MASTER

Extension of the C method for overhanging gratings

Zheng, Yuhang

Award date:
2006

TECHNISCHE UNIVERSITEIT EINDHOVEN
Department of Mathematics and Computer Science

MASTER'S THESIS

Extension of the C method for overhanging gratings

by
Yuhang Zheng

Supervisor:
Dr.Ir. M.J.H.Anthonissen (TUE)
Ir. N.P.van der Aa (TUE)

Eindhoven, The Netherlands
March 2006

Abstract

Periodic structures, called diffraction gratings play an important role in various metrology applications. The traditional C method is an accurate and efficient method for computing the electromagnetic field due to diffraction gratings. It is applicable to a large class of grating surface profiles, and it is perfectly adapted for modeling multi-layer coated gratings. Its convergence is fast and does not strongly depend on the incident polarization or permittivity of the medium. But there is a limitation for the traditional C method: it can only deal with diffraction gratings of which the interface can be described by a function of the periodicity coordinate. For this thesis, we try to find if there is a way to extend the traditional C method to make it applicable for smooth overhanging gratings.

We make a detailed introduction of the project in Chapter 1. The mathematical model is introduced in Chapter 2. In Chapter 3, the traditional C method will be introduced. Chapter 4 is the core part of this thesis. It presents two possible coordinate transformation describing overhanging gratings of trapezoidal shape and it outlines how the traditional C method can be extended to use more general coordinate transformations.

Acknowledgements

I would like to thank a number of people who helped me in the last two years during my study and the writing of this thesis.

I would like to express my deepest gratitude to my supervisors Dr.Ir. M.J.H.Anthonissen and Ir. N.P.van der Aa who directed me on this project. Their comments and suggestions on my work were always valuable. Their serious attitude was motivating me in my difficult times. I really learnt a lot from this project, the working style of a mathematician, the methodology of study, and the technical report writing. My special gratitude goes also to Prof. R.M.M.Matheij, for giving me the opportunity of being a master student in the CASA group.

Special thanks to all my classmates in Eindhoven for the nice environment in which I could study and for the nice time we spent together after study. Thank you Helen, Hong Deng, Lewie, Mary, Nanda and Yevgen. Special thanks goes also to lovely Enna Van Dijk, for her kindness and patience in helping me a lot for the practical things.

My special thanks goes also to my housemates Xuelin Yang, Yi Jin, Lina Sun who helped me with my everyday troubles and with whom I spent a very nice time in Eindhoven.

My deepest gratitude to my friends here. I would like to mention all my friends who made my stay in Eindhoven more enjoyable. My deepest gratitude to Ting Wang, Shaoxian Zhang, Zhonggui Li, Wei Han, Wei Guo, Filip with whom I spent most of my free time, and who helped me in many hard moments.

Last but not least, I thank my parents and grandparents. The constant help and care from them during all these years made this thesis possible. I would like to express my deepest gratitude to them for their love and support.

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Chapter 1

Introduction

As a start of Chapter 1, the background of the project will be introduced first. Then we come to the problem description. In Section 1.3, we will state the goal of the project. In Section 1.4, there is an overview of the thesis.

1.1 Background

To make computer chips, silicon is used as the raw material. We first cut a silicon ingot into slices, called wafers. Then we process each wafer by lapping, polishing, exposing, ashing, baking, etching, etc. Finishing this set of processes, one layer is added onto the wafer. This layer has a certain structure consisting of lines, holes, etc. Then we repeat these processes to add some more layers onto the wafer. Usually, there are thirty to forty layers on one wafer. Since there are several integrated circuits on a wafer, the wafer is cut into small pieces. Each piece is one integrated circuit. The process is shown in Figure 1.2. Finally, we get chips by packing these integrated circuits.

As stated above, a layer is added on the top of another layer. When doing this, each layer should be positioned accurately with respect to each other to obtain high quality circuits. To achieve this, diffraction gratings are used for alignment, which are periodic structures made on the surface of the wafer (see Figure 1.3). However, gratings will damage because of the process of adding layers. This will effect the accuracy of alignment.

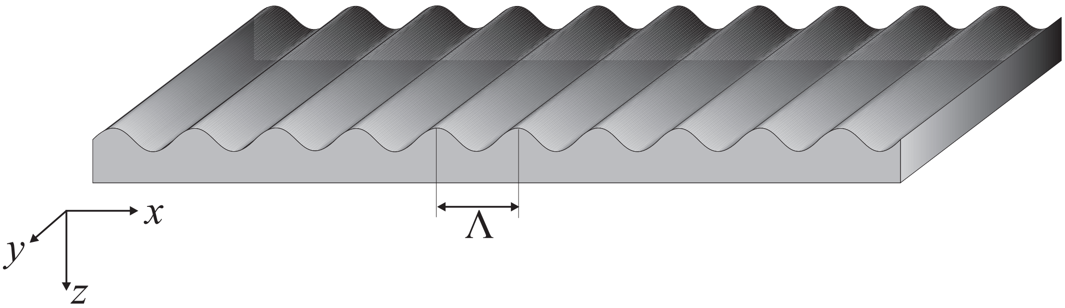

Figure 1.1: Gratings on the markers

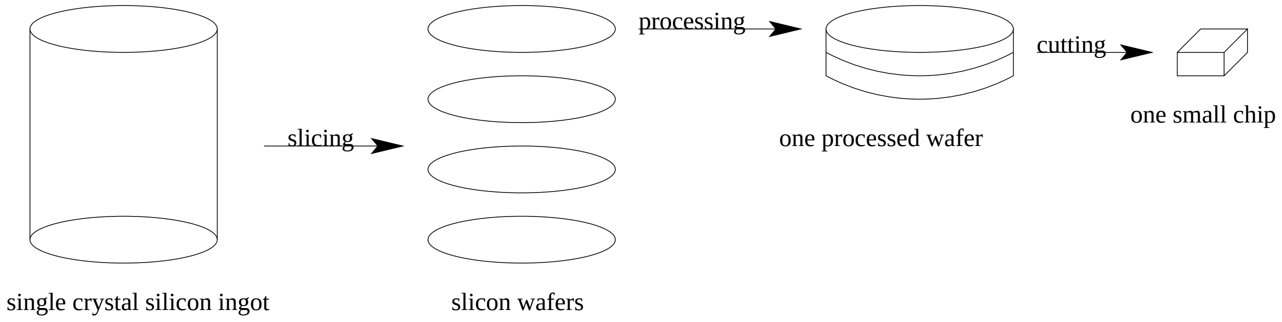

Figure 1.2: Chip making process

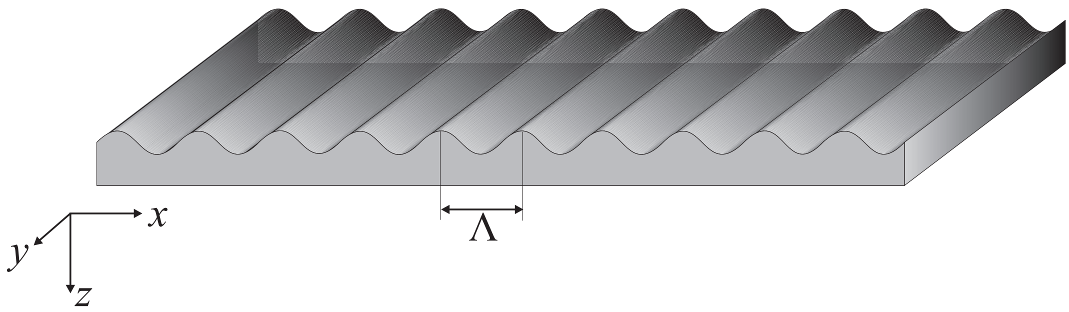

Figure 1.3: Gratings on the markers

To correct for this problem, we have to know:

- the kind of process which caused the damages
- the shape of the damaged gratings

But how to get the results? The problem is that the damaged gratings cannot be seen and measured directly. In practice, we use a laser for measuring: let a laser shoot onto the surface of the grating, and measure the field that is reflected. We can also compute the reflected field for a guessed shape of the grating, because we assume that the incident field and the media properties are given. Comparing the measured and computed reflected fields, we can make a (better) guess for the grating's shape. By iteration, finally we can get a sufficiently accurate result for the grating shape. Combined with the knowledge about the process, its position can be estimated more accurately. The ingenuity of the C method is the introduction of a new coordinate system that not only maps corrugated grating surfaces to planar surfaces, making the matching of boundary conditions easy, but also transforms Maxwell's equations in Fourier space into a matrix eigenvalue problem. Consequently, numerical solution of the grating problem is straightforward.

1.2 Problem description

To compute the field (electromagnetic field) reflected by a diffraction grating, there are several methods. One of them is the C method. The C method is an accurate and efficient method in computing the electromagnetic field for smooth gratings of which the interface

Figure 1.4: Different types of gratings: a non-overhanging grating (left), a binary grating (middle), an overhanging grating (right)

can be described by a continuously differentiable function at each point.

For the C method, we make a coordinate transformation such that the interface between two media becomes a flat line in the new coordinate system. Then the model domain will be separated into two parts, and we get a solution for each medium respectively.

But there is a limitation for the C method as it is applied nowadays: it can only deal with diffraction gratings of which the interface can be described by a function of the periodicity coordinate. Figure 1.4 shows three types of interface, all of which are periodic gratings. On the left is a non-overhanging grating which can be described by a single valued function. In the Figure, shown in the middle is a binary grating which is the extreme case for the C method to compute. And the right grating represents an overhanging grating. We can see that the right one cannot be described by a single valued function, thus the C method cannot be applied to this one.

1.3 Goal of the project

The goal of this master project is to find out if there is a way to extend the C method, such that it is applicable for overhanging gratings as well. Thus in this project, we will only focus on this specific class of gratings: overhanging gratings.

1.4 Overview of the thesis

This thesis will start from introducing some related physical theories about electromagnetism and the mathematical problem in Chapter 2. Then we will explain the C method in detail in Chapter 3. Chapter 4 describes the way to extend the C method for overhanging gratings.

Chapter 2

Mathematical model

In this chapter, we start from Maxwell's equations. Then constitutive relations and the continuity equation will be introduced to simplify Maxwell's equations. In Section 2.4, a mathematical problem will be introduced which the C method solves.

2.1 Maxwell's equations

The C method is based on a classical group of equations: Maxwell's equations. It is used to describe the relationship between electromagnetic fields.

$$\begin{cases} \nabla \cdot \mathbf{D}(\mathbf{x}, t) = \rho(\mathbf{x}, t) \\ \nabla \times \mathbf{E}(\mathbf{x}, t) = -\dfrac{\partial \mathbf{B}(\mathbf{x}, t)}{\partial t} \\ \nabla \cdot \mathbf{B}(\mathbf{x}, t) = 0 \\ \nabla \times \mathbf{H}(\mathbf{x}, t) = \mathbf{J}(\mathbf{x}, t) + \dfrac{\partial \mathbf{D}(\mathbf{x}, t)}{\partial t} \end{cases} \tag{2.1}$$

Here, $\mathbf{D}$ is the electric flux density with unit C/m^2, ρ is the charge density with unit C/m^3, $\mathbf{E}$ is the electric field with unit V/m, $\mathbf{B}$ is the magnetic flux density with unit T, $\mathbf{H}$ is the magnetic field with unit A/m, and $\mathbf{J}$ is the electric current density with unit A/m^2.

2.2 Constitutive relations

In electromagnetism, we have three related physical quantities to describe the media properties: permittivity $\varepsilon(\mathbf{x}, t)$, electrical conductivity $\boldsymbol{\sigma}(\mathbf{x}, t)$, and permeability $\boldsymbol{\mu}(\mathbf{x}, t)$. Here, the constitutive equations which describe the relationship between the basic variables are introduced:

$$\begin{aligned} \mathbf{D}(\mathbf{x}, t) &= \varepsilon(\mathbf{x}, t)\mathbf{E}(\mathbf{x}, t) \\ \mathbf{J}(\mathbf{x}, t) &= \boldsymbol{\sigma}(\mathbf{x}, t)\mathbf{E}(\mathbf{x}, t) \\ \mathbf{B}(\mathbf{x}, t) &= \boldsymbol{\mu}(\mathbf{x}, t)\mathbf{H}(\mathbf{x}, t) \end{aligned} \tag{2.2}$$

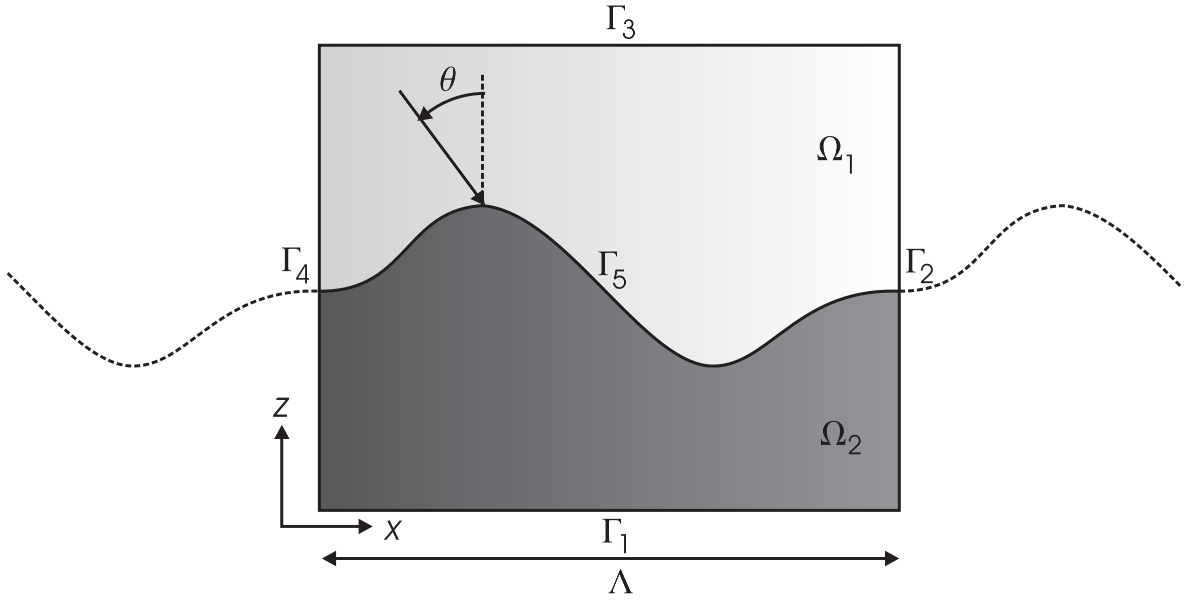

Figure 2.1: Representation of mathematical domain

2.3 Continuity equation

Besides the constitutive equations, also the continuity equation holds:

$$\nabla \cdot \mathbf{J}(\mathbf{x}, t) = -\frac{\partial \rho(\mathbf{x}, t)}{\partial t} \tag{2.3}$$

where ρ is the charge density with unit C/m^3.

2.4 Model Introduction

2.4.1 Assumptions

To describe the model, some assumptions are given. A restriction is made to a two-media grating with a smooth interface. As is illustrated in Figure 2.1, a laser beam is incident on the interface under an angle θ. The grating is assumed to have the following properties:

- Periodic in one direction
  We consider the gratings to be periodic in one direction, along the x-axis. Having this property, we can apply Fourier expansions to the material properties.

- Infinitely many periods
  We assume that for the x-direction, the grating has infinitely many periods. We do this so that we can reduce our model to one period only by imposing periodic boundary conditions.

- Independent of the $y-$direction
  The gratings are considered to be independent of the $y-$direction. With this assumption, we can restrict ourselves to a cross-section of the grating.

In Figure 2.1, there are two different domains: Ω_1 and Ω_2. They represent two media: Ω_1 is usually air and Ω_2 is a kind of material which can be dielectric or metallic. For the materials, we have some additional assumptions. The materials are

- Isotropic
  The material properties $(\varepsilon, \ \sigma, \ \mu)$ are considered to be direction independent.
- Homogeneous
  The material properties are considered to be independent of the space coordinates for each medium separately.
- Time-invariant
  The material properties are considered to be independent of time.
- Non-magnetic
  We consider the permeability of the medium to be equal to the permeability of vacuum, viz. $\mu = \mu_0$.
- Source free
  For the model, we assume that there are no external currents or charges.

In the beginning, the physical quantities $\boldsymbol{\varepsilon}$, $\boldsymbol{\sigma}$, and $\boldsymbol{\mu}$ are tensors depending on space and time. After applying the assumptions, they reduce to scalar constants. Thus we have:

$$\begin{aligned} \boldsymbol{\varepsilon}(\mathbf{x}, t) &= \varepsilon \\ \boldsymbol{\sigma}(\mathbf{x}, t) &= \sigma \\ \boldsymbol{\mu}(\mathbf{x}, t) &= \mu_0 \end{aligned} \tag{2.4}$$

We also have assumptions for both the electric and the magnetic field. The fields are assumed to be

- Time-harmonic
  Since the time of initiation is not important to our model, the fields are assumed to be time harmonic which means we neglect the fact that the field was once initiated. With this assumption, we can eliminate the time derivatives. Then the fields are represented by:

  $$\begin{aligned} \mathbf{E}(\mathbf{x}, t) &= \tilde{\mathbf{E}}(\mathbf{x}) \exp[i\omega t] \\ \mathbf{H}(\mathbf{x}, t) &= \tilde{\mathbf{H}}(\mathbf{x}) \exp[i\omega t] \end{aligned} \tag{2.5}$$

  where ω is the angular frequency with unit s^{-1}.
- Monochromatic
  We regard the field as monochromatic, which means that it has only one wavelength. The case of multiple wavelengths is a superposition of several monochromatic fields. Therefore, we can restrict ourselves to monochromatic fields.
- Finite
  Considering energy, the fields should be finite everywhere.

2.4.2 Mathematical equations

From the assumptions, we know that the constitutive equations are reduced to

$$\begin{aligned} \mathbf{D}(\mathbf{x},t) &= \varepsilon\mathbf{E}(\mathbf{x},t), \\ \mathbf{J}(\mathbf{x},t) &= \sigma\mathbf{E}(\mathbf{x},t) \\ \mathbf{B}(\mathbf{x},t) &= \mu_0\mathbf{H}(\mathbf{x},t) \end{aligned} \tag{2.6}$$

For both domains Ω_1 and Ω_2, Maxwell's equations (2.1) hold. Substituting equations (2.6) into Maxwell's equations (2.1), we get:

$$\begin{cases} \nabla \times \mathbf{E}(\mathbf{x},t) = -\mu_0 \dfrac{\partial \mathbf{H}(\mathbf{x},t)}{\partial t} \\ \nabla \times \mathbf{H}(\mathbf{x},t) = \sigma\mathbf{E}(\mathbf{x},t) + \varepsilon \dfrac{\partial \mathbf{E}(\mathbf{x},t)}{\partial t} \\ \nabla \cdot \mathbf{H}(\mathbf{x},t) = 0 \\ \nabla \cdot \mathbf{E}(\mathbf{x},t) = \dfrac{\rho(\mathbf{x},t)}{\varepsilon} \end{cases} \tag{2.7}$$

To simplify the computation, we want $\nabla \cdot \mathbf{E} = 0$. From the continuity equation (2.3), we know that $\dfrac{\partial \rho}{\partial t} = -\nabla \cdot \mathbf{J}$. With the source free assumption, we can write $\dfrac{\partial \rho}{\partial t} = -\sigma \nabla \cdot \mathbf{E}$. From equation (2.7), we get $\dfrac{\partial \rho}{\partial t} = -\dfrac{\sigma}{\varepsilon}\rho$, thus we have: $\rho \sim e^{-\frac{\sigma}{\varepsilon}t}$. Because of the time-harmonic assumption (2.5), we may take $t \to \infty$, and hence $\rho = 0$, which means $\nabla \cdot \mathbf{E}(\mathbf{x},t) = 0$

From the time-harmonic field assumption, we obtain the following equations for the model:

$$\begin{cases} \nabla \times \tilde{\mathbf{E}}(\mathbf{x}) = -i\omega\mu_0\tilde{\mathbf{H}}(\mathbf{x}) \\ \nabla \times \tilde{\mathbf{H}}(\mathbf{x}) = i\omega(\varepsilon - i\dfrac{\sigma}{\omega})\tilde{\mathbf{E}}(\mathbf{x}) \\ \nabla \cdot \tilde{\mathbf{H}}(\mathbf{x}) = 0 \\ \nabla \cdot \tilde{\mathbf{E}}(\mathbf{x}) = 0 \end{cases} \tag{2.8}$$

These equations are valid for both Ω_1 and Ω_2.

Actually, for the C method, we would like to transform equation (2.8) into a second order differential equation, a generalized Helmholtz equation. The reason for this is that the Helmholtz equation is an easier starting point to introduce the coordinate transformation, which is the core part of the C method.

It is convenient to introduce two new constants: the wave number k, and the refractive index ν.

$$k = \omega\sqrt{\mu_0\varepsilon_0} = \frac{2\pi}{\lambda}, \qquad \nu = \frac{\sqrt{\mu\varepsilon}}{\sqrt{\mu_0\varepsilon_0}} = \sqrt{\frac{\varepsilon}{\varepsilon_0}} \tag{2.9}$$

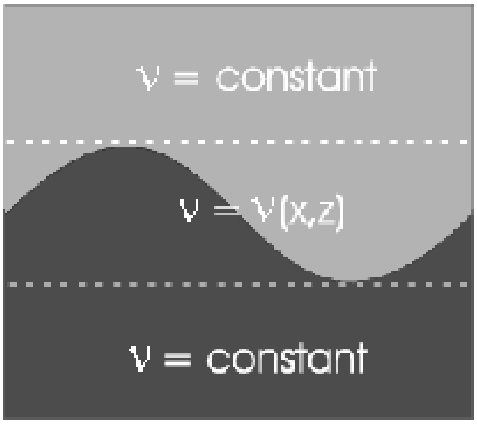

Figure 2.2: Refractive index ν changing with the medium

where λ is the wavelength of the laser, ε_0 is the permittivity of the vacuum. Note that the refractive index ν is different for medium 1 and 2. Thus for the whole domain $\Omega_1 \cup \Omega_2$, we write $\nu(\mathbf{x})$.

For simplicity, we discard the tilde in equation (2.8), and write $\varepsilon - i\frac{\sigma}{\omega}$ as ε, then we obtain from the first two equations of (2.8):

$$\nabla \times (\nabla \times \mathbf{E}) = -i\omega\mu_0(\nabla \times \mathbf{H}) = \omega^2\varepsilon\mu_0\mathbf{E}$$

From mathematics, we know that:

$$\nabla \times (\nabla \times \mathbf{E}) = \nabla(\nabla \cdot \mathbf{E}) - \nabla^2\mathbf{E}$$

From the last equation of (2.8), we know that $\nabla \cdot \mathbf{E} = 0$. By substitution, we get:

$$\nabla(\nabla \cdot \mathbf{E}) - \nabla^2\mathbf{E} = \omega^2\varepsilon\mu_0\mathbf{E} = k^2\nu^2\mathbf{E}$$

Thus we have:

$$\nabla^2\mathbf{E} + k^2\nu^2\mathbf{E} = 0 \tag{2.10}$$

Similarly, we get for the magnetic field:

$$\nabla^2\mathbf{H} + k^2\nu^2\mathbf{H} = 0 \tag{2.11}$$

Since the shapes of both equations (2.10) and (2.11) are the same, we use **F** to represent either **E** or **H**. Hence, we get the generalized form of the Helmoltz equation:

$$\nabla^2\mathbf{F} + k^2\nu^2(\mathbf{x})\mathbf{F} = 0 \tag{2.12}$$

Note that (2.12) reduces to the Helmholtz equation if the refractive index ν is a constant. Thus we can use it for the upper area Ω_1 and the lower area Ω_2 of the domain (see Figure 2.2).

2.4.3 Boundary conditions

Boundary conditions are used to make the solution unique. In Figure 2.1, we can see that there are five boundaries for the model, viz. $\Gamma_1, ..., \Gamma_5$. We use **F** to represent either **E** or **H** and impose the following boundary conditions:

- Γ_1 and Γ_3: outgoing wave condition

$$\lim_{z \to \pm\infty} |\mathbf{F}(x, z)| < \infty, \quad -\frac{\Lambda}{2} < x < \frac{\Lambda}{2} \tag{2.13}$$

  where Λ is the length of one period. Boundaries Γ_1 and Γ_3 represent the boundaries for $z \to \infty$ and $z \to -\infty$. Because the fields are finite everywhere, Γ_1 and Γ_3 have identical boundary conditions, namely the outgoing wave condition.

- Γ_2 and Γ_4: pseudo-periodic boundary condition (Floquet condition)

$$\mathbf{F}(x + \Lambda, z) = \mathbf{F}(x, z) \exp(ik\Lambda \sin\theta), \quad -\frac{\Lambda}{2} < x < \frac{\Lambda}{2}, -\infty < z < \infty, \quad k = \frac{2\pi}{\lambda} \tag{2.14}$$

  Pseudo-periodic means periodic up to a phase correction. The phase correction depends on the incident field which will be discussed in the next section.

- Γ_5: continuity of the field components that are tangential to the interface

$$\begin{aligned} \mathbf{n} \times \left(\mathbf{F}^{I}(x, z) - \mathbf{F}^{II}(x, z)\right) &= \mathbf{0} \\ \Rightarrow \mathbf{F}_t^{I}(x, z) - \mathbf{F}_t^{II}(x, z) &= \mathbf{0}, \quad (x, z) \in \Gamma_5 \end{aligned} \tag{2.15}$$

  We can get this according to the boundary condition at the interface of two media. **n** is the normal of the interface, $\mathbf{F}^{I}$ and $\mathbf{F}^{II}$ denote the fields in the two media respectively.

  We know that the magnetic field has effect on the electric field. Thus we get:

$$\mathbf{G}_n^{I}(x, z) - \mathbf{G}_n^{II}(x, z) = \mathbf{0}, \quad (x, z) \in \Gamma_5 \tag{2.16}$$

  where

$$\mathbf{G} = \begin{cases} n^2\mathbf{E}, & \text{for TM polarization} \\ -\sqrt{\dfrac{\mu}{\varepsilon_0}}\mathbf{H}, & \text{for TE polarization} \end{cases}$$

  This condition will be explained later in next chapter.

2.4.4 Incident field

In this thesis, we only concentrate on two extreme types of incident fields, namely **TE** and **TM** polarized fields. For **TE** polarization, there is only a y component of **E**, viz. E_y. In addition, H_x and H_z should also be considered, since they effect the electric field E_y. Similarly, for **TM** polarization, only H_y, E_x, and E_z are present. Every other linearly polarized light can be considered as a mixture of these two extremes.

