Halfspace Matching: a Domain Decomposition Method for Scattering by 2D Open Waveguides

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Abstract

We study a scattering problem for the Helmholtz equation in 2D, which involves non-parallel open waveguides, by means of the halfspace matching method. This method has formerly been applied to periodic media and homogeneous anisotropic media, and we extend it to open waveguides. It allows the reformulation of the Helmholtz equation in an exterior domain to a set of equations for particular traces of the solution, reducing the overall dimension of the problem by 1, making it accessible for numerical discretisation. We show the well-posedness of the halfspace matching method for a model problem in the exterior of a triangular domain, assuming the presence of absorption. Furthermore, we introduce a numerical discretisation which allows the realisation of transparent boundary conditions by a system of coupled integral equations. To illustrate the practicality of this method, we study a number of optimisation examples involving junctions of open waveguides by means of material optimisation.

Acknowledgements

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Last but not least, I have to thank Anne-Sophie Bonnet-ben Dhia, Sonia Fliss, Christoph Hazard and Antoine Tonnoir: this thesis is nothing but a small extension of their works. My short research stay at ENSTA, Paris, in the spring of 2016 provided critical inputs and ideas, and is a main cause why thesis takes the form it has today. I hope my work will do justice to theirs. I am very grateful that Sonia Fliss agreed to be the third examiner of this thesis.

I want to close with a personal thank to all the living mathematicians, as well as the dead. Ever so often when reading up on a new topic, I was filled with awe in view of the ingenuity, thought, and elegance i glimpsed.

Julian Ott
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Contents

1 Introduction

1.1 Introduction

Open waveguides have become a rather ubiquitous element in many technical applications, in particular in the context of telecommunication technology. Formerly being used mostly for long-distance data communication in the form of optical fibres, their use has been extended to smaller scales. In the last few years, optical chip-to-chip interconnects have been demonstrated to work[54], and the field of integrated nanophotonics is steadily growing.

The dissertation on hand is motivated by these developments, but the situation considered is a much simpler, reduced model distantly related to this topic. Why this?

The critical feature of an *open optical waveguide* is the existence of so-called *guided modes*. These are *time-harmonic* solutions to Maxwell's equations with *unboundedly supported* perturbations of the material coefficients (see [70]). The question of interest is the following: what happens if waveguides of different shape and orientation are linked by some structure?

Within the previous sentences, the mathematical modelling has already been determined: one should study *time-harmonic* Maxwell's equation in $\mathbb{R}^3$ with *unboundedly supported* and *non-separable* perturbations of the homogeneous background material. The key problem is the following. Time-harmonic Maxwell equations need to be completed by a *radiation condition* to ensure uniqueness: in the case of an homogeneous free space, the appropriate one is the Silver–Müller radiation condition (see, for example, [62]).

For open waveguides, this radiation condition will fail, that is, it will not ensure existence and uniqueness any more. How to replace it? The answer to this question is not entirely clear. A number of radiation conditions have been proposed, but so far, no complete analytical study is available (compare also Subsection 1.1.2 below).

So we withdraw from Maxwell's equations before even writing them down, and turn our attention to a simpler problem, which retains many of the problematic features of the Maxwell problem, but gives us more tools to treat it in a tractable fashion: we will consider the *time-harmonic* wave equation in $\mathbb{R}^2$ with *unboundedly supported, non-separable* perturbations.

For a given incident field u_{inc}, we want to consider the problem of finding a solution to

$$\begin{cases} \Delta u(x) + p(x)u(x) = 0 & \text{for } x \in \mathbb{R}^2, \\ u - u_{\text{inc}} & \text{fulfils some radiation condition,} \end{cases}$$

where the function p is strictly larger than 0, and takes only 2 values $p_1 > p_0 > 0$, on the domains as sketched in Figure 1.1. Now again arises the question: what is the proper radiation condition?

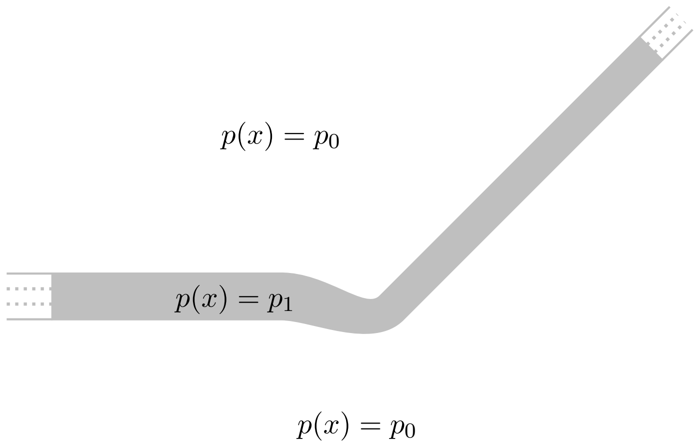

Figure 1.1: Example configuration for the potetial p as considered throughout this thesis.

To avoid creating false hope amongst our readers: we do not give an answer to this question.

We will define a formal radiation condition in Chapter 5, but are far from actually giving a well-posedness result for this problem. It is the problem we wanted to study, but were not able to. However, we will give an overview over results for special cases of this problem in the following section, to convince the reader that it is not as easy at it may seem.

We will instead study a radically simpler problem, namely: find a solution $u \in H^1(\mathbb{R}^2)$ to

$$\Delta u_\epsilon(x) + (p(x) + i\epsilon)u_\epsilon(x) = f(x) \qquad \text{for } x \in \mathbb{R}^2, \tag{1.1.1}$$

where $f \in L^2(\mathbb{R}^2)$ is some given, compactly supported source, and $\epsilon > 0$ is some (small) *absorption parameter*. Note that the radiation condition vanished, since it can be replaced by the condition $u \in H^1(\mathbb{R}^2)$. This problem is radically simpler, since we switched into the resolvent set of $\Delta + p$. It can be seen to be well-posed by different arguments: we will prove the well-posedness in a variational setting with the help of the Lax-Milgram theorem in Section 1.4.

Is this a suitable replacement for the scattering problem? *It is by definition.* Let us elaborate a bit on this point: in many cases (in particular the physical literature), radiation conditions are vaguely introduced by claiming that they "select outgoing waves" or prohibit "sources at infinity". This explanation still sounds very imprecise and vague to the author, and luckily, there are well established alternatives. A way of rigorously justifying radiation conditions is the limit-absorption principle: a solution u to the Helmholtz equation $\Delta u + pu = f$ is *called outgoing*, if the solution u_ϵ of (1.1.1) converges locally to u as $\epsilon \to 0$, $\epsilon > 0$.

The limit-absorption principle is the de-facto standard to justify radiation conditions in a multitude of geometries, since it is applicable in very general settings. For this work, it serves the important task of justifying that we treat the absorptive problem. We will give a short introduction into this principle below in Section 1.3.

For the absorptive problem we will derive an alternative formulation, which admits a numerical implementation. This alternative formulation is called *halfspace matching*, the title of our work. To the authors knowledge, it has been first used by Fliss and Joly in [30] for periodic media, and later by Besse et al [8] for hexagonal media. Later it

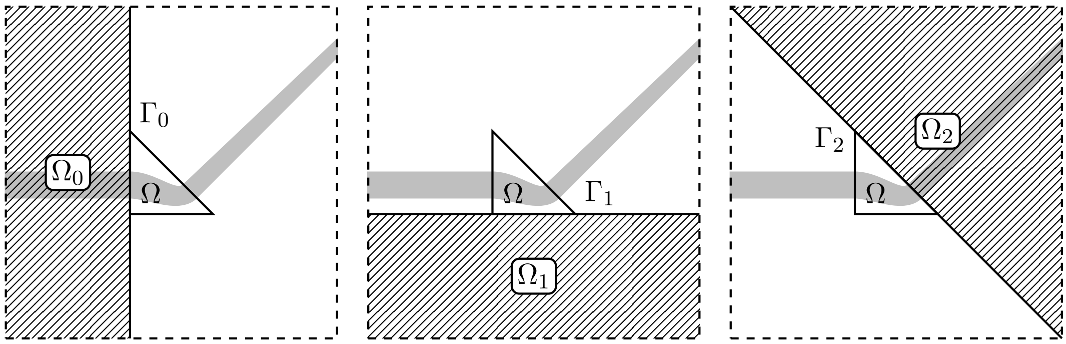

Figure 1.2: The decomposition of the domain $\mathbb{R}^2$ into four, overlapping subdomains: the bounded triangle, and the three (hatched) halfspaces $\Omega_0, \Omega_1,\ \Omega_2$.

has gotten more analytical justification by Tonnoir in [74] (a further publication being prepared [75]). Our main goal is to extend this method to open waveguides. While our study is mostly analytical, we will also show that it works on the numerical side, but only in the form of "experimental numerics".

1.1.1 Overview. Before we outline the remainder of this thesis, let us shortly describe the method of halfspace matching: consider the solution u_ϵ of (1.1.1) for some $\epsilon > 0$. We start by decomposing the full plane into four overlapping sub-domains $\mathbb{R}^2 = \Omega \cup \Omega_0 \cup \Omega_1 \cup \Omega_2$, where Ω is a triangle, and the three domains $\Omega_0, \Omega_1, \Omega_2$ are halfspaces with the boundaries $\Gamma_n = \partial\Omega_n$, $n \in \{0, 1, 2\}$. Figure 1.2 shows how this decomposition of $\mathbb{R}^2$ is done. We gain the following: for halfspaces containing waveguides, there is an explicit solution formula, which maps the Dirichlet trace on the boundary Γ_n to the solution on Ω_n. Accordingly, if this formula is available, one only needs to determine the Dirichlet traces of the three halfspace boundaries $\Gamma_0,\ \Gamma_1$ and Γ_2 and the solution in the triangle Ω. With the help of the solution formula, one also obtains a set of integral equations — called *compatibility equations*— which the traces have to fulfil.

This allows to reduce the problem for the solution on the exterior $\mathbb{R}^2 \setminus \overline{\Omega}$ to a set of integral equations for the traces on the halfspace boundaries, while the problem inside the bounded triangle remains the same. Here, two main questions arise. Firstly: are the resulting compatibility equations well posed? Secondly: can these equations be discretised for a numerical computation of solutions?

The goal of this dissertation is to introduce the method and answer the two questions we just posed. Let us quickly describe how we aim to proceed in this matter.

Chapter 1 Here we will introduce elementary notation and confine the area of topics we expect the reader to be familiar with. Furthermore, a section on the limit-absorption principle is included, were we show that the Sommerfeld radiation condition is insufficient for open waveguides. We will also apply the lemma of Lax–Milgram to show well-posedness for absorptive problems.

Chapter 2 To give the representation formula for a halfspace containing a waveguide, we need a tool of utmost importance for the study of open waveguides: the spectral family associated with the reduced Helmholtz operator. We have decided to include this spectral family together with a complete proof in Chapter 2, since the literature offers a number of representations, which still require some work to obtain the representation as given here. At first reading, most of this chapter can be skipped (in particular the long Section 2.4 containing the proof of the expansion theorem).

Chapter 3 Having the spectral family at hand, it is rather easy to derive the solution formula for a halfspace. To make this discussion rigorous, a careful analysis is required, which is the topic of Chapter 3. Here we will encounter the Dirichlet-to-Dirichlet operators, which will be the operators involved in the compatibility equations, and prove a number of analytical auxiliary theorems.

Chapter 4 At this point, we will finally consider the compatibility equations for the exterior of a triangle. The analytical main result is contained here: the compatibility equations for this case are well-posed in a particular Sobolev space, and consequently, are equivalent to the Helmholtz equation in the exterior of a triangle.

Chapter 5 Here we will describe the numerical discretisation we use, and show a number of convergence examples. Furthermore, we will discuss the non-absorptive case briefly here, and speculate shortly about radiation conditions.

Chapter 6 To give a few colourful pictures, we will give a few ingredients to treat topology/material optimisation problems of waveguide junctions. A few optimisation examples will be shown, and we perform a few design studies.

1.1.2 On scattering in open waveguides. Let us quickly give an overview on works related to scattering in stratified media/open waveguides. In many cases, the two terms are synonymous, since a certain stack of layered media always acts as an open waveguide. Let us start by the monographs of Wilcox [78] and Weder [76], who treat time-dependent scattering in stratified media. The analysis has been refined later on, for example by Debiévre and Pravica [23, 24, 25] and Christiansen [17]. These works already make heavy use of spectral families as the one we introduce in Chapter 2, but deal mostly with time-dependent scattering.

There are a number of works on time-harmonic scattering in the same geometry. There is some study of open waveguides in the Russian literature available (see for example [48, 64] and references therein), which, however, offers no complete analysis of existence and well-posedness.

Rather recently, a few different ansätze have been developed, which allow a proper well-posedness analysis, the first one being contained in works by Xu [79, 80], which has later been extended to 3D geometries [57].

Another strand of work started with the paper by Magnanini and Santosa [58], where they study the Green's function of an open waveguide, which was later refined and turned into a radiation condition for locally perturbed open waveguides by Ciraolo and Magnanini [19, 20], which was extended later on by Ciraolo [18].

Most influential on this dissertation is another group of works: employing the spectral family, Bonnet Ben-Dhia, Hazard and others define a modal radiation condition, which has been employed for defects of open waveguides in 2D [9], as well as for a junction problem of two different parallel waveguides [10]. Similar arguments have also been applied to 3D waveguides by Hazard [40].

We ought to mention the paper by Hanckes and Nédélec [46], where asymptotics of solutions in stratified media are considered.

We close this section by remarking one important point, which complicates this thesis and forces us to consider the absorptive case: none of the well-posedness analysis of the previous references is easily generalisable to *non-parallel* waveguides as shown in Figure 1.1, despite rising interest in this topic.

1.1.3 Numerical methods for open waveguides. To approximate solutions of scattering problems numerically, a common strategy is the following: one truncates the domain and uses some kind of transparent boundary condition to emulate the free space, while the truncated domain is treated, for example, by finite elements. The most commonly used method, also in the context of open waveguides, is the perfectly matched layer (PML), introduced by Berenger [5], which has been later shown by Chew and Weedon [16] to be equivalent to a complex scaling of the exterior solution. For open waveguides, there are some hybrid formulations, which truncate the open waveguide by a PML to obtain a closed waveguide, for which one can then apply mode matching methods (see [35] and references therein).

A newer method are Hardy-space infinite elements (HSIE). Based on the Pole condition [42, 43] by Schmidt, the Hardy space method was already shown to work with closed waveguides [38] and exhibits good convergence for open waveguides [63].

Both PML and HSIE admit much freedom for waveguides in the exterior, and in principle allow the numerical implementation of situations as shown in Figure 1.1.

Also available are boundary integral equation methods in layered media to solve scattering problems, such as the works by Michalski and Zheng [60, 61]. They are, however, restricted to the case of locally perturbed stratified media.

For the readers interested how our method compares to those mentioned, we refer to Subsection 5.4.8 at the end of Chapter 5.

1.2 Notation and a few Basics

We start by listing a number of notations we will frequently use.

Number related notation	
$\mathbb{N}$	The natural numbers
$\mathbb{Z}$	The set of integer numbers
$\mathbb{Z}/m\mathbb{Z}$	The ring of integers modulo m, $m \in \mathbb{N}$
$\mathbb{R}$	The real numbers
$\mathbb{C}$	The complex numbers
$\overline{z}$	The conjugate of a complex number or function $z \in \mathbb{C}$
$\|z\|$	The Euclidean norm of a complex number or vector $z \in \mathbb{C}^d$
$z_1 \cdot z_2$	Dot product $z_1 \cdot z_2 = \sum_{k=1}^{d} z_1 z_2$, for $z_1, z_1 \in C^d$

Topological notation	
$\overline{D}$	Closure of a set (if the topology is clear)
$\mathrm{cl}_{\|\cdot\|_X} D$	Closure of D with respect to the indicated norm
$\cong$	Equivalence of norms

Derivatives	
$\partial_x f$	Derivative of f with respect to x
Δf	Laplacian of f
∇f	Gradient of f
$d\mathcal{F}$	Frechét-derivative of the operator $\mathcal{F}$

1.2.1 Definition. Throughout this thesis, the square root $\sqrt{\cdot}:\mathbb{C}\to\mathbb{C}$ denotes the square root with branch cut along the positive real axis $\{z\in\mathbb{C}:\mathrm{Re}(z)\geq 0,\ \mathrm{Im}(z)=0\}$. For $z=re^{i\theta}$ with $r\geq 0$ and $\theta\in[0,2\pi)$, the square root is given by

$$\sqrt{z}=\sqrt{r}e^{i\theta/2}.$$

$\sqrt{\cdot}$ is holomorphic on $\mathbb{C}\setminus[0,\infty)$, and for $y\geq 0$ the limit coming from the upper halfspace exists and fulfils

$$\lim_{\substack{\epsilon\to 0\\ \epsilon>0}}\sqrt{y+i\epsilon}=\sqrt{y}. \qquad \blacksquare$$

This implies in particular

$$\mathrm{Re}(i\sqrt{\lambda})\leq 0 \text{ for all } \lambda\in\mathbb{C},$$

and $\mathrm{Re}(i\sqrt{\lambda})=0$ if and only if $\lambda\geq 0$.

1.2.2 Derivatives, function spaces. Let us start by introducing the L^2 spaces: if $\Gamma\subset\mathbb{R}^N$ is some (not necessarily smooth) $M\leq N$-dimensional manifold, we denote by

$$L^2(\Gamma):=\{f:\Gamma\to\mathbb{C}:\|f\|_\Gamma<\infty\},$$

the space of (Lebesgue-)measurable functions, whose $L^2(\Gamma)$ scalar product is defined by

$$\langle f,g\rangle_\Gamma=\int_\Gamma f(x)\overline{g}(x)\,\mathrm{d}s(x),$$

with the corresponding norm

$$\|f\|_\Gamma:=\sqrt{\langle f,f\rangle_\Gamma}.$$

Here we denoted by $\mathrm{d}s$ the M-dimensional surface measure of Γ. Occasionally, we will also encounter weighted spaces: let $\mu:\Gamma\to(0,\infty)$ be some weight, then

$$\|f\|^2_{L^2(\Gamma,\mu\mathrm{d}s)}:=\int_\Gamma|f(x)|^2\mu(x)\,\mathrm{d}s(x),$$

and denote by $L^2(\Gamma,\mu\,\mathrm{d}s)=\{f:\Gamma\to\mathbb{C}:\ \|f\|_{L^2(\Gamma,\mu\,\mathrm{d}s)}<\infty\}$ the corresponding L^2 space. In the case that $N=M$ (so that Γ is actually a domain), we denote $\mathrm{d}x=\mathrm{d}s(x)$.

