\beta_s)^2 + \mathcal{O}(m^2))(1+\mathcal{O}(m^2)) - O(m^4)\Big]^{3/2} \\
&= 2(1+d\beta_s)^3 + O(m^2).
\end{aligned} \tag{2.2.93}
$$

Hence, from (2.2.92) and (2.2.93) we obtain that

$$
K^{\mathrm{I}} = \frac{-m\left\{(1+d\beta_s)^3 h^{\mathrm{I}}_{1dd} + (1+d\beta_s)h^{\mathrm{I}}_{1ss} + \beta_s(1+d\beta_s)^2 h^{\mathrm{I}}_{1d} - d\beta_{ss}h^{\mathrm{I}}_{1s}\right\} + \mathcal{O}(m^{5/3})}{2(1+d\beta_s)^3 + O(m^2)}. \tag{2.2.94}
$$

On the other hand, by (1.2.9) we know that surface Laplacian of K^{I} is given by

$$
\begin{aligned}
\Delta_s K^{\mathrm{I}} &= \frac{1}{\sqrt{||X^{\mathrm{I}}_s||^2||X^{\mathrm{I}}_d||^2 - <X^{\mathrm{I}}_s, X^{\mathrm{I}}_d>^2}}\left\{\frac{\partial}{\partial s}\left(\frac{||X^{\mathrm{I}}_d||^2 K^{\mathrm{I}}_s - <X^{\mathrm{I}}_s, X^{\mathrm{I}}_d> K^{\mathrm{I}}_d}{\sqrt{||X^{\mathrm{I}}_s||^2||X^{\mathrm{I}}_d||^2 - <X^{\mathrm{I}}_s, X^{\mathrm{I}}_d>^2}}\right)\right. \\
&\left. + \frac{\partial}{\partial d}\left(\frac{||X^{\mathrm{I}}_s||^2 K^{\mathrm{I}}_d - <X^{\mathrm{I}}_s, X^{\mathrm{I}}_d> K^{\mathrm{I}}_s}{\sqrt{||X^{\mathrm{I}}_s||^2||X^{\mathrm{I}}_d||^2 - <X^{\mathrm{I}}_s, X^{\mathrm{I}}_d>^2}}\right)\right\}.
\end{aligned} \tag{2.2.95}
$$

So in the context of our analysis, the dimensionless surface Laplacian is given by

$$
\begin{aligned}
\Delta_s K^{\mathrm{I}} &= \frac{1}{(1+d\beta_s+\mathcal{O}(m^2))}\Big\{\frac{\partial}{\partial s}\Big(\frac{(1+\mathcal{O}(m^2))K^{\mathrm{I}}_s + \mathcal{O}(m^2)}{1+d\beta_s+\mathcal{O}(m^2)}\Big) \\
&\quad + \frac{\partial}{\partial d}\Big(\frac{((1+d\beta_s)^2+\mathcal{O}(m^2))K^{\mathrm{I}}_d + \mathcal{O}(m^2)}{1+d\beta_s+\mathcal{O}(m^2)}\Big)\Big\} \\
&= \frac{1}{(1+d\beta_s)}\Big\{\frac{\partial}{\partial s}\Big(\frac{K^{\mathrm{I}}_s}{1+d\beta_s}\Big) + \frac{\partial}{\partial d}\Big(\frac{(1+d\beta_s)^2 K^{\mathrm{I}}_d}{1+d\beta_s}\Big)\Big\} + \mathcal{O}(m^2) \\
&= \frac{1}{(1+d\beta_s)}\Big\{\frac{\partial}{\partial s}\Big(\frac{K^{\mathrm{I}}_s}{1+d\beta_s}\Big) + \frac{\partial}{\partial d}\Big((1+d\beta_s)K^{\mathrm{I}}_d\Big)\Big\} + \mathcal{O}(m^2).
\end{aligned} \tag{2.2.96}
$$

As to the normal velocity of the surface X^{I}, we readily obtain that

$$\begin{aligned}
\mathbf{V}^{*\mathrm{I}} &= < {X^*}^{\mathrm{I}}_{t^*}, \frac{{X^*}^{\mathrm{I}}_{s^*} \times {X^*}^{\mathrm{I}}_{d^*}}{||{X^*}^{\mathrm{I}}_{s^*} \times {X^*}^{\mathrm{I}}_{d^*}||} > \\
&= \frac{1}{1 + d\beta_s + \mathcal{O}(m^2)} < ({\varphi^*}^{\mathrm{I}}_{t^*}, {\psi^*}^{\mathrm{I}}_{t^*}, {h^*}^{\mathrm{I}}_{t^*}), ({\psi^*}^{\mathrm{I}}_{s^*}{h^*}^{\mathrm{I}}_{d^*} - {h^*}^{\mathrm{I}}_{s^*}{\psi^*}^{\mathrm{I}}_{d^*}, \\
&\qquad - {\varphi^*}^{\mathrm{I}}_{s^*}{h^*}^{\mathrm{I}}_{d^*} + {h^*}^{\mathrm{I}}_{s^*}{\varphi^*}^{\mathrm{I}}_{d^*}, {\varphi^*}^{\mathrm{I}}_{s^*}{\psi^*}^{\mathrm{I}}_{d^*} - {\psi^*}^{\mathrm{I}}_{s^*}{\varphi^*}^{\mathrm{I}}_{d^*}) > \\
&= \frac{A}{Q}\frac{1}{1 + d\beta_s + \mathcal{O}(m^2)} < (x_t + V + d\beta_t \cos\beta, \xi_x x_t + \xi_t + d\beta_t \sin\beta, \frac{L}{Q} m^{2/3} h^{\mathrm{I}}_{1t}) + \mathcal{O}(m^{5/3}), \\
&\quad (0, 0, -1 - d\beta_s) + m(h^{\mathrm{I}}_{1d}(\xi_x x_s + d\beta_s \sin\beta) + h^{\mathrm{I}}_{1s}\cos\beta, -h^{\mathrm{I}}_{1d}(x_s + d\beta_s\cos\beta) + h^{\mathrm{I}}_{1s}\sin\beta, 0) \\
&\quad + \mathcal{O}(m^{5/3}) > \\
&= \frac{A}{Q}\frac{m}{1 + d\beta_s}\Big\{-(1 + d\beta_s)h^{\mathrm{I}}_{1t} + (x_t + V + d\beta_t\cos\beta)\Big[h^{\mathrm{I}}_{1d}(\xi_x x_s + d\beta_s\sin\beta) + h^{\mathrm{I}}_{1s}\cos\beta\Big] \\
&\quad + (\xi_x x_t + \xi_t + d\beta_t \sin\beta)\Big[-h^{\mathrm{I}}_{1d}(x_s + d\beta_s\cos\beta) + h^{\mathrm{I}}_{1s}\sin\beta\Big]\Big\} + \mathcal{O}(m^{5/3}) \\
&= \frac{A}{Q}\frac{m}{1 + d\beta_s}\Big[-(1 + d\beta_s)h^{\mathrm{I}}_{1t} + (\xi_x x_s x_t + V\xi_x x_s + d\xi_x x_s\beta_t\cos\beta + dx_t\beta_s\sin\beta + dV\beta_s\sin\beta \\
&\quad + d^2\beta_t\beta_s\cos\beta\sin\beta - \xi_x x_t x_s - \xi_t x_s - dx_s\beta_t\sin\beta - d\xi_x x_t\beta_s\cos\beta \\
&\quad - d\xi_t\beta_s\cos\beta - d^2\beta_t\beta_s\sin\beta\cos\beta\big)\, h^{\mathrm{I}}_{1d} \\
&\quad + (x_t\cos\beta + V\cos\beta + d\beta_t\cos^2\beta + \xi_x x_t\sin\beta + \xi_t\sin\beta + d\beta_t\sin^2\beta)h^{\mathrm{I}}_{1s}\Big] + \mathcal{O}(m^{5/3}) \\
&= \frac{A}{Q}\frac{m}{1 + d\beta_s}\Big[-(1 + d\beta_s)h^{\mathrm{I}}_{1t} + (V \underbrace{\xi_x x_s}_{=\sin\beta} + dV\beta_s\sin\beta - \xi_t x_s - d\xi_t\beta_s\cos\beta)h^{\mathrm{I}}_{1d} \\
&\quad + (x_t\frac{1}{\cos\beta} + V\cos\beta + d\beta_t + \xi_t\sin\beta)h^{\mathrm{I}}_{1s}\Big] \\
&= \frac{A}{Q}\frac{m}{1 + d\beta_s}\Big[-(1 + d\beta_s)h^{\mathrm{I}}_{1t} + (V\sin\beta - \xi_t x_s)(1 + d\beta_s)h^{\mathrm{I}}_{1d} \\
&\quad + (x_t\frac{1}{\cos\beta} + V\cos\beta + d\beta_t + \xi_t\sin\beta)h^{\mathrm{I}}_{1s}\Big] + \mathcal{O}(m^{5/3}).
\end{aligned}$$