For **TE** polarization, the incident field is given by the electric field $\mathbf{E}^{inc} = E_y\mathbf{e}_y$, where $\mathbf{e}_y$

is the unit vector for y component. For **TM** polarization, the incident field is given by the magnetic field $\mathbf{H}^{inc} = H_y \mathbf{e}_y$. As in (2.12), we write **F** for both **E** and **H**:

$$\mathbf{F}^{inc} = F_y \mathbf{e}_y \tag{2.17}$$

And we have

$$F_y^{inc}(x,z) \quad = \quad \exp(i\alpha_0 x - i\beta_{0,1} z) \tag{2.18}$$

We defined a grating that is independent of the y direction. Also the incident field is defined independent of the y direction. Thus we can get a conclusion that the whole field is independent of the y direction. This means F_y only depends on the x and z coordinates. Thus we only use the expression $F_y(x,z)$ in the equation. And derivatives with respect to the y coordinate equal zero.

For polarization we use $\mathbf{F}_y$ for **F**, and for the independency of y direction we use $F_y(x,z)$ for **F**.

2.4.5 Mathematical problem

To summarize, we state the complete mathematical problem for the model:

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2} + k^2 \nu^2(x,z)\right) F_y(x,z) = 0, \quad -\frac{\Lambda}{2} < x < \frac{\Lambda}{2}, \qquad -\infty < z < \infty \tag{2.19}$$

$$\begin{cases} \lim_{z\to\pm\infty} |F_y(x,z)| < \infty, & -\frac{\Lambda}{2} < x < \frac{\Lambda}{2}, \\ F_y(x+\Lambda,z) = F_y(x,z)\exp(ik\Lambda\sin\theta), & -\frac{\Lambda}{2} < x < \frac{\Lambda}{2}, \qquad -\infty < z < \infty \\ F_{y,1t}(x,z) - F_{y,2t}(x,z) = 0, & (x,z) \in \Gamma_5 \\ G_{y,1n}(x,z) - G_{y,2n}(x,z) = 0, & (x,z) \in \Gamma_5 \end{cases} \tag{2.20}$$

To solve equation (2.19), we need boundary conditions (2.20) to find a unique solution.

Chapter 3

Description of the C method

In this chapter we explain how the C method solves the mathematical problem (2.19)-(2.20). In Section 3.1, the Rayleigh expansion which can be regarded as a solution above and below the grating will be introduced. In Section 3.2, we will give an overview of the C method. In Section 3.3, we will see the details of the C method.

3.1 Rayleigh expansion

For the mathematical problem (2.19)-(2.20), it is impossible to solve the equation for a general grating directly, thus we make an Ansatz for its solution. From physics, we know that the Rayleigh expansion holds above and below the grating.

From boundary condition (2.14), we know that the field is pseudo-periodic:

$$F_y(x+\Lambda, z) = F_y(x, z)\exp(ik\Lambda\sin\theta) \tag{3.1}$$

Introduce a new field $\tilde{F}_y(x, z) = F_y(x, z)\exp(-ikx\sin\theta)$, then we have:

$$\begin{aligned} \tilde{F}_y(x+\Lambda, z) &= F_y(x+\Lambda, z)\exp(-ik(x+\Lambda)\sin\theta) \\ &= F_y(x+\Lambda, z)\exp(-ikx\sin\theta)\exp(-ik\Lambda\sin\theta) \\ &= F_y(x, z)\exp(-ikx\sin\theta) \\ &= \tilde{F}_y(x, z) \end{aligned}$$

Thus $\tilde{F}_y(x, z)$ is a periodic function and we can therefore apply a Fourier expansion

$$\tilde{F}_y(x, z) = \sum_{n=-\infty}^{\infty} \tilde{F}_{yn}(z)\exp(inKx) \qquad (K = \frac{2\pi}{\Lambda})$$

Thus for the original field, we get:

$$\begin{aligned} F_y(x, z) &= \tilde{F}_y(x, z)\exp(ikx\sin\theta) \\ &= \sum_{n=-\infty}^{\infty} \tilde{F}_{yn}(z)\exp(inKx + ikx\sin\theta) \\ &= \sum_{n=-\infty}^{\infty} \tilde{F}_{yn}(z)\exp(i\alpha_n x) \qquad (\alpha_n = nK + k\sin\theta) \end{aligned} \tag{3.2}$$

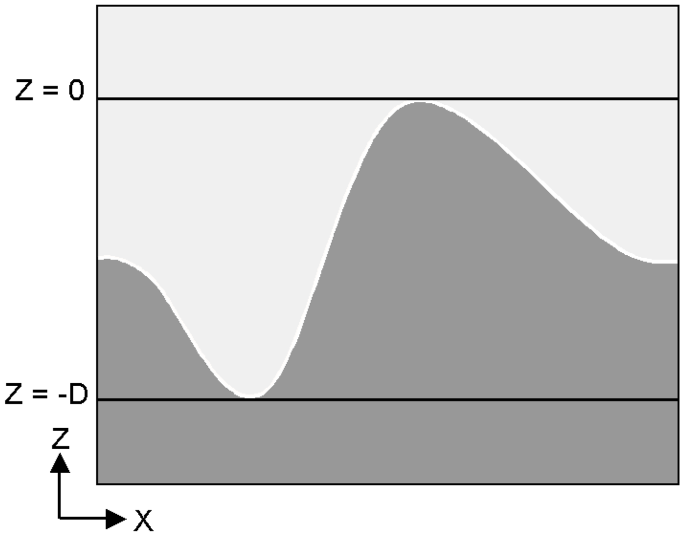

Figure 3.1: Illustration of coordinate transformation

We know that the field should also be related to z. Substitute (3.2) into the Helmholtz equation (2.19) directly, we get the form of the Rayleigh expansion

$$F_y(x,z) = \sum_{n=-\infty}^{\infty} A_n \exp(i\alpha_n x - i\beta_n^I z), \qquad z > 0 \tag{3.3}$$

$$F_y(x,z) = \sum_{n=-\infty}^{\infty} B_n \exp(i\alpha_n x + i\beta_n^{II}(z+D)), \qquad z < -D \tag{3.4}$$

where A_n are the reflected field coefficients, and B_n are the transmitted field coefficients to be determined, D is the height of the grating (See Figure 3.1). And we have $\beta_n^I = \sqrt{k^2\nu_1^2 - \alpha_n^2}$, $\beta_n^{II} = \sqrt{k^2\nu_2^2 - \alpha_n^2}$, where ν_1 and ν_2 are refractive index for the two medium respectively.

Like the Helmholtz equation, the Rayleigh expansion is also only valid above and below the grating where the refractive index ν is a constant. We can see from Figure 2.2 that the refractive index ν is not a constant in the middle area but a function of x and z.

In Figure 2.2, the interface is a curve which is described by $z = a(x)$. But if the interface were a flat line, there would be only two half spaces, and the refractive index would be a constant in both areas. Then we can use two different Rayleigh expansions for the two media and the boundary condition at the interface to get the solution for the entire domain. This gives the inspiration to use a coordinate transformation. Use the coordinate transformation given below:

$$\begin{cases} u = x \\ v = y \\ w = z - a(x) \end{cases} \tag{3.5}$$

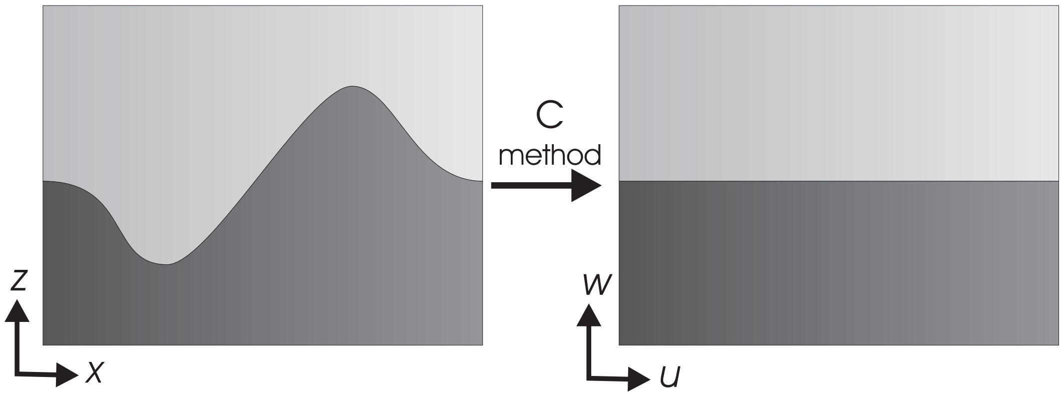

Figure 3.2: Illustration of coordinate transformation

where the function $z = a(x)$ is used to describe the interface. By this transformation, the interface will be transformed into a flat line in the new coordinate system. This process is illustrated in Figure 3.2. This is the core idea for the C method.

In the new coordinate, we introduce a new form for the Rayleigh expansion:

$$F_\nu(u, w) = \sum_{n=-\infty}^{\infty} \tilde{A}_n \exp(i\alpha_n u - i\xi w), \qquad w > 0 \tag{3.6}$$

$$F_\nu(u, w) = \sum_{n=-\infty}^{\infty} \tilde{B}_n \exp(i\alpha_n u + i\xi w), \qquad w < 0 \tag{3.7}$$

with ξ another unknown which will be explained later. The difference for the Rayleigh expansion is that in the original coordinate β is known while now ξ is unknown. Therefore we call (3.6) and (3.7) generalized Rayleigh expansions.

3.2 Overview of the C method

Until now we have already introduced the mathematical problem to be solved and the form of the solution which can be used. We make a coordinate transformation so that the generalized Rayleigh expansion is valid in the whole domain. The problem is how to get the coefficients of the Rayleigh expansion.

After the coordinate transformation, the original equation will no longer be a Helmholtz equation but a generalized version of it.

By substituting the generalized Rayleigh expansion (3.6), (3.7) and the coordinate transformation (3.5) into the generalized Helmholtz equation (2.19), there will be an eigenvalue system (shown later). Solving the eigenvalue system gives eigenvalues and their corresponding eigenvectors.

By using the boundary condition at the interface, we can compute the corresponding coefficients for these eigenvectors.With the eigenvalues, eigenvectors and their corresponding coefficients, we can get the coefficients for the generalized Rayleigh expansion (3.6) and (3.7), which means we get the solution of the mathematical problem.

3.3 Details of the C method

3.3.1 Coordinate transformation

Consider the coordinate transformation as introduced before:

$$\begin{cases} u = x \\ v = y \\ w = z - a(x) \end{cases}$$

Listed below is the process to transform the model equation (2.19) step by step.

- Unit vectors:

$$\begin{cases} \mathbf{e}_x = \dfrac{\partial u}{\partial x}\mathbf{e}_u + \dfrac{\partial v}{\partial x}\mathbf{e}_v + \dfrac{\partial w}{\partial x}\mathbf{e}_w = \mathbf{e}_u - \dot{a}\mathbf{e}_w \\[2ex] \mathbf{e}_y = \dfrac{\partial u}{\partial y}\mathbf{e}_u + \dfrac{\partial v}{\partial y}\mathbf{e}_v + \dfrac{\partial w}{\partial y}\mathbf{e}_w = \mathbf{e}_v \\[2ex] \mathbf{e}_z = \dfrac{\partial u}{\partial z}\mathbf{e}_u + \dfrac{\partial v}{\partial z}\mathbf{e}_v + \dfrac{\partial w}{\partial z}\mathbf{e}_w = \mathbf{e}_w \end{cases} \tag{3.8}$$

  where $\dot{a}$ is the derivative of $a(x)$ with respect to x.

- Partial derivatives:

$$\begin{cases} \dfrac{\partial}{\partial x} = \dfrac{\partial u}{\partial x}\dfrac{\partial}{\partial u} + \dfrac{\partial v}{\partial x}\dfrac{\partial}{\partial v} + \dfrac{\partial w}{\partial x}\dfrac{\partial}{\partial w} = \dfrac{\partial}{\partial u} - \dot{a}\dfrac{\partial}{\partial w} \\[2ex] \dfrac{\partial}{\partial z} = \dfrac{\partial u}{\partial z}\dfrac{\partial}{\partial u} + \dfrac{\partial v}{\partial z}\dfrac{\partial}{\partial v} + \dfrac{\partial w}{\partial z}\dfrac{\partial}{\partial w} = \dfrac{\partial}{\partial w} \\[2ex] \dfrac{\partial^2}{\partial x^2} = \dfrac{\partial}{\partial x}\left(\dfrac{\partial}{\partial x}\right) = \dfrac{\partial}{\partial x}\left(\dfrac{\partial}{\partial u} - \dot{a}\dfrac{\partial}{\partial w}\right) = \dfrac{\partial^2}{\partial u^2} - 2\dot{a}\dfrac{\partial^2}{\partial w \partial u} - \ddot{a}\dfrac{\partial}{\partial w} + \dot{a}^2\dfrac{\partial^2}{\partial w^2} \\[2ex] \dfrac{\partial^2}{\partial z^2} = \dfrac{\partial}{\partial z}\left(\dfrac{\partial}{\partial z}\right) = \dfrac{\partial}{\partial z}\left(\dfrac{\partial}{\partial w}\right) = \dfrac{\partial^2}{\partial w^2} \end{cases} \tag{3.9}$$

- Field components:

$$\begin{cases} \begin{aligned} F_x &= \mathbf{F} \cdot \mathbf{e}_x = (F_u\mathbf{e}_u + F_v\mathbf{e}_v + F_w\mathbf{e}_w) \cdot \mathbf{e}_x \\ &= (F_u\mathbf{e}_u + F_v\mathbf{e}_v + F_w\mathbf{e}_w) \cdot (\mathbf{e}_u - \dot{a}\mathbf{e}_w) = F_u - \dot{a}F_w \\[1ex] F_y &= \mathbf{F} \cdot \mathbf{e}_y = (F_u\mathbf{e}_u + F_v\mathbf{e}_v + F_w\mathbf{e}_w) \cdot \mathbf{e}_y \\ &= (F_u\mathbf{e}_u + F_v\mathbf{e}_v + F_w\mathbf{e}_w) \cdot \mathbf{e}_v = F_v \\[1ex] F_z &= \mathbf{F} \cdot \mathbf{e}_z = (F_u\mathbf{e}_u + F_v\mathbf{e}_v + F_w\mathbf{e}_w) \cdot \mathbf{e}_z \\ &= (F_u\mathbf{e}_u + F_v\mathbf{e}_v + F_w\mathbf{e}_w) \cdot \mathbf{e}_w = F_w \end{aligned} \end{cases} \tag{3.10}$$

Note that the components in the u- and v-direction are tangential to the interface, but the w-component is not normal to the interface. The periodicity is preserved in the u-direction (see Figure 3.2).

When coming to calculation, we should consider each medium separately. Below we will compute the field for Ω_1 (the upper half space) and for Ω_2 (the lower half space). Substitute the coordinate transformation (3.5) into the Helmholtz equation (2.19), using the expression for the partial derivatives (3.9) and field components (3.10), we can get:

$$\begin{aligned} & \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2} + k^2 \nu^2(x,z)\right) F_y(x,z) \\ = & \left(\frac{\partial^2}{\partial u^2} - 2\dot{a}\frac{\partial^2}{\partial w \partial u} - \ddot{a}\frac{\partial}{\partial w} + (1+\dot{a}^2)\frac{\partial^2}{\partial w^2} + k^2\nu_s^2\right) F_v = 0 \end{aligned} \tag{3.11}$$

Note that $s = 1, 2$, and ν_s is a constant for each medium.

3.3.2 Eigenvalue system

In this section, it will be shown that equation (3.11) will result in one eigenvalue system for each medium. We will show this for the two different media separately.

Medium 1

Substitution of the generalized Rayleigh expansion (3.6) for Ω_1 into the generalized Helmholtz equation (3.11) gives:

$$\sum_{n=-\infty}^{\infty} \left(-\alpha_n^2 - 2\dot{a}\xi\alpha_n + \ddot{a}\xi i - \xi^2 - \dot{a}^2\xi^2 + k^2\nu_1^2\right)\tilde{A}_n \exp(i\alpha_n u - i\xi w) = 0 \tag{3.12}$$

Since $\dot{a}$ is a periodic function of u, we can develop it in a Fourier series:

$$\dot{a} = \sum_r \dot{a}_r \exp(-i\frac{2\pi r}{\Lambda}u)$$

In equation (3.12), we have six terms in all. Here we deduce them separately as written below:

1.

$$\sum_{n=-\infty}^{\infty} -\alpha_n^2 \tilde{A}_n \exp(i\alpha_n u - i\xi w) \tag{3.12.1}$$

2.

$$\begin{aligned}
&\sum_{n=-\infty}^{\infty} 2\dot{a}\xi\alpha_n\tilde{A}_n \exp(i\alpha_n u - i\xi w) \\
=&2\sum_n\sum_r \dot{a}_r \exp(-i\frac{2\pi r}{\Lambda}u)\xi\alpha_n\tilde{A}_n\exp(i\alpha_n u - i\xi w) \\
=&2\sum_n\sum_r \dot{a}_r\tilde{A}_n\exp(-i\xi w + iu\frac{2\pi}{\lambda}\nu_1\sin\theta + iu\frac{2\pi(n-r)}{\Lambda})\xi\alpha_n \\
=&2\sum_n\sum_l \dot{a}_{n-l}\tilde{A}_n\exp(i\alpha_l u - i\xi w) \qquad (l := n-r)
\end{aligned} \tag{3.12.2}$$

3.

$$\begin{aligned}
&\sum_{n=-\infty}^{\infty} \ddot{a}\xi i\tilde{A}_n\exp(i\alpha_n u - i\xi w) \\
=&\sum_n\sum_r \frac{2\pi r}{\Lambda}\dot{a}_r\xi\tilde{A}_n\exp(-i\xi w - i\frac{2\pi r}{\Lambda}u + i\alpha_n u) \\
=&\sum_n\sum_r \frac{2\pi r}{\Lambda}\dot{a}_r\xi\tilde{A}_n\exp(-i\xi w - i\alpha_{n-r}u) \\
=&\sum_n\sum_l \frac{2\pi(n-l)}{\Lambda}\xi\dot{a}_{n-l}\tilde{A}_n\exp(i\alpha_l u - i\xi w)
\end{aligned} \tag{3.12.3}$$

4.

$$\sum_{n=-\infty}^{\infty} -\xi^2\tilde{A}_n\exp(i\alpha_n u - i\xi w) \tag{3.12.4}$$

5.

$$\begin{aligned}
&\sum_{n=-\infty}^{\infty} -\dot{a}^2\xi^2\tilde{A}_n\exp(i\alpha_n u - i\xi w) \\
=&-\sum_n\sum_r\sum_p \dot{a}_r\dot{a}_p\xi^2\tilde{A}_n\exp(i\frac{2\pi}{\lambda}\nu_1\sin\theta u + i\frac{2\pi n}{\Lambda}u - i\frac{2\pi(p+r)}{\Lambda}u - i\xi w) \\
=&-\sum_n\sum_r\sum_p \dot{a}_r\dot{a}_p\xi^2\tilde{A}_n\exp(i\alpha_{n+p+r}u - i\xi w) \qquad (k := n+p+r) \\
=&-\sum_n\sum_r\sum_k \dot{a}_r\dot{a}_{k-n-r}\xi^2\tilde{A}_n\exp(i\alpha_k u - i\xi w) \\
=&-\sum_n\sum_l\sum_k \dot{a}_{l-n}\dot{a}_{k-l}\xi^2\tilde{A}_n\exp(i\alpha_k u - i\xi w) \qquad (l\to m,\ k\to n,\ n\to r) \\
=&-\sum_n\sum_m\sum_r \dot{a}_{n-m}\dot{a}_{m-r}\xi^2\tilde{A}_r\exp(i\alpha_n u - i\xi w)
\end{aligned} \tag{3.12.5}$$

6.

$$k^2\nu_1^2\sum_n \tilde{A}_n\exp(i\alpha_n u - i\xi w) \tag{3.12.6}$$

Combining (3.12.2)+(3.12.3), gives:

$$
\begin{aligned}
&2\sum_n\sum_l \dot{a}_{n-l}\tilde{A}_n\exp(i\alpha_l u - i\xi w) + \sum_n\sum_l \frac{2\pi(n-l)}{\Lambda}\xi\dot{a}_{n-l}\tilde{A}_n\exp(i\alpha_l u - i\xi w)\\
&= \sum_n\sum_l(\alpha_n+\alpha_l)\dot{a}_{n-l}\tilde{A}_n\exp(i\alpha_l u - i\xi w)\\
&= \sum_m\sum_n(\alpha_m+\alpha_n)\dot{a}_{n-m}\tilde{A}_m\exp(i\alpha_n u - i\xi w)
\end{aligned}
$$

By substituting (3.12.1) –(3.12.6) into (3.12), we obtain:

$$
\begin{aligned}
&\sum\left(-\alpha_n^2 + 2\dot{a}\xi\alpha_n + \ddot{a}\xi i - \xi^2 - \dot{a}^2\xi^2 + k^2v_1^2\right)\tilde{A}_n\exp(i\alpha_n u - i\xi w)\\
= \quad &\sum -\alpha_n^2\tilde{A}_n\exp(i\alpha_n u - i\xi w) + \sum_m\sum_n(\alpha_m+\alpha_n)\dot{a}_{n-m}\tilde{A}_m\exp(i\alpha_n u - i\xi w)\\
&+\sum -\xi^2\tilde{A}_n\exp(i\alpha_n u - i\xi w) - \sum_n\sum_m\sum_r \dot{a}_{n-m}\dot{a}_{m-r}\xi^2\tilde{A}_r\exp(i\alpha_n u - i\xi w)\\
&+k^2v_1^2\sum_n \tilde{A}_n\exp(i\alpha_n u - i\xi w) = 0
\end{aligned}
\tag{3.13}
$$

Since we cannot compute an infinite system, thus we truncate all infinite sums in the equation to make the sum from $-N$ till N to obtain a finite-dimensional system.

$$
\begin{aligned}
&\sum_{n=-N}^{N}\Bigg(-\alpha_n^2\tilde{A}_n + \xi\sum_{m=-N}^{N}[\![\dot{a}]\!]_{n-m}\alpha_m\tilde{A}_m + \xi\sum_{m=-N}^{N}\alpha_n[\![\dot{a}]\!]_{n-m}\tilde{A}_m\\
&-\xi^2\sum_{m=-N}^{N}\sum_{r=-N}^{N}[\![\dot{a}]\!]_{n-m}[\![\dot{a}]\!]_{m-r}\tilde{A}_r + (-\xi^2+k^2v_1^2)\tilde{A}_n\Bigg)\exp(i\alpha_n u - i\xi w)\\
&= 0
\end{aligned}
\tag{3.14}
$$

In the equation, $[\![\dot{a}]\!]$ is a Toeplitz matrix defined by:

$$
[\![\dot{a}]\!] = \begin{pmatrix} \dot{a}_0 & \dot{a}_{-1} & \cdots & \dot{a}_{-2N}\\ \dot{a}_1 & \dot{a}_0 & \cdots & \dot{a}_{-2N+1}\\ \vdots & \vdots & \ddots & \vdots\\ \dot{a}_{2N} & \dot{a}_{2N-1} & \cdots & \dot{a}_0 \end{pmatrix} \tag{3.15}
$$

In the matrix, we can see that entries are the same for each diagonal, then we make a definition $[\![\dot{a}]\!]_{nm} = [\![\dot{a}]\!]_{n-m}$.

Since the exponential function in (3.14) are linearly independent, we get:

$$
\begin{aligned}
&-\alpha_n^2\tilde{A}_n + \xi\sum_{m=-N}^{N}[\![\dot{a}]\!]_{n-m}\alpha_m\tilde{A}_m + \xi\sum_{m=-N}^{N}[\![\dot{a}]\!]_{n-m}\alpha_n\tilde{A}_m\\
&-\xi^2\sum_{m=-N}^{N}\sum_{r=-N}^{N}[\![\dot{a}]\!]_{n-m}[\![\dot{a}]\!]_{m-r}\tilde{A}_r + (-\xi^2+k^2v_1^2)\tilde{A}_n = 0
\end{aligned}
$$

for all $n = -N, -N+1, \cdots, N$, which is equivalent to

$$(-\alpha_n^2 + k^2\nu_1^2)\tilde{A}_n = \xi \sum_{m=-N}^{N} [\![\dot{a}]\!]_{n-m}(\alpha_m + \alpha_n)\tilde{A}_m + \xi^2\tilde{A}_n + \xi^2 \sum_{m=-N}^{N} \sum_{r=-N}^{N} [\![\dot{a}]\!]_{n-m}[\![\dot{a}]\!]_{m-r}\tilde{A}_r \tag{3.16}$$

Because the generalized "Helmholtz equation" is a second-order partial differential equation, this fact results in terms with ξ, ξ^2 and without ξ. Here we introduce a new quantity Q_n to make the equation first order in ξ:

$$Q_n = \xi\tilde{A}_n \tag{3.17}$$

With this notation, equation (3.16) becomes:

$$(k^2\nu_1^2 - \alpha_n^2)\tilde{A}_n = \xi \sum_{m=-N}^{N} (\alpha_m + \alpha_n)[\![\dot{a}]\!]_{n-m}\tilde{A}_m + \xi\left(Q_n + \sum_{m=-N}^{N} \sum_{r=-N}^{N} [\![\dot{a}]\!]_{n-m}[\![\dot{a}]\!]_{m-r}Q_r \right) \tag{3.18}$$

For the left side of the equation, we know that $k^2\nu_1^2 - \alpha_n^2 = (\beta_n^I)^2$. For the right side, we have two terms.