For the remainder of function spaces defined here, we will give the corresponding notations as used in McLean's book [59], if the reader wants to recheck the precise definition and construction. Let $\Omega\subset\mathbb{R}^N$ be some Lipschitz domain. If $f:\Omega\to\mathbb{C}$ is some function, we denote for any multi-index $\alpha\in\mathbb{N}^N$ the derivative with respect to α by

$$\partial^{|\alpha|}_\alpha f(x):=\partial^{\alpha_1}_{x_1}\ldots\partial^{\alpha_N}_{x_N}f(x):=\frac{\partial^{\alpha_1+\ldots+\alpha_N}f}{\partial x_1^{\alpha_1}\ldots\partial x_N^{\alpha_N}}(x).$$

Note that in general, we use the notion of distributional derivatives. Here we denote by $|\alpha|=\alpha_1+\ldots+\alpha_N$ the order of a multi-index. We then denote by

$$C^\infty_0(\Omega)=\{f:\Omega\to\mathbb{C}:\ \mathrm{supp}(f)\subset\Omega,\ \partial^{|\alpha|}_\alpha f \text{ is continuous for all } \alpha\in\mathbb{N}^N\},$$

the space of smooth functions with compact support in Ω, which corresponds to the space $C^\infty_{\mathrm{comp}}(\Omega)$ or $\mathcal{D}(\Omega)$ from [59]. For $s\geq 0$, the Sobolev-spaces $H^s(\Omega)$ and $H^s_0(\Omega)$ are defined as in [59]. For the construction of the norms, we refer to the reference, and note that the canonical norm for $s = n \in \mathbb{N} \cup \{0\}$ for those spaces is given by

$$\|f\|^2_{H^n(\Omega)} = \sum_{\substack{\alpha\in\mathbb{N}^N\\ |\alpha|\leq n}} \|\partial^{|\alpha|}_\alpha f\|^2_\Omega.$$

Since we will work intensively with trace spaces, we point to a certain peculiarity which we will need to deal with: if $I = (a, b) \subset \mathbb{R}$ is some (possibly unbounded) interval, we need to consider the spaces

$$H^{1/2}(I) \text{ and } H^{1/2}_{00}(I),$$

where the latter corresponds to the space $\tilde{H}^{1/2}(I)$ in [59]. The introduction of the space $H^{1/2}_{00}(I)$ is necessary, since functions from the space $H^{1/2}_0(I)$ cannot necessarily be extended by 0 to obtain a function[1] in $H^{1/2}(\mathbb{R})$. For more information on this issue, we refer to Subsection 3.5.11. Finally, if $\Gamma \subset \mathbb{R}^N$ is a $(N-1)$-dimensional, sufficiently smooth sub-manifold of $\mathbb{R}^N$, we denote by

$$H^s(\Gamma)$$

the corresponding Sobolev space on the boundary. Sufficiently smooth means that Γ is at least $C^{k,1}$-smooth, where $0 \leq s \leq k-1$ and $k \in \mathbb{N} \cup \{0\}$.

1.2.3 Trace operators. Let Ω be some (sufficiently smooth) domain and let $u \in H^s(\Omega)$ be some function. If $\Gamma \subset \overline{\Omega}$ is again some M-dimensional, sufficiently smooth sub-manifold, we denote by

$$u|_\Gamma$$

the trace of u on Γ, which is well defined as a function in $H^{s_0}(\Gamma)$, provided that $0 \leq s_0 \leq s - (N-M)/2$ (see for example [59, Chapter 3]).

1.3 The Limit-Absorption Principle

Since the limit-absorption principle is of great importance for the remainder of this thesis, this section gives an introduction on a few examples.

1.3.1 The limit-absorption principle. Consider the example of the Helmholtz equation in free space

$$\Delta u(x) + \kappa_0 u(x) = f(x) \qquad \text{for } x \in \mathbb{R}^N, \tag{1.3.1}$$

where $\kappa_0 > 0$ is a fixed parameter and $f \in C^\infty_0(\mathbb{R}^N)$ is some given source with compact support. How can one assure uniqueness for (1.3.1)? The answer is classically given by the Sommerfeld radiation condition [71], which states the following: if one looks for solutions of (1.3.1), which additionally fulfil the condition

$$\lim_{r\to\infty} r^{\frac{N-1}{2}} \left(\partial_r - i\sqrt{\kappa_0}\right) u(r\hat{x}) = 0 \qquad \text{for all } |\hat{x}| = 1,\ \hat{x} \in \mathbb{R}^N, \tag{1.3.2}$$

one can show that exactly one solution exists.

[1] Note that one has

$$H^{1/2}_0(I) := \mathrm{cl}_{H^{1/2}(I)} C^\infty_0(I) = H^{1/2}(I),$$

see for example [59, Theorem 3.40].

However, as we will see later, the Sommerfeld radiation condition is restricted to the free $\mathbb{R}^N$ with a constant κ_0, so the following question arises: how can one construct the outgoing solution without the radiation condition?

Or more precisely: if the Sommerfeld radiation condition is not "the right one", what does "outgoing" actually mean?

The answer lies in the limit-absorption principle. It exploits the fact that for any $\epsilon \neq 0$ and given $f \in L^2(\mathbb{R}^N)$, the equation

$$\Delta u_\epsilon(x) + (\kappa_0 + i\epsilon)u_\epsilon(x) = f(x) \qquad \text{for } x \in \mathbb{R}^N,$$

possesses a unique solution in $H^2(\mathbb{R}^2)$ (which we will prove in a more general context in Theorem 1.4.3). The unique outgoing solution can now be constructed by taking the limit $\epsilon \to 0$, coming from above, that is for $\epsilon > 0$. This way, one defines the outgoing solution in the sense of the limit-absorption principle by

$$u(x) = \lim_{\substack{\epsilon \to 0 \\ \epsilon > 0}} u_\epsilon(x) \qquad \text{for } x \in \mathbb{R}^N.$$

It turns out that this definition is equivalent to the Sommerfeld radiation condition in the free space. This argument can be generalised for many operators and geometries, and is practically the standard tool to justify radiation conditions.

For the work at hand, it mainly allows us a trick which enables us to simplify the analytical situation significantly: while being interested in the case that $\epsilon = 0$, we choose $\epsilon > 0$ and obtain very easily the existence and uniqueness of solutions.

1.3.2 The failure of the Sommerfeld radiation condition for an open waveguide. It seems appropriate to illustrate that the Sommerfeld radiation condition fails for open waveguides. Let us construct a counter example in a very particular case of the equation

$$\Delta u_\epsilon(x) + (\kappa_0 + i\epsilon - q(x_1))u(x) = f(x) \qquad \text{for } x \in \mathbb{R}^2, \tag{1.3.3}$$

where $\kappa_0 > 0$, and the function q is given by

$$q(x_1) = \begin{cases} -2 & \text{for } |x_1| < \pi/2, \\ 0 & \text{for } |x_1| > \pi/2. \end{cases}$$

We will construct our solution with a separation of variables ansatz: one easily finds that $u(x) = e^{i\sqrt{\kappa_0+1+i\epsilon}\,x_2}\psi(x_1)$ is a solution to the homogeneous version of (1.3.3), where ψ is given by

$$\psi(x_1) = \begin{cases} \cos(x_1) & \text{for } |x_1| < \pi/2, \\ \frac{e^{\pi/2}}{\sqrt{2}} e^{-|x_1|} & \text{for } |x_1| > \pi/2. \end{cases}$$

Let now $\tilde{f} \in C_0^\infty(\mathbb{R})$, and let us consider the source $f(x) = \psi(x_1)\tilde{f}(x_2)$. We try to solve (1.3.3) by the ansatz

$$u_\epsilon(x) = v_\epsilon(x_2)\psi(x_1).$$

Using that

$$(\partial_{x_1}^2 - q(x_1))\psi(x_1) = \psi(x_1) \qquad \text{for } x_1 \in \mathbb{R},$$

we obtain by inserting our ansatz for u_ϵ into (1.3.3) that v_ϵ must fulfil

$$v_\epsilon''(x_2) + (\kappa_0 + 1 + i\epsilon)v(x_2) = \tilde{f}(x_2) \qquad \text{for } x_2 \in \mathbb{R}.$$

This equation can now easily be solved with the Green's function

$$G_\epsilon(x_2, y_2) = \frac{1}{-2i\sqrt{\kappa_0 + 1 + i\epsilon}} e^{i\sqrt{\kappa_0+1+i\epsilon}\,|x_2-y_2|}.$$

At this point, it is important to recall our choice of the square root in 1.2.1. It is chosen so that $\mathrm{Re}(i\sqrt{\kappa_0 + 1 + i\epsilon}) < 0$, which implies that the exponential in the Green's function is decreasing for $|x| \to \infty$ or $|y| \to \infty$, which indicates that we have chosen the correct root of $\kappa_0 + 1 + i\epsilon$.

Note that this choice is not unique for $\epsilon = 0$: in this case, the only two square roots of $\kappa_0 + 1$ are real, and it is left open which root is the correct one, since both corresponding exponentials do not decay.

Let us get back to finding the function v_ϵ. It is given by

$$v_\epsilon(x_2) = \int\limits_{\mathbb{R}} G_\epsilon(x_2, y_2)\tilde{f}(y_2)\mathrm{d}y_2.$$

One now easily verifies that the solution we obtained

$$u_\epsilon(x) = \psi(x_1) \int\limits_{\mathbb{R}} \frac{e^{i\sqrt{\kappa_0+1+i\epsilon}\,|x_2-y_2|}}{-2i\sqrt{\kappa_0 + 1 + i\epsilon}} \tilde{f}(y_2)\,\mathrm{d}y_2$$

is in $H^2(\mathbb{R}^2)$, and fulfils (1.3.3), so we have found the solution in the case with absorption $\epsilon > 0$.

Let us now establish the outgoing solution in the sense of the limit-absorption principle: since $\tilde{f}$ is compactly supported by assumption, we can simply take the limit by the dominated convergence theorem in

$$\begin{aligned} u_0(x) = \lim_{\substack{\epsilon\to 0\\ \epsilon>0}} u_\epsilon(x) &= \psi(x_1) \int\limits_{\mathbb{R}} \lim_{\substack{\epsilon\to 0\\ \epsilon>0}} \left(\frac{e^{i\sqrt{\kappa_0+1+i\epsilon}\,|x_2-y_2|}}{-2i\sqrt{\kappa_0 + 1 + i\epsilon}} \tilde{f}(y_2) \right) \mathrm{d}y_2 \\ &= \psi(x_1) \int\limits_{\mathbb{R}} \frac{e^{i\sqrt{\kappa_0+1}\,|x_2-y_2|}}{-2i\sqrt{\kappa_0 + 1}} \tilde{f}(y_2)\,\mathrm{d}y_2. \end{aligned}$$

Note that this procedure uniquely determines which square root we have to take for $\sqrt{\kappa_0 + 1}$: it must be the positive square root, since it is the limit of $\sqrt{\kappa_0 + 1 + i\epsilon}$ as $\epsilon \to 0$, $\epsilon > 0$.

We now show that it does not fulfil the Sommerfeld radiation condition: consider the limit $x = (0, x_2)$ as $x_2 \to +\infty$. For x_2 sufficiently large the interval $(-\infty, x_2)$ contains the whole support of $\tilde{f}$, and we have that

$$\begin{aligned} u_0(x) = \psi(0) &\int\limits_{\mathrm{supp}(\tilde{f})} \frac{e^{i\sqrt{\kappa_0+1}\,(x_2-y_2)}}{-2i\sqrt{\kappa_0 + 1}} \tilde{f}(y_2)\,\mathrm{d}y_2 \\ &= e^{i\sqrt{\kappa_0+1}\,x_2} \int\limits_{\mathrm{supp}(\tilde{f})} \frac{e^{-i\sqrt{\kappa_0+1}\,y_2}}{-2i\sqrt{\kappa_0 + 1}} \tilde{f}(y_2)\,\mathrm{d}y_2 \\ &= Ce^{i\sqrt{\kappa_0+1}\,x_2}. \end{aligned}$$

where we used that $x_2 > y_2$ for any $y_2 \in \operatorname{supp}(\tilde{f})$. Let us now check whether or not the Sommerfeld radiation condition (1.3.2) applies. Note that for $x = (x_1, 0)$ the coefficient in the Helmholtz equation (1.3.3) is given by $\kappa_0 + 2$; accordingly, it seems reasonable to choose $\kappa_0 + 2$ or κ_0 instead of κ_0 in the Sommerfeld radiation condition. However, none of the two choices yields the correct result, since we have that

$$\begin{aligned} &|x_2|^{1/2} \left(\partial_{x_2} u_0(0, x_2) - i\sqrt{\kappa_0 + 2}\, u_0(x_2)\right) \\ &\qquad = |x_2|^{1/2} \left(i\sqrt{\kappa_0 + 1} - i\sqrt{\kappa_0 + 2}\right) C e^{i\sqrt{\kappa_0+1}\, x_2}, \end{aligned}$$

which clearly does not converge to 0, even if we replace $\sqrt{\kappa_0 + 2}$ by $\sqrt{\kappa_0}$.

1.3.3 The limit-absorption principle for open waveguides. Let us review quickly a few works, were the limit-absorption principle has been shown to hold for open waveguides. Weder's monograph [76] deals with this issue for stratified media. Similarly, a paper by Boutet de Monvel-Berthier and Dragos [11] deals with this topic. Rather recently, Kirsch and Lechleiter have shown that the limiting absorption principle holds for stratified periodic open waveguides [51].

Let us remark again that all those works are restricted to local perturbations of stratified layers, and do not admit non-parallel waveguides or junctions of differently shaped waveguides.

Correspondingly, there is no result available which can be applied to the situation we are interested in (as in the Situation of Figure 1.1). Later on, in the part concerning numerical examples, we will assume it to hold nonetheless to have a somewhat formal justification for our method.

1.4 Well-Posedness for Absorptive Media

1.4.1 The problem of interest. Let $\Omega \subset \mathbb{R}^N$ be a (possibly unbounded) Lipschitz domain and $q \in L^\infty(\Omega)$ be real-valued. Furthermore, let

$$\kappa \in \mathbb{C} \setminus \mathbb{R}$$

be some arbitrary, non-real complex number.

For given $g \in H^{1/2}(\partial\Omega)$ and $f \in L^2(\Omega)$ we consider the problem of finding a solution $u \in H^1(\Omega)$ of

$$\begin{cases} \Delta u(x) + (\kappa - q(x))u(x) = f(x) & \text{for } x \in \Omega, \\ u(x) = g(x) & \text{for } x \in \partial\Omega. \end{cases} \tag{1.4.1}$$

This problem has to be understood in the variational sense, that is, we say that u fulfils

$$\Delta u(x) + (\kappa - q(x))u(x) = f(x) \qquad \text{for } x \in \Omega,$$

if for any $\psi \in H_0^1(\Omega)$ we have

$$\int_\Omega \nabla u(x) \cdot \nabla \overline{\psi}(x) - (\kappa - q(x))u(x)\overline{\psi}(x)\, \mathrm{d}x = -\int_\Omega f(x)\overline{\psi}(x)\, \mathrm{d}x. \tag{1.4.2}$$

The equality $u(x) = g(x)$ for $x \in \partial\Omega$ has to be understood in the sense of trace operators. The proof of the well-posedness relies on the Lax–Milgram theorem, which reads as follows.

1.4.2 Theorem. Let $b : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$ be a sesquilinear form, that is, linear in the first argument and conjugate linear in the second. Let b be bounded, that is, there exist a constant $c_1 > 0$ such that

$$|b(u, w)| \leq c_1 \|u\|_{\mathcal{H}} \|v\|_{\mathcal{H}} \qquad \text{for all } u, v \in \mathcal{H},$$

and let b be coercive, i.e. there exists $c_2 > 0$ such that

$$\operatorname{Re} b(u, u) \geq c_2 \|u\|^2_{\mathcal{H}} \qquad \text{for all } u \in \mathcal{H}.$$

Then for any conjugate linear, continuous functional $F : \mathcal{H} \to \mathbb{C}$, there exists exactly one solution of

$$b(u, \psi) = F(\psi) \qquad \text{for all } \psi \in \mathcal{H}. \qquad \blacksquare$$

Proof. See [59]. $\blacksquare$

1.4.3 Theorem. Under the assumption of Subsection 1.4.1, there exists exactly one solution $u \in H^1(\Omega)$ of (1.4.1), and the solution operator

$$\mathcal{S} : L^2(\Omega) \times H^{1/2}(\partial\Omega) \to H^1(\Omega), \qquad (f, g) \mapsto u,$$

is continuous. $\blacksquare$

Proof. We start by assuming that $\operatorname{Im}(\kappa) < 0$, since the case $\operatorname{Im}(\kappa) > 0$ can be dealt with analogously. Let us first study a sesquilinear form related to the weak formulation of (1.4.1). Denote $p := -\|q\|_{L^\infty(\Omega)}$. We easily obtain that $\arg(q(x) - \kappa) \leq \arg(p - \kappa) \in [0, \pi)$. In particular, it follows that $\alpha := \arg(p - \kappa)$ cannot be equal to π, since $\operatorname{Im}(\kappa) < 0$. This now implies by elementary calculation that

$$\operatorname{Re}\left(e^{-i\alpha/2}(q(x) - \kappa)\right) \geq \sin(\alpha/2)|\operatorname{Im}(\kappa)| \qquad \text{for all } x \in \mathbb{R}, \tag{1.4.3}$$

(note that $\arg\left(e^{-i\alpha/2}(q(x) - \kappa)\right) < \alpha/2$), as well as

$$\operatorname{Re}\left(e^{-i\alpha/2}\right) \geq \sin(\alpha/2). \tag{1.4.4}$$

We now define the sesquilinear form $b : H^1_0(\Omega) \times H^1_0(\Omega) \to \mathbb{C}$ by

$$b(v, w) := e^{-i\alpha/2} \int_\Omega \nabla v \cdot \nabla \overline{w} + (q - \kappa) u \overline{w} \, \mathrm{d}x.$$

We claim that b is bounded and coercive: by Hölder's and the Cauchy–Schwarz inequality we have

$$|b(v, w)| \leq \max\{1, \|\kappa + q\|_{L^\infty(\Omega)}\} \|v\|_{H^1(\Omega)} \|w\|_{H^1(\Omega)}.$$

Furthermore, to see that b is coercive, consider that for $v \in H^1_0(\Omega)$ we have

$$\begin{aligned}
\operatorname{Re}(b(v, v)) &= \int_\Omega \operatorname{Re}\left(e^{-i\alpha/2}|\nabla v|^2\right) + \operatorname{Re}\left(e^{-i\alpha/2}(q(x) - \kappa)|v|^2\right) \mathrm{d}x \\
&\geq \sin\left(\frac{\alpha}{2}\right) \int_\Omega |\nabla v|^2 \, \mathrm{d}x + \sin\left(\frac{\alpha}{2}\right) |\operatorname{Im}(\kappa)| \int_\Omega |v|^2 \, \mathrm{d}x \\
&\geq \sin\left(\frac{\alpha}{2}\right) \min(|\operatorname{Im}(\kappa)|, 1) \|v\|^2_{H^1(\Omega)},
\end{aligned}$$

where we exploited (1.4.3) and (1.4.4).