Thus, the dimensionless normal velocity to leading order is given by

$$\begin{aligned}
\mathbf{V}^{\mathrm{I}} = \frac{Q}{A}\mathbf{V}^{*\mathrm{I}} &= \frac{m}{1 + d\beta_{0s}}\Big[-(1 + d\beta_{0s})h^{\mathrm{I}}_{1t} + (V_0\sin\beta_0 - \xi_{0t}x_{0s})(1 + d\beta_{0s})h^{\mathrm{I}}_{1d} \\
&\quad + (x_{0t}\frac{1}{\cos\beta_0} + V_0\cos\beta_0 + d\beta_{0t} + \xi_{0t}\sin\beta_0)h^{\mathrm{I}}_{1s}\Big] + \mathcal{O}(m^{5/3}).
\end{aligned} \tag{2.2.97}$$

Now, as we have seen in the Section 2.2.7, since $\xi_0(x,t)$ corresponds to the traveling wave solution given by (2.2.87), which depends on x but not on t, $\xi_{0t} = 0$. Moreover, $x_{0t} = 0$, since x_0 does not depend on t, only $\tilde{x}_0$ depends on t (see fig. 2.2). Hence, we get that

$$\beta_{0t} = (\xi_{0xx}x_{0t} + \xi_{0xt})\cos^2\beta_0 = \xi_{0tx}\cos^2\beta_0 = 0, \tag{2.2.98}$$

and thus, also $\beta_{0t} = 0$. Using these conclusions in (2.2.97), we now get the following expression for dimensionless normal velocity to leading order

$$\mathbf{V}^{\mathrm{I}} = \frac{m}{1+d\beta_{0s}}\Big[-(1+d\beta_{0s})h^{\mathrm{I}}_{1t} + V_0\sin\beta_0(1+d\beta_{0s})h^{\mathrm{I}}_{1d} + V_0\cos\beta_0 h^{\mathrm{I}}_{1s}\Big] + \mathcal{O}(m^{5/3}). \tag{2.2.99}$$

Since, our original dimensional surface diffusion equation, as introduced in Section 1.2, was

$$\mathbf{V}^{*\mathrm{I}} = -B\Delta_{s^*}K^{*\mathrm{I}},$$

after substituting the dimensionless expressions for $\mathbf{V}^{\mathrm{I}}, K^{\mathrm{I}}$, given in (2.2.2), we get

$$\frac{A}{Q}\mathbf{V}^{\mathrm{I}} = -B\frac{1}{Q^3}\Delta_s K^{\mathrm{I}}.$$

Thus, our dimensionless formulation of surface diffusion is given by

$$\mathbf{V}^{\mathrm{I}} = -\frac{B}{AQ^2}\Delta_s K^{\mathrm{I}}. \tag{2.2.100}$$

Finally, substituting (2.2.96) and (2.2.99) into the surface diffusion equation (2.2.100), we obtain that to leading order, the surface diffusion equation for the surface X^{I} is given by

$$\begin{aligned} &h^{\mathrm{I}}_{1t} - V_0\sin\beta_0 h^{\mathrm{I}}_{1d} - \frac{1}{1+d\beta_{0s}}V_0\cos\beta_0 h^{\mathrm{I}}_{1s} \\ &= -\frac{B}{AQ^2}\frac{1}{1+d\beta_{0s}}\left\{\frac{\partial}{\partial s}\left(\frac{K^{\mathrm{I}}_{0s}}{1+d\beta_{0s}}\right) + \frac{\partial}{\partial d}\left((1+d\beta_{0s})K^{\mathrm{I}}_{0d}\right)\right\}, \end{aligned} \tag{2.2.101}$$

where

$$K^{\mathrm{I}}_0 = \frac{(1+d\beta_{0s})^3 h^{\mathrm{I}}_{1dd} + (1+d\beta_{0s})h^{\mathrm{I}}_{1ss} + \beta_{0s}(1+d\beta_{0s})^2 h^{\mathrm{I}}_{1d} - d\beta_{0ss}h^{\mathrm{I}}_{1s}}{2(1+d\beta_{0s})^3}. \tag{2.2.102}$$

(GEOMETRIC INTERPRETATION???)

Remark 1. *Since*

$$[A] = \frac{meter^2}{second}, \quad [B] = \frac{meter^4}{second}$$

we can define a change of variables which scales x by $\overline{x}$ and t by $\overline{t}$, where

$$\overline{x} = \sqrt{\frac{B}{A}} \quad \text{and} \quad \overline{t} = \frac{B}{A^2}. \tag{2.2.103}$$

Substituting these variables into our partial differential equations will eliminate the appearance of A and B in our equations.

2.2.9 Exterior boundary conditions

As to the exterior boundary conditions, we shall demand that the following conditions be satisfied at the boundaries of our domain (see fig. 2.10):

(2.2.104) $$h^{\mathrm{I}}(d,s,t) = \mathcal{O}(m^{4/3}), \quad \text{at } d = Q/2,$$

(2.2.105) $$h^{\mathrm{II}}(d,s,t) = \mathcal{O}(m^{4/3}), \quad \text{at } d = -Q/2,$$

(2.2.106) $$K^{\mathrm{I}}(d,s,t) = \mathcal{O}(m^{5/3}), \quad \text{at } d = Q/2,$$

(2.2.107) $$K^{\mathrm{II}}(d,s,t) = \mathcal{O}(m^{5/3}), \quad \text{at } d = -Q/2.$$

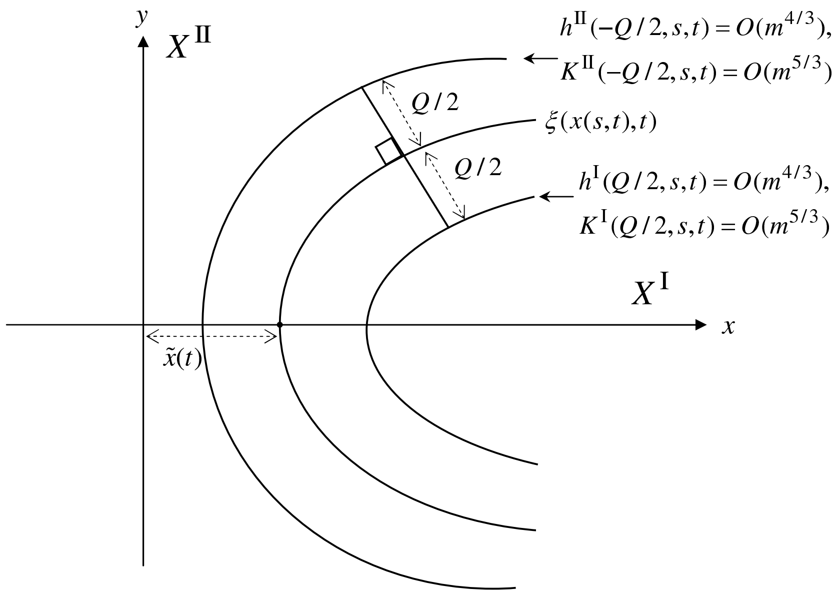

Figure 2.10: Boundary conditions for $d = \pm Q/2$.