- For the first term, $\sum_{m=-N}^{N} (\alpha_m + \alpha_n)[\![\dot{a}]\!]_{n-m}\tilde{A}_m$ is the n-th component of the vector $(\boldsymbol{\alpha}[\![\dot{a}]\!] + [\![\dot{a}]\!]\boldsymbol{\alpha})\tilde{\mathbf{A}}$ if we define $\boldsymbol{\alpha} \in \mathbb{C}^{(2N+1)\times(2N+1)}$ and $\tilde{\mathbf{A}} \in \mathbb{C}^{2N+1}$ in the following way:

$$\boldsymbol{\alpha} = \begin{pmatrix} \alpha_{-N} & & 0 \\ & \ddots & \\ 0 & & \alpha_N \end{pmatrix}, \qquad \tilde{\mathbf{A}} = \begin{bmatrix} \tilde{A}_{-N} \\ \vdots \\ \tilde{A}_N \end{bmatrix}$$

- For the second term, $Q_n + \sum_{m=-N}^{N} \sum_{r=-N}^{N} [\![\dot{a}]\!]_{n-m}[\![\dot{a}]\!]_{m-r}Q_r$ is the n-th component of the vector $(\mathbf{I} + [\![\dot{a}]\!][\![\dot{a}]\!])\tilde{\mathbf{A}}$ if we define $\mathbf{Q_1} \in \mathbb{C}^{2N+1}$ in the following way:

$$\mathbf{Q_1} = \begin{bmatrix} Q_{-N} \\ \vdots \\ Q_N \end{bmatrix}$$

Equation (3.17) can now be written as

$$\mathbf{Q_1} = \xi\tilde{\mathbf{A}} \tag{3.19}$$

Equation (3.18) can now be written as

$$\boldsymbol{\beta_1}^2\tilde{\mathbf{A}} = -\xi(\boldsymbol{\alpha}[\![\dot{a}]\!] + [\![\dot{a}]\!]\boldsymbol{\alpha})\tilde{\mathbf{A}} + \xi(\mathbf{I} + [\![\dot{a}]\!][\![\dot{a}]\!])\mathbf{Q_1} \tag{3.20}$$

with the definition for $\boldsymbol{\beta_1} \in \mathbb{C}^{(2N+1)\times(2N+1)}$ as

$$\boldsymbol{\beta_1} = \begin{pmatrix} \beta^I_{-n} & & 0 \\ & \ddots & \\ 0 & & \beta^I_n \end{pmatrix}$$

Then we get from (3.20):

$$\tilde{\mathbf{A}} = -\boldsymbol{\beta_1}^{-2}\xi(\boldsymbol{\alpha}[\![\dot{a}]\!] + [\![\dot{a}]\!]\boldsymbol{\alpha})\tilde{\mathbf{A}} + \boldsymbol{\beta_1}^{-2}\xi(\mathbf{I} + [\![\dot{a}]\!][\![\dot{a}]\!])\mathbf{Q_1} \tag{3.21}$$

Thus we can get the matrix equation:

$$\xi\mathbf{M_1}\begin{bmatrix} \tilde{\mathbf{A}} \\ \mathbf{Q_1} \end{bmatrix} = \begin{bmatrix} \tilde{\mathbf{A}} \\ \mathbf{Q_1} \end{bmatrix} \tag{3.22}$$

with

$$\mathbf{M_1} = \begin{bmatrix} -\boldsymbol{\beta_1}^{-2}(\boldsymbol{\alpha}[\![\dot{a}]\!] + [\![\dot{a}]\!]\boldsymbol{\alpha}) & \boldsymbol{\beta_1}^{-2}(\mathbf{I} + [\![\dot{a}]\!][\![\dot{a}]\!]) \\ \mathbf{I} & 0 \end{bmatrix}$$

Rewriting equation (3.22), we obtain:

$$\mathbf{M_1}\begin{bmatrix} \mathbf{A} \\ \mathbf{Q_1} \end{bmatrix} = \frac{1}{\xi}\begin{bmatrix} \tilde{\mathbf{A}} \\ \mathbf{Q_1} \end{bmatrix} \tag{3.23}$$

From the definition of an eigenvalue problem, we can regard $\frac{1}{\xi}$ as an eigenvalue of $\mathbf{M_1}$, and $\begin{bmatrix} \tilde{\mathbf{A}} \\ \mathbf{Q_1} \end{bmatrix}$ as its corresponding eigenvector.

When there are values on the diagonal of matrix $\boldsymbol{\beta}_1$ equal to zero, viz. $\beta_{i,1} = 0$ for some $i = -N...N$, then $\boldsymbol{\beta}^{-2}{}_1$ does not exist. Then we transform the system and solve the matrix equation given below:

$$\xi\tilde{\mathbf{M}}_\mathbf{1}\begin{bmatrix} \tilde{\mathbf{A}} \\ \mathbf{Q_1} \end{bmatrix} = \tilde{\boldsymbol{\beta}_1}\begin{bmatrix} \tilde{\mathbf{A}} \\ \mathbf{Q_1} \end{bmatrix} \qquad \Leftrightarrow \qquad \xi\begin{bmatrix} \tilde{\mathbf{A}} \\ \mathbf{Q_1} \end{bmatrix} = \tilde{\mathbf{M}}_\mathbf{1}^{-1}\tilde{\boldsymbol{\beta}_1}\begin{bmatrix} \tilde{\mathbf{A}} \\ \mathbf{Q_1} \end{bmatrix} \tag{3.24}$$

where

$$\tilde{\mathbf{M}}_\mathbf{1} = \begin{bmatrix} -(\boldsymbol{\alpha}[\![\dot{a}]\!] + [\![\dot{a}]\!]\boldsymbol{\alpha}) & \mathbf{I} + [\![\dot{a}]\!][\![\dot{a}]\!] \\ \mathbf{I} & \mathbf{0} \end{bmatrix}, \qquad \tilde{\boldsymbol{\beta}_1} = \begin{bmatrix} \boldsymbol{\beta}_1^2 & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \tag{3.25}$$

However, this will bring us much more work in computing. We first compute the inverse matrix of $\tilde{\mathbf{M}}_\mathbf{1}$ and then compute the eigenvalues and eigenvectors of matrix $\tilde{\mathbf{M}}_\mathbf{1}^{-1}\tilde{\boldsymbol{\beta}_1}$.

Thus we get $\tilde{A}_n$ and ξ for the Rayleigh expansion (3.6) and (3.7). But since there are many values for $\tilde{A}_n$ and ξ, we have to find out the way to match them such that we will get a unique solution. As stated, Boundary conditions will help to do this.

Medium 2

For medium 2, we have a similar process as above. Substituting the generalized Rayleigh expansion for Ω_2 (3.7) into the generalized Helmholtz equation (3.11), then we get:

$$\sum_{n=-\infty}^{\infty}\left(-\alpha_n^2 - 2\dot{a}\xi\alpha_n + \ddot{a}\xi i - \xi^2 - \dot{a}^2\xi^2 + k^2\nu_2^2\right)\tilde{B}_n \exp(i\alpha_n u + i\xi w) = 0 \tag{3.26}$$

By using Fourier expansion for $a(x)$ and truncating the equation into a finite system, we have:

$$\mathbf{M_2}\begin{bmatrix}\tilde{\mathbf{B}}\\ \mathbf{Q_2}\end{bmatrix} = \frac{1}{\xi}\begin{bmatrix}\tilde{\mathbf{B}}\\ \mathbf{Q_2}\end{bmatrix} \tag{3.27}$$

where

$$\mathbf{M_2} = \begin{bmatrix} -\boldsymbol{\beta}_2{}^{-2}(\boldsymbol{\alpha}[\![\dot{a}]\!] + [\![\dot{a}]\!]\boldsymbol{\alpha}) & \boldsymbol{\beta}_2{}^{-2}(\mathbf{I} + [\![\dot{a}]\!][\![\dot{a}]\!]) \\ \mathbf{I} & 0 \end{bmatrix}, \quad \tilde{\mathbf{B}} = \begin{bmatrix}\tilde{B}_{-N}\\ \vdots \\ \tilde{B}_N\end{bmatrix}, \quad \mathbf{Q_2} = \xi\tilde{\mathbf{B}}$$

with

$$\boldsymbol{\beta}_2 = \begin{pmatrix}\beta_{-n}^{II} & & 0\\ & \ddots & \\ 0 & & \beta_n^{II}\end{pmatrix}$$

3.3.3 Boundary condition at the interface

Let us concentrate on the boundary condition for the interface (2.15). With this boundary condition, we know that the tangential components of the fields to the interface are continuous between medium 1 and medium 2. This boundary condition connects the system of medium 1 (3.23) and the system of medium 2 (3.27) together.

Apply this boundary condition to the fields directly, we can get $2N + 1$ equations. But we have $4N + 2$ unknowns in all, thus we should find another $2N + 1$ equations. The equations gotten above are all of the ν component, the other component which is tangential to the interface is the u component, but as has been defined, there is no u component of the **F** field.

It is known that electric fields have effect on magnetic fields, and the other way around. By means of the Maxwell equations (2.8), the electric field can be written as a function of magnetic field components and vice versa. Thus we apply the boundary condition of the interface for the u component of magnetic field, because they will effect the value of the ν component of electric field. Then we will get the other $2N + 1$ equations. With these $4N + 2$ equations we can solve the unknowns to get the unique solution.

Equations for the ν component

For the unity, we write A_n^I for $\tilde{A}_n$ and A_n^{II} for $\tilde{B}_n$ below.

- Fields in medium 1.
  The field in medium 1 is given in Cartesian coordinates by:

$$F_\nu^I(x,z) \quad = \quad F_\nu^{inc}(x,z) + F_\nu^r(x,z)$$

where $F_\nu^{inc}(x,z)$ represents the incident field, and $F_\nu^r(x,z)$ the reflected field. The reflected field is split up into propagating orders which can be measured and evanescent orders which cannot be measured. Then we have $F_\nu^r(x,z) = F_\nu^{prop}(x,z) + F_\nu^{evan}(x,z)$, and we can get:

$$\begin{aligned} F_\nu^I(x,z) &= F_\nu^{inc}(x,z) + F_\nu^{prop}(x,z) + F_\nu^{evan}(x,z) \\ &= \exp[i\alpha_0 x - i\beta_0^I z] + \sum_{n\in U^I} \exp[i\alpha_n x + i\beta_n^I z] A_n^I \\ &\quad + \sum_m \sum_{q\in V^I} \exp[i\alpha_m x + i\rho_{q,1} z] C_q^I \end{aligned} \tag{3.28}$$

where $F_\nu^{prop}(x,z)$ are the fields of the propagating orders, and $F_\nu^{evan}(x,z)$ of the evanescent orders. U^I is the set of indices for the propagating orders and V^I is the set of indices for the evanescent orders and we have $U^I \cup V^I = \{-N, ..., N\}$, $U^I \cap V^I = \varnothing$.

It can be shown that ξ converges to β_n^I for the propagating orders (real eigenvalues). Thus we use β_n^I for ξ in computing. This is not the case for the evanescent orders where the eigenvalues are complex valued only.

In the new coordinate system, the incident term F_ν^{inc} becomes:

$$\begin{aligned} F_\nu^{inc}(u,w) &= \exp(i\alpha_0 u - i\beta_0^I(w + a(u))) \\ &= \exp(-i\beta_0^I a(u)) \exp(i\alpha_0 u - i\beta_0^I w) \end{aligned} \tag{3.29}$$

Take Fourier expansion of $\exp(-i\beta_0^I a(u))$, then we have

$$\begin{aligned} F_\nu^{inc}(u,w) &= \sum_m L_m(-\beta_0^I) \exp(imKu) \exp(i\alpha_0 u - i\beta_0^I w) \\ &= \sum_m L_m(-\beta_0^I) \exp(i\alpha_m u - i\beta_0^I w) \end{aligned} \tag{3.30}$$

where L_m is the Fourier coefficient:

$$L_m(-\beta_0^I) := \frac{1}{\Lambda} \int_0^\Lambda \exp[-i\beta_0^I a(u) - imKu] du$$

In the new coordinate system, the reflected field term F_ν^r becomes:

$$\begin{aligned} F_\nu^r(u,w) &= F_\nu^{prop}(u,w) + F_\nu^{evan}(u,w) \\ &= \sum_{n\in U^I} A_n^I \exp(i\alpha_n u + i\beta_n^I(w + a(u))) + \sum_m \sum_{q\in V^I} \exp[i\alpha_m u + i\rho_{q,1}(w + a(u))] C_q^I \\ &= \sum_{n\in U^I} A_n^I \exp(i\beta_n^I a(u)) \exp(i\alpha_n u + i\beta_n^I w) \\ &\quad + \sum_m \sum_{q\in V^I} \exp[i\alpha_m u + i\rho_{q,1}(w + a(u))] C_q^I \end{aligned} \tag{3.31}$$

Then for the new coordinate system, the field in medium 1 becomes:

$$
\begin{aligned}
F_v^I(u,w) &= \exp[i\alpha_0 u - i\beta_0^I(w + a(u))] + \sum_{n\in U^I} \exp[i\alpha_n u + i\beta_n^I(w + a(u))]A_n^I \\
&\quad + \sum_m \sum_{q\in V^I} \exp[i\alpha_m u + i\rho_{q,1}(w + a(u))]C_q^I \\
&= \exp[-i\beta_0^I a(u)] \exp[i\alpha_0 u - i\beta_0^I w] + \sum_{n\in U^I} \exp[i\beta_n^I a(u)] \exp[i\alpha_n u + i\beta_n^I w]A_n^I \\
&\quad + \sum_m \sum_{q\in V^I} \exp[i\rho_{q,1} a(u)] \exp[i\alpha_m u + i\rho_{q,1} w]C_q^I \\
&= \sum_m L_m(-\beta_0^I) \exp[imKu] \exp[i\alpha_0 u - i\beta_0^I w] \\
&\quad + \sum_m \sum_{n\in U^I} L_m(\beta_n^I) \exp[imKu] \exp[i\alpha_n u + i\beta_n^I w]A_n^I \\
&\quad + \sum_m \sum_{q\in V^I} F_{mq}^I \exp[i\alpha_m u + i\rho_{q,1} w]C_q^I \\
&= \sum_m L_m(-\beta_0^I) \exp[i\alpha_m u - i\beta_0^I w] + \sum_m \sum_{n\in U^I} L_m(\beta_n^I) \exp[i\alpha_{m+n} u + i\beta_n^I w]A_n^I \\
&\quad + \sum_m \sum_{q\in V^I} F_{mq}^I \exp[i\alpha_m u + i\rho_{q,1} w]C_q^I \\
&= \sum_m L_m(-\beta_0^I) \exp[i\alpha_m u - i\beta_0^I w] + \sum_m \sum_{n\in U^I} L_{m-n}(\beta_n^I) \exp[i\alpha_m u + i\beta_n^I w]A_n^I \\
&\quad + \sum_m \sum_{q\in V^I} F_{mq}^I \exp[i\alpha_m u + i\rho_{q,1} w]C_q^I \\
&= \sum_m \exp[i\alpha_m u] \cdot \{L_m(-\beta_0^I) \exp[-i\beta_0^I w] \\
&\quad + \sum_{n\in U^I} L_{m-n}(\beta_n^I) \exp[i\beta_n^I w]A_n^I + \sum_{q\in V^I} F_{mq}^I \exp[i\rho_{q,1} w]C_q^I\} \qquad (3.32)
\end{aligned}
$$

where

$$F_{mq}^I := \exp[i\rho_{q,1} a(u)]$$

- Fields in medium 2.
  The same can be done for medium 2. Note that in medium 2, only a transmitted field is present.

$$\begin{aligned} F_v^{II}(x,z) &= F_v^{prop}(x,z) + F_v^{evan}(x,z) \\ &= \sum_{n \in U^{II}} \exp[i\alpha_n x - i\beta_n^{II} z] A_n^{II} + \sum_m \sum_{q \in V^{II}} \exp[i\alpha_m x + i\rho_{q,2} z] C_q^{II} \end{aligned}$$

  Note that U^{II} is the set of indices of propagating orders and V^{II} is the set of indices of evanescent orders for medium 2, and therefore differ from U^I and V^I.

  Similar to the derivation for $F_v^I(u,w)$, we have:

$$\begin{aligned} F_v^{II}(u,w) = \quad & \sum_m \exp[i\alpha_m u] \cdot \{ \sum_{n \in U^{II}} L_{m-n}(-\beta_n^{II}) \exp[-i\beta_n^{II} w] A_n^{II} + \\ & \sum_{q \in V^{II}} F_{mq}^{II} \exp[i\rho_{q,2} w] C_q^{II} \} \end{aligned} \tag{3.33}$$

  Since only F_v is under consideration, the resulting boundary condition is:

$$F_v^I(u,0) = F_v^{II}(u,0) \tag{3.34}$$

  Substituting the expansions (3.32) and (3.33) into this boundary condition and setting $w = 0$ gives:

$$\begin{aligned} & L_m(-\beta_n^I) + \sum_{n \in U^I} L_{m-n}(\beta_n^I) A_n^I + \sum_{q \in V^I} F_{mq}^I C_q^I \\ = \quad & \sum_{n \in U^{II}} L_{m-n}(-\beta_n^{II}) A_n^{II} + \sum_{q \in V^{II}} F_{mq}^{II} C_q^{II} \end{aligned} \tag{3.35}$$

  This equation can be written in matrix form. Introduce M^I and M^{II} as the number of propagating diffraction orders in media 1 and 2, respectively. Define the following matrices:

  - $\mathbf{F}_{prop}^I \in \mathbb{R}^{(2N+1)\times M^I}$ for the propagating orders in medium 1;
  - $\mathbf{F}_{evan}^I \in \mathbb{R}^{(2N+1)\times(2N+1-M^I)}$ for the evanescent orders in medium 1;
  - $\mathbf{F}_{prop}^{II} \in \mathbb{R}^{(2N+1)\times M^{II}}$ for the propagating orders in medium 2;
  - $\mathbf{F}_{evan}^{II} \in \mathbb{R}^{(2N+1)\times(2N+1-M^{II})}$ for the evanescent orders in medium 2;
  - $\mathbf{F}_0^I \in \mathbb{R}^{(2N+1)\times 1}$ for the incident field.

  The entries of these matrices are given by:

$$(\mathbf{F}_{prop}^I)_{mn} := L_{m-n}(\beta_n^I), \quad n \in U^I \tag{3.36}$$

$$(\mathbf{F}_{evan}^I)_{mq} := F_{mq}, \quad q \in V^I \tag{3.37}$$

$$(\mathbf{F}_{prop}^{II})_{ms} := L_{m-s}(-\beta_{s,2}), \quad s \in U^{II} \tag{3.38}$$

$$(\mathbf{F}_{evan}^{II})_{mt} := F_{mt}, \quad t \in V^{II} \tag{3.39}$$

$$(\mathbf{F}_0^I)_{n1} := L_m(-\beta_0^I) \tag{3.40}$$

The matrix equation then becomes:

$$\begin{bmatrix} \mathbf{F}^{I}_{prop} & \mathbf{F}^{I}_{evan} & -\mathbf{F}^{II}_{prop} & -\mathbf{F}^{II}_{evan} \end{bmatrix} \begin{bmatrix} \mathbf{A}^{I} \\ \mathbf{C}^{I} \\ \mathbf{A}^{II} \\ \mathbf{C}^{II} \end{bmatrix} = -\mathbf{F}^{I}_{0} \tag{3.41}$$

where

$$\mathbf{A}^{I} = \begin{bmatrix} A^{I}_{-N} \\ \vdots \\ A^{I}_{N} \end{bmatrix}, \quad \mathbf{C}^{I} = \begin{bmatrix} C^{I}_{-N} \\ \vdots \\ C^{I}_{N} \end{bmatrix}, \quad \mathbf{A}^{II} = \begin{bmatrix} A^{II}_{-N} \\ \vdots \\ A^{II}_{N} \end{bmatrix}, \quad \mathbf{C}^{II} = \begin{bmatrix} C^{II}_{-N} \\ \vdots \\ C^{II}_{N} \end{bmatrix}$$

This equation is valid for both TE and TM polarization.

Equations for the u-component

Here we want to concentrate on the u-component of magnetic field. We look back at the first two equations of the local Maxwell equations (2.8)

$$\begin{cases} \dfrac{\partial E_y}{\partial z} - \dfrac{\partial E_z}{\partial y} = -i\omega\mu H_x = -ikZH_x \\[2ex] \dfrac{\partial E_z}{\partial x} - \dfrac{\partial E_x}{\partial z} = -i\omega\mu H_y = -ikZH_y \\[2ex] \dfrac{\partial E_x}{\partial y} - \dfrac{\partial E_y}{\partial x} = -i\omega\mu H_z = -ikZH_z \end{cases} \quad \text{and} \quad \begin{cases} \dfrac{\partial H_y}{\partial z} - \dfrac{\partial H_z}{\partial y} = -i\omega\varepsilon E_x = i\dfrac{kn^2}{Z}E_x \\[2ex] \dfrac{\partial H_z}{\partial x} - \dfrac{\partial H_x}{\partial z} = -i\omega\varepsilon E_y = i\dfrac{kn^2}{Z}E_y \\[2ex] \dfrac{\partial H_x}{\partial y} - \dfrac{\partial H_y}{\partial x} = -i\omega\varepsilon E_z = i\dfrac{kn^2}{Z}E_z \end{cases}$$

where Z is the impedance of vacuum: $Z = \sqrt{\frac{\mu_0}{\varepsilon_0}} = \sqrt{\frac{\mu}{\varepsilon_0}}$. Since that the electromagnetic fields are independent of the y-direction, we get:

$$\begin{cases} \dfrac{\partial E_y(x,z)}{\partial z} = -ikZH_x(x,z) \\[2ex] \dfrac{\partial E_z(x,z)}{\partial x} - \dfrac{\partial E_x(x,z)}{\partial z} = -ikZH_y(x,z) \\[2ex] -\dfrac{\partial E_y(x,z)}{\partial x} = -ikZH_z(x,z) \end{cases} \quad \text{and} \quad \begin{cases} \dfrac{\partial H_y(x,z)}{\partial z} = i\dfrac{kn^2}{Z}E_x(x,z) \\[2ex] \dfrac{\partial H_z(x,z)}{\partial x} - \dfrac{\partial H_x(x,z)}{\partial z} = i\dfrac{kn^2}{Z}E_y(x,z) \\[2ex] -\dfrac{\partial H_y(x,z)}{\partial x} = i\dfrac{kn^2}{Z}E_z(x,z) \end{cases}$$

With the coordinate transformation (3.5), we obtain:

$$\begin{aligned} E_u &= \frac{1}{ikn^2}\left[\dot{a}\left(-\frac{\partial ZH_v}{\partial u} + \dot{a}\frac{\partial ZH_v}{\partial w}\right) + \frac{\partial ZH_v}{\partial w}\right] \\ ZH_u &= \frac{1}{ik}\left[\dot{a}\left(\frac{\partial E_v}{\partial u} - \dot{a}\frac{\partial E_v}{\partial w}\right) - \frac{\partial E_v}{\partial w}\right] \end{aligned} \tag{3.42}$$

Since both expressions have a similar form, introduce field G, which is defined as:

$$G_u = \begin{cases} n^2 E_u, & \text{for TM polarization} \\ -ZH_u, & \text{for TE polarization} \end{cases}$$

Substitute the expansions for medium 1 $F_v^I(u,w)$(3.32) and for medium 2 $F_v^{II}(u,w)$(3.33) into equations (3.42) for G_u and set w to be zero, this gives:

$$\begin{aligned}
G_u^I(u,0) &= -\frac{1}{k}\Big[\sum_m [[\dot{a}]]_{n-m}\alpha_m\{L_m(-\beta_n^I) + \sum_{p\in U^I} L_{n-p}\,(\beta_{p,1})A_p^I + \sum_{q\in V^I} F_{nq}^I C_q^I\} \\
&\quad - \sum_m\sum_r [[\dot{a}]]_{n-m}[[\dot{a}]]_{m-r}\{-\beta_n L_r(-\beta_n^I) + \sum_{p\in U^I}\beta_{p,1}L_{r-p}\,(\beta_{p,1}) + \sum_{q\in V^I} F_{rq}^I\rho_{q,1}C_q^I\} \\
&\quad -\{-\beta_n^I L_n\,(-\beta_n^I) + \sum_{p\in U^I}\beta_{p,1}L_{n-p}\,(\beta_{p,1}) + \sum_{q\in V^I} F_{nq}^I\rho_{q,1}C_q^I\}\Big] \\
&= -\frac{1}{k}\sum_m\{[[\dot{a}]]_{n-m}\alpha_m + \left(\delta_{nm} + \sum_r [[\dot{a}]]_{n-r}[[\dot{a}]]_{r-m}\right)\beta_n^I\}L_m(-\beta_n^I) \\
&\quad -\frac{1}{k}\sum_{p\in U^I}\sum_m\{[[\dot{a}]]_{n-m}\alpha_m - \left(\delta_{nm} + \sum_r [[\dot{a}]]_{n-r}[[\dot{a}]]_{r-m}\right)\beta_{p,1}\}L_{m-p}(\beta_{p,1})A_p^I \\
&\quad -\frac{1}{k}\sum_{q\in V^I}\sum_m\{[[\dot{a}]]_{n-m}\alpha_m - \left(\delta_{nm} + \sum_r [[\dot{a}]]_{n-r}[[\dot{a}]]_{r-m}\right)\rho_{q,1}\}F_{mq}^I C_q^I
\end{aligned} \tag{3.43}$$

Similar for medium 2:

$$\begin{aligned}
G_u^{II}(u,0) &= -\frac{1}{k}\Big[\sum_m [[\dot{a}]]_{n-m}\alpha_m\{\sum_{s\in U^{II}} L_{n-s}\,(-\beta_{s,2})A_s^{II} + \sum_{t\in V^{II}} F_{nt}^{II}C_t^{II}\} \\
&\quad - \sum_m\sum_r [[\dot{a}]]_{n-m}[[\dot{a}]]_{m-r}\{\sum_{s\in U^{II}} -\beta_{s,2}L_{r-s}(-\beta_{s,2}) + \sum_{t\in V^{II}} F_{rt}^{II}\rho_{t,2}C_t^{II}\} \\
&\quad -\{\sum_{s\in U^{II}} -\beta_{s,2}L_{n-s}\,(-\beta_{s,2}) + \sum_{t\in V^{II}} F_{nt}^{II}\rho_{t,2}C_t^{II}\}\Big] \\
&= -\frac{1}{k}\sum_{s\in U^{II}}\sum_m\{[[\dot{a}]]_{n-m}\alpha_m - \left(\delta_{nm} + \sum_r [[\dot{a}]]_{n-r}[[\dot{a}]]_{r-m}\right)\beta_{s,2}\}L_{m-s}(-\beta_{s,2}) \\
&\quad -\frac{1}{k}\sum_{t\in U^{II}}\sum_m\{[[\dot{a}]]_{n-m}\alpha_m - \left(\delta_{nm} + \sum_r [[\dot{a}]]_{n-r}[[\dot{a}]]_{r-m}\right)\rho_{t,2}\}F_{mt}^{II}
\end{aligned} \tag{3.44}$$

Since $w = 0$ is already substituted, both equations (3.43) and (3.44) are equal to each other.

$$G_u^I(u,0) = G_u^{II}(u,0) \tag{3.45}$$

This equality can be given in matrix form. Therefore introduce the following matrices:

- $\mathbf{G}_{prop}^I \in \mathbb{R}^{(2N+1)\times M^I}$ for the propagating orders in medium 1;
- $\mathbf{G}_{evan}^I \in \mathbb{R}^{(2N+1)\times(2N+1-M^I)}$ for the evanescent orders in medium 1;
- $\mathbf{G}_{prop}^{II} \in \mathbb{R}^{(2N+1)\times M^{II}}$ for the propagating orders in medium 2;
- $\mathbf{G}_{evan}^{II} \in \mathbb{R}^{(2N+1)\times(2N+1-M^{II})}$ for the evanescent orders in medium 2;
- $\mathbf{G}_0^I \in \mathbb{R}^{(2N+1)\times 1}$ for the incident field.