Let us now consider the problem (1.4.1). We first show uniqueness: let $u \in H^1(\Omega)$ be a solution to (1.4.1) with homogeneous data, that is $g = 0,\ f = 0$. From $g = 0$ we deduce that $u \in H_0^1(\Omega)$, and if we multiply the variational form (1.4.2) by $e^{-\alpha/2}$, we obtain that

$$b(u, \psi) = 0 \qquad \text{for all } \psi \in H_0^1(\Omega).$$

Since b is bounded and coercive, this implies by the Lax-Milgram Lemma that $u = 0$.

Let us now show existence. Fix $g \in H^{1/2}(\partial\Omega)$ and $f \in L^2(\Omega)$. Let $w \in H^1(\Omega)$ be an extension of g, that is, some arbitrary function $w \in H^1(\Omega)$ such that $w|_{\partial\Omega} = g$. We now define the conjugate linear functional $F : H_0^1(\Omega) \to \mathbb{C}$ by

$$F(\psi) = -e^{-i\alpha/2} \int\limits_{\Omega} \nabla w \cdot \nabla\overline{\psi} + (q - \kappa) w\overline{\psi} + f\overline{\psi}\, \mathrm{d}x$$

Again by the Lax–Milgram Lemma, we have exactly one solution $v \in H_0^1(\Omega)$ of

$$b(v, \psi) = F(\psi) \qquad \text{for all } \psi \in H_0^1(\Omega).$$

It is now easy to show that $u := v + w \in H^1(\Omega)$ is a variational solution of (1.4.1). To see the continuity of $\mathcal{S}$, we note that by the Cauchy–Schwarz inequality we have

$$\begin{aligned}
\|u\|_{H^1(\Omega)}^2 &\leq \frac{1}{c_2} |\mathrm{Re}\, b(u, u)| \\
&\leq \frac{1}{c_2} |F(u)| \\
&\leq \frac{1}{c_2} (\|w\|_{H^1(\Omega)} + \|f\|_{L^2(\Omega)}) \|u\|_{H^1(\Omega)} \\
&\leq \frac{1}{c_2} (\tilde{C}\|g\|_{H^{1/2}(\partial\Omega)} + \|f\|_{L^2(\Omega)}) \|u\|_{H^1(\Omega)},
\end{aligned}$$

where we used that there exists a constant $\tilde{C}$ independent of f such that $\|w\|_{H^1(\Omega)} \leq \tilde{C}\|g\|_{H^{1/2}(\partial\Omega)}$, see [59, Theorem 3.37]. ■

2 The Expansion Theorem

2.1 Introduction and References

2.1.1 Introduction. This chapter deals with a technical, albeit essential tool for this thesis: the spectral family of a certain perturbation of the Laplacian.

Spectral families are an important instrument in the study of many differential equations. From the most prominent example one derives a second nomenclature: spectral families are sometimes called *generalised Fourier transforms*. From this wording we derive our notation: we denote by $\mathcal{F}_A$ the transform which diagonalises the self-adjoint operator A.

This diagonalisation of A — specified below — will allow us to give explicit solution formulae in later chapters. Contained in this solution formulae will be the guided modes, which therefore occur naturally as part of the solution. Note that we already stumbled upon those modes in the introductory Section 1.3.

The outline of this chapter is as follows: after a very brief reminder on the *spectral theorem*, we will define the operator A and give its spectral family in Section 2.2, where the main result, Theorem 2.2.12, will be given. The statement of the result will take some room, since a number of definitions and notations have to be clarified first. In particular, certain *generalised eigenfunctions* have to be defined and analysed. We will illustrate our main theorem by deriving the conventional 1D Fourier transform from it.

Afterwards, we will consider the so-called Pekeris profile in Section 2.3. For this case we will give explicit formulae for the generalised eigenfunctions and show how to determine the ordinary eigenfunctions, which will be heavily employed in the remainder of the thesis, in particular in the numerical examples.

The last Section 2.4 will be devoted to the proof of Theorem 2.2.12. Since we have chosen a rather elementary proof, this will take some pages: much of it will consist of technical lemmata, which can be skipped at first reading. We refer to the remarks at the beginning of Section 2.4.

2.1.2 References and historical remarks. The representation of the spectral family with the help of generalised eigenfunctions has received vast amounts of attention due to its outstanding importance for the field of mathematical physics. It is an underlying, basic notion in classical quantum mechanics, and of critical importance for many different partial differential equations.

Particularly well studied is the theory of Sturm–Liouville problems. It is concerned with differential operators on sub-intervals of $\mathbb{R}$ and has received much attention during the last century, with one of the first important works being Weyl's paper [77]. Those eigenfunction expansions have been further developed and studied for example by Titchmarch [73] and Kodaira [52]. Also worth mentioning is the book of Coddington [22] as a standard reference on this type of expansion.

A critical point of interest is the choice of the generalised eigenfunctions: a second order ordinary differential equation of the form

$$u''(x) + q(x)u(x) = 0 \qquad \text{for } x \in \mathbb{R}$$

always has two linearly independent solutions, which serve as a kind of basis functions in the associated spectral family. Depending on the choice of these eigenfunctions, the obtained formulae can be rather complicated involving (matrix–valued) weights, which leads to the question: how can one choose suitable solutions to obtain simple expansions?

The answer turns out to lie in scattering theory: if we choose the two solutions as scattered waves corresponding to particular incident fields, the weights involved in the spectral family become very simple. This definition of the generalised eigenfunctions is well known, in particular for (in some sense compact) perturbations of the Laplacian on $\mathbb{R}^n$: the first work in this direction probably coming from Ikebe [45], which was refined later on, where we note in particular the paper by Agmon [1].

The differential operator considered in this chapter has been thoroughly studied in the context of layered media scattering. In fact, a much more general version is commonly considered there. We will restrict ourselves to mention only a few works, which served as a basis for this chapter. We have to start with Wilcox' monograph [78], from where our representation can be deduced, his generalised eigenfunctions being similarly defined as in our case. Secondly, we want to mention the paper by Magnanini and Santosa [58], where the classical Titchmarch theory of eigenfunction expansions has been applied under the additional assumption that the potential q is axially symmetric. Their work uses a more classical choice of generalised eigenfunctions (as for example in [73, 22]), which gives a more complicated representation involving weights.

2.2 The Operator A and Spectral Family $\mathcal{F}_A$

We will start by recalling the spectral theorem.

2.2.1 Theorem. Let H be a Hilbert space, and let $A : H \supset D(A) \to H$ be a self-adjoint operator. Then there exists a measure space $(\Lambda, \mathrm{d}\mu)$, an unitary operator $\mathcal{F}_A : H \to L^2(\Lambda, \mathrm{d}\mu)$ and a real valued function $\hat{\lambda} : \Lambda \to \mathbb{R}$ such that

$$Au = \mathcal{F}_A^{-1}(\hat{\lambda}\mathcal{F}_A u), \qquad \text{for all } u \in D(A),$$

where $\hat{\lambda}\mathcal{F}_A u$ denotes the (point-wise) product of the two functions $\hat{\lambda},\ \mathcal{F}_A u : \Lambda \to \mathbb{C}$, that is $(\hat{\lambda}\mathcal{F}_A u)(m) = \hat{\lambda}(m)\mathcal{F}_A u(m)$ for all $m \in \Lambda$. Furthermore, it holds that

$$u \in D(A) \text{ if and only if } \hat{\lambda}\mathcal{F}_A u \in L^2(\Lambda, \mathrm{d}\mu). \qquad \blacksquare$$

In this form, Theorem 2.2.12 can be found in [67, Chapter VIII.3]. The goal of this chapter is to give and prove an explicit representation of the *generalised Fourier transform* for a particular operator A. Let us define this operator.

2.2.2 Definition and Assumption. Let $A : L^2(\mathbb{R}) \supset H^2(\mathbb{R}) \to L^2(\mathbb{R})$ be defined for $f \in C_0^\infty(\mathbb{R})$ by

$$Af(x) := -\Delta f(x) + q(x)f(x) \qquad \text{for } x \in \mathbb{R},$$

with the function $q : \mathbb{R} \to \mathbb{R}$ given by

$$q(x) = \begin{cases} q_- & \text{if } x < a, \\ q_0(x) & \text{if } a < x < b, \\ q_+ & \text{if } b < x, \end{cases}$$

where $a, b \in \mathbb{R}$, $a < b$, $q_0 : (a, b) \to \mathbb{R}$ is an $L^\infty(a, b)$ function and $q_-, q_+ \in \mathbb{R}$ are constants. We also define $q_m := \operatorname{essinf}(q_0)$ and assume $q_m \le q_- \le q_+$. ■

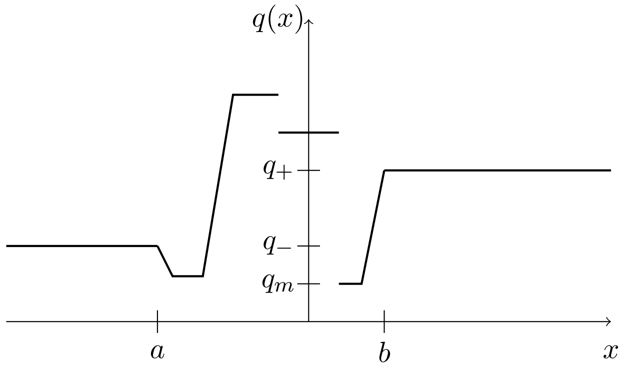

Figure 2.1: Example profile for q.

Note that the assumption $q_- \le q_+$ can actually be dropped: by mirroring the x-coordinate, q_- and q_+ can be exchanged. We make it nonetheless to simplify a few notations later on. Let us quickly state the spectral properties of A, and let us recall that the spectrum of A is defined by

$$\sigma(A) = \mathbb{C} \setminus \{\lambda \in \mathbb{C} : \text{The operator } \lambda I - A \text{ is boundedly invertible}\}.$$

The point spectrum is defined by

$$\sigma_p(A) := \{\lambda \in \mathbb{C} : \text{There exists } u \in H^2(\mathbb{R}) \text{ such that } Au = \lambda u\},$$

while the continuous spectrum is given by

$$\begin{aligned}\sigma_c(A) := \{\lambda \in \mathbb{C} : (\lambda I - A) : H^2(\mathbb{R}) \to L^2(\mathbb{R}) \text{ is not surjective,} \\ \text{but } \mathcal{R}(\lambda I - A) \text{ is dense in } L^2(\mathbb{R})\}.\end{aligned}$$

The residual spectrum will be empty for our case, so we have no need to define it. Also note that we are dealing with unbounded self-adjoint operators here.

2.2.3 Theorem. A is self-adjoint. We have $\sigma(A) = \sigma_p(A) \cup \sigma_c(A)$, where

(a) The point spectrum is finite (and possibly empty) $\sigma_p(A) = \{\lambda_1, \ldots, \lambda_N\} \subset (q_m, q_-)$, where $N \in \mathbb{N} \cup \{0\}$. For any $\lambda_n \in \sigma_p(A)$, the corresponding eigenspace has dimension one.

(b) $\sigma_c(A) = [q_-, +\infty)$. ■

Proof. The self-adjointness follows by the Rellich–Kato theorem [68, Theorem X.12] since $-\Delta : L^2(\mathbb{R}) \supset H^2(\mathbb{R}) \to L^2(\mathbb{R})$ is selfadjoint and since the operator $B : L^2(\mathbb{R}) \to L^2(\mathbb{R}),\ u \mapsto qu$, is bounded in $L^2(\mathbb{R})$ (B is $-\Delta$-bounded with relative bound 0). (a) can be found in Lemma 2.4.4, while (b) is given by Lemma 2.4.6 below. ■

We continue by defining the measure space $(\Lambda, \mathrm{d}\mu)$ from Theorem 2.2.1 for our operator A. For this, we will need the notion of a disjoint union of sets.

2.2.4 Definition. Let $A_1, \ldots, A_n$ be arbitrary sets. Then the *disjoint union* of $A_1, \ldots, A_n$ is defined by

$$A_1 \dot\cup \ldots \dot\cup A_n := \{(k, x) : k \in \{1, \ldots, n\},\ x \in A_k\}.$$ ■

Let us quickly illustrate this notion for readers not familiar with it. For example, the disjoint union $(0,\infty) \dot\cup (0,\infty)$ can be considered as a two–fold copy of $(0,\infty)$: if we take some $m \in (0,\infty) \dot\cup (0,\infty)$, then it can be considered as a positive number, coming either from the first copy of $(0,\infty)$, i.e. $m = (1, x)$, or the second, that is $m = (2, x)$, where $x \in (0,\infty)$. To give a bit more illustration, consider some function $f \in (L^2(0,\infty))^2 \cong L^2(0,\infty) \times L^2(0,\infty)$. It can be considered as a vector valued function $f : (0,\infty) \to \mathbb{C}^2$ by denoting $f(x) = (f_1(x), f_2(x))^\top$. However, it can also be canonically identified with a function $\hat{f} : (0,\infty) \dot\cup (0,\infty) \to \mathbb{C}$. If $(k, x) \in (0,\infty) \dot\cup (0,\infty)$ is some element of the disjoint union (that is, $k \in \{1, 2\},\ x \in (0,\infty)$), we can set $\hat{f}(k, x) := f_k(x)$, to obtain a canonical identification between vector valued functions on $(0,\infty)$ and scalar valued functions on $(0,\infty) \dot\cup (0,\infty)$.

Similarly, one can consider $f \in L^2(A_1) \times \ldots \times L^2(A_n)$ as a scalar valued function on the disjoint union: if $f = (f_k)_{k=1}^n$, where $f_k \in L^2(A_k)$, then we define $\hat{f} : A_1 \dot\cup \ldots \dot\cup A_n \to \mathbb{C}$ by $\hat{f}(k, x) := f_k(x)$, where our notation stems from.

2.2.5 Definition. We define

$$\Lambda := \sigma_p(A) \dot\cup (q_+, \infty) \dot\cup (q_-, \infty).$$

For a function $f : \Lambda \to \mathbb{C}$ defined on Λ, we denote by $f^p : \sigma_p(A) \to \mathbb{C}$ the part defined on $\sigma_p(A) \subset \Lambda$, by $f^+ : (q_+, \infty) \to \mathbb{C}$ the part defined on $(q_+, \infty) \subset \Lambda$ and by $f^- : (q_-, \infty)$ the part defined on $(q_-, \infty) \subset \Lambda$. For abbreviation we write $f = (f^p, f^+, f^-)$. Furthermore, we define the measure $\mathrm{d}\mu$ by

$$\int_\Lambda f(m)\,\mathrm{d}\mu(m) := \sum_{n=1}^N f^p(\lambda_n) + \frac{1}{2\pi} \sum_{\sigma \in \{\pm\}} \int_{q_\sigma}^\infty f^\sigma(\lambda) \frac{\mathrm{d}\lambda}{2\sqrt{\lambda - q_\sigma}},$$

where $f : \Lambda \to \mathbb{C}$ is an arbitrary (Lebesgue-)measurable function. Lastly we define the spectral identity $\hat\lambda : \Lambda \to \mathbb{R}$ by $\hat\lambda = (\hat\lambda^p, \hat\lambda^+, \hat\lambda^-)$, where $\hat\lambda^p(\lambda_n) = \lambda_n$, $\hat\lambda^+(\lambda) = \lambda$ and $\hat\lambda^-(\lambda) = \lambda$. ■

How can we now understand Λ? It is a "version" of the spectrum, which takes into account the "multiplicity" of its elements. Each eigenvalue λ_n only appears once, since its multiplicity is 1 by Theorem 2.2.3. If $\lambda \in \sigma_c(A)$ is some value in the continuous spectrum, there are two possible cases: if $\lambda \in (q_-, q_+]$, then there exists only one point in Λ associated to λ: that is, there exists one linearly independent "generalised eigenfunction" associated to λ. If $\lambda \in (q_+, \infty)$, there exist two, that is, λ has in a sense of "multiplicity" 2. Note that we do not give a precise definition of "generalised eigenfunction" here, and emphasise that the last remark is more of a motivational explanation.

We can now define a few function spaces on Λ.

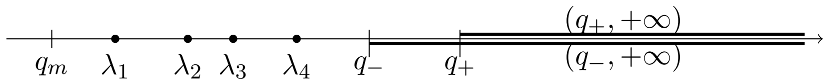

Figure 2.2: Sketch of the Λ. It consists of three parts: the point spectrum $\sigma_p(A) = \{\lambda_1, \ldots, \lambda_N\}$ (the dots in the figure) and the two intervalls $(q_-, +\infty)$ and (q_+, ∞) (the two thick lines).

2.2.6 Definition. Set

$$C_0^\infty(\Lambda) := \left\{ f : \Lambda \to \mathbb{C} : f^+ \in C_0^\infty(q_+, \infty),\ f^- \in C_0^\infty(q_-, \infty) \right\}.$$

For $f, g \in C_0^\infty(\Lambda)$ we define the scalar product

$$\langle f, g \rangle_\Lambda := \int_\Lambda f(m)\overline{g}(m)\,\mathrm{d}\mu(m),$$

with the corresponding norm

$$\|f\|^2_{L^2(\Lambda,\mathrm{d}\mu)} := \langle f, f \rangle_\Lambda,$$

and the corresponding space

$$L^2(\Lambda, \mathrm{d}\mu) := \{f : \Lambda \to \mathbb{C} \text{ measurable} : \|f\|_{L^2(\Lambda,\mathrm{d}\mu)} < \infty\} = \overline{C_0^\infty(\Lambda)}. \qquad \blacksquare$$

With these definitions, we have the spectral space $L^2(\Lambda, \mathrm{d}\mu)$ available. The generalised Fourier transform $\mathcal{F}_A$ will appear as an integral operator with a particular kernel $\Psi : \Lambda \times \mathbb{R} \to \mathbb{C}$. It will be defined with the help of solutions to scattering problems on the real line, for which we introduce a few additional preliminaries in the following lemmata.