ALTERNATIVELY MORE COMPLICATED BC MAY BE FOUND (FOR DETAILED EXPLANATION SEE **exterior bc.jpg** FILE)

We shall now write out the expression for the conditions (2.2.106)–(2.2.107) explicitly. Substituting $d = Q/2$ into $K_0^j,\ j = \mathrm{I}, \mathrm{II}$ given in (2.2.102), namely

$$K_0^j = \frac{(1+d\beta_{0s})^3 h^j_{1dd} + (1+d\beta_{0s})h^j_{1ss} + \beta_{0s}(1+d\beta_{0s})^2 h^j_{1d} - d\beta_{0ss}h^j_{1s}}{2(1+d\beta_{0s})^3}, \quad j = \mathrm{I}, \mathrm{II},$$

we see that conditions (2.2.106), (2.2.107) may be written as

$$h^{\mathrm{I}}_{1dd}(Q/2,s,t) + \frac{1}{(1+\frac{Q}{2}\beta_{0s})^2}h^{\mathrm{I}}_{1ss}(Q/2,s,t) + \frac{\beta_{0s}}{(1+\frac{Q}{2}\beta_{0s})}h^{\mathrm{I}}_{1d}(Q/2,s,t)$$
$$-\frac{Q}{2}\frac{\beta_{0ss}}{(1+\frac{Q}{2}\beta_{0s})^3}h^{\mathrm{I}}_{1s}(Q/2,s,t) = 0,$$

and

$$h^{\rm II}_{1\ dd}(-Q/2,s,t) + \frac{1}{(1-\frac{Q}{2}\beta_{0s})^2} h^{\rm II}_{1\ ss}(-Q/2,s,t) + \frac{\beta_{0s}}{(1-\frac{Q}{2}\beta_{0s})} h^{\rm II}_{1\ d}(-Q/2,s,t)$$
$$+\frac{Q}{2}\frac{\beta_{0ss}}{(1-\frac{Q}{2}\beta_{0s})^3} h^{\rm II}_{1\ s}(-Q/2,s,t) = 0,$$

respectively.

Finally, using the conditions (2.2.104)–(2.2.105) which imply that all derivatives with respect to s of $h^{\rm I}_1$ vanish at $d = Q/2$ and of $h^{\rm II}_1$ vanish for $d = -Q/2$, we obtain that the conditions (2.2.106), (2.2.107) may be written out explicitly as

(2.2.108) $$h^{\rm I}_{1dd}(Q/2,s,t) = -\frac{\beta_{0s}}{(1+\frac{Q}{2}\beta_{0s})} h^{\rm I}_{1d}(Q/2,s,t),$$

(2.2.109) $$h^{\rm II}_{1\ dd}(-Q/2,s,t) = -\frac{\beta_{0s}}{(1-\frac{Q}{2}\beta_{0s})} h^{\rm II}_{1\ d}(-Q/2,s,t),$$

respectively.

In addition to the boundary conditions (2.2.104)–(2.2.107), we can add “artificial” geometrical boundary conditions at $s = 5Q$, namely that our three surfaces $X^{\rm I}$, $X^{\rm II}$ and $X^{\rm III}$ are symmetric with respect to the plane located at $s = 5Q$. These conditions imply that the functions ξ, h^j, $j = {\rm I}, {\rm II}$, and u are symmetric with respect to $s = 5Q$. Hence

(2.2.110a) $$\xi_x(x(s,t),t) = 0, \quad \text{at } s = 5Q,$$

(2.2.110b) $$h^{\rm I}_s(d,s,t) = 0, \quad \text{at } s = 5Q,$$

(2.2.110c) $$h^{\rm II}_s(d,s,t) = 0, \quad \text{at } s = 5Q,$$

(2.2.110d) $$u_s(s,z,t) = 0, \quad \text{at } s = 5Q,$$

and similarly all partial derivatives with respect to s of odd order of ξ, h^j, $j = {\rm I}, {\rm II}$, and u are anti-symmetric functions with respect to the plane $s = 5Q$, and thus vanish at $s = 5Q$, and their partial derivatives with respect to s of even order are symmetric functions with respect to the plane $s = 5Q$. We emphasize that if $\xi_x = 0$ at some $x = \hat{x}$, then $\xi_s = \xi_x x_s = 0$ at $x = \hat{x}$, since $x_s(\hat{x}) = \frac{1}{\sqrt{1+\xi_x^2(\hat{x})}} = 1$.

As we shall show in the continuation of this section, the conditions (2.2.110) together with the assumptions about the even and the odd derivatives with respect to s of ξ, h^j, $j = {\rm I}, {\rm II}$, and u, imply that the leading order of $K^{\rm I}$, $K^{\rm II}$, which is $\mathcal{O}(m)$, and orders $\mathcal{O}(1)$ and $\mathcal{O}(m^{2/3})$ of $K^{\rm III}$ are symmetric functions with respect to the plane $s = 5Q$. This will lead to the conclusion that no mass flux (up to order $\mathcal{O}(m^2)$ for $K^{\rm I}$, $K^{\rm II}$, and up to order $\mathcal{O}(m)$ for $K^{\rm III}$) enters, or exits via the boundary of our domain located at $s = 5Q$, namely

$$< \tilde{\tau}^j, \nabla_s K^j > (d,s,t) = \mathcal{O}(m^2), \quad \text{for } s = 5Q, \quad j = {\rm I}, {\rm II},$$

and

$$< \tilde{\tau}^{\text{III}}, \nabla_s K^{\text{III}} > (s,z,t) = \mathcal{O}(m), \quad \text{for } s = 5Q,$$

where $\tilde{\tau}^j$ is the unit exterior tangent vector to the surface X^j, $j = \text{I}, \text{II}, \text{III}$ at $s = 5Q$ (see fig. 2.11).

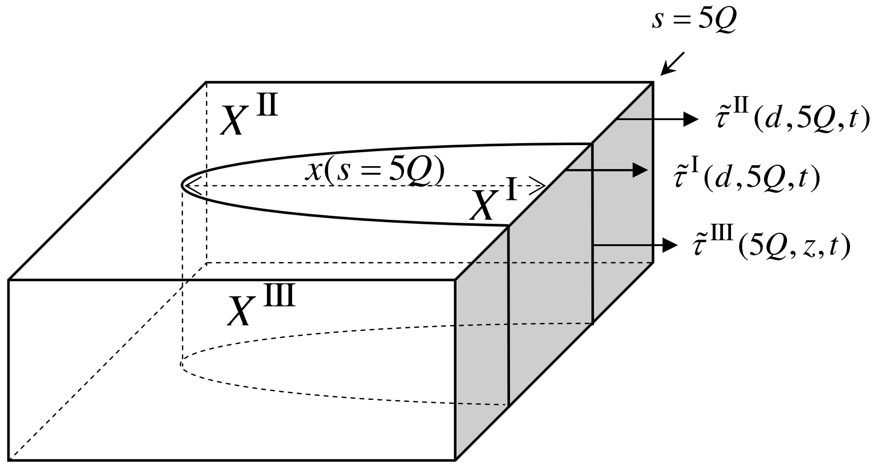

Figure 2.11: The exterior tangent vectors $\tilde{\tau}^{\text{I}}$, $\tilde{\tau}^{\text{II}}$ and $\tilde{\tau}^{\text{III}}$ at $s = 5Q$, to the surfaces X^{I}, X^{II} and X^{III}, respectively.