The entries of these matrices are given by:

$$
\begin{aligned}
(G^{I}_{prop})_{np} &= \frac{1}{k}\sum_{m}\{[[\dot{a}]]_{n-m}\alpha_m L_{m-p}(\beta_{p,1}) - \left(\delta_{nm} + \sum_{r}[[\dot{a}]]_{n-r}[[\dot{a}]]_{r-m}\right) \\
&\quad L_{m-p}(\beta_{p,1})\beta_{p,1}\}, \quad p \in U^{I} && (3.46)\\
(G^{I}_{evan})_{nq} &= \frac{1}{k}\sum_{m}\{[[\dot{a}]]_{n-m}\alpha_m F_{mq} \\
&\quad -\left(\delta_{nm} + \sum_{r}[[\dot{a}]]_{n-r}[[\dot{a}]]_{r-m}\right)F_{mq}\rho_{q,1}\}, \quad q \in V^{I} && (3.47)\\
(G^{II}_{prop})_{ns} &= \frac{1}{k}\sum_{m}\{[[\dot{a}]]_{n-m}\alpha_m L_{m-s}(\beta_{s,2}) - \left(\delta_{nm} + \sum_{r}[[\dot{a}]]_{n-r}[[\dot{a}]]_{r-m}\right) \\
&\quad L_{m-s}(\beta_{s,2})\beta_{s,2}\}, \quad s \in U^{II} && (3.48)\\
(G^{II}_{evan})_{nt} &= \frac{1}{k}\sum_{m}\{[[\dot{a}]]_{n-m}\alpha_m F_{mt} \\
&\quad -\left(\delta_{nm} + \sum_{r}[[\dot{a}]]_{n-r}[[\dot{a}]]_{r-m}\right)F_{mt}\rho_{t,2}\}, \quad t \in V^{II} && (3.49)\\
(G^{I}_{0})_{n1} &= \frac{1}{k}\sum_{m}\{[[\dot{a}]]_{n-m}\alpha_m L_{m}(-\beta^{I}_{0}) + \left(\delta_{nm} + \sum_{r}[[\dot{a}]]_{n-r}[[\dot{a}]]_{r-m}\right) \\
&\quad L_{m}(-\beta^{I}_{0})\beta^{I}_{0}\} && (3.50)
\end{aligned}
$$

This matrix equation then becomes:

$$
\begin{bmatrix} \mathbf{G}^{I}_{prop} & \mathbf{G}^{I}_{evan} & -\mathbf{G}^{II}_{prop} & -\mathbf{G}^{II}_{evan} \end{bmatrix}
\begin{bmatrix} \mathbf{A}^{I} \\ \mathbf{C}^{I} \\ \mathbf{A}^{II} \\ \mathbf{C}^{II} \end{bmatrix} = -\mathbf{G}^{I}_{0} \qquad (3.51)
$$

Combining with equation for F_v (68) and equation for G_u (79) gives:

$$
\begin{bmatrix} \mathbf{F}^{I}_{prop} & \mathbf{F}^{I}_{evan} & -\mathbf{F}^{II}_{prop} & -\mathbf{F}^{II}_{evan} \\ \mathbf{G}^{I}_{prop} & \mathbf{G}^{I}_{evan} & -\mathbf{G}^{II}_{prop} & -\mathbf{G}^{II}_{evan} \end{bmatrix}
\begin{bmatrix} \mathbf{A}^{I} \\ \mathbf{C}^{I} \\ \mathbf{A}^{II} \\ \mathbf{C}^{II} \end{bmatrix} = \begin{bmatrix} -\mathbf{F}^{I}_{0} \\ -\mathbf{G}^{I}_{0} \end{bmatrix} \qquad (3.52)
$$

Solving the system gives coefficients $\mathbf{A}^{I}$, $\mathbf{C}^{I}$, $\mathbf{A}^{II}$ and $\mathbf{C}^{II}$. In general, only $\mathbf{A}^{I}$ is important, since these coefficients correspond to the reflected field that can be measured.

3.4 Conclusion

Figure 3.3 shows the steps of the traditional C method. With the traditional C method, we finally get the reflected field for both media.

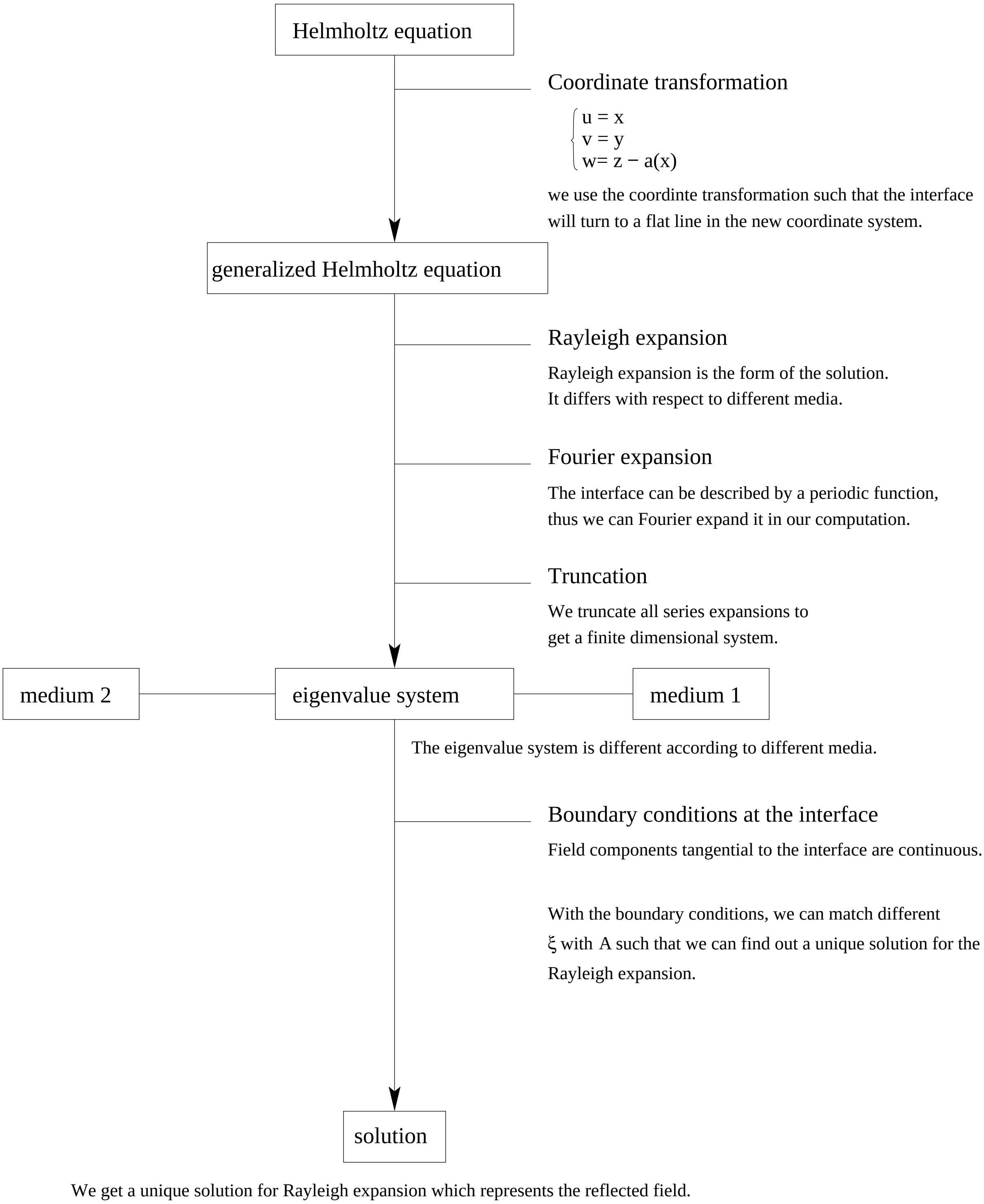

Figure 3.3: Scheme for the traditional C method

Chapter 4

Extension of the C method

In this chapter, we try to extend the C method to overhanging gratings. As has been said, the reason why the C method cannot be used for overhanging gratings is because overhanging gratings cannot be described by a single valued function and thus the coordinate transformation of the traditional C method cannot change into a flat line. So the core of the extension is to generalize the C method with another coordinate transformation such that the interface can be described by a flat line in the new coordinate system.

As the grating is independent of the y direction, there are two degrees of freedom to describe the grating. For a given overhanging grating, we construct a set of non-intersecting lines to cover the model domain (see Figure 4.1). Note that in the figure, the interface is bold and is described by $w = 0$ in the new coordinate system. The lines we make should be non-intersecting everywhere so that for each point inside the domain there is only one line passing through it. The overhanging lines will gradually change into flat lines on the boundary ($z \to \pm\infty$).

With these lines, we can find two parameters, say u and w, to describe the domain. Originally, we use x and z to locate the point. Now there will be one line passing through the given point, and we use w to specify the line, and u to locate the exact position of the point

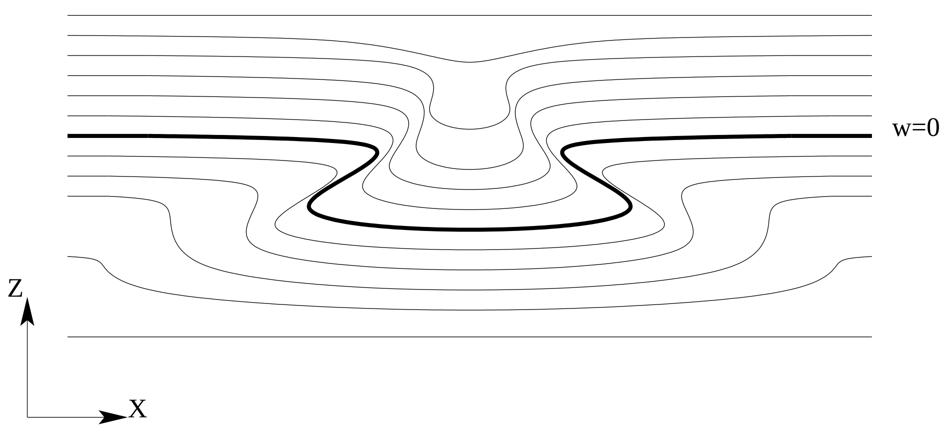

Figure 4.1: Non-intersecting lines in the domain

on that line. By doing this, we get our new coordinate system $u - w$. In the new coordinate system, the interface will be a flat line.

In Section 4.1, we study overhanging trapezoidal lines. This is meant as a start for smooth overhanging gratings. We show two ways to build the new coordinate transformation. In Section 4.2, we turn back to study the coordinate transformation of smooth overhanging gratings. In Section 4.3, we derive the generalized Helmholtz equation (2.19) for the new coordinate system. In Section 4.4, we conclude by giving the scheme for the extension of the C method, and future work will be stated.

4.1 Overhanging trapezoidal lines

In this section we will concentrate on a situation for which the coordinate transformation can be found relatively easy is easy to study: symmetric overhanging trapezoidal lines (see Figure 4.2). We will try to draw trapezoidal lines to cover the domain. Of course, these trapezoidal lines should not intersect.

We can see from Figure 4.2 that any trapezoidal line is composed by five lines. Since it is symmetric, we will concentrate on only half of the domain.

For each half trapezoidal line, we see that there are two points to connect the three lines, namely turning points p and q. We can obtain a unique trapezoidal line through these two corresponding turning points. This gives us the idea that if we have functions to describe the outlines of the two turning points, then we can cover the domain with non-intersecting trapezoidal lines. Thus we try to find functions for the outlines of the two turning points.

4.1.1 Outlines of the turning points described by Gaussian curves

Outlines for the turning points

We want to have the disconnected trapezoidal lines to become flat towards $z \to \pm\infty$ and to be overhanging when $z \to 0$. Here we will introduce the idea to describe the outlines by Gaussian curves (see Figure 4.3). In the figure, PS and QT represent the two outlines and they must satisfy the following requirements:

1. PS and QT should get closer to the boundary $x = \pm\frac{\Lambda}{2}$ when z goes to $\pm\infty$, but cannot exceed the boundary.
2. PS and QT should not intersect each other.
3. Assume there is a point $p(x_2, z_2)$ moving on the left curve PS, its corresponding point $q(x_1, z_1)$ is moving on the right curve QT. Originally, p and q should be on a flat line PQ ($z \to \infty$). When p moves from P to A, q moves from Q to B, and AB is a vertical line. When p reaches C, q reaches D. For the first part (PC and QD), p moves slower than q. Then p moves to S and q moves to T. When p gets to E, q gets to F, and EF is a vertical line like AB. For the second part (CS and DT), p moves faster than q, and ST is also a flat line ($z \to -\infty$).

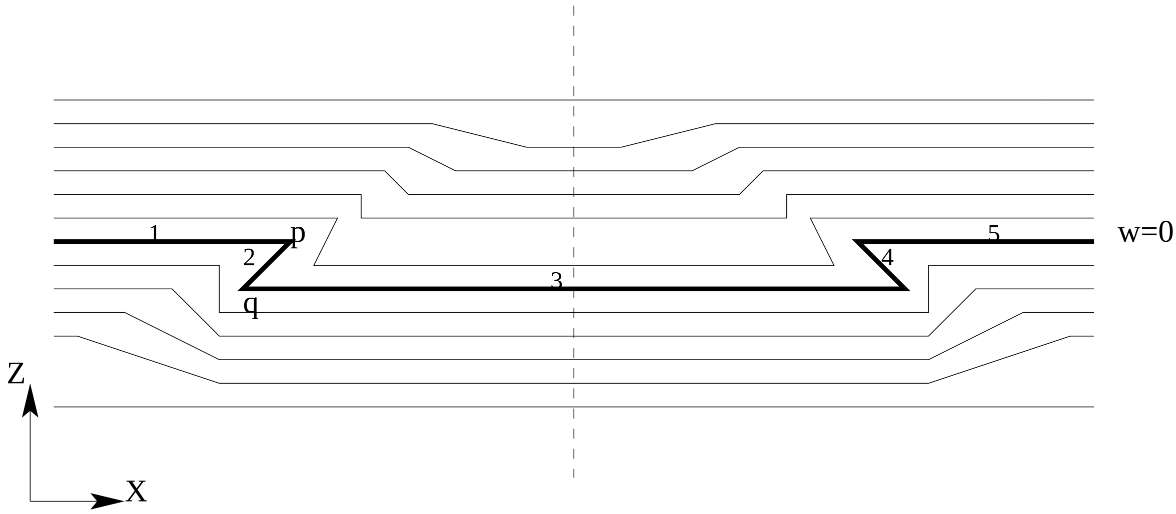

Figure 4.2: Symmetric overhanging trapezoidal lines

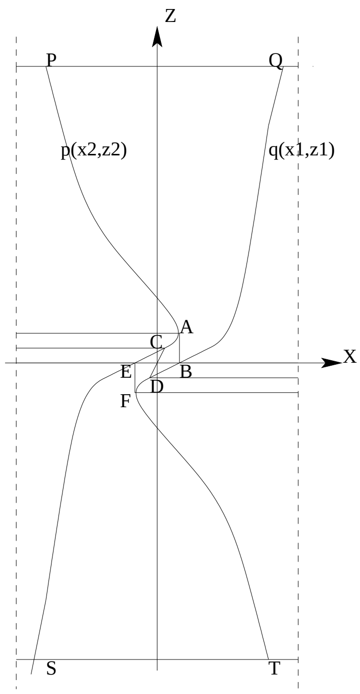

Figure 4.3: Outlines of the turning points described by Gaussian curves 1

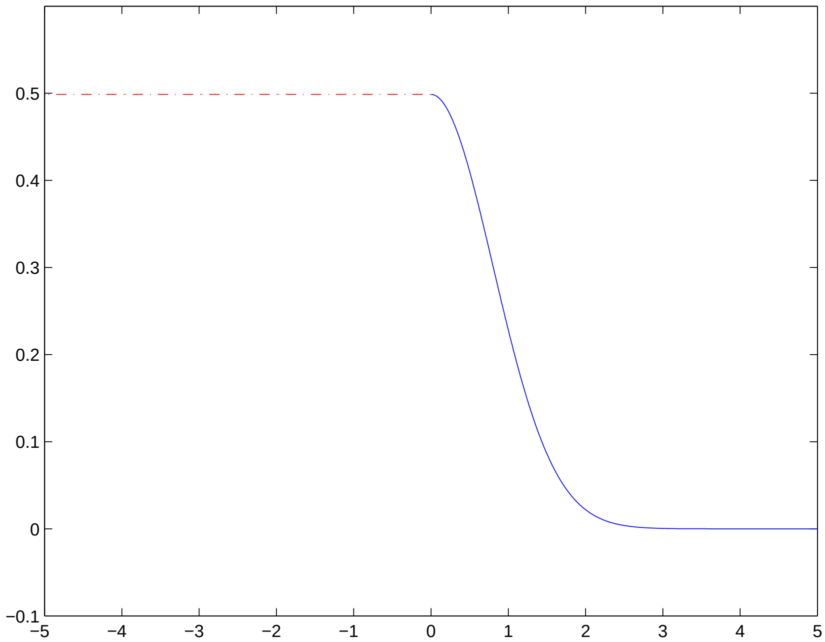

Figure 4.4: Combination of a Gaussian curve $(x \geqslant 0)$ and a flat line $(x < 0)$

With the conditions and the figure, we think of PS and QT as symmetric lines: PA is the same as TF, and AS is the same as FQ.

We can make curve PS by combining two parts PA and AS. There is one thing to be stated here: we want the resulting shape to be continuously differentiable such that the implementation of the C method should go smoothly. The function of the Gaussian curve is $z(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp(\frac{-x^2}{2\sigma^2})$, and we have $z'(0) = 0$. Then we have an easier way to build the curve: change the other part to be a horizontal line. Since they have the same slope at $x = 0$, thus we can combine them together (see Figure 4.4), and it is continuously differentiable along the whole curve. Furthermore, with this curve we can satisfy the requirements as well.

Figure 4.5 shows the easier version of Figure 4.3 where we make PA and FT two vertical lines. In the figure, p moves on PS and q moves on QT. When p moves from P to A, q moves from Q to B. For this part, their speed for the z direction is equal, so we will always get a flat line. Then p goes to C and q goes to D. For this part (AC and BD), p moves slower than q. Then it continues that p moves to E, and q moves to F. For this part (CE and DF), p moves faster than q. For the last part (ES and FT), the situation is like the first part: we will get flat lines in this part.

Functions for the outlines

As we have already said, the function for each curve is continuously differentiable. Also, we can see from Figure 4.5, that both PS and QT are symmetric with respect to the original

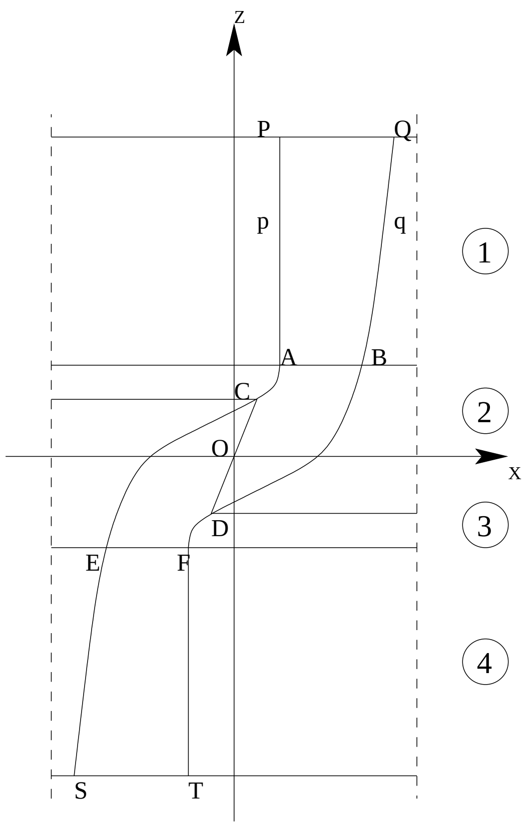

Figure 4.5: Outlines of the turning points described by Gaussian curves 2

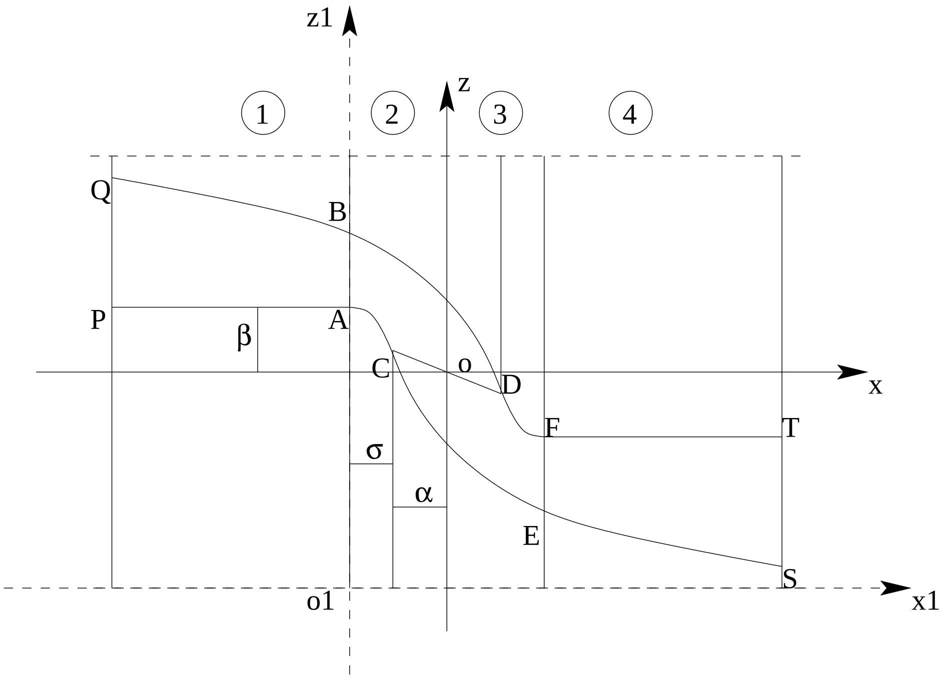

Figure 4.6: Outlines of the turning points described by Gaussian curves 3

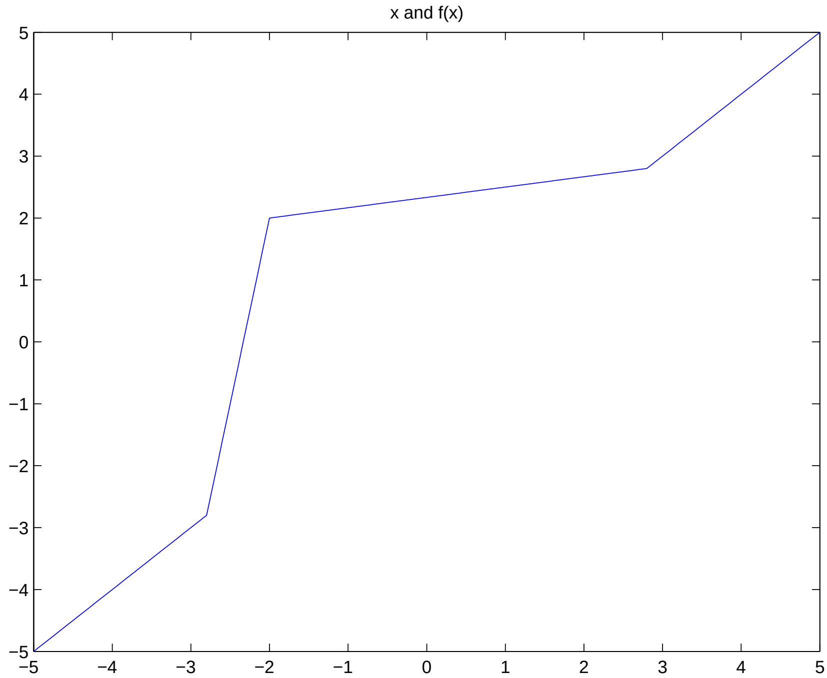

Figure 4.7: The relation between x and $f(x)$

O. From Figure 4.4, we know that we can get PS by moving the two axes x and z in the figure. Doing that, we will have a new coordinate system. Then we can get QT by taking the symmetric function of PS in the new coordinate system.

For convenience, we refer to Figure 4.6. In the figure, there are two pairs of coordinates: $x - z$ and $x1 - z1$. $x1 - z1$ is the original coordinate as we have seen in Figure 4.4, and $x - z$ is the new coordinate after we have moved the x and z axes. We use the new coordinate system to make it easier to write out the function of TQ, as we can see that TQ is symmetric with PS according to the new origin o. In the new coordinate system, the function of PS will be changed. In the figure, we separate each curve into four parts by their different relative speed. The position of p is denoted by $(x, \psi(x))$. If we denote the x coordinate of q by $f(x)$, then q has position $(f(x), -\psi(-f(x)))$ due to the symmetry. In addition, there are three constants in the figure: σ, α and β, where σ is the constant from the function of the Gaussian curve, α and β are two constants we created.

Figure 4.7 is given to show the relation between x and $f(x)$. It can also show the relative speed of p and q. We can see clearly that for the first part and the last part, the plot represents the function $f(x) = x$, which corresponds to Part 1 and Part 4 in Figure 4.6. For Part 2, $f(x)$ changes faster and the other way around for Part 3. Thus we write out the functions of both curves in the new coordinate system $x - z$:

1. $x \in (-\infty, -\sigma-\alpha)$, $f(x) \in (-\infty, -\sigma-\alpha)$

PA:	x	$\psi(x) = \beta$
QB:	$f(x) = x$	$-\psi(-f(x)) = -\frac{1}{\sqrt{2\pi}\sigma}\exp(\frac{-(-f(x)+\sigma+\alpha)^2}{2\sigma^2}) + \frac{1}{\sqrt{2\pi}\sigma} - \beta$

2. $x \in (-\sigma-\alpha, -\alpha)$, $f(x) \in (-\sigma-\alpha, \alpha)$

AC:	x	$\psi(x) = \frac{1}{\sqrt{2\pi}\sigma}\exp(\frac{-(x+\sigma+\alpha)^2}{2\sigma^2}) - \frac{1}{\sqrt{2\pi}\sigma} + \beta$
BD:	$f(x) = \frac{2\alpha+\sigma}{\sigma}(x+\alpha)+\alpha$	$-\psi(-f(x)) = -\frac{1}{\sqrt{2\pi}\sigma}\exp(\frac{-(-f(x)+\sigma+\alpha)^2}{2\sigma^2}) + \frac{1}{\sqrt{2\pi}\sigma} - \beta$

3. $x \in (-\alpha, \sigma+\alpha)$, $f(x) \in (\alpha, \sigma+\alpha)$

CE:	x	$\psi(x) = \frac{1}{\sqrt{2\pi}\sigma}\exp(\frac{-(x+\sigma+\alpha)^2}{2\sigma^2}) - \frac{1}{\sqrt{2\pi}\sigma} + \beta$
DF:	$f(x) = \frac{\sigma}{2\alpha+\sigma}(x+\alpha)+\alpha$	$-\psi(-f(x)) = -\frac{1}{\sqrt{2\pi}\sigma}\exp(\frac{-(-f(x)+\sigma+\alpha)^2}{2\sigma^2}) + \frac{1}{\sqrt{2\pi}\sigma} - \beta$

4. $x \in (\sigma+\alpha, \infty)$, $f(x) \in (\sigma+\alpha, \infty)$

ES:	x	$\psi(x) = \frac{1}{\sqrt{2\pi}\sigma}\exp(\frac{-(x+\sigma+\alpha)^2}{2\sigma^2}) - \frac{1}{\sqrt{2\pi}\sigma} + \beta$
FT:	$f(x) = x$	$-\psi(-f(x)) = -\beta$

With these functions, we make a program to draw the two curves and the trapezoidal lines passing through the turning points (see Figure 4.8).