2.2.7 Lemma. Let $\lambda > q_-$, $\lambda \neq q_+$, and consider a solution $u \in H^2_{\mathrm{loc}}(\mathbb{R})$ of

$$\Delta u(x) + (\lambda - q(x))u(x) = 0 \qquad \text{for } x \in \mathbb{R}. \tag{2.2.1}$$

Then u must have the form

$$u(x) = \begin{cases} \alpha_1 e^{i\sqrt{\lambda - q_-}\ x} + \alpha_2 e^{-i\sqrt{\lambda - q_-}\ x} & \text{for } x < a, \\ \alpha_3 e^{i\sqrt{\lambda - q_+}\ x} + \alpha_4 e^{-i\sqrt{\lambda - q_+}\ x} & \text{for } x > b, \end{cases} \tag{2.2.2}$$

with some coefficients $\alpha_1, \ldots, \alpha_4 \in \mathbb{C}$. They fulfil

$$\begin{aligned} &\mathrm{Re}(\sqrt{\lambda - q_-})|\alpha_1|^2 + \mathrm{Re}(\sqrt{\lambda - q_+})|\alpha_4|^2 \\ &\qquad = \mathrm{Re}(\sqrt{\lambda - q_-})|\alpha_2|^2 + \mathrm{Re}(\sqrt{\lambda - q_+})|\alpha_3|^2. \end{aligned} \tag{2.2.3}$$

This relation will be called the *energy conservation equation.* $\blacksquare$

Proof. The representation of the solution follows immediately, considering that $\lambda - q(x) = \lambda - q_-$ for any $x < a$ (and $\lambda - q(x) = \lambda - q_+$ for $x > b$). If we multiply (2.2.1) by $\overline{u}(x)$, integrate from a to b and use partial integration, we obtain

$$0 = u'(b)\overline{u}(b) - u'(a)\overline{u}(a) + \int_a^b -|u'(x)|^2 + (\lambda - q(x))|u(x)|^2\,\mathrm{d}x.$$

If we take the imaginary part of the last equation, the integral vanishes. The remainder

$$0 = \operatorname{Im}\left[u'(b)\overline{u}(b) - u'(a)\overline{u}(a)\right]$$

can be easily recomputed with the help of the representations for $x < a$ and $x > b$ to obtain the energy conservation (2.2.3). ■

2.2.8 Definition. Let $\lambda > q_-$, $\lambda \neq q_+$, and let $u \in H^2_{\mathrm{loc}}(\mathbb{R})$ be a solution of (2.2.1) on $\mathbb{R} \setminus (a, b)$. We say that u is *outgoing* if it has the form

$$u(x) = \begin{cases} \alpha_2 e^{-i\sqrt{\lambda - q_-}\, x} & \text{for } x < a, \\ \alpha_3 e^{i\sqrt{\lambda - q_+}\, x} & \text{for } x > b, \end{cases}$$

where $\alpha_2, \alpha_3 \in \mathbb{C}$ are some complex coefficients. ■

2.2.9 Lemma. (Unique continuation principle) Let $u \in H^2_{\mathrm{loc}}(\mathbb{R})$ be a solution to (2.2.1), and let there exist a non-empty open interval $I \subset \mathbb{R}$ such that $u(x) = 0$ for $x \in I$. Then $u(x) = 0$ for all $x \in \mathbb{R}$. ■

Proof. Let $I = (c, d)$. Then $u|_{(-\infty,c)}$ fulfils

$$\begin{cases} \Delta u + (\lambda - q)u = 0 & \text{in } (-\infty, c), \\ \quad u(c) = 0 = u'(c), \end{cases}$$

since $u \in H^2_{\mathrm{loc}}(\mathbb{R})$, and since u vanishes to the right of c on (c, d). This problem has a unique solution by the Picard-Lindelöf theorem (for further references regarding L^∞-coefficients, we refer to Section 2.4), which is obviously given by $u = 0$ on $(-\infty, c)$. The same way one can confirm that u vanishes also on (d, ∞). ■

2.2.10 Lemma. Let $\lambda > q_-$, $\lambda \neq q_+$ and let $u_{\mathrm{i}} \in H^2_{\mathrm{loc}}(\mathbb{R} \setminus (a, b))$ be given by

$$u_{\mathrm{i}}(x) = \begin{cases} c_1 e^{i\sqrt{\lambda - q_-}\, x} & \text{for } x < a, \\ c_4 e^{-i\sqrt{\lambda - q_+}\, x} & \text{for } x > b, \end{cases}$$

where c_1, $c_4 \in \mathbb{C}$ are arbitrary coefficients. Then there exists exactly one solution $u \in H^2_{\mathrm{loc}}(\mathbb{R})$ of (2.2.1) such that

$$u - u_{\mathrm{i}} \text{ is outgoing .}$$ ■

Proof. Let us show uniqueness: let u_1 and u_2 be two solutions fulfilling (2.2.1) such that $u_k - u_{\mathrm{i}}$ is outgoing, $k \in \{1, 2\}$. Then $w = u_1 - u_2$ is also outgoing, implying that $\alpha_1 = \alpha_4 = 0$, where $\alpha_1, \ldots, \alpha_4$ are the coefficients of w in the expansion (2.2.2). We have by the energy conservation (2.2.3)

$$0 = \operatorname{Re}(\sqrt{\lambda - q_-})|\alpha_2|^2 + \operatorname{Re}(\sqrt{\lambda - q_+})|\alpha_3|^2.$$

Note that both terms are non-negative, that $\operatorname{Re}\left(\sqrt{\lambda - q_-}\right) > 0$ and that $\operatorname{Re}\left(\sqrt{\lambda - q_+}\right) \geq 0$. Note that $\sqrt{\lambda - q_+}$ might be imaginary, but cannot be real and negative. This implies that at least $\alpha_3 = 0$, which in turn yields that $w(x) = 0$ for $x > b$. The unique continuation principle now implies $w = 0$.

To see the existence of the solution, we now restrict ourselves to the incident field $c_1 = 1,\ c_4 = 0$ and to the case $\lambda \in (q_-, q_+)$. The other cases can be treated analogously. Let us denote by $w \in H^2_{\mathrm{loc}}(\mathbb{R})$ the unique solution of (2.2.1) such that

$$w'(b) = i\sqrt{\lambda - q_+}, \quad w(b) = 1,$$

and let again $\alpha_1, \dots, \alpha_4$ be its coefficients. By the Picard–Lindelöf theorem, w exists and is unique. Clearly, $\alpha_3 = 1,\ \alpha_4 = 0$. We obtain by the energy conservation equation that

$$\mathrm{Re}(\sqrt{\lambda - q_-})|\alpha_1|^2 = \mathrm{Re}(\sqrt{\lambda - q_-})|\alpha_2|^2,$$

so that $\alpha_1 \neq 0 \neq \alpha_2$, since otherwise the unique continuation principle would imply $w = 0$. One can now easily verify that $u(x) := \alpha_1^{-1} w(x)$ fulfils the Helmholtz equation, while $u - u_{\mathrm{i}}$ is outgoing. ■

With these preliminaries, we can now define the kernel of the generalised Fourier transform.

2.2.11 Definition. We define the function $\Psi : \Lambda \times \mathbb{R} \to \mathbb{C},\ \Psi = (\Psi^p, \Psi^+, \Psi^-)$ as follows: for $\lambda_n \in \sigma_p(A)$, let $\Psi^p : \sigma_p(A) \times \mathbb{R} \to \mathbb{C}$ be defined by

$$\Psi^p(\lambda_n, x) = \frac{\phi_n(x)}{\|\phi_n\|_{L^2(\mathbb{R})}},$$

where ϕ_n is a nontrivial eigenfunction for the eigenvalue λ_n (recall that λ_n has multiplicity 1 by Theorem 2.2.3).

Let $\sigma \in \{\pm\}$. Then we define $\Psi^\sigma : (q_\sigma, \infty) \times \mathbb{R} \to \mathbb{C}$ as follows: for $\lambda > q_\sigma$, let $\Psi^\sigma(\lambda, \cdot\,)$ be the unique solution to

$$\begin{cases} \Delta_x \Psi^\sigma(\lambda, x) + (\lambda - q(x))\Psi^\sigma(\lambda, x) = 0 & \text{for } x \in \mathbb{R}, \\ \Psi^\sigma(\lambda, \cdot\,) - u_i^\sigma & \text{is outgoing,} \end{cases}$$

where the incident field is given by either

$$u_i^-(x) = \begin{cases} e^{i\sqrt{\lambda - q_-}x} & \text{if } x < a, \\ 0 & \text{if } b < x, \end{cases}$$

or

$$u_i^+(x) = \begin{cases} 0 & \text{if } x < a, \\ e^{-i\sqrt{\lambda - q_+}x} & \text{if } b < x, \end{cases}$$

depending on σ. For any $\lambda_n \in \sigma_p(A)$, we call $\Psi^p(\lambda_n, \cdot\,)$ a *normalised eigenfunction*, while for $\lambda \in \sigma_c(A)$, we call $\Psi^+(\lambda, \cdot\,)$ and $\Psi^-(\lambda, \cdot\,)$ *generalised eigenfunctions.* ■

2.2.12 Theorem. For $\Psi : \Lambda \times \mathbb{R} \to \mathbb{C}$ as defined in Definition 2.2.11, we define $\mathcal{F}_A : L^2(\mathbb{R}) \to L^2(\Lambda, \mathrm{d}\mu)$ for $f \in C_0^\infty(\mathbb{R})$ and $m \in \Lambda$ by

$$\mathcal{F}_A f(m) = \int_{\mathbb{R}} f(x)\overline{\Psi}(m, x)\,\mathrm{d}x.$$

It is unitary, i.e. we have the Parseval's relation for $f, g \in L^2(\mathbb{R})$,

$$\langle f, g\rangle_{\mathbb{R}} = \langle \mathcal{F}_A f, \mathcal{F}_A g\rangle_\Lambda \tag{2.2.4}$$

and its inverse $\mathcal{F}_A^{-1} : L^2(\Lambda, \mathrm{d}\mu) \to L^2(\mathbb{R})$ is defined for $\tilde{f} \in C_0^\infty(\Lambda)$ by

$$\mathcal{F}_A^{-1}\tilde{f}(x) = \int_\Lambda \Psi(m,x)\tilde{f}(m)\,\mathrm{d}\mu(m).$$

It diagonalizes A, i.e.

$$Af = \mathcal{F}_A^{-1}\hat{\lambda}\mathcal{F}_A f$$

for any $f \in H^2(\mathbb{R})$. Here $\hat{\lambda}\mathcal{F}_A f$ denotes the point-wise product of $\hat{\lambda}$ with $\mathcal{F}_A f$. ■

Proof. The proof is (almost) contained in Section 2.4 below. We point out that the different parts of the Theorem are proved at the end of this chapter in Lemmata 2.4.12 and 2.4.13, and point also to the remarks of Subsection 2.4.14. ■

2.2.13 Example. To illustrate the expansion theorem, let us use it to derive the Fourier inversion formula: when $q(x) = 0$ for all $x \in \mathbb{R}$, we obtain $Af = -\Delta f$, so we will end up diagonalizing the Laplacian. We set $a = b = 0$ and $q_- = q_+ = q_m = 0$, so in this case, Theorem 2.2.3 yields $\sigma_p(A) = \emptyset$, and $\sigma_c(A) = [0,\infty)$. To determine $\Psi^\pm(\lambda,\,\cdot\,)$ we have to find for $\lambda > 0$ the solution of $\Delta_x\Psi^+(\lambda,\,\cdot\,) + \lambda\Psi^+(\lambda,\,\cdot\,) = 0$ such that

$$\Psi^+(\lambda,x) = \begin{cases} \alpha e^{i\sqrt{\lambda}x} & \text{if } x < 0, \\ e^{i\sqrt{\lambda}\,x} + \beta e^{-i\sqrt{\lambda}x} & \text{if } x > 0. \end{cases}$$

Clearly, this implies $\Psi^+(\lambda,x) = e^{i\sqrt{\lambda}x}$ for all $x \in \mathbb{R}$. Likewise we obtain $\Psi^-(\lambda,x) = e^{-i\sqrt{\lambda}\,x}$. From Theorem 2.2.12 we obtain for any $f \in L^2(\mathbb{R})$

$$f(x) = (\mathcal{F}_A^{-1}\mathcal{F}_A f)(x) = \int_\Lambda \Psi(m,x) \int_\mathbb{R} \overline{\Psi}(m,y)f(y)\,\mathrm{d}y\,\mathrm{d}\mu(m).$$

Applying the definition of the spectral space $(\Lambda, \mathrm{d}\mu)$, we can write the right hand side integral by

$$\begin{aligned} f(x) &= \frac{1}{2\pi}\int_0^\infty \Psi^+(\lambda,x) \int_\mathbb{R} \overline{\Psi}^+(\lambda,y)f(y)\,\mathrm{d}y\frac{\mathrm{d}\lambda}{2\sqrt{\lambda}} \\ &\quad + \frac{1}{2\pi}\int_0^\infty \Psi^-(\lambda,x) \int_\mathbb{R} \overline{\Psi}^-(\lambda,y)f(y)\,\mathrm{d}y\frac{\mathrm{d}\lambda}{2\sqrt{\lambda}} \\ &= \frac{1}{2\pi}\int_0^\infty e^{i\sqrt{\lambda}x} \int_\mathbb{R} e^{-i\sqrt{\lambda}x} f(y)\,\mathrm{d}y\frac{\mathrm{d}\lambda}{2\sqrt{\lambda}} \\ &\quad + \frac{1}{2\pi}\int_0^\infty e^{-i\sqrt{\lambda}x} \int_\mathbb{R} e^{i\sqrt{\lambda}x} f(y)\,\mathrm{d}y\frac{\mathrm{d}\lambda}{2\sqrt{\lambda}} \end{aligned}$$

We now substitute $\xi = \sqrt{\lambda}$ in the first and $\xi = -\sqrt{\lambda}$ in the second integral to obtain

$$f(x) = \frac{1}{2\pi}\int_0^\infty e^{i\xi x} \int_\mathbb{R} e^{-i\xi x} f(y)\,\mathrm{d}y\,\mathrm{d}\xi + \frac{1}{2\pi}\int_{-\infty}^0 e^{i\xi x} \int_\mathbb{R} e^{-i\xi x} f(y)\,\mathrm{d}y\,\mathrm{d}\xi,$$

which, not so surprisingly, turns out to be the Fourier inversion formula.

2.3 The Pekeris Profile

In this section we consider a special profile q, which admits a (mostly) explicit representation of the eigenfunctions and generalised eigenfunctions. Its name originates from Pekeris' paper [65], where it has been studied for the first time. Due to its explicit form, it will be the foundation of the numerical examples we will show in later chapters, where we will need to implement $\mathcal{F}_A$. Let $a < b$ and consider for (arbitrary) constants $q_m < q_- \leq q_+$ the profile

$$q(x) = \begin{cases} q_- & \text{for } x < a, \\ q_m & \text{for } a < x < b, \\ q_+ & \text{for } b < x. \end{cases}$$

We only demand $q_m < q_-$ to obtain a point spectrum by Theorem 2.2.3, which will be shown to be non-empty under the given assumptions. If $q_m \geq q_-$, the calculations below can be carried out as shown, too. However, in this case the point spectrum $\sigma_p(A)$ is empty, and the corresponding part can be skipped. To determine the spectral family of $A = -\Delta + q$, we fix some $\lambda \in \mathbb{R} \setminus \{q_+, q_-, q_m\}$ and study solutions $u \in H^2_{\mathrm{loc}}(\mathbb{R})$ of the equation $(-\Delta + q - \lambda)u = 0$; due to the piecewise constant coefficients they have the form

$$u(x) = \begin{cases} \alpha_1 e^{i\sqrt{\lambda - q_-}(x-a)} + \alpha_2 e^{-i\sqrt{\lambda - q_-}(x-a)} & \text{if } x < a, \\ \alpha_3 e^{i\sqrt{\lambda - q_m}\,x} + \alpha_4 e^{-i\sqrt{\lambda - q_m}\,x} & \text{if } a < x < b, \\ \alpha_5 e^{i\sqrt{\lambda - q_+}(x-b)} + \alpha_6 e^{-i\sqrt{\lambda - q_+}(x-b)} & \text{if } b < x, \end{cases} \tag{2.3.1}$$

where $\alpha_1, \ldots, \alpha_6 \in \mathbb{C}$ are some complex coefficients. To proceed, we need a few abbreviations, and define the following quantities for $\sigma \in \{-, +, m\}$

$$\mu_\sigma(\lambda) := \sqrt{\lambda - q_\sigma},\ p_a(\lambda) := e^{i\sqrt{\lambda - q_m}\,a},\ p_b(\lambda) := e^{i\sqrt{\lambda - q_m}\,b}.$$

To shorten notation, we omit the argument λ in the following for the five functions defined in the last line. Since we demand that $u \in H^2_{\mathrm{loc}}(\mathbb{R})$, u and u' are continuous (by Sobolev-embedding). Setting $x = a$ and $x = b$ in the representations of u, we obtain that the coefficients $\alpha_1, \ldots, \alpha_6$ must fulfil the following set of equations:

$$\begin{aligned} \alpha_1 + \alpha_2 &= p_a\alpha_3 + p_a^{-1}\alpha_4, \\ \alpha_5 + \alpha_6 &= p_b\alpha_3 + p_b^{-1}\alpha_4, \\ \mu_-\alpha_1 - \mu_-\alpha_2 &= \mu_m p_a\alpha_3 + \mu_m p_a^{-1}\alpha_4, \\ \mu_+\alpha_5 - \mu_+\alpha_6 &= \mu_m p_b\alpha_3 + \mu_m p_b^{-1}\alpha_4. \end{aligned} \tag{2.3.2}$$

Solving the first and second equation for α_2 and α_5, and inserting the result into the third and fourth equations, we obtain the following system of equations for $\alpha_3, \alpha_4, \alpha_1, \alpha_6$, which we write in matrix-vector form

$$\begin{pmatrix} (\mu_- + \mu_m)p_a & (\mu_- - \mu_m)p_a^{-1} \\ (\mu_+ - \mu_m)p_b & (\mu_+ + \mu_m)p_b^{-1} \end{pmatrix} \begin{pmatrix} \alpha_3 \\ \alpha_4 \end{pmatrix} = \begin{pmatrix} 2\mu_-\alpha_1 \\ 2\mu_+\alpha_6 \end{pmatrix}. \tag{2.3.3}$$

Let us denote the left hand side matrix by $B = B(\lambda)$, and let

$$\begin{aligned} d(\lambda) &= \det(B(\lambda)) \\ &= (\mu_- + \mu_m)(\mu_+ + \mu_m)p_a p_b^{-1} - (\mu_- - \mu_m)(\mu_+ - \mu_m)p_b p_a^{-1} \end{aligned} \tag{2.3.4}$$

denote its determinant. We have to determine (a) the point spectrum, and the corresponding normalised eigenfunctions and (b) the generalised eigenfunctions (see Definition 2.2.11). Let us do both.