In order to prove that K_0^{I}, K_0^{II} and $\tilde{K}^{\text{III}}$ (where K_0^j, $j = \text{I}, \text{II}$ are the leading orders of K^j, $j = \text{I}, \text{II}$, respectively, and $\tilde{K}^{\text{III}}$ is K^{III} up to the order $\mathcal{O}(m^{4/3})$) are symmetric functions with respect to the plane $s = 5Q$, let us consider β which was introduced in (2.1.4), namely

$$\beta(s,t) = \arctan \xi_x(x(s,t),t).$$

In view of the assumptions (2.2.110), it is easy to see that

$$\beta(s,t) = 0, \quad \text{for } s = 5Q,$$

and that β is an anti-symmetric function in s, with respect to the plane $s = 5Q$, since

$$\begin{aligned} \beta(5Q + \Delta s, t) &= \arctan \xi_x(x(5Q + \Delta s, t), t) = \arctan\left[-\xi_x(x(5Q - \Delta s, t), t)\right] \\ &= -\arctan \xi_x(x(5Q - \Delta s, t), t) = -\beta(5Q - \Delta s, t). \end{aligned}$$

Hence, all odd derivatives of β with respect to s are symmetric functions and all even derivatives of β with respect to s are anti-symmetric functions.

Therefore, we have obtained that all terms which appear in K_0^j, $j = \text{I}, \text{II}$ given in (2.2.102), namely in

$$K_0^j = \frac{(1 + d\beta_{0s})^3 h_{1dd}^j + (1 + d\beta_{0s}) h_{1ss}^j + \beta_{0s}(1 + d\beta_{0s})^2 h_{1d}^j - d\beta_{0ss} h_{1s}^j}{2(1 + d\beta_{0s})^3}, \quad j = \text{I}, \text{II},$$

are symmetric functions with respect to $s = 5Q$, since they are the products of symmetric functions, except the term $d\beta_{0ss} h_{1s}^j$, which is a symmetric function because it is a product of two anti-symmetric functions. So, it follows that K_0^{I} and K_0^{II} are symmetric functions with respect to $s = 5Q$.

As to $\tilde{K}^{\mathrm{III}}$, using Taylor expansion in $m^{2/3}$ of

$$\frac{a + bm^{2/3}}{(c + dm^{2/3})^{3/2}} \sim \frac{a}{c^{3/2}} - \frac{1}{2}m^{2/3}\frac{3ad - 2bc}{c^{5/2}} + \mathcal{O}(m^{4/3}),$$

by (2.2.67), we obtain that $\tilde{K}^{\mathrm{III}}$ can be written as

$$\begin{aligned}\tilde{K}^{\mathrm{III}} &= \frac{-\xi_{xx}x_s^3 + m^{2/3}(D_{2uu} + 3\bar{u}_1\xi_{xx}x_s^3) + \mathcal{O}(m^{4/3})}{2\left[(1 - 2m^{2/3}\bar{u}_1) + \mathcal{O}(m^{4/3})\right]^{3/2}} \\ &= -\frac{\xi_{xx}x_s^3}{2} - \frac{1}{2}m^{2/3}\frac{6\bar{u}_1\xi_{xx}x_s^3 - 2D_{2uu} - 6\bar{u}_1\xi_{xx}x_s^3}{2} + \mathcal{O}(m^{4/3}) \\ &= -\frac{\xi_{xx}}{2(1+\xi_x^2)^{3/2}} + \frac{1}{2}m^{2/3}D_{2uu} + \mathcal{O}(m^{4/3}).\end{aligned} \tag{2.2.111}$$

We recall that by our assumption ξ is a symmetric function with respect to $s = 5Q$, hence ξ_x is an anti-symmetric with respect to $s = 5Q$, leading that both ξ_{xx} and ξ_x^2 are symmetric functions with respect to $s = 5Q$, and therefore the first term of (2.2.111) is a symmetric function with respect to $s = 5Q$.

Finally, D_{2uu} is a symmetric function with respect to $s = 5Q$, since by (2.2.81) D_{2uu} may be expressed as

$$D_{2uu} = -\frac{1}{2}\left[h_{1d}^{\mathrm{I}}(0,s,t) + h_{1\ d}^{\mathrm{II}}(0,s,t)\right] - 2h_{1s}^{\mathrm{I}}(0,s,t)\cot\beta_0,$$

and by our assumption $h_{1d}^j(0,s,t)$, $j = \mathrm{I,II}$ are both symmetric functions with respect to $s = 5Q$, and the product of $h_{1s}^{\mathrm{I}}(0,s,t)$ and $\cot\beta_0$ is a symmetric function with respect to $s = 5Q$ since both of its components are anti-symmetric functions with respect to $s = 5Q$. Hence, we conclude that K^{III} is a symmetric function up to order $\mathcal{O}(m^{4/3})$.

As to the mass fluxes in the direction perpendicular to d at the boundary $s = 5Q$ of X^{I}, X^{II}, we readily obtain that

$$\tilde{\tau}^j = \frac{X_s^j - < X_s^j, X_d^j > X_d^j}{||X_s^j - < X_s^j, X_d^j > X_d^j||}, \quad j = \mathrm{I,II}. \tag{2.2.112}$$

Hence, we get that the mass fluxes are given by

$$< \tilde{\tau}^j, K^j > = \frac{- < X_s^j, X_d^j > K_d^j + ||X_d^j||^2 K_s^j}{||X_s^j||^2||X_d^j||^2 - < X_s^j, X_d^j >^2} < \tilde{\tau}^j, X_s^j >, \quad j = \mathrm{I,II},$$

and using (2.2.91a)–(2.2.91c), which were obtained for the surface diffusion equation, we find that

$$< \tilde{\tau}^j, K^j > = \frac{1}{(1 + d\beta_{0s})^2} < \tilde{\tau}^j, X_s^j > K_s^j + \mathcal{O}(m^2), \quad j = \mathrm{I,II}, \tag{2.2.113}$$

where using (2.2.112) and appealing again to (2.2.91a) we get

$$< \tilde{\tau}^j, X^j_s >= \frac{||X^j_s||^2 - < X^j_s, X^j_d >^2}{||X^j_s - < X^j_s, X^j_d > X^j_d||} = ||X^j_s|| + \mathcal{O}(m^2) = 1 + d\beta_{0s} + \mathcal{O}(m^2), \quad j = \mathrm{I}, \mathrm{II}.$$

Thus,

$$< \tilde{\tau}^j, K^j >= \frac{1}{1 + d\beta_{0s}} K^j_s + \mathcal{O}(m^2), \quad j = \mathrm{I}, \mathrm{II}.$$

Finally, since the leading order of K^j, $j = \mathrm{I}, \mathrm{II}$ are symmetric functions with respect to the plane $s = 5Q$, the leading orders of K^j_s, $j = \mathrm{I}, \mathrm{II}$ are anti-symmetric function with respect to $s = 5Q$, namely $K^j_s = mK^j_{0s} + \mathcal{O}(m^2) = \mathcal{O}(m^2)$, $j = \mathrm{I}, \mathrm{II}$ for $s = 5Q$. So, we obtain that

$$< \tilde{\tau}^j, K^j > (d, 5Q, t) = \mathcal{O}(m^2), \quad j = \mathrm{I}, \mathrm{II},$$

i.e., there is no mass flux via X^j, $j = \mathrm{I}, \mathrm{II}$ up to order $\mathcal{O}(m^2)$ perpendicular to the plane $s = 5Q$.

Similarly, since

$$\tilde{\tau}^{\mathrm{III}} = \frac{X^{\mathrm{III}}_s - < X^{\mathrm{III}}_s, X^{\mathrm{III}}_z > X^{\mathrm{III}}_z}{||X^{\mathrm{III}}_s - < X^{\mathrm{III}}_s, X^{\mathrm{III}}_z > X^{\mathrm{III}}_z||}, \tag{2.2.114}$$

using (2.2.64a)–(2.2.64c), which were proved in the section of mean curvature equation, we get from

$$< \tilde{\tau}^{\mathrm{III}}, X^{\mathrm{III}}_s >= \frac{||X^{\mathrm{III}}_s||^2 - < X^{\mathrm{III}}_s, X^{\mathrm{III}}_z >^2}{||X^{\mathrm{III}}_s - < X^{\mathrm{III}}_s, X^{\mathrm{III}}_z > X^{\mathrm{III}}_z||} = ||X^{\mathrm{III}}_s|| + \mathcal{O}(m) = 1 + \mathcal{O}(m),$$

that,

$$< \tilde{\tau}^{\mathrm{III}}, K^{\mathrm{III}}_s >= \frac{- < X^{\mathrm{III}}_s, X^{\mathrm{III}}_z > K^{\mathrm{III}}_z + ||X^{\mathrm{III}}_z||^2 K^{\mathrm{III}}_s}{||X^{\mathrm{III}}_s||^2 ||X^{\mathrm{III}}_z||^2 - < X^{\mathrm{III}}_s, X^{\mathrm{III}}_z >^2} < \tilde{\tau}^{\mathrm{III}}, X^{\mathrm{III}}_s >= K^{\mathrm{III}}_s + \mathcal{O}(m).$$

Now, since K^{III}_s is an anti-symmetric function up to the order $\mathcal{O}(m^{4/3})$, we obtain that

$$< \tilde{\tau}^{\mathrm{III}}, K^{\mathrm{III}}_s > (5Q, z, t) = \mathcal{O}(m),$$

thus, there is no mass flux also via X^{III}, up to order $\mathcal{O}(m)$, in the direction perpendicular to the plane $s = 5Q$.