Note that the coordinate system for Figure 4.6 is x, z exchanged from Figure 4.2. The reason we use the coordinate system shown in Figure 4.6 is for the convenience to get the functions. Beneath we will turn back to use the coordinate system shown in Figure 4.2.

Functions by u and w

We have built outlines for the two turning points by Gaussian curve. Now we want to construct a new coordinate system $u-w$ in which the interface will change into a flat line such that the generalized Rayleigh expansion can be used. We will use (u, w) to describe a point inside the domain instead of (x, z) in the new coordinate system. w is to indicate the trapezoidal line which passes through the point, which means w corresponds to the Gaussian curve. u is used to locate the exact point on that line. We use (x_1, z_1) and (x_2, z_2) to express the two turning points below, with them we can determine the trapezoidal line. Taking w as z (see Figure 4.5), we have:

1. $w \in (\sigma+\alpha, \infty)$

$$x_1(w) = -\frac{1}{\sqrt{2\pi}\sigma}\exp(\frac{-(w+\sigma+\alpha)^2}{2\sigma^2}) + \frac{1}{\sqrt{2\pi}\sigma} - \beta$$
$$x_2(w) = \beta$$

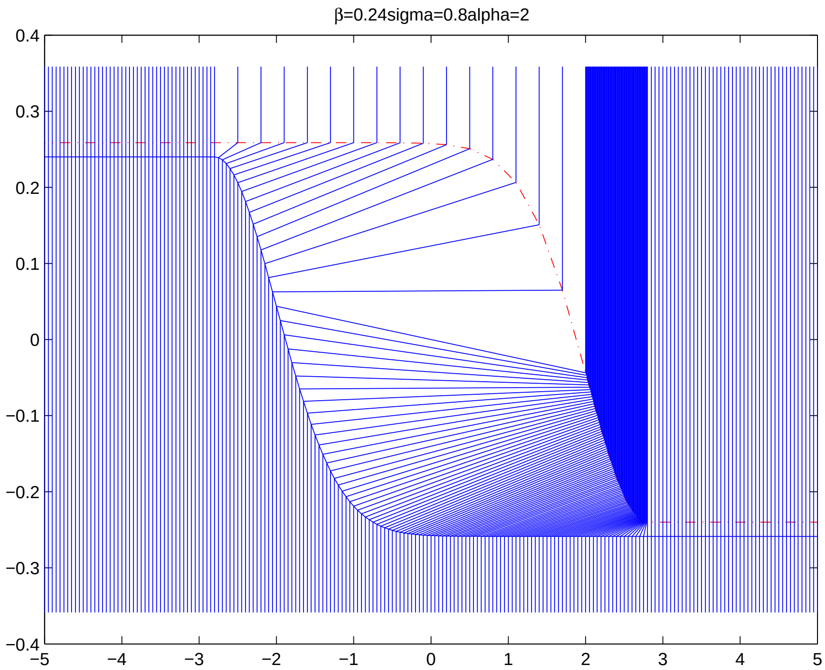

Figure 4.8: Trapezoidal lines for $\beta = 0.24$, $\sigma = 0.8$, $\alpha = 2$

$$z_1(w) = w$$
$$z_2(w) = w$$

2. $w \in (-\alpha, \sigma + \alpha]$

$$x_1(w) = -\frac{1}{\sqrt{2\pi}\sigma}\exp(\frac{-(w+\sigma+\alpha)^2}{2\sigma^2}) + \frac{1}{\sqrt{2\pi}\sigma} - \beta$$
$$x_2(w) = \frac{1}{\sqrt{2\pi}\sigma}\exp(\frac{-(-z_2(w)+\sigma+\alpha)^2}{2\sigma^2}) - \frac{1}{\sqrt{2\pi}\sigma} + \beta$$
$$z_1(w) = w$$
$$z_2(w) = \frac{\sigma}{2\alpha+\sigma}(w+\alpha) + \alpha$$

3. $w \in (-\sigma - \alpha, -\alpha]$

$$x_1(w) = -\frac{1}{\sqrt{2\pi}\sigma}\exp(\frac{-(w+\sigma+\alpha)^2}{2\sigma^2}) + \frac{1}{\sqrt{2\pi}\sigma} - \beta$$
$$x_2(w) = \frac{1}{\sqrt{2\pi}\sigma}\exp(\frac{-(-z_2(w)+\sigma+\alpha)^2}{2\sigma^2}) - \frac{1}{\sqrt{2\pi}\sigma} + \beta$$
$$z_1(w) = w$$
$$z_2(w) = \frac{2\alpha+\sigma}{\sigma}(w+\alpha) + \alpha$$

4. $w \in (-\infty, -\sigma - \alpha]$

$$x_1(w) = -\beta$$
$$x_2(w) = \frac{1}{\sqrt{2\pi}\sigma}\exp(\frac{-(-w+\sigma+\alpha)^2}{2\sigma^2}) - \frac{1}{\sqrt{2\pi}\sigma} + \beta$$
$$z_1(w) = w$$
$$z_2(w) = w$$

By taking $u \in [0,\ 1]$, we have:

$$x(w,u) = \begin{cases} -\frac{1}{\sqrt{2\pi}\sigma} + \beta + \frac{u}{u_0}(x_2(w) + \frac{1}{\sqrt{2\pi}\sigma} - \beta), & 0 \leqslant u \leqslant u_0 \\ x_2(w) + \frac{u-u_0}{u_1-u_0}(x_1(w) - x_2(w)), & u_0 < u \leqslant u_1 \\ x_1(w) + \frac{u-u_1}{1-u_1}(\frac{1}{\sqrt{2\pi}\sigma} - \beta - x_1(w)), & u_1 < u \leqslant 1 \end{cases} \tag{4.1}$$

$$z(w,u) = \begin{cases} z_2(w), & 0 \leqslant u \leqslant u_0 \\ z_2(w) - \frac{u-u_0}{u_1-u_0}(z_2(w) - z_1(w)), & u_0 < u \leqslant u_1 \\ z_1(w), & u_1 < u \leqslant 1 \end{cases} \tag{4.2}$$

where u_0 and u_1 are two constants and they satisfy the condition $0 \leqslant u_0 < u_1 \leqslant 1$.

Family of lines

We now discuss how to generate a whole family of trapezoidal lines when a single one is given.

When one trapezoidal line is given, we know the coordinates of the two turning points (x_1, z_1) and (x_2, z_2). Then we get the value of w, since w is always equal to z_1.

As analyzed above, the outline is described by four parts. For each part, we have four expressions $x_1(w)$, $x_2(w)$, $z_1(w)$, $z_2(w)$. Mostly our interest is on overhanging trapezoidal lines, thus when an overhanging trapezoidal line is given, we set $w = -\alpha$. This means that we take the given line as the co-boundary line of both part 2 and part 3. Of course we can do this because the set of lines are created by us according to the given line.

Since the line is both in part 2 and part 3, we can use the expression group for either part. From the equation for $x_1(w)$ or $x_2(w)$, we can get the relation between β and σ. Take one as known, then we have the corresponding value of the other.

Knowing these constants, we can construct a family of trapezoidal lines to cover the domain, which means we can use (u, w) to describe the domain, where $w \in (-\infty, \infty)$ and $u \in [0,\ 1]$.

Changing a point from (x, z) to (u, w)

Equations (4.1) and (4.2) give x and z as functions of u and w. We will now show how we may obtain u and w for a given point (x, z) in the computational domain, viz. from (x, z) to (u, w). Suppose one point is given as (x_0, z_0), then we should take the following steps:

1. Change (x_0, z_0) to (x_3, z_3).
   Take $x_3 = -z_0$ and $z_3 = x_0$, then we have $(x_3, z_3) = (-z_0, x_0)$. We do this because we want to use the function $\psi(x)$ for the old coordinate (see Figure 4.6).

2. Check which part the point (x_3, z_3) belongs to.
   As we want to use the equation groups (4.1) and (4.2), there are three equations for either x or z, we should know which equation to use. That means for a half trapezoidal line (see Figure 4.2), we should know which line (1, 2, and 3) the point (x_3, z_3) belongs to. We do this by substituting x_3 into the two curve functions and we can obtain $\psi(x_3)$ and $-\psi(-x_3)$. Then we compare z_3 with them to see which part (x_3, z_3) belongs to. Then we can choose the exact equation to use.

3. Get (u, w).
   For each particular part, we have two equations for u and w. For example, if it is in the middle part, we have

$$\begin{cases} x = x_2(w) + \dfrac{u - u_0}{u_1 - u_0}(x_1(w) - x_2(w)) \\ \\ z = z_2(w) - \dfrac{u - u_0}{u_1 - u_0}(z_2(w) - z_1(w)) \end{cases}$$

   In the equation group, we have two unknowns u and w. We can solve the equations by Newton's Method. Then we get (u_0, w_0) for the given point (x_0, z_0).

By performing these three steps, we can transfer any point (x, z) inside the domain into its new coordinate (u, w).

Constraints for the constants

To ensure that there is no intersection for all the trapezoidal lines, there should be some constraints for the constants σ, α and β (see Figure 4.6). Note that only in the old coordinate system do we have overhanging gratings, thus we will analyse the constraints under the old coordinate system.

- For the first part, QB should always be above PA. We can see that the lowest point for QB is B. Thus we have $\beta < -\frac{1}{2\sqrt{2\pi}\sigma}\exp(\frac{-2(\sigma+\alpha)^2}{\sigma^2}) + \frac{1}{2\sqrt{2\pi}\sigma}$.

- For the second part, point C should always be above the x axis, otherwise there will be no overhanging trapezoidal lines which are the focus of the project. Thus we have $\beta > -\frac{1}{\sqrt{2\pi}\sigma}\exp(-\frac{1}{2}) + \frac{1}{\sqrt{2\pi}\sigma}$.

- We set $\Delta = (-\frac{1}{2\sqrt{2\pi}\sigma}\exp(\frac{-2(\sigma+\alpha)^2}{\sigma^2}) + \frac{1}{2\sqrt{2\pi}\sigma}) - (-\frac{1}{\sqrt{2\pi}\sigma}\exp(-\frac{1}{2}) + \frac{1}{\sqrt{2\pi}\sigma})$. And we use it to check α and σ since Δ should always be bigger than 0.

  Before continuing to talk about the next constraint, we here discuss the relation between the value of a turning angle ϕ of a trapezoidal line and the value of w (see

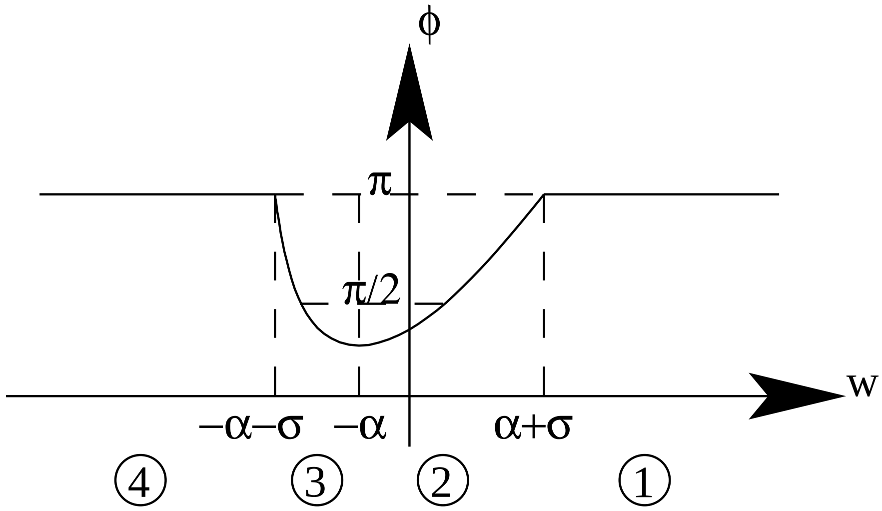

Figure 4.9: The relation between ϕ and w

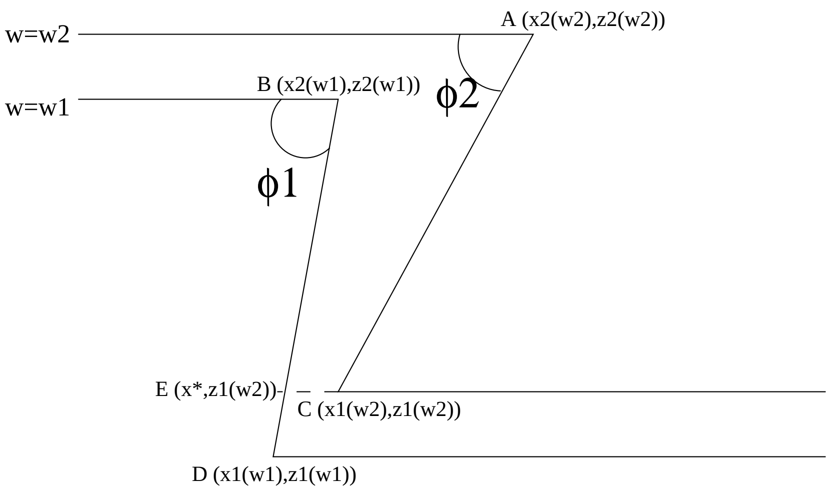

Figure 4.10: Two neighboring trapezoidal lines

Figure 4.9). The four parts inside are divided in the same way as shown in Figure 4.6. From the figure, we can see that $\phi = \pi$ when $w \leq -\alpha - \sigma$ and $w \geq \alpha + \sigma$. ϕ will get its minimum when $w = -\alpha$, and this minimum is smaller than $\frac{\pi}{2}$. In part 2 ϕ increases when w turns bigger, while in part 3 ϕ decreases when w becomes larger. Note that the value of ϕ changes faster in part 3 than in part 2.

Take two neighboring trapezoidal lines as shown in Figure 4.10. Assume we have $w = w_2$ for the upper line and $w = w_1$ for the lower one. For these two lines, we have the coordinate for the four turning points A, B, C, D, and we have two turning angles ϕ_1 and ϕ_2. We can see that points A and B are on the same outline of turning points, while points C and D are on the other turning-curve. In the figure, ϕ_1 is larger than ϕ_2, and w_2 is bigger than w_1. Comparing with Figure 4.9, we know that the situation in Figure 4.10 is taken from part 3.

Note that two trapezoidal lines will never intersect in the parts 1, 2, and 4. Thus we will only focus on the situation when ϕ decreases from π to its minimum, which means $w \in (-\alpha - \sigma, -\alpha)$.

From Figure 4.10 we see that to ensure that there will be no intersection, point C must be at the right side of BD and should not touch BD. Let $E(x^*, z_1(w_2))$ be the point which has the same z coordinate as point C and is on BD. We must ensure that $x^* < x_1(w_2)$. From the coordinate of B and D, we can write out the function for BD:

$$y_{BD} := \frac{z_1(w_1) - z_2(w_1)}{x_1(w_1) - x_2(w_1)}(x - x_1(w_1)) + z_1(w_1). \tag{4.3}$$

Because E is on this line, we can get:

$$\begin{aligned}
z_1(w_2) &= \frac{z_1(w_1) - z_2(w_1)}{x_1(w_1) - x_2(w_1)}(x^* - x_1(w_1)) + z_1(w_1) \\
\Leftrightarrow z_1(w_2) - z_1(w_1) &= \frac{z_1(w_1) - z_2(w_1)}{x_1(w_1) - x_2(w_1)}(x^* - x_1(w_1)) \\
\Leftrightarrow (x^* - x_1(w_1)) &= \frac{x_1(w_1) - x_2(w_1)}{z_1(w_1) - z_2(w_1)}(z_1(w_2) - z_1(w_1)) \\
\Leftrightarrow x^* &= x_1(w_1) + \frac{x_1(w_1) - x_2(w_1)}{z_1(w_1) - z_2(w_1)}(z_1(w_2) - z_1(w_1)) \qquad (4.4)
\end{aligned}$$

The requirement $x^* < x_1(w_2)$ gives:

$$\begin{aligned}
x_1(w_1) + (x_1(w_1) - x_2(w_1))\frac{z_1(w_2) - z_1(w_1)}{z_1(w_1) - z_2(w_1)} &< x_1(w_2) \\
\Leftrightarrow (x_1(w_1) - x_2(w_1))\frac{z_1(w_2) - z_1(w_1)}{z_1(w_1) - z_2(w_1)} &< x_1(w_2) - x_1(w_1) \\
\Rightarrow \frac{x_2(w_1) - x_1(w_1)}{z_2(w_1) - z_1(w_1)} &< \frac{x_1(w_2) - x_1(w_1)}{z_1(w_2) - z_1(w_1)}, \quad (z_1(w_2) - z_1(w_1) > 0)
\end{aligned} \tag{4.5}$$

For part 3 $w \in (-\sigma - \alpha, -\alpha]$, we have:

$$\begin{aligned}
x_1(w_1) &= -\frac{1}{\sqrt{2\pi}\sigma}\exp(\frac{-(w_1+\sigma+\alpha)^2}{2\sigma^2}) + \frac{1}{\sqrt{2\pi}\sigma} - \beta \\
x_2(w_1) &= \frac{1}{\sqrt{2\pi}\sigma}\exp(\frac{-(-z_2(w_1)+\sigma+\alpha)^2}{2\sigma^2}) - \frac{1}{\sqrt{2\pi}\sigma} + \beta \\
z_1(w_1) &= w_1 \\
z_2(w_1) &= \frac{2\alpha+\sigma}{\sigma}(w_1+\alpha) + \alpha \\
x_1(w_2) &= -\frac{1}{\sqrt{2\pi}\sigma}\exp(\frac{-(w_2+\sigma+\alpha)^2}{2\sigma^2}) + \frac{1}{\sqrt{2\pi}\sigma} - \beta \\
z_1(w_2) &= w_2
\end{aligned}$$

Then we obtain by calculation:

$$\begin{aligned}
\frac{x_2(w_1)-x_1(w_1)}{z_2(w_1)-z_1(w_1)} &= \frac{\frac{1}{2\sqrt{2\pi}}[\exp(\frac{-(w_1+\sigma+\alpha)^2}{2\sigma^2}) + \exp(\frac{-(-z_2(w_1)+\sigma+\alpha)^2}{2\sigma^2})] - \frac{1}{\sqrt{2\pi}} + \beta\sigma}{\alpha^2+\alpha w_1+\sigma\alpha} \\
\frac{x_1(w_2)-x_1(w_1)}{z_1(w_2)-z_1(w_1)} &= \frac{\frac{1}{\sqrt{2\pi}}[\exp(\frac{-(w_2+\sigma+\alpha)^2}{2\sigma^2}) - \exp(\frac{-(w_1+\sigma+\alpha)^2}{2\sigma^2})]}{\sigma w_1 - \sigma w_2}
\end{aligned}$$

- This gives us another constraint:

$$\frac{(\frac{1}{2}[\exp(\frac{-(w_1+\sigma+\alpha)^2}{2\sigma^2}) + \exp(\frac{-(-z_2(w_1)+\sigma+\alpha)^2}{2\sigma^2})] + \sqrt{2\pi}\beta\sigma - 1)(\sigma w_1 - \sigma w_2)}{(\exp(\frac{-(w_2+\sigma+\alpha)^2}{2\sigma^2}) - \exp(\frac{-(w_1+\sigma+\alpha)^2}{2\sigma^2}))(\alpha w_1+\alpha^2+\alpha\sigma)} < 1 \tag{4.6}$$

We can put the given α, β, σ inside to see if it is smaller than 1. But there is one problem: there are two w values (w_1 and w_2) inside, how to choose w_1 and w_2 as they should be adjacent to each other.

To solve this problem, we will use a limit argument. Take $w_1 = w$, $w_2 = w + h$, substitution into (4.5) gives:

$$\frac{x_2(w)-x_1(w)}{z_2(w)-z_1(w)} < \frac{x_1(w+h)-x_1(w)}{z_1(w+h)-z_1(w)} = \frac{\frac{x_1(w+h)-x_1(w)}{h}}{\frac{z_1(w+h)-z_1(w)}{h}}$$

and we let $h \to 0$, this gives:

$$\frac{x_2(w)-x_1(w)}{z_2(w)-z_1(w)} < \frac{x_1'(w)}{z_1'(w)} \tag{4.7}$$

The inequality (4.7) is a general constraint such that two neighboring trapezoidal lines do not intersect.

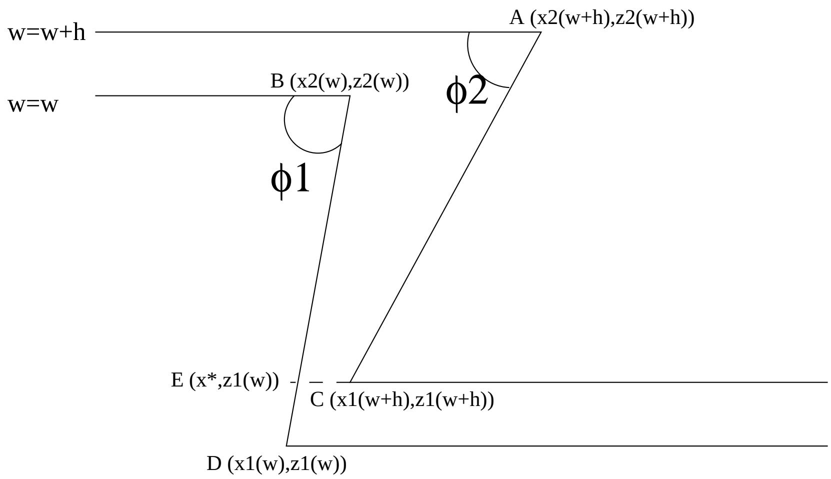

Figure 4.11: Limitation of two neighboring trapezoidal lines

Theorem 4.1

Assume there are two arbitrary trapezoidal lines AC and BD (see Figure 4.11), the coordinates of the points A, B, C and D are $(x2(w+h), z2(w+h))$, $(x2(w), z2(w))$, $(x1(w+h), z1(w+h))$, and $(x1(w), z1(w))$ respectively. When $h \to 0$, AC and BD become two neighboring lines. The constraint for not intersecting is:

$$\frac{x_2(w) - x_1(w)}{z_2(w) - z_1(w)} < \frac{x_1'(w)}{z_1'(w)} \tag{4.8}$$

♯

We define two functions $f_1(w)$ and $f_2(w)$ here:

$$f_1(w) := \frac{x_2(w) - x_1(w)}{z_2(w) - z_1(w)}$$
$$f_2(w) := \frac{x_1'(w)}{z_1'(w)}$$

Note that $f_1(w)$ and $f_2(w)$ are both functions of w.

For part 3, we have for $f_1(w)$:

$$\begin{cases} x_2(w) - x_1(w) = \frac{1}{\sqrt{2\pi}\sigma}\exp(\frac{-(-z_2(w)+\sigma+\alpha)^2}{2\sigma^2}) + \frac{1}{\sqrt{2\pi}\sigma}\exp(\frac{-(w+\sigma+\alpha)^2}{2\sigma^2}) - \frac{2}{\sqrt{2\pi}\sigma} + 2\beta \\ z_2(w) - z_1(w) = \frac{2\alpha}{\sigma}(w+\sigma+\alpha) \end{cases}$$

$$\Rightarrow f_1(w) = \frac{x_2(w) - x_1(w)}{z_2(w) - z_1(w)} = \frac{\exp(\frac{-(-z_2(w)+\sigma+\alpha)^2}{2\sigma^2}) + \exp(\frac{-(w\sigma+\alpha)^2}{2\sigma^2}) - 2 + 2\sqrt{2\pi}\beta\sigma}{2\sqrt{2\pi}\alpha(w+\sigma+\alpha)} \tag{4.9}$$

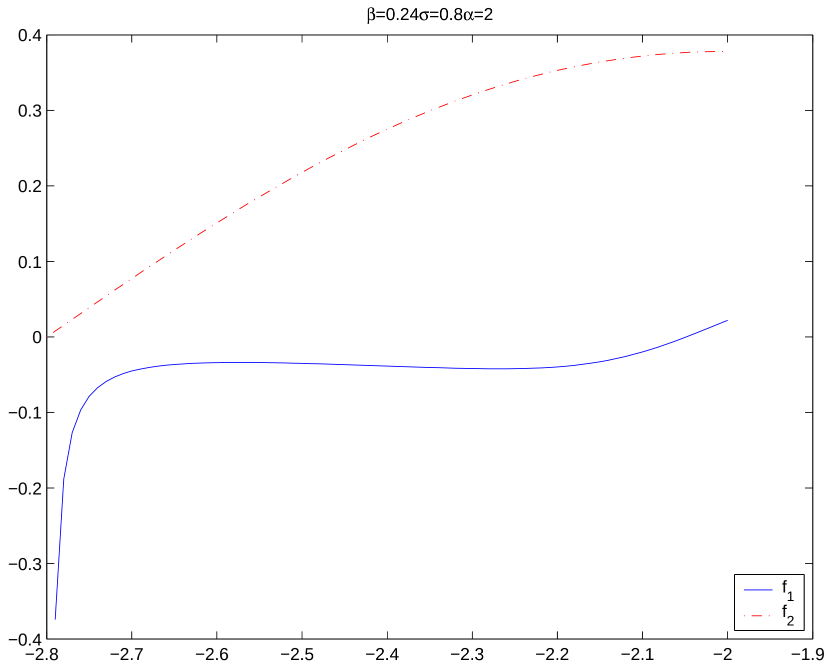

Figure 4.12: Figure for $f_1(w)$ and $f_2(w)$ for Gaussian curve for part 3

and for $f_2(w)$:

$$\begin{cases} x_1'(w) = \dfrac{w+\sigma+\alpha}{\sqrt{2\pi}\sigma^3}\exp(\dfrac{-(w+\sigma+\alpha)^2}{2\sigma^2}) \\ z_1'(w) = 1 \end{cases}$$

$$\Rightarrow f_2(w) = \frac{w+\sigma+\alpha}{\sqrt{2\pi}\sigma^3}\exp(\frac{-(w+\sigma+\alpha)^2}{2\sigma^2}) \tag{4.10}$$

Thus we have:

$$f_1(w) < f_2(w) \Rightarrow$$
$$\frac{\exp(\frac{-(-z_2(w)+\sigma+\alpha)^2}{2\sigma^2}) + \exp(\frac{-(w+\sigma+\alpha)^2}{2\sigma^2}) - 2 + 2\sqrt{2\pi}\beta\sigma}{\frac{2\alpha}{\sigma^3}(w+\sigma+\alpha)^2} < \exp(\frac{-(w+\sigma+\alpha)^2}{2\sigma^2}) \tag{4.11}$$

For this equality there is only w inside, and we can use it instead of (4.6) as the constraint to ensure that there will be no intersection. In Figure 4.12, we plot f_1 and f_2 for given α, β, σ for part 3 to check the inequality (4.11). We can see that for part 3, $f_1(w)$ is always smaller than $f_2(w)$, which means that the constants we take fulfill the constraints, and there will be no intersection. This can be shown in Figure 4.8 as we take the same value $\beta = 0.24$, $\sigma = 0.8$, $\alpha = 2$, and there is no intersection in between.