2.3.1 Eigenfunctions. We have to search for eigenvalue/eigenvector pairs $\lambda \in \mathbb{R}$, $u \in H^2(\mathbb{R})$. By Theorem 2.2.3, we only have to consider $\lambda \in (q_m, q_-)$. For such λ the terms corresponding to α_1 and α_6 in (2.3.1) increase exponentially, and hence $\alpha_1 = \alpha_6 = 0$ must vanish for u to be in $H^2(\mathbb{R})$. This implies by (2.3.3) that

$$B(\lambda)\begin{pmatrix}\alpha_3\\ \alpha_4\end{pmatrix} = 0,$$

and this may happen only if $d(\lambda) = \det(B(\lambda)) = 0$. One easily sees that for any $\lambda \in (q_m, q_-)$ such that $d(\lambda) = 0$, any element of the Kernel $(\hat\alpha_3, \hat\alpha_4) \in \mathcal{N}(B(\lambda))$ generates an $H^2(\mathbb{R})$ eigenfunction, so determining all zeros of d is equivalent to determining the point spectrum (for more details, we refer to the proof of Lemma 2.4.4). Let us rewrite $d(\lambda) = 0$ in a fashion that allows numerical computation of *all* zeros: by easy manipulation of equation (2.3.4), we obtain that $d(\lambda) = 0$ is equivalent to

$$\frac{\mu_m + \mu_-}{\mu_m - \mu_-}\,\frac{\mu_m + \mu_+}{\mu_m - \mu_+}\,\frac{p_a^2}{p_b^2} = 1. \tag{2.3.5}$$

Note that for $\lambda \in (q_m, q_-)$ we have $\mu_m = \sqrt{\lambda - q_m} > 0$, while $\mu_\sigma = \sqrt{\lambda - q_\sigma} = i\sqrt{q_\sigma - \lambda} \in i(0,\infty)$, so that $\overline{\mu_m + \mu_\sigma} = \mu_m - \mu_\sigma$. Since $|p_a| = |p_b| = 1$, the left hand side of (2.3.4) is always a complex number of modulus one, and we only have to check whether the arguments of the two sides of the equality are equal. Elementary calculation now yields

$$\begin{aligned}\theta(\lambda) &:= \arg\left(\frac{\mu_m + \mu_-}{\mu_m - \mu_-}\,\frac{\mu_m + \mu_+}{\mu_m - \mu_+}\,\frac{p_a^2}{p_b^2}\right)\\ &= 2\,\mathrm{atan}\left(\sqrt{\frac{q_+ - \lambda}{\lambda - q_m}}\right) + 2\,\mathrm{atan}\left(\sqrt{\frac{q_- - \lambda}{\lambda - q_m}}\right) - 2(b-a)\sqrt{\lambda - q_m}.\end{aligned}$$

Hence (2.3.5) is fulfilled if and only if

$$\theta(\lambda) = 2\pi n \tag{2.3.6}$$

for some $n \in \mathbb{Z}$. Note that θ is bounded on $[q_m, q_-]$ and continuous, and one easily sees that it is also strictly decreasing. Hence, for any

$$n \in \left(\theta(q_-)(2\pi)^{-1}\ ,\ \theta(q_m)(2\pi)^{-1}\right) \cap \mathbb{Z}$$

there exists exactly one solution of $\theta(\lambda) = 2\pi n$. Numerically, one can find those by solving (2.3.6) for all suitable $n \in \mathbb{Z}$ by Newton's method. Denote this finite set of solutions (that is, the eigenvalues of A) by $\{\lambda_1, \dots, \lambda_N\}$, ordered ascendingly. For each $n \in \{1, \dots, N\}$, the Kernel $\mathcal{N}(B(\lambda_n))$ has dimension 1, since $B(\lambda_n)$ is a 2×2 matrix and easily seen to be non-zero. Let $(\alpha_3, \alpha_4)^\top \in \mathcal{N}(B(\lambda_n)) \setminus \{0\}$ be some vector. After setting $\alpha_1 = \alpha_6 = 0$, we can retrieve α_2 and α_5 from the first two equations (2.3.2), and arrive at a full coefficient vector $\alpha_1, \dots, \alpha_6$. (2.3.1) then yields an eigenfunction u.

To obtain the normalised eigenfunction $\Psi^p(\lambda_n,\cdot\,)$ corresponding to λ_n, one calculates straightforwardly

$$\begin{aligned}\|u\|^2_{L^2(\mathbb{R})} =&(b-a)\left(|\alpha_3|^2+|\alpha_4|^2\right)+\frac{1}{\mu_m}\mathrm{Im}\left(\alpha_3\overline{\alpha}_4(p_b^2-p_a^2)\right)\\ &+\frac{1}{2|\mu_-|}\left|\alpha_3 p_a+\alpha_4 p_a^{-1}\right|^2+\frac{1}{2|\mu_+|}\left|\alpha_3 p_b+\alpha p_b^{-1}\right|^2.\end{aligned}$$

Hence, the corresponding real eigenfunction is given by

$$\Psi^p(\lambda_n,x)=\sqrt{\frac{\overline{\alpha}_4|\alpha_3|}{\alpha_3|\alpha_4|}}\;\|u\|^{-1}_{L^2(\mathbb{R})}\;u(x)\qquad\text{for } x\in\mathbb{R},$$

where the factor under the square root ensures that $\Psi^p(\lambda_n,\cdot\,)$ is real.

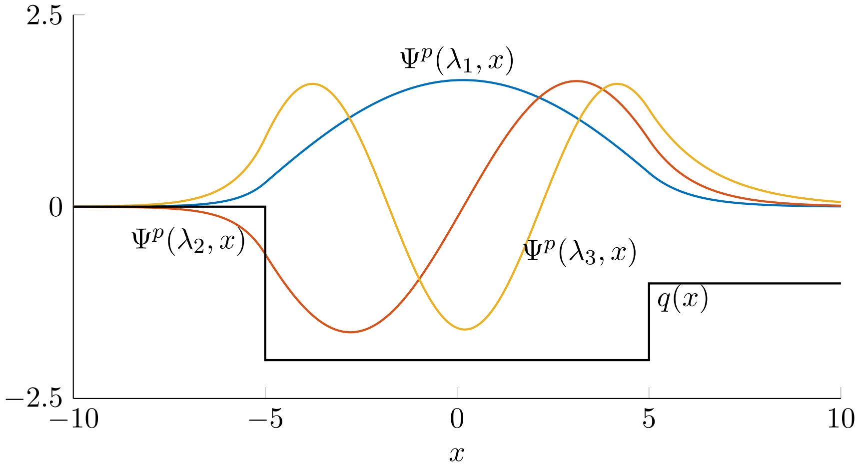

Figure 2.3: Sketch of all proper eigenfunctions (in total 3) of A, for a given Pekeris–profile, also sketched ($a=-5,\ b=5,\ q_-=0,\ q_m=-2,\ q_+=-1$). The functions are sinusoidal for $x\in(-5,5)$, and exponential elsewhere.

2.3.2 Generalised eigenfunctions. One easily checks that for $\lambda>q_-$ the determinant $d(\lambda)$ cannot vanish, since the absolute value of the numerator in (2.3.5) is strictly larger than the denominator. Accordingly, $B=B(\lambda)$ is invertible, and for fixed known α_1,α_6, we can retrieve from (2.3.3) the coefficients α_3,α_4 by

$$\begin{aligned}\begin{pmatrix}\alpha_3\\ \alpha_4\end{pmatrix}&=B^{-1}\begin{pmatrix}2\mu_-\alpha_1\\ 2\mu_+\alpha_6\end{pmatrix}\\ &=\frac{1}{d(\lambda)}\begin{pmatrix}2\mu_-(\mu_++\mu_m)p_b^{-1} & 2\mu_+(\mu_m-\mu_-)p_a^{-1}\\ 2\mu_-(\mu_m-\mu_+)p_b & 2\mu_+(\mu_-+\mu_m)p_a\end{pmatrix}\begin{pmatrix}\alpha_1\\ \alpha_6\end{pmatrix},\end{aligned}\tag{2.3.7}$$

while we can retrieve α_2,α_5 from the remaining coefficients from the first two equations of (2.3.3), namely by

$$\begin{aligned}\alpha_2&=p_a\alpha_3+p_a^{-1}\alpha_4-\alpha_1,\\ \alpha_5&=p_b\alpha_3+p_b^{-1}\alpha_4-\alpha_6.\end{aligned}\tag{2.3.8}$$

Let $\lambda > q_-$, and consider the generalised eigenfunction $\Psi^-(\lambda,\,\cdot\,)$ from Definition 2.2.11. It solves $(-\Delta - \lambda + q)\Psi^-(\lambda,\,\cdot\,) = 0$ and it must have the form

$$\Psi^-(\lambda, x) = \begin{cases} c_- e^{-i\sqrt{\lambda - q_-}\ x} + e^{i\sqrt{\lambda-q_-}\ x}, & \text{if } x < a, \\ c_+ e^{i\sqrt{\lambda - q_+}\ x} & \text{if } x > b. \end{cases}$$

By comparing coefficients, we obtain that $\Psi^-(\lambda,\,\cdot\,)$ corresponds to u with $\alpha_1 = e^{i\sqrt{\lambda-q_-}\ a}$ and $\alpha_6 = 0$. The remaining coefficients $\alpha_2, \dots, \alpha_5$ then follow from (2.3.7) and (2.3.8). Similarly, one easily sees that for $\lambda > q_+$, the second eigenfunction $\Psi^+(\lambda,\,\cdot\,)$ is obtained in the same fashion by comparing coefficients and finding that $\alpha_1 = 0$ and $\alpha_6 = e^{i\sqrt{\lambda-q_+}\ b}$.

2.3.3 Definition. Let us introduce the function

$$\alpha : \Lambda \to \mathbb{C}^6.$$

For a given $m \in \Lambda$, it gives the coefficients $\alpha_1, \dots, \alpha_6 \in \mathbb{C}$ of the corresponding eigenfunction $\Psi(m,\,\cdot\,)$, expanded as in (2.3.1). ∎

Note that all formulae we calculated are explicit in terms of elementary function, provided, one has determined the point spectrum. This will allow us to implement the transformation of the operator $\mathcal{F}_A$.

2.4 Proof of the Expansion Theorem

2.4.1 Overview. Our goal is to prove Theorem 2.2.12. This, however, will take some space, and we want to start by giving an overview over the proof and by introducing some elementary notation from spectral theory (for an introduction into those topics, we will generally refer to [67, Chapter VII and VIII]). Let us denote the resolvent of the operator A for $\lambda \in \mathbb{C} \setminus \mathbb{R}$ by

$$R_\lambda := (A - \lambda)^{-1}.$$

Since A is self-adjoint by Theorem 2.2.3, the resolvent $R_\lambda : L^2(\mathbb{R}) \to H^2(\mathbb{R})$ is bounded for any non-real λ. For some bounded interval $I \subset \mathbb{R}$, denote by $P_I : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ the spectral projection associated with A. The core of our proof now rests in two steps: firstly, we can compute $P_{(a,b)}$ for $a < b$ with the help of Stone's formula (see for example [67, Theorem VII.13 and Remark after Theorem VIII.6])

$$\frac{1}{2}(P_{[a,b]} f + P_{(a,b)} f) = \frac{1}{2\pi i} \lim_{\epsilon \to 0} \int_a^b R_{\lambda + i\epsilon} f - R_{\lambda - i\epsilon} f \,\mathrm{d}\lambda. \tag{2.4.1}$$

Once a representation for the spectral projection is found, we will use that for any $f \in L^2(\mathbb{R})$ we have that (see [67, Remark after Theorem VIII.5])

$$f = \lim_{\rho \to \infty} P_{(-\rho,\rho)} f.$$

This allows us to obtain a rather complicated representation of the identity. It will turn out, however, that this representation is nothing but the inversion formula $f = \mathcal{F}_A^{-1} \mathcal{F}_A f$ from Theorem 2.2.12, which will afterwards yield the remaining properties of the theorem. We can now structure the remainder of this section as follows.

(1) We need to study the resolvent R_λ very precisely. To do this, we will derive a representation of the resolvent with a Green's function, that is, we will find $G_\lambda : \mathbb{R} \times \mathbb{R} \to \mathbb{C}$ such that

$$R_\lambda f(x) = \int_{\mathbb{R}} G_\lambda(x,y) f(y) \,\mathrm{d}y \qquad \text{for } x \in \mathbb{R}.$$

G_λ will be expressed with the help of two particular solutions $v_\lambda^\pm$ of the Helmholtz equation, which are introduced in Subsection 2.4.2 and are studied in Lemmata 2.4.3 and 2.4.4. The Green's function will be given in Lemma 2.4.5.

(2) To take the limit $\epsilon \to 0$ in Stone's formula (2.4.1), we will prepare a number of auxiliary results: this will be the topic of Lemmata 2.4.6 to 2.4.9. We can then give the core argument of this section, which is contained in the proof of Lemma 2.4.10, where we apply Stone's formula and take the limit $\epsilon \to 0$.

(3) The remainder of the section will be concerned with proving the claims of Theorem 2.2.12.

2.4.2 Two special solutions. For $\lambda \in \mathbb{C}$, we define v_λ^+ and v_λ^- as the unique solutions of

$$-\Delta v_\lambda^\pm(x) - (\lambda - q(x)) v_\lambda^\pm(x) = 0 \qquad \text{for } x \in \mathbb{R} \tag{2.4.2}$$

such that

$$\begin{aligned} v_\lambda^+(a) = 1,\ \partial_x v_\lambda^+(a) &= -i\sqrt{\lambda - q_-}, \\ \text{and} \quad v_\lambda^-(b) = 1,\ \partial_x v_\lambda^-(b) &= i\sqrt{\lambda - q_+}. \end{aligned} \tag{2.4.3}$$

Those functions are both well-defined by Lemma 2.4.3 below. For $\lambda \in \mathbb{C} \setminus \{q_+\}$ we have that

$$v_\lambda^+(x) = \begin{cases} e^{-i\sqrt{\lambda - q_-}(x-a)} & \text{if } x < a, \\ \beta_\lambda^+ e^{i\sqrt{\lambda - q_+}(x-b)} + \alpha_\lambda^+ e^{-i\sqrt{\lambda - q_+}(x-b)} & \text{if } x > b, \end{cases} \tag{2.4.4}$$

while for $\lambda \in \mathbb{C} \setminus \{q_-\}$

$$v_\lambda^-(x) = \begin{cases} \alpha_\lambda^- e^{i\sqrt{\lambda - q_-}(x-a)} + \beta_\lambda^- e^{-i\sqrt{\lambda - q_-}(x-a)} & \text{if } x < a, \\ e^{i\sqrt{\lambda - q_+}(x-b)} & \text{if } x > b, \end{cases} \tag{2.4.5}$$

where $\alpha_\lambda^+, \alpha_\lambda^-, \beta_\lambda^+, \beta_\lambda^- \in \mathbb{C}$ are some complex coefficients. Let us point at the most important feature of these two functions: if $\lambda \in \mathbb{C} \setminus [q_-, \infty)$, $v_\lambda^+(x)$ decays exponentially as $x \to -\infty$, while $v_\lambda^-(x)$ decays exponentially as $x \to +\infty$. We furthermore define the Wronskian of the two functions as

$$w_\lambda := W(v_\lambda^+, v_\lambda^-)(x) = v_\lambda^+(x)\partial_x v_\lambda^-(x) - (\partial_x v_\lambda^+)(x) v_\lambda^-(x), \tag{2.4.6}$$

Note that the Wronskian w_λ does not depend on $x \in \mathbb{R}$. This can be easily seen by differentiating the right hand side of (2.4.6) with respect to x and utilising that v_λ^+ and v_λ^- both fulfil (2.4.2). The Wronskian can be easily expressed with the coefficients of (2.4.4) and (2.4.5) as follows

$$w_\lambda = -2i\sqrt{\lambda - q_-}\ \alpha_\lambda^- = -2i\sqrt{\lambda - q_+}\ \alpha_\lambda^+, \tag{2.4.7}$$

whenever the quantities on the right are defined; this follows by applying the definition of the Wronskian (2.4.6) to the representation for $x < a$ (or $x > b$) after a bit of straightforward calculation.

The existence and uniqueness of the two solutions would follow immediately if we had assumed that the coefficient q is continuous, since then the well-know Picard–Lindelöf theorem applies. We will give the corresponding result for a more general situation in the following.

2.4.3 Definition and Lemma. Let $q \in L^\infty(\mathbb{R})$. For $\lambda \in \mathbb{C}$, let $\tilde{\psi}_\lambda, \hat{\psi}_\lambda : \mathbb{R} \to \mathbb{C}$ be the solutions to

$$-\Delta\psi_\lambda(x) + q(x)\psi_\lambda(x) = \lambda\psi_\lambda(x) \qquad \text{for } x \in \mathbb{R},$$

such that

$$\tilde{\psi}_\lambda(a) = 1,\ \partial_x\tilde{\psi}_\lambda(a) = 0, \quad \text{and} \quad \hat{\psi}_\lambda(a) = 0,\ \partial_x\hat{\psi}_\lambda(a) = 1.$$

$\tilde{\psi}_\lambda, \hat{\psi}_\lambda$ are well defined and for any bounded interval $I \subset \mathbb{R}$, the mappings $\mathbb{C} \to H^2(I),\ \lambda \mapsto \tilde{\psi}_\lambda$ and $\mathbb{C} \to H^2(I),\ \lambda \mapsto \hat{\psi}_\lambda$ are entire[1]. In particular, the matrix

$$T_\lambda = \begin{pmatrix} t_{11}(\lambda) & t_{12}(\lambda) \\ t_{21}(\lambda) & t_{22}(\lambda) \end{pmatrix} := \begin{pmatrix} \tilde{\psi}_\lambda(b) & \hat{\psi}_\lambda(b) \\ \partial_x\tilde{\psi}_\lambda(b) & \partial_x\hat{\psi}_\lambda(b) \end{pmatrix}$$

is an entire function of λ, that is, all entries t_{nm} are entire functions $(n, m \in \{1, 2\})$. For any $\lambda \in \mathbb{C}$ we have that $\det(T_\lambda) \neq 0$.

Furthermore, the mappings $\mathbb{C} \setminus [q_-, +\infty) \to H^2(I),\ \lambda \mapsto v_\lambda^\pm$, are holomorphic on their domain and can be continuously extended such that for any $\lambda > 0$ the limits

$$\lim_{\substack{\epsilon \to 0 \\ \epsilon > 0}} v^\pm_{\lambda + i\epsilon} = v^\pm_\lambda,$$

exist, where the convergence takes place in $H^2(I)$. ■

Proof. For the fact that $\lambda \mapsto \tilde{\psi}_\lambda,\ \lambda \mapsto \hat{\psi}_\lambda$ are entire functions and well-defined, we refer to [50, Section 4.2], where those statements are proved for $q \in L^2(I)$, which is clearly the case if $q \in L^\infty(\mathbb{R})$. To see that the determinant cannot vanish, let us note the meaning of the matrix T_λ: if we have some solution U of (2.4.2) with $U(a) = c_1 \in \mathbb{C}$, $\partial_x U(a) = c_2 \in \mathbb{C}$, we obtain that $U = c_1\tilde{\psi}_\lambda + c_2\hat{\psi}_\lambda$, so that

$$\begin{pmatrix} U(b) \\ \partial_x U(b) \end{pmatrix} = \begin{pmatrix} c_1\tilde{\psi}_\lambda(b) + c_2\hat{\psi}_\lambda(b) \\ c_1\partial_x\tilde{\psi}_\lambda(b) + c_2\partial_x\hat{\psi}_\lambda(b) \end{pmatrix} = T_\lambda \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}.$$

Thus the matrix T_λ maps the Dirichlet and Neumann boundary data at a to the Dirichlet and Neumann boundary data at b. Now assume $\det(T_\lambda) = 0$, so that we have some $c \in \mathbb{C}^2 \setminus \{0\}$ such that $T_\lambda c = 0$. Then the function $U = c_1\tilde{\psi}_\lambda + c_2\hat{\psi}_\lambda$ solves (2.4.2) and

$$\begin{pmatrix} U(b) \\ \partial_x U(b) \end{pmatrix} = T_\lambda c = 0.$$

This, however, implies that $U = 0$ everywhere by the unique continuation principle, so that we obtain $c = 0$. This gives a contradiction.