2.2.10 Summary of all equations and boundary conditions that have been obtain in this chapter

The equations that have been obtained from the motion by the mean curvature of surface X^{III}, (see (2.2.81) and (2.2.82)), are

$$D_1 \equiv 0, \tag{2.2.115}$$

$$D_{2uu}(s, u(s, z, t), t) = -\frac{1}{2}\left[h^{\mathrm{I}}_{1d}(0, s, t) + h^{\mathrm{II}}_{1\,d}(0, s, t)\right] - 2h^{\mathrm{I}}_{1s}(0, s, t) \cot \beta_0, \tag{2.2.116}$$

and

(2.2.117)
$$V_0\xi_{1x} + V_1\xi_{0x} - \xi_{1t} = -\frac{\xi_{1xx}}{2(1+{\xi_{0x}}^2)} + \frac{\xi_{0xx}\xi_{0x}\xi_{1x}}{(1+{\xi_{0x}}^2)^2} - \frac{1}{4}\big[h^{\mathrm{I}}_{1d}(0,s,t) + h^{\mathrm{II}}_{1\,d}(0,s,t)\big]\sqrt{1+\xi_{0x}^2} - h^{\mathrm{I}}_{1s}(0,s,t)\frac{\xi_{0x}}{\sqrt{1+\xi_{0x}^2}}.$$

The equations for surface diffusion of the surfaces X^{I} and X^{II}, according to (2.2.101) and (2.2.102), can be stated as

$$\begin{aligned} &h^j_{1t} - V_0\sin\beta_0 h^j_{1d} - \frac{1}{1+d\beta_{0s}}V_0\cos\beta_0 h^j_{1s} \\ &= -\frac{B}{AQ^2}\frac{1}{1+d\beta_{0s}}\left\{\frac{\partial}{\partial s}\left(\frac{K^j_{0s}}{1+d\beta_{0s}}\right) + \frac{\partial}{\partial d}\left((1+d\beta_{0s})K^j_{0d}\right)\right\}, \quad j = \mathrm{I},\mathrm{II}, \end{aligned} \tag{2.2.118}$$

where

$$K^j_0 = \frac{(1+d\beta_{0s})^3 h^j_{1dd} + (1+d\beta_{0s})h^j_{1ss} + \beta_{0s}(1+d\beta_{0s})^2 h^j_{1d} - d\beta_{0ss}h^j_{1s}}{2(1+d\beta_{0s})^3}, \quad j = \mathrm{I},\mathrm{II}. \tag{2.2.119}$$

Along the "groove root," we have the continuity conditions, which, as we have seen in (2.2.25) and (2.2.33), may be expressed by

$$h^{\mathrm{I}}_1(0,s,t) = h^{\mathrm{II}}_1(0,s,t) = \bar{u}_1(s,t), \quad D_2(s,\bar{u}(s,t),t) = 0, \tag{2.2.120}$$

and

$$h^{\mathrm{I}}_{1dd}(0,s,t) - h^{\mathrm{II}}_{1\,dd}(0,s,t) = -\frac{\xi_{0xx}}{(1+\xi_{0x}^2)^{3/2}}(x(s,t),t). \tag{2.2.121}$$

In addition, we have the balance of mass flux, which by (2.2.48), can be written in the form

$$h^{\mathrm{I}}_{1ddd}(0,s,t) - h^{\mathrm{II}}_{1\,ddd}(0,s,t) = \frac{\xi_{0xx}^2}{(1+\xi_{0x}^2)^3}(x(s,t),t), \tag{2.2.122}$$

and Young's law, which by (2.2.54) and (2.2.60), may be stated as

$$h^{\mathrm{I}}_{1d}(0,s,t) - h^{\mathrm{II}}_{1\,d}(0,s,t) = 1, \tag{2.2.123}$$

and

$$D_{2u}(s,\bar{u}(s,t),t) = -\frac{1}{2}\big[h^{\mathrm{I}}_{1d}(0,s,t) + h^{\mathrm{II}}_{1\,d}(0,s,t)\big] - 2h^{\mathrm{I}}_{1s}(0,s,t)\cot\beta_0. \tag{2.2.124}$$

Finally, we have the exterior boundary conditions for the boundaries located at $d = \pm Q/2$, which according to (2.2.104)–(2.2.105), and (2.2.108)–(2.2.109) can be stated as

$$\begin{aligned} &h^{\mathrm{I}}_1(Q/2,s,t) = h^{\mathrm{II}}_1(-Q/2,s,t) = 0, \\ &h^{\mathrm{I}}_{1dd}(Q/2,s,t) = -\frac{\beta_{0s}}{(1+\frac{Q}{2}\beta_{0s})}h^{\mathrm{I}}_{1d}(Q/2,s,t), \\ &h^{\mathrm{II}}_{1\,dd}(-Q/2,s,t) = -\frac{\beta_{0s}}{(1-\frac{Q}{2}\beta_{0s})}h^{\mathrm{II}}_{1\,d}(-Q/2,s,t). \end{aligned} \tag{2.2.125}$$

And, we have the geometrical assumption about the boundary located at $s = 5Q$, namely, that the functions ξ, h^j, $j = \mathrm{I}, \mathrm{II}$, and u are symmetric functions with respect to the plane located at $s = 5Q$.

2.3 Finding the solution to the leading order for D

As we have already seen in the previous sections,

$$D_1 \equiv 0.$$

Thus, in this section we shall solve the equation for D_2, given in (2.2.116), namely

$$D_{2uu}(s, u(s, z, t), t) = -\frac{1}{2}\left[h^{\mathrm{I}}_{1d}(0, s, t) + h^{\mathrm{II}}_{1\,d}(0, s, t)\right] - 2h^{\mathrm{I}}_{1s}(0, s, t)\cot\beta_0, \tag{2.3.1}$$

together with the boundary conditions, which appear in (2.2.120) and (2.2.124), namely

$$D_{2u}(s, \bar{u}(s, t), t) = -\frac{1}{2}\left[h^{\mathrm{I}}_{1d}(0, s, t) + h^{\mathrm{II}}_{1\,d}(0, s, t)\right] - 2h^{\mathrm{I}}_{1s}(0, s, t)\cot\beta_0, \tag{2.3.2a}$$

and

$$D_2(s, \bar{u}(s, t), t) = 0. \tag{2.3.2b}$$

Integration of (2.3.1) with respect to u yields

$$D_{2u}(s, u(s, z, t), t) = -\left\{\frac{1}{2}\left[h^{\mathrm{I}}_{1d}(0, s, t) + h^{\mathrm{II}}_{1\,d}(0, s, t)\right] + 2h^{\mathrm{I}}_{1s}(0, s, t)\cot\beta_0\right\}u + C_1, \tag{2.3.3}$$

where C_1 is an arbitrary constant of integration. Substituting the boundary condition (2.3.2a), which is given at $z = \bar{u}(s, t)$ so at $u = \frac{\bar{u}}{\bar{u}} = 1$, into (2.3.3) leads

$$\begin{aligned} D_{2u}(s, u(s, \bar{u}, t), t) &= -\left\{\frac{1}{2}\left[h^{\mathrm{I}}_{1d}(0, s, t) + h^{\mathrm{II}}_{1\,d}(0, s, t)\right] + 2h^{\mathrm{I}}_{1s}(0, s, t)\cot\beta_0\right\} + C_1 \\ &= -\frac{1}{2}\left[h^{\mathrm{I}}_{1d}(0, s, t) + h^{\mathrm{II}}_{1\,d}(0, s, t)\right] - 2h^{\mathrm{I}}_{1s}(0, s, t)\cot\beta_0, \end{aligned} \tag{2.3.4}$$

yielding that

$$C_1 = 0.$$

Thus, from (2.3.3) we obtain that D_2 satisfies the equation

$$D_{2u}(s, u(s, z, t), t) = -\left\{\frac{1}{2}\left[h^{\mathrm{I}}_{1d}(0, s, t) + h^{\mathrm{II}}_{1\,d}(0, s, t)\right] + 2h^{\mathrm{I}}_{1s}(0, s, t)\cot\beta_0\right\}u. \tag{2.3.5}$$