With these constraints, we can pick constants to ensure that there will be non-intersecting lines.

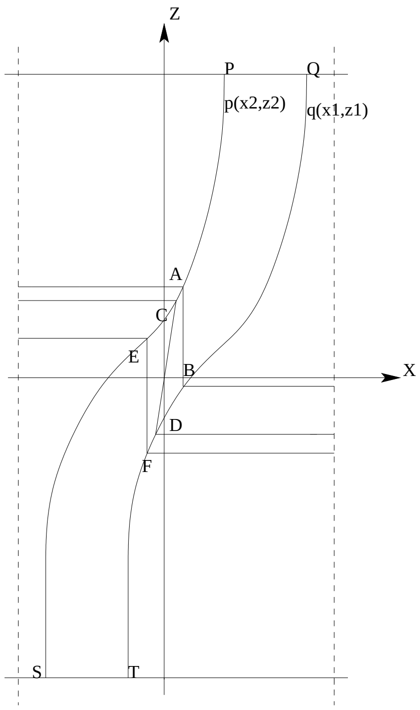

Figure 4.13: Outlines of the turning points described by tangential functions

4.1.2 Outlines of the turning points described by tangential functions

Since the function with the Gaussian curve is very complicated, this will bring us much computational trouble in the remainder of implementing the C method. We want to find more simple functions to describe the outlines of the turning points. Here we will introduce the idea to describe the outlines of the turning points by tangential functions (see Figure 4.13).

Outlines for the turning points

In Figure 4.13, we use PS and QT to represent the two outlines and the requirements for them to fulfill are similar as we have seen for Gaussian curve.

Functions for the outlines

For the two outlines, we use the tangential function $z = \tan(x)$ to draw one of the outlines and make a coordinate translation to get the other one. Note that we make a scaling on x from $(-\frac{\Lambda}{2}, 0)$ to $(-\frac{\pi}{2}, \frac{\pi}{2})$. There are two moving points p and q on the curves PS and QT. We use $(x_1(x), z_1(x))$ to represent the translated curve QT where x_1 denotes the x component and z_1 denotes the z component. Similarly, we use $(x_2(x), z_2(x))$ for the original curve PS.

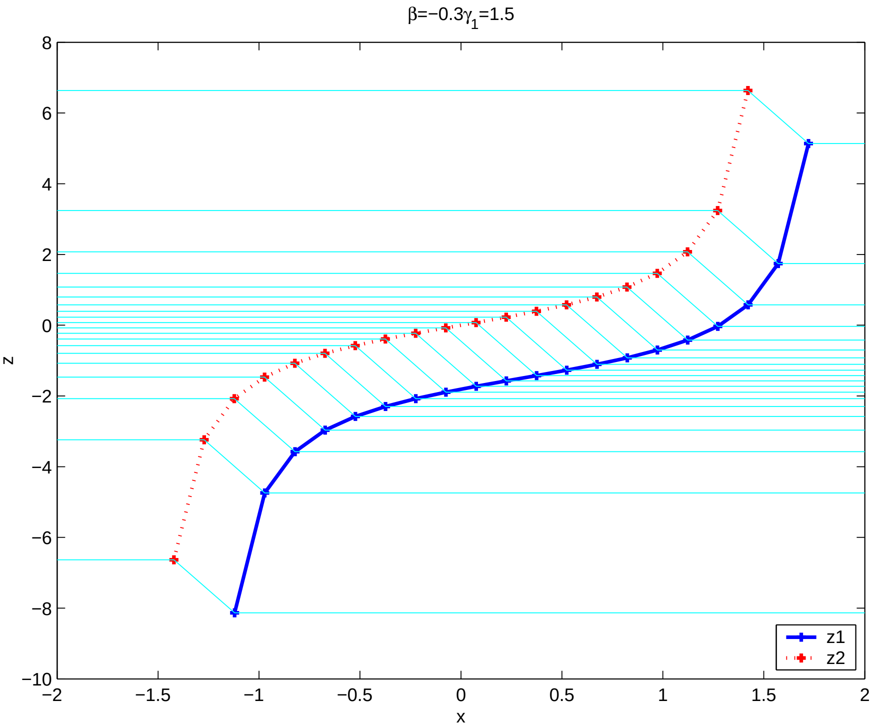

Figure 4.14: Turning points as $z_2 = \tan(x)$ and $z_1 = \tan(x) - \gamma_1$

We first try :

$$\begin{cases} x_1 = x - \beta \\ z_1 = \tan(x) - \gamma_1 \\ x_2 = x \\ z_2 = \tan(x) \end{cases} \tag{4.12}$$

where β, and γ_1 are constants, $x_1, x_2 \in (-\frac{\pi}{2}, \frac{\pi}{2})$, and $z_1, z_2 \in (-\infty, \infty)$.

Figure 4.14 shows a solid line which represents the original curve $z_2 = \tan(x)$, and a dotted line which represents the translated curve $z_1 = \tan(x) - \gamma_1$. For these two outlines, we take N pairs of corresponding points. Connecting these corresponding points, we can get N trapezoidal lines. As the translated line is just the result of moving the original line, the two lines have the same shape and the same distance between each pair of two corresponding points. This brings us a problem: when $|x|$ goes to $\frac{\pi}{2}$, we will not get flat lines there. Actually we want the vertical distance $\Delta z = z_1 - z_2$ to be maximal when x equals zero. On the other hand, when $|x|$ goes to $\frac{\pi}{2}$, we expect Δz to become zero. So we shall make some changes for the translated line in the zdirection.

$y = \cos(x)$ is such a function that when x changes from $-\frac{\pi}{2}$ to 0 to $\frac{\pi}{2}$, y corresponds from 0 to 1 to 0. This function can help us to get the behavior we want for the zdirection. Thus we have the idea to apply the function $y = \cos(x)$ to improve the translated curve z_1 for the

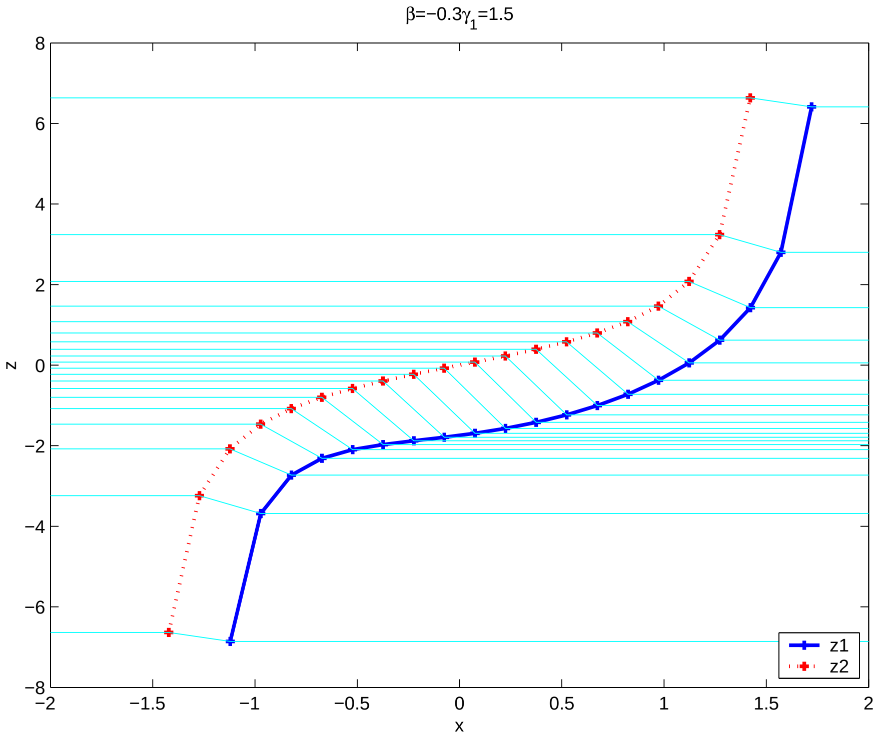

Figure 4.15: Turning points as $z_2 = \tan(x)$ and $z_1 = \tan(x) - \gamma_1 \cos(x)$

zdirection.

The second attempt:

$$\begin{cases} x_1 = x - \beta \\ z_1 = \tan(x) - \gamma_1 \cos(x) \\ x_2 = x \\ z_2 = \tan(x) \end{cases} \tag{4.13}$$

We can see in Figure 4.15 that the dotted line now represents the curve $z_1 = \tan(x) - \gamma_1 \cos(x)$. But there is still one problem: we cannot get overhanging trapezoidal lines. This is because we do the same change for the xdirection for all points. So there should be some changes for the x direction too.

For the x direction, we want the trapezoidal lines to be overhanging ($x_1 < x_2$) only when $|x|$ is small. When $|x|$ goes to $\frac{\pi}{2}$, we want to have $x_2 < x_1$, which means that the lines are not overhanging. This behavior is similar to the change we have implemented for the zdirection, so we try the same method: put inside a function $y = \cos(x)$ to improve the translated line z_1 for the x direction.

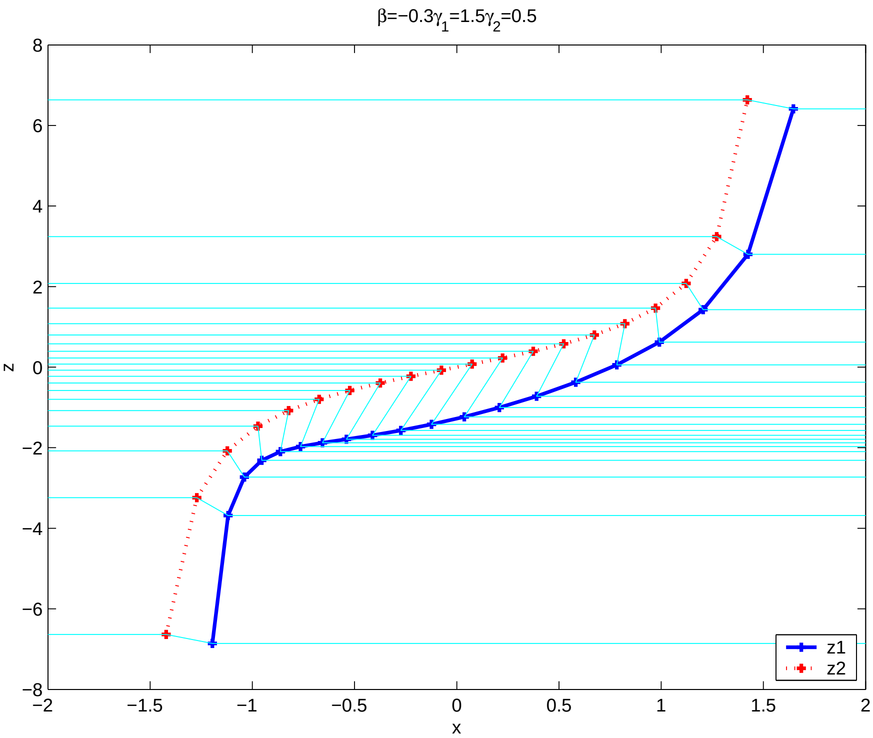

Figure 4.16: Turning points as $z_2 = \tan(x)$ and $z_1 = \tan(x) - \gamma_1 \cos(x)$

The third attempt:

$$\begin{cases} x_1 = x - \beta - \gamma_2 \cos(x) \\ z_1 = \tan(x) - \gamma_1 \cos(x) \\ x_2 = x \\ z_2 = \tan(x) \end{cases} \tag{4.14}$$

where γ_2 is also a constant.

Figure 4.16 shows the dotted line which stands for the translated curve $z_1 = \tan(x) - \gamma_1 \cos(x)$. In the figure, there are overhanging trapezoidal lines when $|x|$ is around zero, flat lines when $|x|$ goes to $\frac{\pi}{2}$, and all the trapezoidal lines do not intersect each other.

Now we can say that we can draw non-intersecting trapezoidal lines to cover the whole domain, and there are overhanging trapezoidal lines inside for a specific selection of constants.

Functions by u and w

Here we introduce a new parameter first: s. $s \in (-\frac{\pi}{2}, \frac{\pi}{2})$ is the parameter to indicate which line is under consideration. With s, we can determine the coordinate of the two turning points which means we get the trapezoidal line passing through:

$$\begin{cases} x_1(s) = s - \beta - \gamma_2 \cos(s) \\ z_1(s) = \tan(s) - \gamma_1 \cos(s) \\ x_2(s) = s \\ z_2(s) = \tan(s) \end{cases} \tag{4.15}$$

For the new coordinate transformation, we want to have one parameter which is from $-\infty$ to ∞, thus we introduce a new parameter $w = \tan(s)$. As $s \in (-\frac{\pi}{2}, \frac{\pi}{2})$, we have $w \in (-\infty, \infty)$. Then we can get from (4.15):

$$\begin{cases} x_1(w) = \arctan w - \beta - \gamma_2 \cos(\arctan w) \\ z_1(w) = w - \gamma_1 \cos(\arctan w) \\ x_2(w) = \arctan w \\ z_2(w) = w \end{cases} \tag{4.16}$$

To locate the position of a point on the trapezoidal line determined by w, we need another parameter u $(0 < u < 1)$ to indicate where we are on the line. With u and w, we have:

$$x(u,w) = \begin{cases} -\frac{\pi}{2} + \frac{u}{u_0}(\arctan w + \frac{\pi}{2}), & 0 \leqslant u \leqslant u_0 \\ \arctan w + \frac{u - u_0}{u_1 - u_0}(x_1(w) - \arctan w), & u_0 < u \leqslant u_1 \\ x_1(w) + \frac{u - u_1}{1 - u_1}(\frac{\pi}{2} - x_1(w)), & u_1 < u \leqslant 1 \end{cases} \tag{4.17}$$

$$z(u,w) = \begin{cases} w, & 0 \leqslant u \leqslant u_0 \\ w - \frac{u - u_0}{u_1 - u_0}(w - z_1(w)), & u_0 < u \leqslant u_1 \\ z_1(w), & u_1 < u \leqslant 1 \end{cases} \tag{4.18}$$

where u_0 and u_1 are two constants and they satisfy the condition $(0 \leqslant u_0 < u_1 \leqslant 1)$.

Family of lines

The way to generate a whole family of trapezoidal lines when a single one is given is similar as for the Gaussian curve. We get the value of w, since $w = z_2$, then we can get $\gamma_1 = \frac{w - z_1}{\cos(\arctan w)}$. Also we get the relation for β and γ_2. If we assume one is known and we get all the constants and can build a set of trapezoidal lines to cover the domain.

From (x, z) to (u, w)

Equation (4.17) and (4.18) give x and z as functions of u and w. To get the new coordinate (u, w), we have a similar method as shown for the Gaussian curve. Suppose one point is given as (x_0, z_0), then we take the following steps:

1. Check which part the point (x_0, z_0) belongs to.
2. Get (u, w).

Constraints for the constants

As we want to make all the lines non-intersecting, there are some constraints for the three constants β, γ_1, and γ_2.

- In Figure 4.13, we see that the translated line QT should always lie under the original line PS. According to (4.15), this means $\forall s \neq 0$, $z_1(s) < z_2(s)$ and we can get $\gamma_1 > 0$.
- We do not have overhanging gratings when $s \to \pm\frac{\pi}{2}$, then we have for $s = \pm\frac{\pi}{2}$, $x_2(s) < x_1(s)$, and we can get $\beta < 0$.
- We have overhanging gratings when $s \to 0$, then we have for $s = 0$, $x_2(s) > x_1(s)$, and we can get $\gamma_2 > -\beta$. Note that $\gamma_2 = -\beta$ gives the limit situation for binary gratings (see Figure 1.4 middle).
- Theorem 4.1 is another constraint that must be fulfilled. From (4.8), we have

$$\frac{x_2(w) - x_1(w)}{z_2(w) - z_1(w)} < \frac{x_1'(w)}{z_1'(w)}$$

Similarly, we define $f_1(w)$ and $f_2(w)$:

$$f_1(w) := \frac{x_2(w) - x_1(w)}{z_2(w) - z_1(w)} = \frac{x_2(w) - x_1(w)}{z_2(w) - z_1(w)} = \frac{\beta + \gamma_2 \cos(\arctan w)}{\gamma_1 \cos(\arctan w)}$$
$$f_2(w) := \frac{x_1'(w)}{z_1'(w)} = \frac{1 + \gamma_2 \sin(\arctan w)}{\gamma_1 \sin(\arctan w) + 1 + w^2}$$

Then we get

$$f_1(w) < f_2(w) \Rightarrow \frac{\beta + \gamma_2 \cos(\arctan w)}{\gamma_1 \cos(\arctan w)} < \frac{1 + \gamma_2 \sin(\arctan w)}{\gamma_1 \sin(\arctan w) + 1 + w^2} \quad (4.19)$$

We regard (4.19) as the fourth constraint. In Figure 4.17, we plot f_1 and f_2 for given γ_1, γ_2, β to check the inequality (4.19). We can see that $f_1(w)$ is always smaller than $f_2(w)$ for $w \in (-\infty, 0]$. Thus $\gamma_1 = 1.5$, $\gamma_2 = 0.5$, $\beta = -0.3$ can be used as the constants for the equations (4.16).

4.2 Smooth overhanging gratings

4.2.1 Function and constraints

Having studied trapezoidal lines, now we want to return to smooth overhanging gratings (see Figure 4.18). The function for the grating is given as:

$$\begin{cases} x(u) = au + b\sin(4\pi u) \\ z(u) = \frac{c}{2} + \frac{c}{2}\cos(2\pi u) \end{cases} \quad (4.20)$$

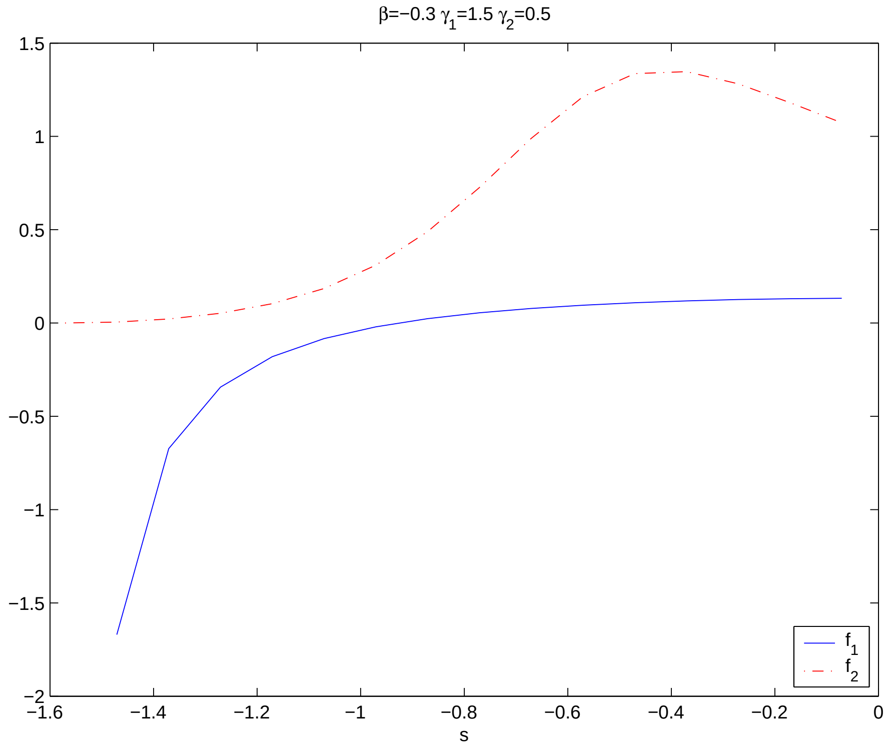

Figure 4.17: Figure for $f_1(w)$ and $f_2(w)$ for tangential functions

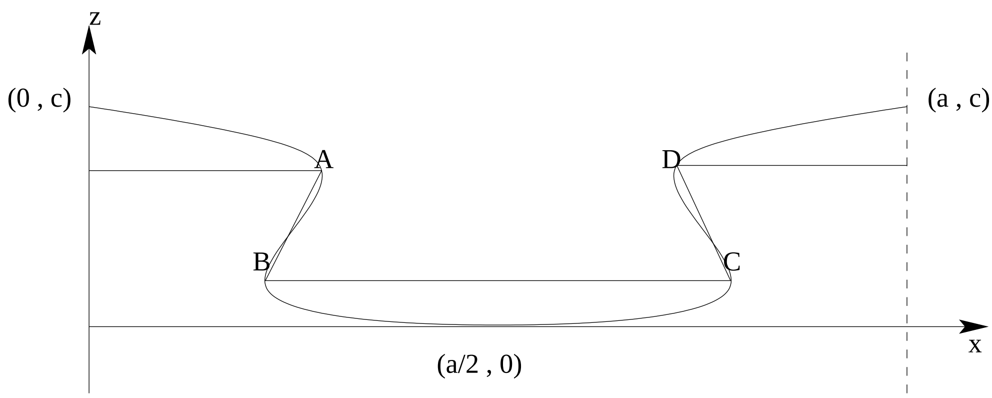

Figure 4.18: Smooth overhanging gratings

where a,b and c and three given constants, and they describe the shape of the grating. The function depends on the variable u. We can see from the figure that there are four turning points: A, B, C, and D. For these turning points, we have:

$$\frac{dx}{dz} = 0 \qquad \Rightarrow \qquad \frac{\frac{dx}{du}}{\frac{dz}{du}} = 0 \qquad \Rightarrow \qquad x'(u) = 0$$

Thus we have: $x'(u) = a + 4\pi b \cos(4\pi u) = 0$. And therefore:

$$\begin{aligned} u_1 &= \frac{1}{4\pi} \arccos(-\frac{a}{4\pi b}) \\ u_2 &= \frac{1}{2} - \frac{1}{4\pi} \arccos(-\frac{a}{4\pi b}) \\ u_3 &= \frac{1}{2} + \frac{1}{4\pi} \arccos(-\frac{a}{4\pi b}) \\ u_4 &= 1 - \frac{1}{4\pi} \arccos(-\frac{a}{4\pi b}) \end{aligned}$$

Then there will be two situations:

1. $0 < \frac{1}{4\pi} \arccos(-\frac{a}{4\pi b}) < \frac{1}{4}$

   In this case, we will have $u_1 < u_2 < u_3 < u_4$, then we can get for the four points:

$$\begin{aligned} A: \quad x_A &= \frac{a}{4\pi} \arccos(-\frac{a}{4\pi b}) + b \sin(\arccos(-\frac{a}{4\pi b})) \\ z_A &= \frac{c}{2} + \frac{c}{2} \cos(\frac{1}{2} \arccos(-\frac{a}{4\pi b})) \\ B: \quad x_B &= \frac{a}{2} - \frac{a}{4\pi} \arccos(-\frac{a}{4\pi b}) - b \sin(\arccos(-\frac{a}{4\pi b})) \\ z_B &= \frac{c}{2} - \frac{c}{2} \cos(\frac{1}{2} \arccos(-\frac{a}{4\pi b})) \\ C: \quad x_C &= \frac{a}{2} + \frac{a}{4\pi} \arccos(-\frac{a}{4\pi b}) + b \sin(\arccos(-\frac{a}{4\pi b})) \\ z_C &= \frac{c}{2} - \frac{c}{2} \cos(\frac{1}{2} \arccos(-\frac{a}{4\pi b})) \\ D: \quad x_D &= a - \frac{a}{4\pi} \arccos(-\frac{a}{4\pi b}) - b \sin(\arccos(-\frac{a}{4\pi b})) \\ z_D &= \frac{c}{2} + \frac{c}{2} \cos(\frac{1}{2} \arccos(-\frac{a}{4\pi b})) \end{aligned}$$

   For this situation, we have from the figure:

$$\begin{cases} u_A < u_B < u_C < u_D \\ z_A = z_D > z_B = z_C \end{cases} \qquad \Rightarrow \qquad 0 < \arccos(-\frac{a}{4\pi b}) < \pi \tag{4.21}$$

   Also, we have:

$$x_B < x_A < x_D < x_C \quad \Rightarrow \quad \frac{a}{4} < \frac{a}{4\pi} \arccos(-\frac{a}{4\pi b}) + b \sin(\arccos(-\frac{a}{4\pi b})) < \frac{a}{2} \tag{4.22}$$

   (4.21) and (4.22) are the constraints for a and b.