[1] Recall that an entire function is a function $\mathbb{C} \to \mathbb{C}$, which is holomorphic on the entirety of $\mathbb{C}$.

To see that the statements for v_λ^+ hold, note that

$$v_\lambda^+ = \psi_\lambda - i\sqrt{\lambda - q_-}\ \hat{\psi}_\lambda,$$

so that the differentiability properties of the square root (Definition 1.2.1) are inherited. ■

The following lemma characterises the point spectrum of A with the help of the Wronskian w_λ and gives a number of technical properties. The proof is rather long and technical and not very rich in instructive details, so the reader can safely skip it at first reading.

2.4.4 Lemma. $w_\lambda : \mathbb{C} \setminus [q_-, +\infty) \to \mathbb{C}$ is holomorphic, and can be continuously extended so that the one sided limits

$$\lim_{\substack{\lambda\to\mu\\ \mathrm{Im}(\lambda)>0}} w_\lambda = w_\mu \qquad \text{for } \mu \in [q_-, \infty)$$

exist. We furthermore have:

(a) $\sigma_p(A) = \{\lambda \in \mathbb{C} : w_\lambda = 0\} \setminus \{q_-\} \subset (q_m, q_-)$.

(b) $\sigma_p(A) = \{\lambda_1, \dots, \lambda_N\}$ is a finite (but possibly empty) set (i.e. $N \in \mathbb{N} \cup \{0\}$).

(c) If $w_{q_-} = 0$, then we have for λ in some neighbourhood of q_-

$$w_\lambda = C\sqrt{\lambda - q_-} + \mathcal{O}(|\lambda - q_-|),$$

with $C \in \mathbb{C} \setminus \{0\}$. ■

Proof. Let us rewrite w_λ with the help of T_λ: We have that

$$w_\lambda = \det\begin{pmatrix} v_\lambda^+(b) & v_\lambda^-(b) \\ \partial_x v_\lambda^+(b) & \partial_x v_\lambda^-(b)\end{pmatrix} = \det\left[\ T_\lambda \begin{pmatrix} v_\lambda^+(a) \\ \partial_x v_\lambda^+(a)\end{pmatrix} \middle| \begin{pmatrix} v_\lambda^-(b) \\ \partial_x v_\lambda^-(b)\end{pmatrix}\ \right].$$

Exploiting the boundary conditions for $v_\lambda^\pm$ in (2.4.3), we can more explicitly calculate

$$\begin{aligned} w_\lambda &= \det\left[\ T_\lambda \begin{pmatrix} 1 \\ -i\sqrt{\lambda - q_-}\end{pmatrix} \middle| \begin{pmatrix} 1 \\ i\sqrt{\lambda - q_+}\end{pmatrix}\ \right] \\ &= -t_{21}(\lambda) + i\sqrt{\lambda - q_+}\ t_{22}(\lambda) \\ &\quad + i\sqrt{\lambda - q_-}\ t_{11}(\lambda) + \sqrt{\lambda - q_+}\sqrt{\lambda - q_-}\ t_{12}(\lambda). \end{aligned} \tag{2.4.8}$$

Since t_{nm} are entire functions of λ, we obtain that $\lambda \mapsto w_\lambda$ is holomorphic whenever the two square roots $\sqrt{\cdot - q_\pm}$ are holomorphic. This yields the continuity as well as the continuous extension of the one sided limits for real $\lambda \geq q_-$ (compare also the choice of the square root in Definition 1.2.1). Let us now show the three assertions (a)-(c).

(a) To show the equivalence of the sets, we split the proof further into two parts.

(i) We firstly show that $\sigma_p(A)$ is contained in (q_m, q_-) and subset of $\{\lambda \in \mathbb{C} : w_\lambda = 0\}$. Let $\lambda \in \sigma_p(A)$ be an eigenvalue, which implies that $\lambda \in \mathbb{R}$, since A is self-adjoint.

Let $U \in H^2(\mathbb{R})$ be the corresponding eigenfunction, which can be expanded in the form (if $\lambda \notin \{q_+, q_-\}$):

$$U(x) = \begin{cases} c_1 e^{i\sqrt{\lambda - q_-}(x-a)} + c_2 e^{-i\sqrt{\lambda-q_-}(x-a)} & \text{if } x < a, \\ c_3 e^{i\sqrt{\lambda-q_+}(x-b)} + c_4 e^{-i\sqrt{\lambda-q_+}(x-b)} & \text{if } x > b. \end{cases}$$

If $\lambda > q_-$, then both terms for $x < a$ do not decay, and hence $U = 0$ on $(-\infty, a)$, which implies that $U = 0$ everywhere by the unique continuation principle, a contradiction. By the same argument we can rule out $\lambda \in \{q_+, q_-\}$, with the terms for $x < a$ (or $x > b$) replaced by $c_1 + c_2 x$. Hence this is not possible, and there are no eigenvalues larger than q_-.

Let $\lambda < q_-$. The terms after the coefficients c_1 and c_4 increase exponentially on their domains, and since $U \in H^2(\mathbb{R})$, we obtain $c_1 = c_4 = 0$, so that

$$U(x) = \begin{cases} c_2 e^{-i\sqrt{\lambda-q_-}(x-a)} & \text{if } x < a, \\ c_3 e^{i\sqrt{\lambda-q_+}(x-b)} & \text{if } x > b. \end{cases} \tag{2.4.9}$$

Comparing coefficients for $x < a$, we obtain $U(x) = c_2 v_\lambda^+(x)$, while by comparing coefficients for $x > b$, we obtain $U(x) = c_3 v_\lambda^-(x)$. Since $c_2 \neq 0 \neq c_3$, this implies that v_λ^+ and v_λ^- are linearly dependent, and hence $w_\lambda = 0$. This shows that $\sigma_p(A) \subset \{\lambda \in \mathbb{C} : w_\lambda = 0\}$.

Let us show that $\lambda \leq q_m$ cannot be an eigenvalue: multiplying $AU(x) = \lambda U(x)$ by $\overline{U}(x)$, integrating over $\mathbb{R}$ and using integration by parts we obtain

$$\int_{\mathbb{R}} |\partial_x U|^2 + (q(x) - \lambda)|U|^2 \,\mathrm{d}x = 0.$$

Since $q(x) - \lambda \geq 0$ for almost all $x \in \mathbb{R}$, this implies that $\int_{\mathbb{R}} |\partial_x U|^2 \,\mathrm{d}x = 0$, so U must be constant, which implies $U = 0$ since $U \in H^2(\mathbb{R})$. Thus, we have shown that $\sigma_p(A) \subset (q_m, q_-)$.

(ii) Let us now prove that $\sigma_p(A) \supset \{\lambda \in \mathbb{C} : w_\lambda = 0\} \setminus \{q_-\}$, i.e. that any zero of w_λ (except q_-) is also an eigenvalue: let $\lambda \in \mathbb{C}$ be such that $w_\lambda = 0$. So v_λ^+ and v_λ^- are linearly dependent, and we have $c \in \mathbb{C}$ such that $v_\lambda^+ = c v_\lambda^-$, from which we obtain by comparing coefficients for $x < a$ and $x > b$ that v_λ^+ must be of the form (2.4.9).

If $\lambda \in \mathbb{C} \setminus [q_-, +\infty)$, any solution U of the form (2.4.9) is an eigenfunction, since it decays exponentially as $x \to \pm\infty$. Hence $v_\lambda^\pm$ are eigenfunctions, implying $\lambda \in \sigma_p(A)$.

If $\lambda > q_-$, $\lambda \neq q_+$, we can apply the energy conservation relation (2.2.3) to $v_\lambda^+ = c v_\lambda^-$ to obtain

$$\mathrm{Re}(\sqrt{\lambda - q_-}) + \mathrm{Re}(\sqrt{\lambda - q_+})|\beta_\lambda^+|^2 = 0,$$

where β_λ^+ is the coefficient in the expansion (2.4.4). This gives a contradiction, since the first term is strictly larger than zero, while the second larger or equal zero.

Note that we have not considered the behaviour of the Wronskian at q_+: it holds that $w_{q_+} \neq 0$, which will be shown at the end of the proof.

(b) Let us prove that there exist only finitely many eigenvalues, that is, solutions to $w_\lambda = 0$. Since all zeros are contained in the bounded interval $(q_m, q_-]$, it is sufficient to show that there are no accumulation points of zeros in $[q_m, q_-]$. Let us rewrite w_λ as

$$w_\lambda = i\sqrt{\lambda - q_-}\Bigg(\frac{-t_{21}(\lambda) + it_{11}(\lambda)\sqrt{\lambda - q_+}}{i\sqrt{\lambda - q_-}} - \Big(t_{21}(\lambda) - it_{12}(\lambda)\sqrt{\lambda - q_+}\Big)\Bigg),$$

so that $\lambda \in (-\infty, q_-)$ solves $w_\lambda = 0$ if and only if

$$0 = \frac{g(\lambda)}{i\sqrt{\lambda - q_-}} - h(\lambda), \tag{2.4.10}$$

where the functions g and h are defined by

$$\begin{aligned} g(\lambda) &:= -t_{21}(\lambda) + it_{11}(\lambda)\sqrt{\lambda - q_+}, \\ h(\lambda) &:= -t_{22}(\lambda) + it_{12}(\lambda)\sqrt{\lambda - q_+}. \end{aligned}$$

Now assume there exists an infinite sequence $(\lambda_j)_{j\in\mathbb{N}}$ of solutions to (2.4.10). Since all zeros of (2.4.10) are contained in $(q_m, q_-]$ and since the right hand side of (2.4.10) is holomorphic on $\{\lambda \in \mathbb{C} : \mathrm{Re}(\lambda) < q_-\}$, the sequence $(\lambda_j)_{j\in\mathbb{N}}$ must converge to q_-. Here we used that holomorphic functions cannot have accumulation points in the interior of their domain.

Let us now consider the right hand side of (2.4.10) around q_-: since g and h are holomorphic in a neighbourhood of q_-, there exist holomorphic functions $\tilde{g}$ and $\tilde{h}$ as well as $p_1,\ p_2 \in \mathbb{N} \cup \{0\}$ such that

$$\begin{aligned} g(\lambda) &= (\lambda - q_-)^{p_1}\tilde{g}(\lambda), \\ h(\lambda) &= (\lambda - q_-)^{p_2}\tilde{h}(\lambda), \end{aligned}$$

for λ in a neighbourhood of q_-. Inserting those into (2.4.10) for $\lambda = \lambda_j$, we obtain

$$0 = \frac{g(\lambda_j)}{i\sqrt{\lambda_j - q_-}} - h(\lambda_j) = \frac{(\lambda_j - q_-)^{p_1}\tilde{g}(\lambda_j)}{i\sqrt{\lambda_j - q_-}} - (\lambda_j - q_-)^{p_2}\tilde{h}(\lambda_j),$$

which can be reformulated after a straightforward manipulation to

$$\tilde{h}(\lambda_j) = (\lambda_j - q_-)^{p_1 - p_2 - \frac{1}{2}}\tilde{g}(\lambda_j).$$

Let us take the limit $j \to +\infty$ in this equations. The left hand side converges to $\tilde{h}(q_-) \neq 0$, while the right hand side converges either to 0 (if $p_1 - p_2 - 1/2 > 0$) or to $\pm\infty$ (if $p_1 - p_2 - 1/2 < 0$), depending on the sign of $g(q_-) \neq 0$. In any case, this gives a contradiction.

(c) Let now $w_{q_-} = 0$. We will again only consider the case $q_- < q_+$, since the case $q_+ = q_-$ is simpler. Rewriting (2.4.8), we obtain

$$\begin{aligned} w_\lambda = {} & -t_{21}(\lambda) + it_{11}(\lambda)\sqrt{\lambda - q_+} \\ & + i\sqrt{\lambda - q_-}\Big(t_{22}(\lambda) - it_{12}(\lambda)\sqrt{\lambda - q_+}\Big). \end{aligned} \tag{2.4.11}$$

Setting $\lambda = q_-$, we obtain from $w_{q_-} = 0$

$$t_{21}(q_-) = it_{11}(q_-)\sqrt{q_- - q_+}.$$

This implies that $t_{22}(q_-) - it_{12}(q_-)\sqrt{q_- - q_+} \neq 0$: assume on the contrary, that also $t_{22}(q_-) - it_{12}(q_-)\sqrt{q_- - q_+} = 0$. Then

$$\begin{aligned}\det T_{q_-} &= t_{11}(q_-)t_{22}(q_-) - t_{12}(q_-)t_{21}(q_-)\\ &= t_{11}(q_-)it_{12}(q_-)\sqrt{q_- - q_+} - t_{12}(q_-)it_{11}(q_-)\sqrt{q_- - q_+}\\ &= 0,\end{aligned}$$

which cannot happen by Definition and Lemma 2.4.3. Hence we have for λ in a neighbourhood of q_-

$$\begin{aligned}-t_{21}(\lambda) + it_{11}(\lambda)\sqrt{\lambda - q_+} &= \mathcal{O}(|\lambda - q_-|),\\ t_{22}(\lambda) - it_{12}(\lambda)\sqrt{\lambda - q_+} &= C + \mathcal{O}(|\lambda - q_-|),\end{aligned}$$

where $C = t_{22}(q_-) - it_{12}(q_-)\sqrt{q_- - q_+} \neq 0$. Note that both functions on the left are holomorphic in a neighbourhood of q_-, and allow a zeroth order Taylor expansion with an error in $\mathcal{O}(|\lambda - q_-|)$. Accordingly

$$\begin{aligned}w_\lambda &= \mathcal{O}(|\lambda - q_-|) + \sqrt{\lambda - q_-}(C + \mathcal{O}(|\lambda - q_-|))\\ &= C\sqrt{\lambda - q_-} + \mathcal{O}(|\lambda - q_-|).\end{aligned}$$

Note also that this approximation holds despite w_λ being discontinuous around q_-, since the square root $\sqrt{\lambda - q_-}$ is discontinuous as a complex function there. As a function on $\mathbb{R}$, however, w_λ is continuous.

Let us finish the proof by picking up the last morsel, namely that $w_{q_+} \neq 0$. Assume that $w_{q_+} = 0$, and consider $\lambda \in (q_-, q_+)$: note that for these λ, the first two summands in (2.4.11) are real, while the third summand is strictly imaginary. Thus from the continuity on the positive real axis we have $w_\lambda \to 0$ as $\lambda \to q_+$ from the left, and obtain

$$-t_{21}(\lambda) + it_{11}(\lambda)\sqrt{\lambda - q_+} \to 0 \quad \text{and} \quad t_{22}(\lambda) - it_{12}(\lambda)\sqrt{\lambda - q_+} \to 0$$

as $\lambda \to q_+$, $\lambda < q_+$. This, however, implies that $t_{21}(q_+) = 0$ and $t_{22}(q_+) = 0$, which again implies $\det(T_{q_+}) = 0$, which is forbidden by Definition and Lemma 2.4.3. ■

We can now give the Green's function of the operator A for the whole resolvent set.

2.4.5 Lemma. For any $\lambda \in \mathbb{C} \setminus (\sigma_p(A) \cup [q_-, \infty))$ and $f \in C_0^\infty(\mathbb{R})$, we have

$$R_\lambda f(x) = \int_{\mathbb{R}} G_\lambda(x, y) f(y)\,\mathrm{d}y,$$

where

$$G_\lambda(x, y) = \frac{1}{w_\lambda}\begin{cases} v_\lambda^+(x)v_\lambda^-(y) & \text{if } x < y,\\ v_\lambda^-(x)v_\lambda^+(y) & \text{if } y < x.\end{cases}$$ ■

Proof. We will only sketch the proof here, since the construction is a standard tool in the theory of ordinary differential equations (see for example [73, Section 1.4]). Note that for $\lambda \in \mathbb{C} \setminus (\sigma_p(A) \cup [q_-, +\infty))$, G_λ is well defined. Define

$$\begin{aligned} u(x) &:= \int_{\mathbb{R}} G_\lambda(x,y) f(y)\,\mathrm{d}y \\ &= \frac{1}{w_\lambda} v_\lambda^-(x) \int_{-\infty}^{x} v_\lambda^+(y) f(y)\,\mathrm{d}y + \frac{1}{w_\lambda} v_\lambda^+(x) \int_{x}^{+\infty} v_\lambda^-(y) f(y)\,\mathrm{d}y. \end{aligned}$$

Firstly, note that u fulfils

$$-\Delta u(x) + (q(x) - \lambda) u(x) = f(x) \qquad \text{for } x \in \mathbb{R},$$

as can be verified via a straightforward calculation: apply Δ to the right hand side of the definition of u, and exploit the fundamental theorem of calculus as well as the fact that $v_\lambda^\pm$ solve the homogeneous equation (2.4.2), and keep in mind the definition of the Wronskian (2.4.6). It remains to show that $u \in L^2(\mathbb{R})$. Since clearly $u \in L^2_{\mathrm{loc}}(\mathbb{R})$ (in fact, u is easily seen to be continuous), we only check the asymptotics of u, exemplarily for the first term on the right hand side. Since $\lambda \in \mathbb{C} \setminus [q_-, \infty)$, we have that $v_\lambda^+(x) \to 0$ as $x \to -\infty$, and $v_\lambda^-(x) \to 0$ as $x \to +\infty$ with exponential decay. Now, let us take the limit $x \to +\infty$ in the first term

$$I_1(x) = v_\lambda^-(x) \int_{-\infty}^{x} v_\lambda^+(y) f(y)\,\mathrm{d}y.$$

If x is large enough, $(-\infty, x)$ will contain $\mathrm{supp}(f)$, and the integral will stay constant. Thus we obtain that that $I_1(x) = C v_\lambda^-(x) \to 0$ exponentially as $x \to \infty$ for some constant $C \in \mathbb{C}$. On the other hand, if we take the limit $x \to -\infty$, we will obtain $(-\infty, x) \cap \mathrm{supp}(f) = \emptyset$ for sufficiently small x, and hence $I_1(x) = 0$. The analogous argument for the second term gives that $u(x)$ converges exponentially to zero as $x \to \pm\infty$, and hence $u \in L^2(\mathbb{R})$, which finishes the proof. ■

We proceed by showing that the continuous spectrum is the interval $[q_-, \infty)$.