Now, integrating (2.3.5), we get that

$$D_2(s, u(s, z, t), t) = -\frac{1}{4}\left\{\left[h^{\mathrm{I}}_{1d}(0, s, t) + h^{\mathrm{II}}_{1\,d}(0, s, t)\right] + 4h^{\mathrm{I}}_{1s}(0, s, t)\cot\beta_0\right\}u^2 + C_2, \tag{2.3.6}$$

where C_2 is an arbitrary constant of integration. Substituting the boundary condition (2.3.2b), which is as previously given at $z = \bar{u}$, hence at $u = 1$, into (2.3.6), we find that

$$(2.3.7) \quad D_2(s, u(s, \bar{u}, t), t) = -\frac{1}{4}\Big\{\big[h^{\mathrm{I}}_{1d}(0, s, t) + h^{\mathrm{II}}_{1\,d}(0, s, t)\big] + 4h^{\mathrm{I}}_{1s}(0, s, t)\cot\beta_0\Big\} + C_2 = 0,$$

which leads

$$C_2 = \frac{1}{4}\Big\{\big[h^{\mathrm{I}}_{1d}(0, s, t) + h^{\mathrm{II}}_{1\,d}(0, s, t)\big] + 4h^{\mathrm{I}}_{1s}(0, s, t)\cot\beta_0\Big\}.$$

Thus, (2.3.6) implies that, the solution to the problem (2.3.1)–(2.3.2) is given by

$$(2.3.8) \quad D_2(s, u(s, z, t), t) = -\frac{1}{4}\Big\{\big[h^{\mathrm{I}}_{1d}(0, s, t) + h^{\mathrm{II}}_{1\,d}(0, s, t)\big] + 4h^{\mathrm{I}}_{1s}(0, s, t)\cot\beta_0\Big\}(u^2 - 1).$$

2.4 Finding solutions for $V_1(t)$ and $\xi_1(x, t)$

Consider the equation (2.2.117), which was obtained from the motion by mean curvature of the surface X^{III}. It is easily verified that (2.2.117) may be expressed in the following manner

$$(2.4.1) \qquad \xi_{1t} = L(\xi_1) + V_1\xi_{0x} + G(h^{\mathrm{I}}_1, h^{\mathrm{II}}_1),$$

where L is the linear operator defined by

$$(2.4.2) \qquad L(\xi_1) = \Big[\frac{\xi_{1x}}{2(1 + \xi_{0x}^2)}\Big]_x + V_0\xi_{1x},$$

and where G is given by

$$(2.4.3) \qquad G(h^{\mathrm{I}}_1, h^{\mathrm{II}}_1) = \frac{1}{4}\big[h^{\mathrm{I}}_{1d}(0, s, t) + h^{\mathrm{II}}_{1\,d}(0, s, t)\big]\sqrt{1 + \xi_{0x}^2} + h^{\mathrm{I}}_{1s}(0, s, t)\frac{\xi_{0x}}{\sqrt{1 + \xi_{0x}^2}}.$$

Our purpose in this section is to obtain from (2.4.1) an expression for V_1 which does not depend on ξ_1, and an equation for ξ_1 which does not depend on V_1.

First, we shall integrate the equation (2.4.1) with respect to x, $0 \le x < \infty$, to obtain

$$(2.4.4) \quad \int_0^\infty \xi_{1t}dx = \int_0^\infty \Big[\frac{\xi_{1x}}{2(1 + \xi_{0x}^2)}\Big]_x dx + \int_0^\infty V_0\xi_{1x}dx + \int_0^\infty V_1\xi_{0x}dx + \int_0^\infty G(h^{\mathrm{I}}_1, h^{\mathrm{II}}_1)dx.$$

If we denote by $\bar{\xi}_1(t)$,

$$(2.4.5) \qquad \bar{\xi}_1(t) = \int_0^\infty \xi_1(x, t)dx,$$

and formally interchange the integration with respect to x and the differentiation with respect to t, from (2.4.4) we get that

$$(2.4.6) \qquad \bar{\xi}_{1t} = \Big[\frac{\xi_{1x}}{2(1 + \xi_{0x}^2)}\Big]\Big|_{x=0}^{\infty} + V_0\xi_1\Big|_{x=0}^{\infty} + V_1\xi_0\Big|_{x=0}^{\infty} + \int_0^\infty G(h^{\mathrm{I}}_1, h^{\mathrm{II}}_1)dx.$$

Assuming the following boundary conditions (I SHOULD ADD THEM SOMEWHERE WITH EXPLANATION ...)

(2.4.7a) $$\xi_1(0) = 0,$$

(2.4.7b) $$\xi_1(x) \sim o(e^{-\frac{\pi}{4}x}), \quad \text{at } x >> 1,$$

(2.4.7c) $$\lim_{x\to 0} \frac{\xi_{1x}}{\xi_{0x}^2}(x) = 0,$$

(2.4.7d) $$\xi_{1x}(x) \sim o(e^{-\frac{\pi}{4}x}), \quad \text{at } x >> 1,$$

and using the boundary conditions of ξ_0, which are known since ξ_0 coincides with the traveling wave solution (2.2.88), namely

(2.4.8a) $$\xi_0(0) = 0,$$

(2.4.8b) $$\lim_{x\to\infty} \xi_0(x) = 1,$$

(2.4.8c) $$\lim_{x\to\infty} \xi_{0x}(x) \sim o(e^{-\frac{\pi}{2}x}),$$

substituted to (2.4.6), lead

(2.4.9) $$\bar{\xi}_{1t} = V_1 + \int_0^\infty G(h_1^{\mathrm{I}}, h_1^{\mathrm{II}})dx.$$

Now, if we subtract (2.4.9) multiplied by ξ_{0x}, namely

$$\xi_{0x}\bar{\xi}_{1t} = \xi_{0x}V_1 + \xi_{0x}\int_0^\infty G(h_1^{\mathrm{I}}, h_1^{\mathrm{II}})dx,$$

from (2.4.1), we get that

(2.4.10) $$\xi_{1t} = L(\xi_1) + \xi_{0x}\bar{\xi}_{1t} + G(h_1^{\mathrm{I}}, h_1^{\mathrm{II}}) - \xi_{0x}\int_0^\infty G(h_1^{\mathrm{I}}, h_1^{\mathrm{II}})dx.$$

As we shall explain in the following section, there exists a solution to the equation

(2.4.11) $$\xi_{1t} = L(\xi_1) + G(h_1^{\mathrm{I}}, h_1^{\mathrm{II}}) - \xi_{0x}\int_0^\infty G(h_1^{\mathrm{I}}, h_1^{\mathrm{II}})dx,$$

together with the boundary conditions (2.4.7) and the initial condition

(2.4.12) $$\xi_1(x, 0) = \xi_1^0(x).$$

This solution surely satisfies (2.4.10) where $\bar{\xi}_{1t} = 0$, together with the boundary conditions (2.4.7) and the initial condition (2.4.12), or in other words there exists a solution to the problem

$$\xi_{1t} = L(\xi_1) + \xi_{0x}\bar{\xi}_{1t} + G(h_1^{\mathrm{I}}, h_1^{\mathrm{II}}) - \xi_{0x}\int_0^\infty G(h_1^{\mathrm{I}}, h_1^{\mathrm{II}})dx, \tag{2.4.13a}$$

$$\xi_1(0) = 0, \tag{2.4.13b}$$

$$\xi_1(x) \sim o(e^{-\frac{\pi}{4}x}), \quad \text{at } x >> 1, \tag{2.4.13c}$$

$$\lim_{x\to 0}\frac{\xi_{1x}}{\xi_{0x}^2}(x) = 0, \tag{2.4.13d}$$

$$\xi_{1x}(x) \sim o(e^{-\frac{\pi}{4}x}), \quad \text{at } x >> 1, \tag{2.4.13e}$$

$$\xi_1(x, 0) = \xi_1^0(x), \tag{2.4.13f}$$

with $\bar{\xi}_{1t} = 0$.