2. $\frac{1}{4} < \frac{1}{4\pi} \arccos(-\frac{a}{4\pi b}) < \frac{1}{2}$

In this case, we will have $u_2 < u_1 < u_4 < u_3$, then the coordinate of the points will change as:

$$
\begin{aligned}
A: \quad x_A &= \frac{a}{2} - \frac{a}{4\pi}\arccos(-\frac{a}{4\pi b}) - b\sin(\arccos(-\frac{a}{4\pi b})) \\
z_A &= \frac{c}{2} - \frac{c}{2}\cos(\frac{1}{2}\arccos(-\frac{a}{4\pi b})) \\
B: \quad x_B &= \frac{a}{4\pi}\arccos(-\frac{a}{4\pi b}) + b\sin(\arccos(-\frac{a}{4\pi b})) \\
z_B &= \frac{c}{2} + \frac{c}{2}\cos(\frac{1}{2}\arccos(-\frac{a}{4\pi b})) \\
C: \quad x_C &= a - \frac{a}{4\pi}\arccos(-\frac{a}{4\pi b}) - b\sin(\arccos(-\frac{a}{4\pi b})) \\
z_C &= \frac{c}{2} + \frac{c}{2}\cos(\frac{1}{2}\arccos(-\frac{a}{4\pi b})) \\
D: \quad x_D &= \frac{a}{2} + \frac{a}{4\pi}\arccos(-\frac{a}{4\pi b}) + b\sin(\arccos(-\frac{a}{4\pi b})) \\
z_D &= \frac{c}{2} - \frac{c}{2}\cos(\frac{1}{2}\arccos(-\frac{a}{4\pi b}))
\end{aligned}
$$

For this situation, we have from the figure:

$$
\begin{cases} u_A < u_B < u_C < u_D \\ z_A = z_D > z_B = z_C \end{cases} \Rightarrow \quad \pi < \arccos(-\frac{a}{4\pi b}) < 2\pi \qquad (4.23)
$$

Also, we have:

$$
x_B < x_A < x_D < x_C \quad \Rightarrow \quad 0 < \frac{a}{4\pi}\arccos(-\frac{a}{4\pi b}) + b\sin(\arccos(-\frac{a}{4\pi b})) < \frac{a}{4} \qquad (4.24)
$$

(4.23) and (4.24) are an other set of constraints for a and b.

In practice, we find that c must be positive, otherwise, the figure will be upside down.

4.2.2 Gaussian curves and tangential functions for smooth overhanging gratings

Gaussian curves as the outlines of the turning points

Substitute the function for overhanging gratings (4.20) into functions for the outlines described by Gaussian curves (4.1) and (4.2), together with the functions for the two turning points, we can get a set of smooth gratings instead of trapezoidal lines to cover the whole domain. It must fulfill all the constraints for the constants for Gaussian curves. To ensure that there will be no intersections, there should be some additional constraints.

Tangential functions as the outlines of the turning points

Similarly, substitute the function for overhanging gratings (4.20) into functions for the outlines described by tangential functions (4.17) and (4.18), together with the function for the two turning points (4.16), we can get the smooth gratings for the domain also. Of course the constraints for the constants for tangential functions must be fulfilled and there should be some additional constraints such that there will be no intersections.

4.3 Transformation of the Helmholtz equation

As shown in Section 3.3, the Helmholtz equation (2.19) will transfer into an eigenvalue system. In this section, we will derive the system for the coordinate transformation we introduced in Section 4.1.

4.3.1 Helmholtz equation for the general coordinate transformation

Here we consider the general coordinate transformation:

$$\begin{cases} u = f(x,z) \\ v = y \\ w = g(x,z) \end{cases} \tag{4.25}$$

As shown in Chapter 3, we only consider the u and w coordinate. Suppose the function under consideration is $\varphi = \varphi(u,w)$. Then the derivatives of φ are

$$\begin{cases} \dfrac{\partial\varphi}{\partial x} = \dfrac{\partial\varphi}{\partial u}\dfrac{\partial u}{\partial x} + \dfrac{\partial\varphi}{\partial w}\dfrac{\partial w}{\partial x} \\ \dfrac{\partial\varphi}{\partial z} = \dfrac{\partial\varphi}{\partial u}\dfrac{\partial u}{\partial z} + \dfrac{\partial\varphi}{\partial w}\dfrac{\partial w}{\partial z} \\ \dfrac{\partial^2\varphi}{\partial x^2} = \dfrac{\partial}{\partial x}\left(\dfrac{\partial\varphi}{\partial u}\dfrac{\partial u}{\partial x} + \dfrac{\partial\varphi}{\partial w}\dfrac{\partial w}{\partial x}\right) = \dfrac{\partial^2\varphi}{\partial u^2}\cdot(\dfrac{\partial f}{\partial x})^2 + \dfrac{\partial^2\varphi}{\partial u\partial w}\cdot\dfrac{\partial g}{\partial x}\cdot\dfrac{\partial f}{\partial x} + \dfrac{\partial\varphi}{\partial u}\cdot\dfrac{\partial^2 f}{\partial x^2} \\ \qquad +\dfrac{\partial^2\varphi}{\partial w^2}\cdot(\dfrac{\partial g}{\partial x})^2 + \dfrac{\partial^2\varphi}{\partial w\partial u}\cdot\dfrac{\partial f}{\partial x}\cdot\dfrac{\partial g}{\partial x} + \dfrac{\partial\varphi}{\partial w}\cdot\dfrac{\partial^2 g}{\partial x^2} \\ \dfrac{\partial^2\varphi}{\partial z^2} = \dfrac{\partial}{\partial z}\left(\dfrac{\partial\varphi}{\partial u}\dfrac{\partial u}{\partial z} + \dfrac{\partial\varphi}{\partial w}\dfrac{\partial w}{\partial z}\right) = \dfrac{\partial^2\varphi}{\partial u^2}\cdot(\dfrac{\partial f}{\partial z})^2 + \dfrac{\partial^2\varphi}{\partial u\partial w}\cdot\dfrac{\partial g}{\partial z}\cdot\dfrac{\partial f}{\partial z} + \dfrac{\partial\varphi}{\partial u}\cdot\dfrac{\partial^2 f}{\partial z^2} \\ \qquad +\dfrac{\partial^2\varphi}{\partial w^2}\cdot(\dfrac{\partial g}{\partial z})^2 + \dfrac{\partial^2\varphi}{\partial w\partial u}\cdot\dfrac{\partial f}{\partial z}\cdot\dfrac{\partial g}{\partial z} + \dfrac{\partial\varphi}{\partial w}\cdot\dfrac{\partial^2 g}{\partial z^2} \end{cases} \tag{4.26}$$

By substitution into the Helmholtz equation (2.19), we get the generalized Helmoltz equation for the new coordinate system (4.25):

$$\begin{aligned} &\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2} + k^2\nu_1^2(x,z)\right)\tilde{A}_n \exp(i\alpha_n u - i\xi w) \\ = \quad & -\alpha_n^2\tilde{A}_n \exp(i\alpha_n u - i\xi w)\cdot(\frac{\partial f}{\partial x})^2 + \alpha_n\xi\tilde{A}_n \exp(i\alpha_n u - i\xi w)\cdot\frac{\partial g}{\partial x}\cdot\frac{\partial f}{\partial x} \\ & +i\alpha_n\tilde{A}_n \exp(i\alpha_n u - i\xi w)\cdot\frac{\partial^2 f}{\partial x^2} - \xi^2\tilde{A}_n \exp(i\alpha_n u - i\xi w)\cdot(\frac{\partial g}{\partial x})^2 \\ & +\alpha_n\xi\tilde{A}_n \exp(i\alpha_n u - i\xi w)\cdot\frac{\partial f}{\partial x}\cdot\frac{\partial g}{\partial x} - i\xi\tilde{A}_n \exp(i\alpha_n u - i\xi w)\cdot\frac{\partial^2 g}{\partial x^2} \\ & -\alpha_n^2\tilde{A}_n \exp(i\alpha_n u - i\xi w)\cdot(\frac{\partial f}{\partial z})^2 + \alpha_n\xi\tilde{A}_n \exp(i\alpha_n u - i\xi w)\cdot\frac{\partial g}{\partial z}\cdot\frac{\partial f}{\partial z} \\ & +i\alpha_n\tilde{A}_n \exp(i\alpha_n u - i\xi w)\cdot\frac{\partial^2 f}{\partial z^2} - \xi^2\tilde{A}_n \exp(i\alpha_n u - i\xi w)\cdot(\frac{\partial g}{\partial z})^2 \\ & +\alpha_n\xi\tilde{A}_n \exp(i\alpha_n u - i\xi w)\cdot\frac{\partial f}{\partial z}\cdot\frac{\partial g}{\partial z} - i\xi\tilde{A}_n \exp(i\alpha_n u - i\xi w)\cdot\frac{\partial^2 g}{\partial z^2} \\ & +k^2\nu_1^2\tilde{A}_n \exp(i\alpha_n u - i\xi w) = 0 \end{aligned} \tag{4.27}$$

Of course the generalized Helmoltz equation (4.27) is a generalization of equation (3.12). Here, we use the coordinate transformation (3.5) to check whether (2.19) becomes (3.12). From (3.5), we have $f(x,z) = x$, $g(x,z) = z - a(x)$, then we can get:

$$\frac{\partial f}{\partial x} = 1,\ \frac{\partial f}{\partial z} = 0,\ \frac{\partial f^2}{\partial x^2} = 0,\ \frac{\partial f^2}{\partial z^2} = 0$$
$$\frac{\partial g}{\partial x} = -\dot{a}(x),\ \frac{\partial g}{\partial z} = 1,\ \frac{\partial g^2}{\partial x^2} = -\ddot{a}(x),\ \frac{\partial g^2}{\partial z^2} = 0$$

Substituting these into (4.27) gives

$$\begin{aligned}
&\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2} + k^2 \nu_1^2(x,z)\right) \sum_{n=-\infty}^{\infty} \tilde{A}_n \exp(i\alpha_n u - i\xi w) \\
= \quad & -\alpha_n^2 \sum_{n=-\infty}^{\infty} \tilde{A}_n \exp(i\alpha_n u - i\xi w) - 2\alpha_n \xi \dot{a} \sum_{n=-\infty}^{\infty} \tilde{A}_n \exp(i\alpha_n u - i\xi w) \\
& -\xi^2 \sum_{n=-\infty}^{\infty} \tilde{A}_n \exp(i\alpha_n u - i\xi w) + i\xi\ddot{a} \sum_{n=-\infty}^{\infty} \tilde{A}_n \exp(i\alpha_n u - i\xi w) \\
& -\xi^2 \dot{a}^2 \sum_{n=-\infty}^{\infty} \tilde{A}_n \exp(i\alpha_n u - i\xi w) + k^2 \nu_1^2 \sum_{n=-\infty}^{\infty} \tilde{A}_n \exp(i\alpha_n u - i\xi w) \\
= \quad & \sum_{n=-\infty}^{\infty} \left(-\alpha_n^2 - 2\dot{a}\xi\alpha_n + \ddot{a}\xi i - \xi^2 - \dot{a}^2\xi^2 + k^2\nu_1^2\right) \tilde{A}_n \exp(i\alpha_n u - i\xi w) = 0
\end{aligned}$$

This is same as (3.12). This gives us confidence that (4.27) can be used as the equation for general coordinate transformation.

4.3.2 Periodicity

As we want to use Fourier expansions, we have to explore which terms are periodic. In equation (4.27), we have eight terms: $\frac{\partial f}{\partial x}$, $\frac{\partial f}{\partial z}$, $\frac{\partial g}{\partial x}$, $\frac{\partial g}{\partial z}$, $\frac{\partial^2 f}{\partial x^2}$, $\frac{\partial f^2}{\partial z^2}$, $\frac{\partial^2 g}{\partial x^2}$, and $\frac{\partial^2 g}{\partial z^2}$. In Appendix A we will show for Gaussian curve as outlines of turning points that all these terms are periodic with respect to the u coordinate, thus Fourier expansions can be used.

4.4 Conclusion and future work

For the generalized coordinate transformation, we also have a scheme for the C method, viz. extension of the C method (see Figure 4.19). From the figure, we can see that this scheme is similar to the scheme for the traditional C method. With the different coordinate transformation, we get a different eigenvalue system. Note that the incident field has been changed for the new coordinate transformation. Thus the boundary conditions also have some changes.

For the future work, we have several things to do:

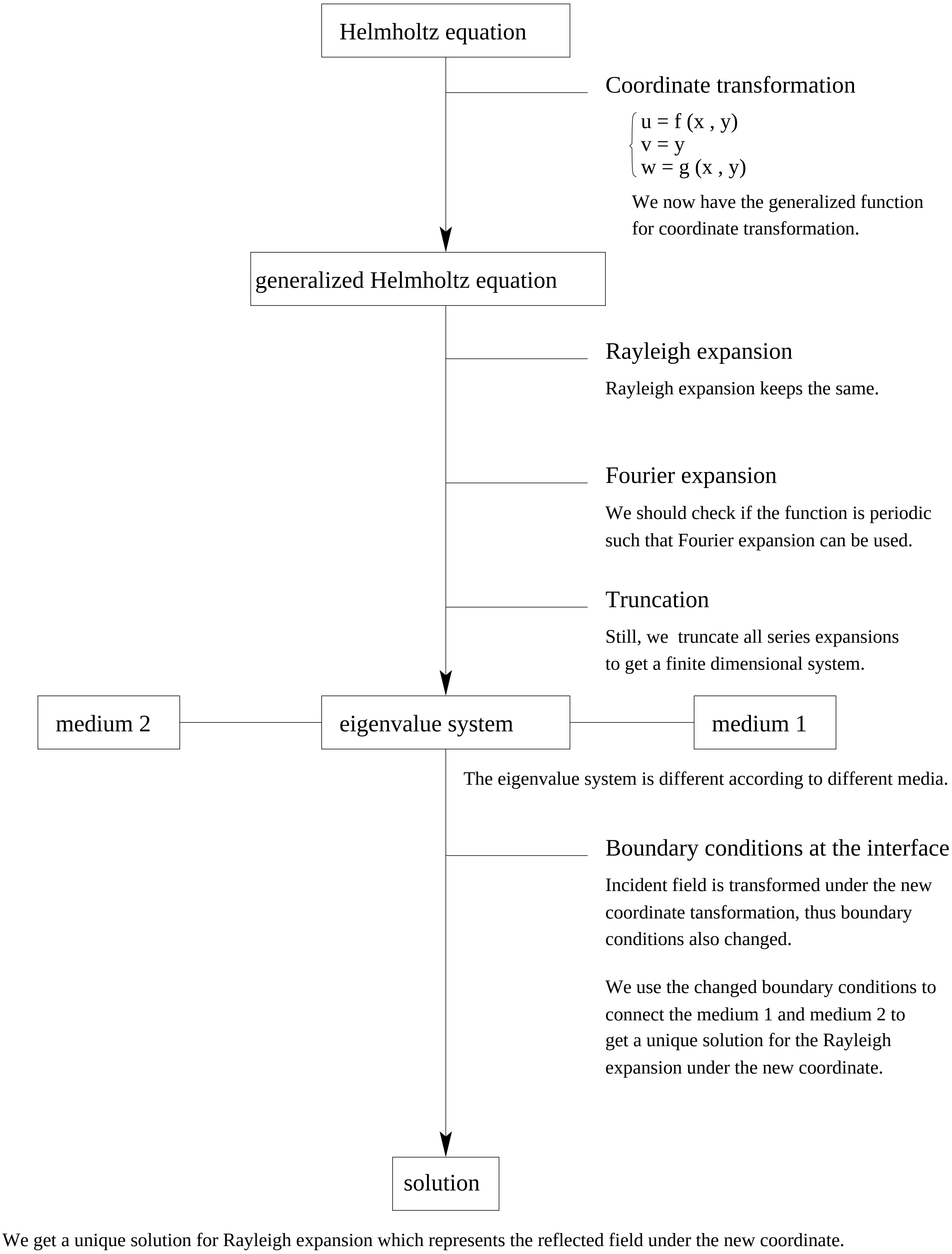

Figure 4.19: Scheme for extension of the C method

1. Additional constraints for the smooth gratings not to intersect should be found.
   As stated in Section 4.2.2, we want the smooth gratings not to intersect, there must be some additional constraints to ensure this both for Gaussian curves and for tangential functions.

2. The incident field should be transformed.
   The incident field must change under the new coordinate transformation. Thus we should find the new form of the incident field to substitute into the generalized Helmholtz equation (4.27). We do this because the incident field plays a role in the boundary conditions.

3. Check for the periodicity for the eight terms for tangential function.
   In Appendix A, we have checked the periodicity for Gaussian curves, thus the terms can be Fourier expanded for this situation. If we want to use the tangential function as outlines of the turning points, we should check the periodicity first. The process is similar as what we did for the Gaussian curve.

4. Solve the new eigenvalue system.
   We will get a new eigenvalue system with new boundary conditions. The process to solve it is similar as stated in Section 3.3.

Appendix A

Proof for the periodicity

A.1 Periodicity proof for Gaussian curve as the outlines of the turning points

For the general coordinate transformation, we have the functions:

$$\begin{cases} u = f(x, z) \\ w = g(x, z) \\ x = F(w, u) \\ z = G(w, u) \end{cases} \tag{A.1}$$

For Gaussian curve shaped turning points, we use functions for the outlines described by Gaussian curves (4.1) and (4.2) for the coordinate transformation (A.1). Note that we have different expressions for x and z when w belongs to different regions, thus we should discuss for w.

Here we expand (4.1) for the whole grating as we set $u \in [0, 2]$, then we have:

$$x(w, u) = F(w, u) = \begin{cases} -\frac{1}{\sqrt{2\pi}\sigma} + \beta + \frac{u}{u_0}(x_2(w) + \frac{1}{\sqrt{2\pi}\sigma} - \beta), & 0 \leqslant u \leqslant u_0 \\ x_2(w) + \frac{u - u_0}{u_1 - u_0}(x_1(w) - x_2(w)), & u_0 < u \leqslant u_1 \\ x_1(w) + \frac{u - u_1}{1 - u_1}(\frac{1}{\sqrt{2\pi}\sigma} - \beta - x_1(w)), & u_1 < u \leqslant u_2 \\ \frac{1}{\sqrt{2\pi}\sigma} - \beta + \frac{u - u_2}{u_3 - u_2}(x_3(w) - \frac{1}{\sqrt{2\pi}\sigma} + \beta), & u_2 < u \leqslant u_3 \\ x_3(w) - \frac{u - u_3}{u_4 - u_3}(x_3(w) - x_4(w)), & u_3 < u \leqslant u_4 \\ x_4(w) + \frac{u - u_4}{2 - u_4}(\frac{3}{\sqrt{2\pi}\sigma} - 3\beta - x_4(w)), & u_4 < u \leqslant 2 \end{cases} \tag{A.2}$$

$$z(w,u) = G(w,u) = \begin{cases} z_2(w), & 0 \leqslant u \leqslant u_0 \\ z_2(w) - \dfrac{u-u_0}{u_1-u_0}(z_2(w)-z_1(w)), & u_0 < u \leqslant u_1 \\ z_1(w), & u_1 < u \leqslant u_2 \\ z_3(w), & u_2 < u \leqslant u_3 \\ z_3(w) + \dfrac{u-u_3}{u_4-u_3}(z_4(w)-z_3(w)), & u_3 < u \leqslant u_4 \\ z_4(w), & u_4 < u \leqslant 2 \end{cases} \tag{A.3}$$

where $x_3(w) = 2(\frac{1}{\sqrt{2\pi}\sigma} - \beta) - x_1(w)$, $x_4(w) = 2(\frac{1}{\sqrt{2\pi}\sigma} - \beta) - x_2(w)$.

- $\dfrac{\partial F}{\partial u} = \dfrac{1}{\frac{\partial f}{\partial x}}$

  $w \in (-\infty, -\sigma - \alpha]$

$$\frac{\partial F}{\partial u} = \begin{cases} \dfrac{3}{\sqrt{2\pi}\sigma}\exp(\dfrac{-(-w+\sigma+\alpha)^2}{2\sigma^2}), & 0 \leqslant u \leqslant u_0 \\ -\sigma\beta + \dfrac{3}{\sqrt{2\pi}\sigma} - \dfrac{3}{\sqrt{2\pi}\sigma}\exp(\dfrac{-(-w+\sigma+\alpha)^2}{2\sigma^2}), & u_0 < u \leqslant u_1 \\ \dfrac{3}{\sqrt{2\pi}\sigma}, & u_1 < u \leqslant u_3 \\ -\sigma\beta + \dfrac{3}{\sqrt{2\pi}\sigma} - \dfrac{3}{\sqrt{2\pi}\sigma}\exp(\dfrac{-(-w+\sigma+\alpha)^2}{2\sigma^2}), & u_3 < u \leqslant u_4 \\ \dfrac{3}{\sqrt{2\pi}\sigma}\exp(\dfrac{-(-w+\sigma+\alpha)^2}{2\sigma^2}), & u_4 < u \leqslant 2 \end{cases} \tag{A.4}$$

$w \in (-\sigma - \alpha, -\alpha]$

$$\frac{\partial F}{\partial u} = \begin{cases} \frac{3}{\sqrt{2\pi}\sigma}\exp(\frac{-(-z_2(w)+\sigma+\alpha)^2}{2\sigma^2}), & 0 \leqslant u \leqslant u_0 \\ -\sigma\beta + \frac{\sigma}{\sqrt{2\pi}\sigma} \\ -\frac{3}{\sqrt{2\pi}\sigma}[\exp(\frac{-(w+\sigma+\alpha)^2}{2\sigma^2}) - \exp(\frac{-(-z_2(w)+\sigma+\alpha)^2}{2\sigma^2})], & u_0 < u \leqslant u_1 \\ \frac{3}{\sqrt{2\pi}\sigma}\exp(\frac{-(w+\sigma+\alpha)^2}{2\sigma^2}), & u_1 < u \leqslant u_3 \\ -\sigma\beta + \frac{\sigma}{\sqrt{2\pi}\sigma} \\ -\frac{3}{\sqrt{2\pi}\sigma}[\exp(\frac{-(w+\sigma+\alpha)^2}{2\sigma^2}) - \exp(\frac{-(-z_2(w)+\sigma+\alpha)^2}{2\sigma^2})], & u_3 < u \leqslant u_4 \\ \frac{3}{\sqrt{2\pi}\sigma}\exp(\frac{-(-z_2(w)+\sigma+\alpha)^2}{2\sigma^2}), & u_4 < u \leqslant 2 \end{cases} \quad \text{(A.5)}$$

where $z_2(w) = \frac{2\alpha+\sigma}{\sigma}(w+\alpha)+\alpha$.

$w \in (-\alpha, \sigma + \alpha]$

$$\frac{\partial F}{\partial u} = \begin{cases} \frac{3}{\sqrt{2\pi}\sigma}\exp(\frac{-(-z_2(w)+\sigma+\alpha)^2}{2\sigma^2}), & 0 \leqslant u \leqslant u_0 \\ -\sigma\beta + \frac{\sigma}{\sqrt{2\pi}\sigma} \\ -\frac{3}{\sqrt{2\pi}\sigma}[\exp(\frac{-(w+\sigma+\alpha)^2}{2\sigma^2}) - \exp(\frac{-(-z_2(w)+\sigma+\alpha)^2}{2\sigma^2})], & u_0 < u \leqslant u_1 \\ \frac{3}{\sqrt{2\pi}\sigma}\exp(\frac{-(w+\sigma+\alpha)^2}{2\sigma^2}), & u_1 < u \leqslant u_3 \\ -\sigma\beta + \frac{\sigma}{\sqrt{2\pi}\sigma} \\ -\frac{3}{\sqrt{2\pi}\sigma}[\exp(\frac{-(w+\sigma+\alpha)^2}{2\sigma^2}) - \exp(\frac{-(-z_2(w)+\sigma+\alpha)^2}{2\sigma^2})], & u_3 < u \leqslant u_4 \\ \frac{3}{\sqrt{2\pi}\sigma}\exp(\frac{-(-z_2(w)+\sigma+\alpha)^2}{2\sigma^2}), & u_4 < u \leqslant 2 \end{cases} \quad \text{(A.6)}$$

where $z_2(w) = \frac{\sigma}{2\alpha+\sigma}(w+\alpha)+\alpha$.

$w \in (\sigma + \alpha, \infty]$

$$\frac{\partial F}{\partial u} = \begin{cases} \frac{3}{\sqrt{2\pi}\sigma}, & 0 \leqslant u \leqslant u_0 \\ -\sigma\beta + \frac{3}{\sqrt{2\pi}\sigma} - \frac{3}{\sqrt{2\pi}\sigma}\exp(\frac{-(w+\sigma+\alpha)^2}{2\sigma^2}), & u_0 < u \leqslant u_1 \\ \frac{3}{\sqrt{2\pi}\sigma}\exp(\frac{-(w+\sigma+\alpha)^2}{2\sigma^2}), & u_1 < u \leqslant u_3 \\ -\sigma\beta + \frac{3}{\sqrt{2\pi}\sigma} - \frac{3}{\sqrt{2\pi}\sigma}\exp(\frac{-(w+\sigma+\alpha)^2}{2\sigma^2}), & u_3 < u \leqslant u_4 \\ \frac{3}{\sqrt{2\pi}\sigma}, & u_4 < u \leqslant 2 \end{cases} \tag{A.7}$$

We can see that for all w, $\frac{\partial F}{\partial u}$ is periodic with respect to u, which means $\frac{\partial f}{\partial x}$ is also periodic with respect to u.

- $\frac{\partial F}{\partial w} = \frac{1}{\frac{\partial g}{\partial x}}$

  $w \in (-\infty, -\sigma - \alpha]$

$$\frac{\partial F}{\partial w} = \begin{cases} \frac{3u}{\sigma^2}(-w+\sigma+\alpha)\frac{1}{\sqrt{2\pi}\sigma}\exp(\frac{-(-w+\sigma+\alpha)^2}{2\sigma^2}), & 0 \leqslant u \leqslant u_0 \\ (2-3u)\frac{1}{\sqrt{2\pi}\sigma^3}(-w+\sigma+\alpha)\exp(\frac{-(-w+\sigma+\alpha)^2}{2\sigma^2}), & u_0 < u \leqslant u_1 \\ 0, & u_1 < u \leqslant u_3 \\ (4-3u)\frac{1}{\sqrt{2\pi}\sigma^3}(-w+\sigma+\alpha)\exp(\frac{-(-w+\sigma+\alpha)^2}{2\sigma^2}), & u_3 < u \leqslant u_4 \\ (3u-6)\frac{1}{\sqrt{2\pi}\sigma^3}(-w+\sigma+\alpha)\exp(\frac{-(-w+\sigma+\alpha)^2}{2\sigma^2}), & u_4 < u \leqslant 2 \end{cases} \tag{A.8}$$

$w \in (-\sigma - \alpha, -\alpha]$

$$\frac{\partial F}{\partial w} = \begin{cases} \frac{3u}{\sqrt{2\pi}\sigma^4}(-z_2(w) + \sigma + \alpha)(2\alpha + \sigma)\exp(\frac{-(-z_2(w) + \sigma + \alpha)^2}{2\sigma^2}), & 0 \leqslant u \leqslant u_0 \\ \frac{1}{\sqrt{2\pi}\sigma^4}(-z_2(w) + \sigma + \alpha)(2\alpha + \sigma)\exp(\frac{-(-z_2(w) + \sigma + \alpha)^2}{2\sigma^2}) \\ +(3u-1)\frac{1}{\sqrt{2\pi}\sigma^4}[\sigma(w + \sigma + \alpha)\exp(\frac{-(w + \sigma + \alpha)^2}{2\sigma^2}) \\ -(-z_2(w) + \sigma + \alpha)(2\alpha + \sigma)\exp(\frac{-(-z_2(w) + \sigma + \alpha)^2}{2\sigma^2})], & u_0 < u \leqslant u_1 \\ (3-3u)\frac{1}{\sqrt{2\pi}\sigma^3}(w + \sigma + \alpha)\exp(\frac{-(w + \sigma + \alpha)^2}{2\sigma^2}), & u_1 < u \leqslant u_3 \\ -\frac{1}{\sqrt{2\pi}\sigma^3}(w + \sigma + \alpha)\exp(\frac{-(w + \sigma + \alpha)^2}{2\sigma^2}) \\ +(3u-4)\frac{1}{\sqrt{2\pi}\sigma^4}[\sigma(w + \sigma + \alpha)\exp(\frac{-(w + \sigma + \alpha)^2}{2\sigma^2}) \\ -(-z_2(w) + \sigma + \alpha)(2\alpha + \sigma)\exp(\frac{-(-z_2(w) + \sigma + \alpha)^2}{2\sigma^2})], & u_3 < u \leqslant u_4 \\ (3u-6)\frac{1}{\sqrt{2\pi}\sigma^4}(-z_2(w) + \sigma + \alpha)(2\alpha + \sigma)\exp(\frac{-(-z_2(w) + \sigma + \alpha)^2}{2\sigma^2}), & u_4 < u \leqslant 2 \end{cases} \quad \text{(A.9)}$$

where $z_2(w) = \frac{2\alpha + \sigma}{\sigma}(w + \alpha) + \alpha$.