2.4.6 Lemma. It holds that

$$\sigma_c(A) = [q_-, +\infty)$$ ■

Proof. By the proof of Lemma 2.4.5, we obtain that the resolvent set $\rho(A) = \{\lambda \in \mathbb{C} : R_\lambda : L^2(\mathbb{R}) \to H^2(\mathbb{R})$, exists, is continuous and bijective$\}$ must contain the set $\mathbb{C} \setminus (\sigma_p(A) \cup [q_-, +\infty))$. We are done if we can show that $[q_-, \infty) \subset \sigma(A)$. Let $\lambda \in (q_-, \infty)$, and for $n \in \mathbb{N}$ let $u_n \in H^2(\mathbb{R})$ be a cut-off of v_λ^+ such that

$$u_n(x) := \begin{cases} 0 & \text{if } x < -n-1, \\ v_\lambda^-(x) & \text{if } -n < x < n, \\ 0 & \text{if } n+1 < x, \end{cases}$$

with extensions on the two intervals $(-n-1, -n)$ and $(n, n+1)$ such that $u_n \in C^2(\mathbb{R})$. Note that $Au_n(x) = \lambda u_n(x)$ for $x \in (-n, n)$, and the extensions can be constructed in a fashion so that $\|Au_n - \lambda u_n\|_{L^2(\mathbb{R})}$ stays bounded, since v_λ^-, $\partial_x v_\lambda^-$ are continuous and bounded on $\mathbb{R}$. Thus

$$\frac{\|Au_n - \lambda u_n\|_{L^2(\mathbb{R})}}{\|u_n\|_{L^2(\mathbb{R})}} \to 0 \qquad \text{as } n \to \infty,$$

which implies by Weyl's criterion [67, Theorem VII.12] that $\lambda \in \sigma(A)$. The Lemma then follows by taking the characterisation of $\sigma_p(A)$ of Lemma 2.4.4 and the closedness of the spectrum into account. ■

The following Lemma gives another technical property for the Wronskian, which will be needed for the integrals related to the singularities of the Green's function.

2.4.7 Lemma. Let $\lambda_n \in \sigma_p(A)$, so that $cv_{\lambda_n}^+ = v_{\lambda_n}^-$ for some $c \neq 0$. Then

$$[\partial_\lambda w_\lambda]|_{\lambda=\lambda_n} = -c\|v_{\lambda_n}^+\|_{L^2(\mathbb{R})}^2. \qquad ■$$

Proof. For some function f depending on λ, we denote by an overdot the derivative with respect to λ, that is $\dot{f} := \partial_\lambda f$. We aim to compute for some $y \in \mathbb{R}$

$$\dot{w}_\lambda = \partial_\lambda W(v_\lambda^+, v_\lambda^-)(y) = W(\dot{v}_\lambda^+, v_\lambda^-)(y) + W(v_\lambda^+, \dot{v}_\lambda^-)(y).$$

We explicitly denoted the dependence on the point $y \in \mathbb{R}$, since the terms on the right hand side depend on y, while the left hand side is constant (as a function of y). First note that from differentiating (2.4.2) with respect to λ we obtain that

$$-\Delta\dot{v}_\lambda^+(x) - (\lambda - q(x))\dot{v}_\lambda^+(x) = v_\lambda^+(x) \qquad \text{for } x \in \mathbb{R}, \tag{2.4.12}$$

while from differentiating (2.4.4) we obtain that

$$\dot{v}_\lambda^+(x) = -\frac{i(x-a)}{2\sqrt{\lambda - q_-}} e^{-i\sqrt{\lambda-q_-}(x-a)} \qquad \text{for } x < a. \tag{2.4.13}$$

With the help of (2.4.2) and (2.4.12), one easily verifies by straightforward calculation that for any $x \in \mathbb{R}$

$$\partial_x W(\dot{v}_\lambda^+, v_\lambda^-)(x) = -v_\lambda^+(x)v_\lambda^-(x).$$

Setting $\lambda = \lambda_n$ in this equation and integrating with respect to x form $y_0 < y$ to y we obtain by the fundamental theorem of calculus

$$W(\dot{v}_{\lambda_n}^+, v_{\lambda_n}^-)(y) - W(\dot{v}_{\lambda_n}^+, v_{\lambda_n}^-)(y_0) = -\int_{y_0}^{y} v_{\lambda_n}^+(x)v_{\lambda_n}^-(x)\,\mathrm{d}x.$$

Since $v_{\lambda_n}^-(x) = cv_{\lambda_n}^+(x)$ and $\dot{v}_{\lambda_n}^-(x)$ as well as their derivatives converge to 0 as $x \to -\infty$, as can be seen from (2.4.4) and (2.4.13), we can take the limit $y_0 \to -\infty$ in the last equation to obtain

$$W(\dot{v}_{\lambda_n}^+, v_{\lambda_n}^-)(y) = -\int_{-\infty}^{y} v_{\lambda_n}^+(x)v_{\lambda_n}^-(x)\,\mathrm{d}x = -c\int_{-\infty}^{y} |v_{\lambda_n}^+(x)|^2\,\mathrm{d}x.$$

Note that we used the fact that $v^+_{\lambda_n}(x) \in \mathbb{R}$ for any $x \in \mathbb{R}$, since the PDE as well as the boundary conditions for $v^+_{\lambda_n}$ are real (due to $\lambda_n \in (q_m, q_-)$ by Lemma 2.4.4). Similarly, one can prove that

$$W(v^+_{\lambda_n}, \dot{v}^-_{\lambda_n})(y) = -c \int_y^\infty |v^+_{\lambda_n}(x)|^2 \, \mathrm{d}x,$$

so that we obtain by adding the last two equations

$$\dot{w}_\lambda = -c \int_{\mathbb{R}} |v^+_{\lambda_n}(x)|^2 \, \mathrm{d}x,$$

which ends the proof. ■

We have to clarify the relation between the expansion basis $\Psi^\pm(\lambda, \cdot)$ and our solutions $v^\pm_\lambda$.

2.4.8 Lemma. For any $\sigma \in \{\pm\}$ and $\lambda \in (q_\sigma, \infty)$ it holds that

$$\frac{v^\sigma_\lambda(x)}{|a^\sigma_\lambda|} = c^\sigma_\lambda \Psi^\sigma(\lambda, x) \qquad \text{for } x \in \mathbb{R},$$

with $|c^\sigma_\lambda| = 1$. Furthermore, there exist constants C_1, C_2 such that for all $m \in \Lambda$ and $x \in \mathbb{R}$

$$|\Psi(m, x)| < C_1, \ |\partial_x \Psi(m, x)| < C_2 \left(1 + \sqrt{|\hat{\lambda}(m)|}\right). \tag{2.4.14}$$

■

Proof. Note that

$$\frac{v^\sigma_\lambda(x)}{|a^\sigma_\lambda|} = c^\sigma_\lambda \Psi^\sigma(\lambda, x) \qquad \text{for } x \in \mathbb{R},$$

with $|c^\sigma_\lambda| = 1$ follows easily by comparing the coefficients of Ψ^- (see Definition 2.2.11) and v^-_λ (see (2.4.4)), and similarly for Ψ^+ and v^+_λ. For the proper eigenfunctions, the statement simply holds by definition.

It remains to show that the bounds for the (generalised) eigenfunctions as well as their derivatives hold. Let us first recall that the mappings $\mathbb{R} \times \mathbb{R} \to \mathbb{C}$, $(\lambda, x) \mapsto v^\sigma_\lambda(x)$ are continuous. Also, note that α^σ_λ cannot vanish for $\lambda \in [q_\sigma, \infty)$: considering v^-_λ, one obtains for $\lambda \in (q_-, q_+)$ that there holds the energy conservation property (2.2.3)

$$\sqrt{\lambda - q_-} |\alpha^-_\lambda|^2 = \sqrt{\lambda - q_-} |\beta^-_\lambda|^2,$$

so that $\alpha^-_\lambda = 0$ would yield $\beta^-_\lambda = 0$, giving $v^-_\lambda = 0$, and by the unique continuation principle, a contradiction. This argument can be continued to obtain that $\lim_{\lambda \to q_-} |\alpha^-_\lambda| \neq 0$, since this would imply that $v^-_{q_-}$ would vanish. The same can be shown for $\lambda \in [q_+, \infty)$. Here we have by (2.2.3) that

$$\sqrt{\lambda - q_-} |\alpha^-_\lambda|^2 = \sqrt{\lambda - q_+} + \sqrt{\lambda - q_-} |\beta^-_\lambda|^2,$$

which implies by the same argument as before that α^-_λ stays away from zero.

Hence the continuity and boundedness of the coefficients of v^-_λ is inherited by the coefficients of $\Psi^-(\lambda, \cdot)$. Furthermore, considering the asymptotics of $\Psi^-(\lambda, x)$ as $x \to \pm\infty$ with help of (2.4.5), one obtains that the bounds (2.4.14) hold for all $x \in \mathbb{R}$ and for

λ on any bounded subset. The critical point is to estimate the terms as $\lambda \to +\infty$. We refer to [50, Theorem 4.5]: from this theorem it easily follows that for any $x \in (a,b)$ one has

$$|v_\lambda^-(x) - e^{-\sqrt{\lambda-q_-}(x-a)}| \le \frac{C}{1+\sqrt{|\lambda|}},$$
$$\text{and } |\partial_x v_\lambda^-(x) - \partial_x e^{-\sqrt{\lambda-q_-}(x-a)}| \le \frac{C}{1+\sqrt{|\lambda|}},$$

so that one obtains the bounds (2.4.14) immediately for $x \in (a,b)$, while they follow for $x > b$ and $x < a$ directly by (2.4.5) (Here we used again that α_λ^- cannot vanish). For $\Psi^+(\lambda,\,\cdot)$, the proof is the same. Note that the estimates for the proper eigenfunctions $\Psi^p(\lambda_n,\,\cdot\,)$ are also easily seen to hold. ■

The definition of the generalised eigenfunctions will play a crucial role in then following lemma. In fact, this is a critical step of the whole process: we rewrite the imaginary part of the Green's function for $\lambda \in (q_-,\infty)$ with help of the generalised eigenfunctions.

2.4.9 Lemma. For any $x, y \in \mathbb{R}$ and real λ, we have the following representations

$$G_\lambda(x,y) - \overline{G}_\lambda(x,y) = \begin{cases} 0 & \text{if } \lambda \in (-\infty,q_-)\setminus\sigma_p(A), \\[2ex] \dfrac{\Psi^-(\lambda,x)\overline{\Psi}^-(\lambda,y)}{-2i\sqrt{\lambda-q_-}} & \text{if } \lambda \in (q_-,q_+), \\[2ex] \displaystyle\sum_{\sigma\in\{\pm\}} \frac{\Psi^\sigma(\lambda,x)\overline{\Psi}^\sigma(\lambda,y)}{-2i\sqrt{\lambda-q_\sigma}} & \text{if } \lambda \in (q_+,+\infty). \end{cases}$$

■

Proof. We only consider the case $x > y$, since the case $x < y$ then follows by symmetry. We have to recompute

$$G_\lambda(x,y) - \overline{G}_\lambda(x,y) = \frac{1}{w_\lambda} v_\lambda^-(x) v_\lambda^+(y) - \frac{1}{\overline{w}_\lambda} \overline{v}_\lambda^-(x)\overline{v}_\lambda^+(y).$$

We will consider the three cases for λ:

(a) If $\lambda \in (-\infty,q_-)\setminus\sigma_p(A)$, then $w_\lambda, v_\lambda^\pm$ are all strictly real, hence it follows that

$$G_\lambda(x,y) - \overline{G}_\lambda(x,y) = 0.$$

(b) Let $\lambda \in (q_-,q_+)$. Then v_λ^- is real, as can be seen from (2.4.4) for $x < a$, and the fact that (2.4.2) has strictly real coefficients. Accordingly, it follows from (2.4.4) for $x > b$ that $\alpha_\lambda^- = \overline{\beta}_\lambda^-$. In other words, $v_\lambda^- = \overline{v}_\lambda^-$.

Since $\overline{v}_\lambda^+$ solves the eigenvalue equation (2.4.2), it must be a linear combination of v_λ^- and v_λ^+. Here we obtain by comparing coefficients for $x < a$

$$\begin{aligned} \overline{v}_\lambda^+(x) &= e^{i\sqrt{\lambda-q_-}\ (x-a)} \\ &= \frac{1}{\alpha_\lambda^-}\left(\alpha_\lambda^- e^{i\sqrt{\lambda-q_-}\ (x-a)} + \beta_\lambda^- e^{-i\sqrt{\lambda-q_-}\ (x-a)}\right) - \frac{\beta_\lambda^-}{\alpha_\lambda^-} e^{-i\sqrt{\lambda-q_a}\ (x-a)} \\ &= \frac{1}{\alpha_\lambda^-} v_\lambda^-(x) - \frac{\beta_\lambda^-}{\alpha_\lambda^-} v_\lambda^+(x). \end{aligned}$$

So with help of the representation for w_λ from equation (2.4.7) it follows

$$G_\lambda(x,y) - \overline{G}_\lambda(x,y) = \frac{1}{w_\lambda} v_\lambda^-(x) v_\lambda^+(y) - \frac{1}{\overline{w}_\lambda} \overline{v}_\lambda^-(x) \overline{v}_\lambda^+(y)$$

$$= v_\lambda^-(x) \left(\frac{1}{w_\lambda} v_\lambda^+(x) - \frac{1}{\overline{w}_\lambda} \left(\frac{1}{\alpha_\lambda^-} v_\lambda^-(x) - \frac{\beta_\lambda^-}{\alpha_\lambda^-} v_\lambda^+(x) \right) \right)$$

$$= v_\lambda^-(x) \frac{1}{2i\sqrt{\lambda - q_-}} \left(\frac{1}{-\alpha_\lambda^-} v_\lambda^+(x) - \frac{1}{\overline{\alpha}_\lambda^-} \frac{1}{\alpha_\lambda^-} v_\lambda^-(x) + \frac{1}{\overline{\alpha}_\lambda^-} \frac{\beta_\lambda^-}{\alpha_\lambda^-} v_\lambda^+(x) \right).$$

Since $\alpha_\lambda^- = \overline{\beta}_\lambda^-$ the terms inside the bracket with $v_\lambda^+(x)$ cancel out, and we obtain

$$G_\lambda(x,y) - \overline{G}_\lambda(x,y) = \frac{1}{-2i\sqrt{\lambda - q_-} |\alpha_\lambda^i|^2} v_\lambda^-(x) \overline{v}_\lambda^-(y),$$

where we used again that v_λ^- is real. Applying Lemma 2.4.8 yields the representation.

(c) Now let $\lambda > q_+$. In this case, neither v_λ^+ nor v_λ^- are real, so we have to calculate the representation of both conjugates $\overline{v}_\lambda^+$ and $\overline{v}_\lambda^-$. By comparing coefficients for $x < a$, we obtain

$$\overline{v}_\lambda^+(x) = e^{i\sqrt{\lambda - q_-}(x-a)} = \frac{1}{\alpha_\lambda^-} v_\lambda^-(x) - \frac{\beta_\lambda^-}{\alpha_\lambda^-} v_\lambda^+(x).$$

Similarly, we can obtain another representation by comparing the coefficients for $x > b$, which yields (we omit the details of the calculations here):

$$\overline{v}_\lambda^+(x) = \frac{|\alpha_\lambda^+|^2 - |\beta_\lambda^+|^2}{\alpha_\lambda^+} v_\lambda^-(x) + \frac{\overline{\beta}_\lambda^+}{\alpha_\lambda^+} v_\lambda^+(x).$$

If we compare the two different representations for $\overline{v}_\lambda^+$, we obtain by considering the coefficients in front of v_λ^+ on the right hand side that

$$\frac{\overline{\beta}_\lambda^+}{\alpha_\lambda^+} = -\frac{\beta_\lambda^-}{\alpha_\lambda^-}. \tag{2.4.15}$$

Repeating the same procedure for $\overline{v}_\lambda^-$, we end up with the following "conjugation matrix":

$$\begin{pmatrix} \overline{v}_\lambda^-(x) \\ \overline{v}_\lambda^+(x) \end{pmatrix} = \begin{pmatrix} -\frac{\beta_\lambda^+}{\alpha_\lambda^+} & \frac{1}{\alpha_\lambda^+} \\ \frac{1}{\alpha_\lambda^-} & -\frac{\beta_\lambda^-}{\alpha_\lambda^-} \end{pmatrix} \begin{pmatrix} v_\lambda^-(x) \\ v_\lambda^+(x) \end{pmatrix} =: K \begin{pmatrix} v_\lambda^-(x) \\ v_\lambda^+(x) \end{pmatrix}.$$

Note that taking the conjugate of the last equation one obtains $K^{-1} = \overline{K}$. Let us use the conjugation matrix K to rewrite the Greens function

$$G_\lambda(x,y) - \overline{G}_\lambda(x,y) = \frac{1}{w_\lambda} v_\lambda^-(x) v_\lambda^+(y) - \frac{1}{\overline{w}_\lambda} \overline{v}_\lambda^-(x) \overline{v}_\lambda^+(y)$$

$$= \begin{pmatrix} v_\lambda^-(x) \\ v_\lambda^+(x) \end{pmatrix}^\top \begin{pmatrix} 0 & 1/w_\lambda \\ 0 & 0 \end{pmatrix} \begin{pmatrix} v_\lambda^-(y) \\ v_\lambda^+(y) \end{pmatrix} + \begin{pmatrix} \overline{v}_\lambda^-(x) \\ \overline{v}_\lambda^+(x) \end{pmatrix}^\top \begin{pmatrix} 0 & 1/\overline{w}_\lambda \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \overline{v}_\lambda^-(y) \\ \overline{v}_\lambda^+(y) \end{pmatrix}$$

$$= \begin{pmatrix} v_\lambda^-(x) \\ v_\lambda^+(x) \end{pmatrix}^\top \left[\begin{pmatrix} 0 & 1/w_\lambda \\ 0 & 0 \end{pmatrix} \overline{K} + K^\top \begin{pmatrix} 0 & 1/\overline{w}_\lambda \\ 0 & 0 \end{pmatrix} \right] \begin{pmatrix} \overline{v}_\lambda^-(y) \\ \overline{v}_\lambda^+(y) \end{pmatrix},$$

where we used K to transform the $v_\lambda^\pm$ vector on the right in the first summand, and on the left for the second summand. Explicitly calculating the matrix in the middle we obtain

$$G_\lambda(x,y) - \overline{G}_\lambda(x,y) = \begin{pmatrix} v_\lambda^-(x) \\ v_\lambda^+(x) \end{pmatrix}^\top \begin{pmatrix} \frac{1}{w_\lambda \overline{\alpha}_\lambda^-} & \frac{\beta_\lambda^+}{\overline{w}_\lambda \alpha_\lambda^+} - \frac{\overline{\beta}_\lambda^-}{w_\lambda \overline{\alpha}_\lambda^-} \\ 0 & -\frac{1}{\overline{w}_\lambda \alpha_\lambda^+} \end{pmatrix} \begin{pmatrix} \overline{v}_\lambda^-(y) \\ \overline{v}_\lambda^+(y) \end{pmatrix}. \tag{2.4.16}$$

Let us recalculate each of the entries. We have by (2.4.7)

$$\frac{1}{w_\lambda \overline{\alpha}_\lambda^-} = \frac{1}{-2i\sqrt{\lambda - q_-}|\alpha_\lambda^-|^2} \quad \text{and} \quad -\frac{1}{\overline{w}_\lambda \alpha_\lambda^+} = \frac{1}{-2i\sqrt{\lambda - q_+}|\alpha_\lambda^+|^2}.$$

For the third coefficient we can calculate with the help of (2.4.15) and (2.4.7):

$$\begin{aligned} \frac{\beta_\lambda^+}{\overline{w}\alpha_\lambda^+} - \frac{\overline{\beta}_\lambda^-}{w\overline{\alpha}_\lambda^-} &= \frac{\beta_\lambda^+}{\overline{w}\alpha_\lambda^+} + \frac{\beta_\lambda^+}{w\overline{\alpha}_\lambda^+} \\ &= \beta_\lambda^+ \left(\frac{1}{2i\sqrt{\lambda - q_+}|\alpha_\lambda^+|^2} + \frac{1}{-2i\sqrt{\lambda - q_+}|\alpha_\lambda^+|^2} \right) \\ &= 0. \end{aligned}$$

Plugging this into (2.4.16) and applying Lemma 2.4.8 ends the proof.