In Section 2.6 we shall show that the problem (2.4.13) has a unique solution, this will prove that the solution of (2.4.13) must satisfy $\bar{\xi}_{1t} = 0$, which using (2.4.9) yields

$$V_1 = -\int_0^\infty G(h_1^{\mathrm{I}}, h_1^{\mathrm{II}})dx. \tag{2.4.14}$$

2.5 Existence of the solutions to the equation (2.4.11)

Consider the equation

$$\xi_{1t} = L(\xi_1) + G(h_1^{\mathrm{I}}, h_1^{\mathrm{II}}) - \xi_{0x}\int_0^\infty G(h_1^{\mathrm{I}}, h_1^{\mathrm{II}})dx, \tag{2.5.1}$$

where L is the linear operator defined by

$$L(\xi_1) = \Big[\frac{\xi_{1x}}{2(1+\xi_{0x}^2)}\Big]_x + V_0\xi_{1x}. \tag{2.5.2}$$

In this section we shall explain why there exist solutions to the equation (2.5.1), and will find boundary conditions which must be satisfied by these solutions.

First, we shall show that there exists a change of variables, which converts L to the self-adjoint operator. Indeed, consider the arc-length parametrization of ξ_0, denote it by s,

$$s \equiv \int_{\tilde{x}(t)}^{x} \sqrt{1+{\xi_{0x}}^2(\check{x}, t)}\,d\check{x}, \tag{2.5.3}$$

so, s_x is given by

$$s_x = \sqrt{1+{\xi_{0x}}^2(x,t)}, \tag{2.5.4}$$

and, therefore x_s can be expressed as

$$x_s = \frac{1}{\sqrt{1+{\xi_{0x}}^2(x,t)}}. \tag{2.5.5}$$

Hence, using the chain rule we readily obtain that

$$\xi_{1x} = \xi_{1s} s_x = \xi_{1s}\sqrt{1+{\xi_{0x}}^2(x,t)}, \tag{2.5.6}$$

and therefore one may write the operator L as follows

$$\begin{aligned} L(\xi_1) &= \Big[\frac{\xi_{1s}}{2\sqrt{1+\xi_{0x}^2}}\Big]_x + V_0\xi_{1x} \\ &= \sqrt{1+\xi_{0x}^2}\Big[\frac{\xi_{1s}}{2\sqrt{1+\xi_{0x}^2}}\Big]_s + \sqrt{1+\xi_{0x}^2}V_0\xi_{1s} \\ &= \frac{\xi_{1ss}}{2} + \xi_{1s}\sqrt{1+\xi_{0x}^2}\Big(-\frac{\xi_{0x}\xi_{0xx}x_s}{2(1+\xi_{0x}^2)^{3/2}} + V_0\Big) \\ &= \frac{\xi_{1ss}}{2} + \xi_{1s}\sqrt{1+\xi_{0x}^2}\Big(-\frac{\xi_{0x}\xi_{0xx}}{2(1+\xi_{0x}^2)^2} + V_0\Big). \end{aligned} \tag{2.5.7}$$

Now, using the equation which is satisfied by $\xi_0(x)$, namely

$$V_0\xi_{0x} = -\frac{\xi_{0xx}}{2(1+\xi_{0x}^2)},$$

we get from (2.5.7) that

$$\begin{aligned} L(\xi_1) &= \frac{\xi_{1ss}}{2} + \xi_{1s}\sqrt{1+\xi_{0x}^2}\Big(\frac{V_0\xi_{0x}^2}{1+\xi_{0x}^2} + V_0\Big) \\ &= \frac{\xi_{1ss}}{2} + \xi_{1s}V_0\frac{1+2\xi_{0x}^2}{1+\xi_{0x}^2}\sqrt{1+\xi_{0x}^2}. \end{aligned} \tag{2.5.8}$$

Next, recalling that (see (1.3.29), with $Q = 1$)

$$\xi_{0x} = \frac{e^{-\frac{\pi}{2}x}}{\sqrt{1-e^{-\pi x}}}, \tag{2.5.9}$$

we readily obtain that

$$\frac{1+2\xi_{0x}^2}{1+\xi_{0x}^2} = 1 + e^{-\pi x},$$

which substituted to (2.5.8), yields

$$L(\xi_1) = \frac{\xi_{1ss}}{2} + \xi_{1s}V_0(1+e^{-\pi x})\sqrt{1+\xi_{0x}^2}. \tag{2.5.10}$$

Hence, if want to express the operator L in the form

$$L(\xi_1) = \frac{1}{p(s)}\big(p(s)\xi_{1s}\big)_s, \tag{2.5.11}$$

in which case L may be self-adjoint with respect to the inner product $<,>_p =$ ... (TO COMPLETE THE DEF...), from (2.5.10) we conclude that

$$\frac{p_s}{p} = 2V_0(1+e^{-\pi x})\sqrt{1+\xi_{0x}^2},$$

or in other words

$$\frac{dp}{p} = 2V_0(1+e^{-\pi x})\sqrt{1+{\xi_0}_x^2}ds,$$

which, integrated yields

$$\ln(p) = 2V_0\int(1+e^{-\pi x})\sqrt{1+{\xi_0}_x^2}ds = 2V_0\int(1+e^{-\pi x})\sqrt{1+{\xi_0}_x^2}\frac{ds}{dx}dx = 2V_0\int(1+e^{-\pi x})(1+{\xi_0}_x^2)dx.$$

Finally, using (2.5.9), which tells us that

$$1+{\xi_0}_x^2 = \frac{1}{1-e^{-\pi x}}, \tag{2.5.12}$$

we get that

$$\begin{aligned}\ln(p) &= 2V_0\int(1+e^{-\pi x})(1+{\xi_0}_x^2)dx = 2V_0\int\frac{1+e^{-\pi x}}{1-e^{-\pi x}}dx = 2V_0\int\big(1+\frac{2e^{-\pi x}}{1-e^{-\pi x}}\big)dx \\ &= 2V_0\big(x+\frac{2}{\pi}\ln(1-e^{-\pi x})\big).\end{aligned}$$

Thus,

$$p(s) = e^{2V_0\left(x+\frac{2}{\pi}\ln(1-e^{-\pi x})\right)} = e^{2V_0 x}(1-e^{-\pi x})^{\frac{4V_0}{\pi}}, \tag{2.5.13}$$

and, recalling that in our case $V_0 = \pi/4$, as was explained in (2.2.89) or equivalently in (1.3.25) under the assumptions that $Q = 1$ and $A = \frac{1}{2}$, we obtain that

$$p(s) = e^{\frac{\pi}{2}x}(1-e^{-\pi x}). \tag{2.5.14}$$

To conclude this discussion, we see that the operator L may be written in the form (2.5.11), where $p(s)$ is given by (2.5.14). In order to ensure that such L will be self-adjoint, we shall require some boundary conditions for ξ_1. Using Green's formula (ADD REFERENCE), we know that.........