$w \in (-\alpha,\ \sigma+\alpha]$

$$\frac{\partial F}{\partial w} = \begin{cases} \frac{3u}{\sqrt{2\pi\sigma^4}}(-z_2(w)+\sigma+\alpha)(2\alpha+\sigma)\exp(\frac{-(-z_2(w)+\sigma+\alpha)^2}{2\sigma^2}), & 0 \leqslant u \leqslant u_0 \\ \frac{1}{\sqrt{2\pi\sigma^4}}(-z_2(w)+\sigma+\alpha)(2\alpha+\sigma)\exp(\frac{-(-z_2(w)+\sigma+\alpha)^2}{2\sigma^2}) \\ +(3u-1)\frac{1}{\sqrt{2\pi\sigma^4}}[\sigma(w+\sigma+\alpha)\exp(\frac{-(w+\sigma+\alpha)^2}{2\sigma^2}) \\ -(-z_2(w)+\sigma+\alpha)(2\alpha+\sigma)\exp(\frac{-(-z_2(w)+\sigma+\alpha)^2}{2\sigma^2})], & u_0 < u \leqslant u_1 \\ (3-3u)\frac{1}{\sqrt{2\pi\sigma^3}}(w+\sigma+\alpha)\exp(\frac{-(w+\sigma+\alpha)^2}{2\sigma^2}), & u_1 < u \leqslant u_3 \\ -\frac{1}{\sqrt{2\pi\sigma^3}}(w+\sigma+\alpha)\exp(\frac{-(w+\sigma+\alpha)^2}{2\sigma^2}) \\ +(3u-4)\frac{1}{\sqrt{2\pi\sigma^4}}[\sigma(w+\sigma+\alpha)\exp(\frac{-(w+\sigma+\alpha)^2}{2\sigma^2}) \\ -(-z_2(w)+\sigma+\alpha)(2\alpha+\sigma)\exp(\frac{-(-z_2(w)+\sigma+\alpha)^2}{2\sigma^2})], & u_3 < u \leqslant u_4 \\ (3u-6)\frac{1}{\sqrt{2\pi\sigma^4}}(-z_2(w)+\sigma+\alpha)(2\alpha+\sigma)\exp(\frac{-(-z_2(w)+\sigma+\alpha)^2}{2\sigma^2}), & u_4 < u \leqslant 2 \end{cases} \tag{A.10}$$

where $z_2(w) = \frac{\sigma}{2\alpha+\sigma}(w+\alpha)+\alpha$.

$w \in (\sigma+\alpha,\ \infty]$

$$\frac{\partial F}{\partial w} = \begin{cases} 0, & 0 \leqslant u \leqslant u_0 \\ (3u-1)\frac{1}{\sqrt{2\pi\sigma^3}}(w+\sigma+\alpha)\exp(\frac{-(w+\sigma+\alpha)^2}{2\sigma^2}), & u_0 < u \leqslant u_1 \\ (3-3u)\frac{1}{\sqrt{2\pi\sigma^3}}(w+\sigma+\alpha)\exp(\frac{-(w+\sigma+\alpha)^2}{2\sigma^2}), & u_1 < u \leqslant u_3 \\ (3u-5)\frac{1}{\sqrt{2\pi\sigma^3}}(w+\sigma+\alpha)\exp(\frac{-(w+\sigma+\alpha)^2}{2\sigma^2}), & u_3 < u \leqslant u_4 \\ 0, & u_4 < u \leqslant 2 \end{cases} \tag{A.11}$$

We can see that for all w, $\frac{\partial F}{\partial w}$ is periodic with respect to u, which means $\frac{\partial g}{\partial x}$ is also periodic with respect to u.

- $\dfrac{\partial G}{\partial u} = \dfrac{1}{\frac{\partial f}{\partial z}}$

  $w \in (-\infty, -\sigma - \alpha]$

$$\frac{\partial G}{\partial u} = 0, \qquad 0 \leqslant u \leqslant 2 \tag{A.12}$$

  $w \in (-\sigma - \alpha, -\alpha]$

$$\frac{\partial G}{\partial u} = \begin{cases} 0, & 0 \leqslant u \leqslant u_0 \\ -\dfrac{3\alpha}{\sigma}(2w + 2\alpha + \sigma), & u_0 < u \leqslant u_1 \\ 0, & u_1 < u \leqslant u_3 \\ \dfrac{3\alpha}{\sigma}(2w + 2\alpha + \sigma), & u_3 < u \leqslant u_4 \\ 0, & u_4 < u \leqslant 2 \end{cases} \tag{A.13}$$

  $w \in (-\alpha, \sigma + \alpha]$

$$\frac{\partial G}{\partial u} = \begin{cases} 0, & 0 \leqslant u \leqslant u_0 \\ -6\alpha\dfrac{\alpha + \sigma - w}{2\alpha + \sigma}, & u_0 < u \leqslant u_1 \\ 0, & u_1 < u \leqslant u_3 \\ 6\alpha\dfrac{\alpha + \sigma - w}{2\alpha + \sigma}, & u_3 < u \leqslant u_4 \\ 0, & u_4 < u \leqslant 2 \end{cases} \tag{A.14}$$

  $w \in (\sigma + \alpha, \infty)$

$$\frac{\partial G}{\partial u} = 0, \qquad 0 \leqslant u \leqslant 2 \tag{A.15}$$

  We can see that for all w, $\dfrac{\partial G}{\partial u}$ is periodic with respect to u, which means $\dfrac{\partial f}{\partial z}$ is also periodic with respect to u.

Similarly, we can prove that $\dfrac{\partial g}{\partial z}$ is periodic with respect to u. Furthermore, we can easily prove that all the second order derivatives are periodic with respect to u by these formulas. Thus all the terms are periodic with respect to u, and we can use Fourier expansions for all of them.

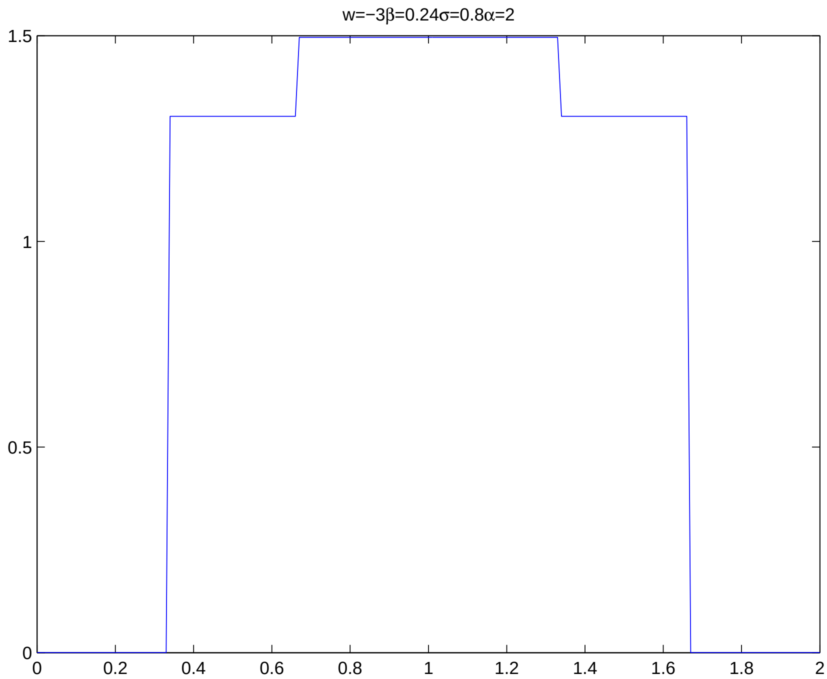

Figure A.1: Relation between $\frac{\partial F}{\partial u}$ and u when $w = -3$

Below we will take a specific set of constants to draw the figures to see the periodicity:

- $\frac{\partial f}{\partial x} = \frac{1}{\frac{\partial F}{\partial u}}$

  $w \in (-\infty, -\sigma - \alpha]$

  Figure A.1 shows the relation between $\frac{\partial F}{\partial u}$ and u when $w = -3$. From the figure, we can see that $\frac{\partial F}{\partial u}$ is periodic with respect to u, which means $\frac{\partial f}{\partial x}$ is periodic with respect to u.

  $w \in (-\sigma - \alpha, -\alpha]$

  Figure A.2 shows that $\frac{\partial f}{\partial x}$ is periodic with respect to u.

  $w \in (-\alpha, \sigma + \alpha]$

  Figure A.3 shows that $\frac{\partial f}{\partial x}$ is periodic with respect to u.

  $w \in (-\sigma - \alpha, \infty]$

  Figure A.4 shows that $\frac{\partial f}{\partial x}$ is periodic with respect to u.

  Thus we get $\frac{\partial f}{\partial x}$ is periodic with respect to u for all w.

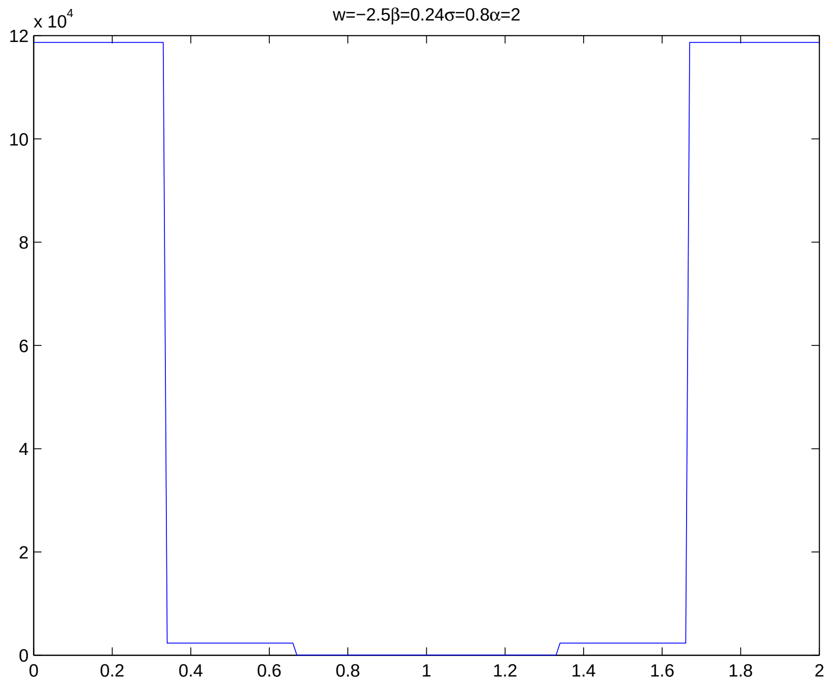

Figure A.2: Relation between $\frac{\partial F}{\partial u}$ and u when $w = -2.5$

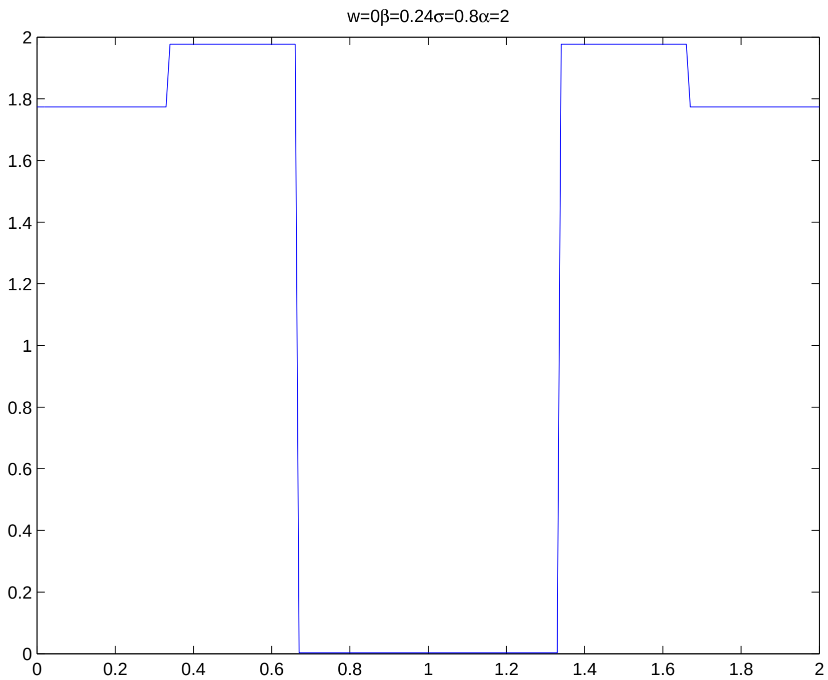

Figure A.3: Relation between $\frac{\partial F}{\partial u}$ and u when $w = 0$

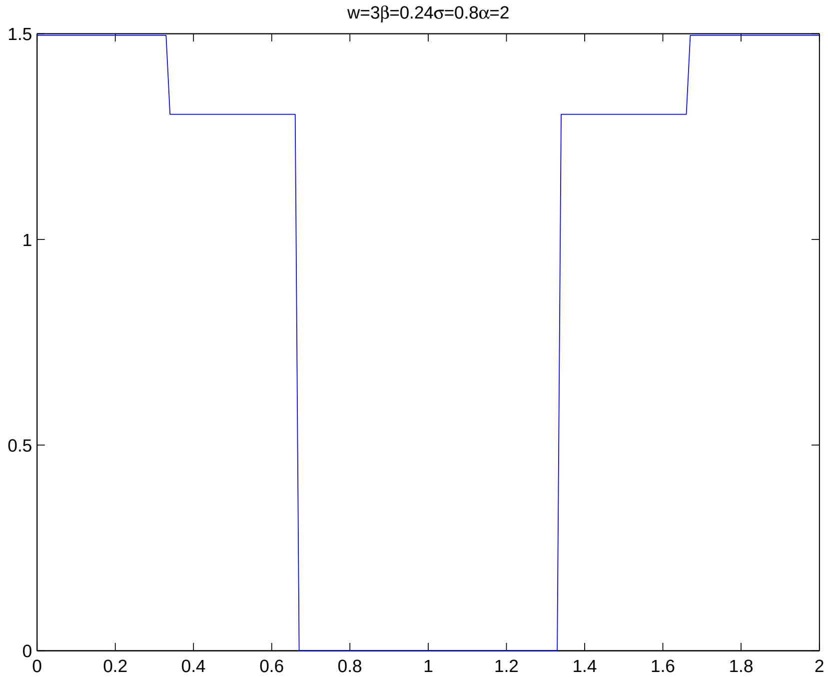

Figure A.4: Relation between $\frac{\partial F}{\partial u}$ and u when $w = 3$

- $\frac{\partial f}{\partial z} = \frac{1}{\frac{\partial G}{\partial u}}$

  $w \in (-\infty, -\sigma - \alpha]$

  $$\frac{\partial G}{\partial u} = 0, \qquad 0 \leq u \leq 2$$

  $\frac{\partial G}{\partial u}$ is periodic with respect to u, which means $\frac{\partial f}{\partial z}$ is periodic with respect to u.

  $w \in (-\sigma - \alpha, -\alpha]$

  Figure A.5 shows that $\frac{\partial f}{\partial z}$ is periodic with respect to u.

  $w \in (-\alpha, \sigma + \alpha]$

  Figure A.6 shows that $\frac{\partial f}{\partial z}$ is periodic with respect to u.

  $w \in (-\sigma - \alpha, \infty]$

  $$\frac{\partial G}{\partial u} = 0, \qquad 0 \leq u \leq 2$$

  $\frac{\partial G}{\partial u}$ is periodic with respect to u, which means $\frac{\partial f}{\partial z}$ is periodic with respect to u.

  Thus we get $\frac{\partial f}{\partial z}$ is periodic with respect to u for all w.

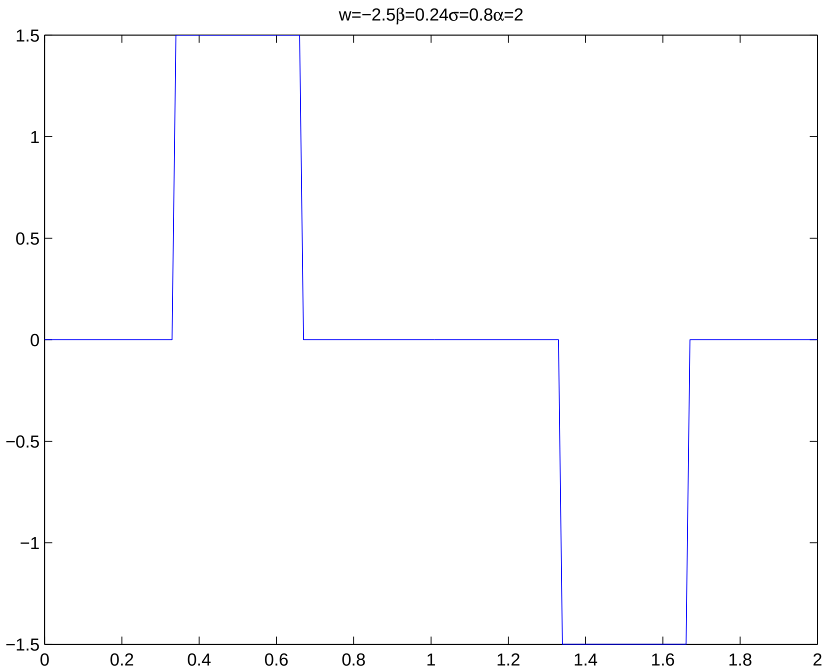

Figure A.5: Relation between $\frac{\partial G}{\partial u}$ and u when $w = -2.5$

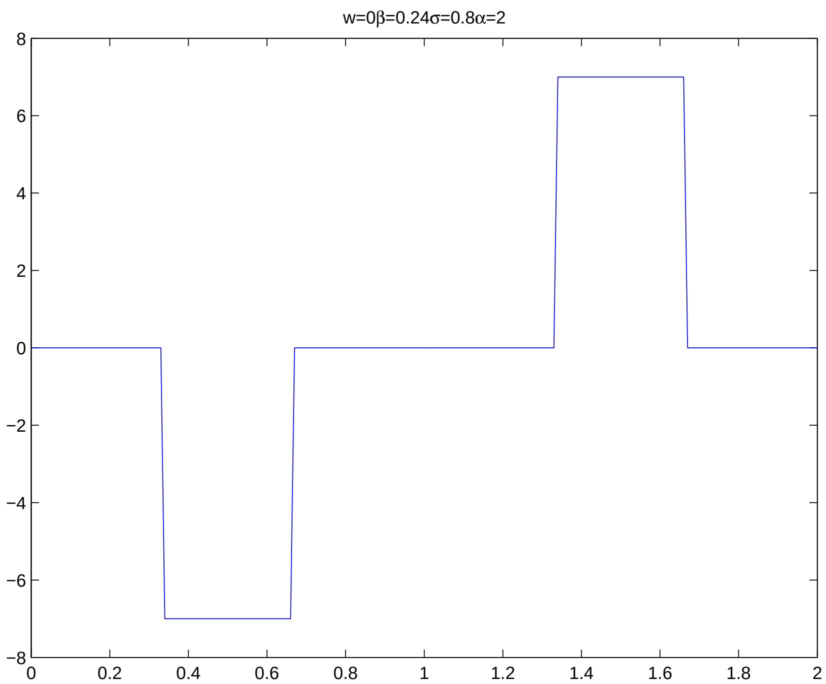

Figure A.6: Relation between $\frac{\partial G}{\partial u}$ and u when $w = 0$

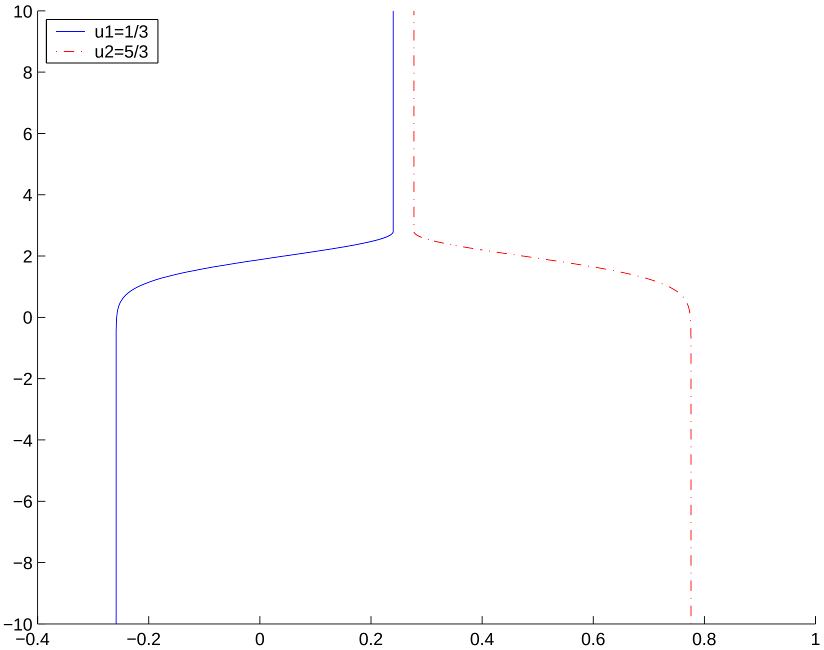

Figure A.7: Different values of u for w

- $\frac{\partial g}{\partial x} = \frac{\partial w}{\partial x}$

  Figure A.7 shows two different lines for different values of u, where $u_1 = \frac{1}{3}$ and $u_2 = \frac{5}{3}$. From Figure A.7, we know that we can get one line for each specific u value. For $u = 0$ and $u = 2$, the vectors for x are different.

$$\begin{cases} x = (-\frac{1}{\sqrt{2\pi\sigma}} + \beta)\begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}, & u = 0 \\ x = (\frac{3}{\sqrt{2\pi\sigma}} - 3\beta)\begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}, & u = 2 \end{cases} \tag{A.16}$$

  But as shown in (A.16), the element for x keeps the same. Thus we have for both $u = 0$ and $u = 2$, $\frac{\partial g}{\partial x} = \frac{\partial w}{\partial x} = \infty$. Thus we get $\frac{\partial g}{\partial x}$ is periodic with respect to u for all w.

- $\frac{\partial g}{\partial z} = \frac{\partial w}{\partial z}$

  For $u = 0$ and $u = 2$, we can easily know that $\frac{\partial w}{\partial z}$ are the same. Thus $\frac{\partial g}{\partial z}$ is periodic with respect to u.

- $\frac{\partial f^2}{\partial x^2}, \frac{\partial f^2}{\partial z^2}, \frac{\partial g^2}{\partial x^2}, \frac{\partial g^2}{\partial z^2}$

For these second order derivatives, we cannot get the figure easily, but from the formulas, we know that they are all periodic with respect to u.

Appendix B

Symbols

The following table lists the used symbols.

Symbol	Meaning
t	Time. Dimension s in S.I. units.
$\mathbf{D}$	Electric flux density. Dimension C/m^2 in S.I. units.
ρ	Charge density. Dimension C/m^3 in S.I. units.
$\mathbf{E}$	Electric field. Dimension V/m in S.I. units.
$\mathbf{B}$	Magnetic flux density. Dimension T in S.I. units.
$\mathbf{H}$	Magnetic field. Dimension A/m in S.I. units.
$\mathbf{J}$	Electric current density. Dimension A/m^2 in S.I. units.
ε	Permittivity. Dimension C/mV in S.I. units.
σ	Electrical conductivity. Dimension A/mV in S.I. units.
μ	Permeability. Dimension mT/A in S.I. units.
ω	Angular frequency. Dimension s^{-1} in S.I. units.
λ	Wave length. Dimension m in S.I. units.
Λ	Grating period. Dimension m in S.I. units.
k	Wave number. Dimension m^{-1} in S.I. units.
ν	Refractive index.
$\mathbf{F}$	Either for **E** or **H**.
$\mathbf{e}_i$	Unit vector for i direction, $i = x,\ y,\ z$.
K	$K = \frac{2\pi}{\Lambda}$.
α_n	$\alpha_n = nK + k\sin\theta$.
β_n^I	$\beta_n^I = \sqrt{k^2\nu_1^2 - \alpha_n^2}$.
A_n	Reflected field coefficients.
B_n	Transmitted field coefficients.
D	Height of the grating. Dimension m in S.I. units.
$a(x)$	The function of the interface.
ξ	$\frac{1}{\xi}$ is the eigenvalue of the system, and $\xi \to \beta_n^I$ in media 1 for propagating orders.
$\dot{a}$	The first derivative of a with respect to u.
$\ddot{a}$	The second derivative of a with respect to u.

Symbol	Meaning
$\tilde{A}_n$	Reflected field coefficients for the new coordinate.
$\tilde{B}_n$	Transmitted field coefficients for the new coordinate.
Q_n	$Q_n = \xi \tilde{A}_n$.
A_n^I	$A_n^I = \tilde{A}_n$.
A_n^{II}	$A_n^{II} = \tilde{B}_n$.
F^{inc}	Incident field.
F^r	Reflected field.
F^I	Field for medium 1.
F^{II}	Field for medium 2.
F^{prop}	Field for propagating orders.
F^{evan}	Field for evanescent orders.

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