2.6 Uniqueness of the solutions to the problem (2.4.13)

Suppose that ${\xi_1}_a(x,t)$ and ${\xi_1}_b(x,t)$ are arbitrary solutions of the problem (2.4.13), in this section we shall show that they must coincide. For this purpose, define w,

$$w(x,t) \equiv {\xi_1}_a(x,t) - {\xi_1}_b(x,t), \tag{2.6.1}$$

so due to the assumption that $\xi_{1a}(x,t)$ and $\xi_{1b}(x,t)$ solve the problem (2.4.13), w solves the problem

(2.6.2a) $$w_t = L(w) + \xi_{0x}\bar{w}_t,$$

(2.6.2b) $$w(0,t) = 0, \quad \text{for } 0 < t < T$$

(2.6.2c) $$w(x,t) \sim o(e^{-\frac{\pi}{4}x}), \quad \text{at } x >> 1, \quad \text{for } 0 < t < T$$

(2.6.2d) $$\lim_{x\to 0} \frac{w_x}{\xi_{0x}^2}(x,t) = 0, \quad \text{for } 0 < t < T$$

(2.6.2e) $$w_x(x,t) \sim o(e^{-\frac{\pi}{4}x}), \quad \text{at } x >> 1, \quad \text{for } 0 < t < T$$

(2.6.2f) $$w(x,0) = 0, \quad \text{for } 0 \le x < \infty.$$

Making the inner product $< .,. >_p$ of the equation (2.6.2a) with w leads to

(2.6.3) $$\int_0^\infty w w_t p(s) ds = \int_0^\infty w L(w) p(s) ds + \int_0^\infty w \bar{w}_t \xi_{0x} p(s) ds.$$

Now, using (2.5.4), (2.5.9), (2.5.12), and (2.5.14), we pay attention that

(2.6.4)

$$\xi_{0x} p(s) ds = \xi_{0x} p(s) \frac{ds}{dx} dx = \xi_{0x} p(s) \sqrt{1 + {\xi_{0x}}^2} dx = \frac{e^{-\frac{\pi}{2}x}}{\sqrt{1 - e^{-\pi x}}} e^{\frac{\pi}{2}x} (1 - e^{-\pi x}) \frac{1}{\sqrt{1 - e^{-\pi x}}} dx = dx.$$

Thus, since $\bar{w}_t$ does not depend on x, using the definition (2.4.5), substituting (2.6.4) into the second integral appearing in the right hand side of (2.6.3), we readily obtain that

(2.6.5) $$\int_0^\infty w \bar{w}_t \xi_{0x} p(s) ds = \int_0^\infty w \bar{w}_t dx = \bar{w}_t \int_0^\infty w(x,t) dx = \bar{w}\bar{w}_t.$$

As to the first term in the right hand side of (2.6.3), since $L(w)$ is linear self-adjoint operator of the form (2.5.11) we get that

$$w L(w) p(s) = p(s) w \frac{1}{p(s)} \big(p(s) w_s\big)_s = w \big(p(s) w_s\big)_s,$$

which integrated by parts yields

(2.6.6) $$\int_0^\infty w L(w) p(s) ds = \int_0^\infty w \big(p(s) w_s\big)_s ds = w \big(p(s) w_s\big)\Big|_0^\infty - \int_0^\infty p(s) w_s^2 ds.$$

Next, using the boundary conditions (2.6.2b)–(2.6.2e) satisfied by w, in particular meaning that

$$w_x(x,t) \sim o(\xi_{0x}^2) = o(x^{-1}), \quad \text{at } x << 1,$$

and hence

$$w_s(x,t) = w_x(x,t) x_s \sim x^{1/2} o(x^{-1}) = o(x^{-1/2}), \quad \text{at } x << 1,$$

and observing that $p(s)$ satisfies

$$p(s) \sim x, \quad \text{at } x << 1,$$
$$p(s) \sim e^{\frac{\pi}{2}x}, \quad \text{at } x >> 1,$$

we obtain that

$$w\big(p(s)w_s\big)\Big|_0^\infty = \lim_{x\to\infty} e^{\frac{\pi}{2}x} o(e^{-\frac{\pi}{4}x}) o(e^{-\frac{\pi}{4}x}) - 0 \lim_{x\to 0} x x^{-1/2} = 0,$$

and hence

$$\int_0^\infty w L(w) p(s) ds = -\int_0^\infty p(s) w_s^2 ds. \tag{2.6.7}$$

Finally, substituting our findings (2.6.5) and (2.6.7) into (2.6.3) we obtain that

$$\int_0^\infty w w_t p(s) ds = -\int_0^\infty p(s) w_s^2 ds + \bar{w}\bar{w}_t, \tag{2.6.8}$$

which integrated with respect to t, $0 < t < T$ yields

$$\frac{1}{2}\int_0^T \int_0^\infty (w^2)_t p(s) ds dt = -\int_0^T \int_0^\infty p(s) w_s^2 ds dt + \frac{1}{2}\int_0^T (\bar{w}^2)_t dt, \tag{2.6.9}$$

and after formal interchange of integration with respect to t and integration with respect to x, and applying the initial condition (2.6.2f), we get that

$$\frac{1}{2}\int_0^\infty w^2(T) p(s) ds = -\int_0^T \int_0^\infty p(s) w_s^2 ds dt + \frac{1}{2}\bar{w}^2(T). \tag{2.6.10}$$

Next, using the identity

$$p^{-1}(s) x_s = e^{-\frac{\pi}{2}x}(1-e^{-\pi x})^{-1}\frac{1}{\sqrt{1+{\xi_{0x}}^2}} = e^{-\frac{\pi}{2}x}(1-e^{-\pi x})^{-1}\sqrt{1-e^{-\pi x}} = \frac{e^{-\frac{\pi}{2}x}}{\sqrt{1-e^{-\pi x}}} = \xi_{0x},$$

Hölder inequality (TO ADD REFERENCE...) and the boundary conditions (2.4.8a) and (2.4.8b) of ξ_0, we obtain that for every t holds the following inequality:

(2.6.11)

$$\begin{aligned}
\bar{w}^2(t) &= \Big(\int_0^\infty w(x,t) dx\Big)^2 = \Big(\int_0^\infty w(x,t) p^{1/2}(s) p^{-1/2}(s) x_s ds\Big)^2 \\
&\underbrace{\leq}_{\text{Hölder inequlity}} \Big(\int_0^\infty w^2(s,t) p(s) ds\Big)\Big(\int_0^\infty p^{-1}(s) x_s^2 ds\Big) \\
&= \Big(\int_0^\infty w^2(s,t) p(s) ds\Big)\Big(\int_0^\infty p^{-1}(s) x_s^2 s_x dx\Big) = \Big(\int_0^\infty w^2(s,t) p(s) ds\Big)\Big(\int_0^\infty p^{-1}(s) x_s dx\Big) \\
&= \Big(\int_0^\infty w^2(s,t) p(s) ds\Big)\Big(\int_0^\infty \xi_{0x} dx\Big) = \Big(\int_0^\infty w^2(s,t) p(s) ds\Big)\Big(\xi_0(x)\Big|_0^\infty\Big) = \int_0^\infty w^2(s,t) p(s) ds.
\end{aligned}$$

In particular for $t = T$ we have that

$$\bar{w}^2(T) \leq \int_0^\infty w^2(s,T) p(s) ds,$$

and since

$$-\int_0^T \int_0^\infty p(s) w_s^2 ds dt \leq 0,$$

we obtain that the left hand side of the equation (2.6.10) is greater than the right hand side of the same equations, unless

$$w_s(s,t) \equiv 0, \quad \text{for all } 0 \leq s < \infty \text{ and } 0 < t \leq T.$$

This, together with the boundary condition (2.6.2b) and the initial condition (2.6.2f) for w, surely implies that

$$w(s,t) \equiv 0, \quad \text{for all } 0 \leq s < \infty \text{ and } 0 \leq t \leq T,$$

meaning, by the definition (2.6.1) of w, that the solutions $\xi_{1_a}(x,t)$ and $\xi_{1_b}(x,t)$ of (2.4.13) coincide, thus uniqueness of the solutions to the problem (2.4.13) follows.

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