∎

We are finally done with technical preliminaries, and can apply Stone's formula.

2.4.10 Lemma. For any $f \in C_0^\infty(\mathbb{R})$ and any $h_1 < h_2$ with $h_1, h_2 \notin \sigma_p(A)$ we have

$$\begin{aligned} &\frac{1}{2}\big(P_{(h_1,h_2)} f(x) + P_{[h_1,h_2]} f(x)\big) \\ &= \sum_{\lambda_n \in (h_1,h_2)} \Psi^p(\lambda_n, x)\langle f, \Psi^p(\lambda_n, \cdot\,)\rangle_{\mathbb{R}} \\ &\quad + \frac{1}{2\pi} \sum_{\sigma \in \{\pm\}} \int_{\max\{h_1,q_\sigma\}}^{\max\{h_2,q_\sigma\}} \Psi^\sigma(\lambda, x)\langle f, \Psi^\sigma(\lambda, \cdot\,)\rangle_{\mathbb{R}} \frac{\mathrm{d}\lambda}{2\sqrt{\lambda - q_\sigma}}. \end{aligned}$$

∎

Proof. We assume that $h_1 < q_-$ and $q_+ < h_2$ for simplicity, to have all relevant terms appear in the calculation. We rewrite Stone's formula into two parts, which we will

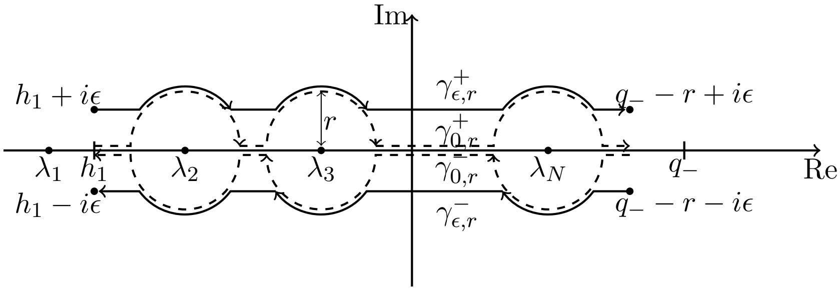

Figure 2.4: The paths $\gamma^+_{\epsilon,r}, \gamma^-_{\epsilon,r}, \gamma^+_{0,r}, \gamma^-_{0,r}$ from the proof of Lemma 2.4.10.

consider separately

$$\begin{aligned}
\frac{1}{2}\big(P_{(h_1,h_2)}f(x) + P_{[h_1,h_2]}f(x)\big) &= \frac{1}{2\pi i}\lim_{\epsilon\to 0}\int_{h_1}^{h_2} R_{\lambda+i\epsilon}f(x) - R_{\lambda-i\epsilon}f(x)\,\mathrm{d}\lambda \\
&= \frac{1}{2\pi i}\Bigg(\lim_{\epsilon\to 0}\int_{h_1}^{q_- - r} R_{\lambda+i\epsilon}f(x) - R_{\lambda-i\epsilon}f(x)\,\mathrm{d}\lambda \\
&\qquad + \lim_{\epsilon\to 0}\int_{q_- - r}^{h_2} R_{\lambda+i\epsilon}f(x) - R_{\lambda-i\epsilon}f(x)\,\mathrm{d}\lambda\Bigg) \\
&= \frac{1}{2\pi i}(I_1 + I_2),
\end{aligned}$$

where $r > 0$ is sufficiently small such that $\sigma_p(A) \subset (-\infty, q_- - r)$. We rewrite I_1 as follows

$$I_1 = \lim_{\epsilon\to 0}\left(\int_{\gamma^+_{\epsilon,r}} R_\lambda f(x)\,\mathrm{d}\lambda + \int_{\gamma^-_{\epsilon,r}} R_\lambda f(x)\,\mathrm{d}\lambda\right),$$

where $\gamma^+_{\epsilon,r}$ and $\gamma^-_{\epsilon,r}$ are the paths as shown in Figure 2.4, which go from $h_1 + i\epsilon$ to $-q_m - r + i\epsilon$ (and from $-q_m - r - i\epsilon$ to $h_1 - i\epsilon$, respectively) and avoid the singularities of $G_\lambda(x,y)$ at the elements of the point spectrum. Taking the limit $\epsilon \to 0$, and noting that the parts of $\gamma^+_{0,r}$ and $\gamma^-_{0,r}$ on the real line cancel each other out, we obtain

$$I_1 = \int_{\gamma^+_{0,r}} R_\lambda f(x)\,\mathrm{d}\lambda + \int_{\gamma^-_{0,r}} R_\lambda f(x)\,\mathrm{d}\lambda = \sum_{\lambda_n\in(h_1,-q_m)}\int_{\lambda_n + rS^1} R_\lambda f(x)\,\mathrm{d}\lambda,$$

where $\lambda_n + rS^1 = \{z \in \mathbb{C} : z = \lambda_n + re^{-i\theta}, \theta \in (0, 2\pi)\}$ denotes the clockwise circlic path around λ_n with radius r. In other words, we have to calculate the residuals of $R_\lambda f(x)$ at the eigenvalues λ_n. Representing the resolvent (Lemma 2.4.5) by the Green's function and using Fubini's Theorem we obtain

$$
\begin{aligned}
\int\limits_{\lambda_n+rS^1} R_\lambda f(x)\,\mathrm{d}\lambda &= \int\limits_{\lambda_n+rS^1}\int\limits_{\mathbb{R}} G_\lambda(x,y)f(y)\,\mathrm{d}y\,\mathrm{d}\lambda \\
&= \int\limits_{-\infty}^{x}\int\limits_{\lambda_n+rS^1} \frac{1}{w_\lambda} v_\lambda^-(x)v_\lambda^+(y)\,\mathrm{d}\lambda\, f(y)\,\mathrm{d}y \\
&\quad + \int\limits_{x}^{+\infty}\int\limits_{\lambda_n+rS^1} \frac{1}{w_\lambda} v_\lambda^+(x)v_\lambda^-(y)\,\mathrm{d}\lambda\, f(y)\,\mathrm{d}y.
\end{aligned}
\tag{2.4.17}
$$

Let us take the limit $r \to 0$ of the first integral: the mapping $\lambda \mapsto v_\lambda^\pm(x)$ converges (uniformly with respect to x in some compact subset) as $\lambda \to \lambda_n$ by Lemma 2.4.3. However, $1/w_\lambda$ is singular, but we have $w_\lambda = (\partial_\lambda w_{\lambda_n})\cdot(\lambda-\lambda_n)+\mathcal{O}(|\lambda-\lambda_n|^2)$ by Taylor expansion around λ_n, where $\partial_\lambda w_{\lambda_n} = -c\|v_{\lambda_n}^+\|_{L^2(\mathbb{R})}^2 \neq 0$ by Lemma 2.4.7 ($c \in \mathbb{C}\setminus\{0\}$ being the constant from the very same lemma), so that

$$
\begin{aligned}
\int\limits_{\lambda_n+rS^1} \frac{1}{w_\lambda} v_\lambda^-(x)v_\lambda^+(y)\,\mathrm{d}\lambda &= \int\limits_0^{2\pi} \frac{1}{(\partial_\lambda w_{\lambda_n})re^{-i\theta}+\mathcal{O}(r^2)} v_\lambda^-(x)v_\lambda^+(y)(-ire^{-i\theta})\,\mathrm{d}\theta \\
&= -\frac{2\pi i}{\partial_\lambda w_{\lambda_n}} v_{\lambda_n}^-(x)v_{\lambda_n}^+(y), \qquad \text{by letting } r\to 0.
\end{aligned}
$$

In view of $v_{\lambda_n}^- = cv_{\lambda_n}^+$ (see again Lemma 2.4.7), we obtain that

$$
\begin{aligned}
-\frac{2\pi i}{\partial_\lambda w_{\lambda_n}} v_{\lambda_n}^+(x)v_{\lambda_n}^-(y) &= -\frac{2\pi i}{-c\|v_{\lambda_n}^+\|_{L^2(\mathbb{R})}^2}\left(cv_{\lambda_n}^+(x)\right)v_{\lambda_n}^+(y) \\
&= 2\pi i \Psi^p(\lambda_n,x)\Psi^p(\lambda_n,y),
\end{aligned}
$$

since $\Psi^p(\lambda_n,x) = \|v_{\lambda_n}^+\|_{L^2(\mathbb{R})}^{-1} v_{\lambda_n}^+(x)$ is the normalised eigenfunction corresponding to λ_n (see Theorem 2.2.3). Performing the same calculation for the second integral of (2.4.17), we obtain that we can rewrite (2.4.17) as

$$
\begin{aligned}
&\int\limits_{\lambda_n+rS^1} R_\lambda f(x)\,\mathrm{d}\lambda \\
&= 2\pi i \int\limits_{-\infty}^{x} \Psi^p(\lambda_n,x)\Psi^p(\lambda_n,y)f(y)\,\mathrm{d}y + 2\pi i \int\limits_{x}^{\infty} \Psi^p(\lambda_n,x)\Psi^p(\lambda_n,y)f(y)\,\mathrm{d}y \\
&= 2\pi i\ \Psi^p(\lambda_n,x)\langle f, \Psi^p(\lambda_n,\,\cdot\,)\rangle_{\mathbb{R}}
\end{aligned}
$$

where we used that $\Psi^p(\lambda_n,\,\cdot\,)$ is strictly real, that is $\Psi^p(\lambda_n,\,\cdot\,) = \overline{\Psi}^p(\lambda_n,\,\cdot\,)$. So we arrive at our final result for I_1, namely that

$$
I_1 = 2\pi i \sum_{\substack{n\in\{1,\dots,N\}\\ \lambda_n\in(h_1,-q_m)}} \Psi^p(\lambda_n,x)\langle f, \Psi^p(\lambda_n,\,\cdot\,)\rangle_{\mathbb{R}}.
$$

Now let us consider I_2, given by

$$I_2 = \lim_{\epsilon\to 0}\left(\int_{q_--r}^{h_2} R_{\lambda+i\epsilon}f(x)\,\mathrm{d}\lambda - \int_{q_--r}^{h_2} R_{\lambda-i\epsilon}f(x)\,\mathrm{d}\lambda\right).$$

Let us consider the first integral, and recall we still keep $x \in \mathbb{R}$ fixed. By Lemma 2.4.5 we have

$$\lim_{\epsilon\to 0}\int_{q_--r}^{h_2} R_{\lambda+i\epsilon}f(x)\,\mathrm{d}\lambda = \lim_{\epsilon\to 0}\int_{q_--r}^{h_2}\int_{\mathbb{R}} G_{\lambda+i\epsilon}(x,y)f(y)\,\mathrm{d}y\,\mathrm{d}\lambda.$$

We want to exchange integration and limit. The dominated convergence theorem tells us that this is possible, provided we find some integrable $g : [q_- - r, h_2]\times \operatorname{supp}(f) \to \mathbb{R}$ such that

$$|G_{\lambda+i\epsilon}(x,y)f(y)| \le g(\lambda,y) \qquad \text{for all } \lambda \in [q_- - r, h_2], y \in \operatorname{supp}(f) \text{ and } \epsilon \in [0,\epsilon_0].$$

Since the two functions $(\lambda, x) \mapsto v_\lambda^\pm(x)$ are continuous on the compact set

$$M = \{(\lambda_0 + i\epsilon, x) \in \mathbb{C}\times\mathbb{R} : \lambda_0 \in [q_- - r, h_2],\ \epsilon \in [0,\epsilon_0],\ x \in \operatorname{supp}(f)\}$$

by Lemma 2.4.3, we obtain a constant $B > 0$ such that

$$|v^\pm_{\lambda+i\epsilon}(y)| \le B \qquad \text{for all } \lambda \in [q_- - r, h_2],\ y \in \operatorname{supp}(f) \text{ and } \epsilon \in [0,\epsilon_0],$$

and it follows that

$$|G_{\lambda+i\epsilon}(x,y)f(y)| \le \frac{B^2\|f\|_{L^\infty(\mathbb{R})}}{|w_{\lambda+i\epsilon}|},$$

so we only have to find a majorant for $1/|w_{\lambda+i\epsilon}|$. The map $\lambda \mapsto w_\lambda$ is continuous for $\lambda \in \hat{M} = \{\lambda \in \mathbb{C} : \mathrm{Re}(\lambda) \in [q_- - r, h_2],\ \mathrm{Im}(\lambda) \in [0,\epsilon_0]\}$, and it can only be zero at q_-. If w_λ has no zero at q_-, we are done, since then $1/|w_\lambda| \le C$ for $\lambda \in \hat{M}$, and we have found a majorant. Assume that $w_{q_-} = 0$. Then we have according to Lemma 2.4.4 (c) some constant $C \in \mathbb{C}\setminus\{0\}$ such that for $\lambda + i\epsilon$ in a neighbourhood of q_-:

$$\frac{1}{|w_{\lambda+i\epsilon}|} = \frac{1}{|C\sqrt{\lambda + i\epsilon - q_-} + \mathcal{O}(|\lambda + i\epsilon - q_-|)|} \le \frac{\tilde{C}}{\sqrt{|\lambda - q_-|}},$$

where the last estimate can be seen by elementary calculation, provided that the neighbourhood is small enough. Outside this neighbourhood $\lambda \mapsto w_\lambda$ is continuous and has no zeros, hence $1/w_\lambda \le \hat{C}$. So we obtain that

$$\frac{1}{|w_{\lambda+i\epsilon}|} \le \frac{\tilde{C}}{\sqrt{|\lambda - q_-|}} + \hat{C} \qquad \text{for any } \lambda \in [q_- - r, h_2], \epsilon \in [0,\epsilon_0].$$

The right hand side is integrable, and hence we have found the majorant

$$g(\lambda,y) = B^2\|f\|_{L^\infty(\mathbb{R})}\left(\frac{\tilde{C}}{\sqrt{|\lambda - q_-|}} + \hat{C}\right),$$

which is integrable on $[q_- - r, h_2] \times \operatorname{supp}(f)$. By the dominated convergence theorem we now obtain

$$\lim_{\epsilon\to 0} \int_{q_- - r}^{h_2} R_{\lambda+i\epsilon} f(x)\,\mathrm{d}\lambda = \int_{q_- - r}^{h_2} \int_{\mathbb{R}} G_\lambda(x,y) f(y)\,\mathrm{d}y\,\mathrm{d}\lambda.$$

For the second integral in I_2, we cannot do the very same procedure, since $G_{\lambda-i\epsilon}(x,y)$ does not converge to $G_\lambda(x,y)$ as $\epsilon \to 0$, since the square root is chosen precisely so that the jump happens at the point $\epsilon = 0$. However, since A has purely real coefficients, one easily verifies that we must have $G_\lambda(x,y) = \overline{G}_{\overline{\lambda}}(x,y)$, so that

$$\begin{aligned}\lim_{\epsilon\to 0} \int_{q_- - r}^{h_2} R_{\lambda-i\epsilon} f(x)\,\mathrm{d}\lambda &= \lim_{\epsilon\to 0} \int_{q_- - r}^{h_2} \int_{\mathbb{R}} \overline{G}_{\lambda+i\epsilon}(x,y) f(y)\,\mathrm{d}y\,\mathrm{d}\lambda \\ &= \int_{q_- - r}^{h_2} \int_{\mathbb{R}} \overline{G}_\lambda(x,y) f(y)\,\mathrm{d}y\,\mathrm{d}\lambda.\end{aligned}$$

From this now follows

$$I_2 = \int_{q_-}^{h_2} \int_{\mathbb{R}} \left(G_\lambda(x,y) - \overline{G}_\lambda(x,y)\right) f(y)\,\mathrm{d}y\,\mathrm{d}\lambda,$$

where we used that $G_\lambda(x,y) = \overline{G}_\lambda(x,y)$ for $\lambda < q_-$. An application of Lemma 2.4.9 to rewrite $G_\lambda(x,y) - \overline{G}_\lambda(x,y)$ and trivial rearrangements now end the proof. ■

2.4.11 Corollary. For $\rho > \|q\|_{L^\infty(\mathbb{R})}$ and $f \in C_0^\infty(\mathbb{R})$ we have

$$\begin{aligned}P_{(-\rho,\rho)} f(x) = &\sum_{n=1}^{N} \Psi^p(\lambda_n, x)\langle f, \Psi^p(\lambda_n,\,\cdot\,)\rangle_{\mathbb{R}} \\ &+ \frac{1}{2\pi} \sum_{\sigma=\pm} \int_{q_\sigma}^{\rho} \Psi^\sigma(\lambda, x)\langle f, \Psi^\sigma(\lambda,\,\cdot\,)\rangle_{\mathbb{R}} \frac{\mathrm{d}\lambda}{2\sqrt{\lambda - q_\sigma}}.\end{aligned}$$

Furthermore, $P_{(-\rho,\rho)} f \to f$ in $L^2(\mathbb{R})$ as $\rho \to \infty$. ■

Proof. For $\rho > \|q\|_{L^\infty(\mathbb{R})}$, the interval $(-\rho,\rho)$ contains the whole point spectrum, and hence the sum over the proper eigenfunctions contains all of them. Since the integrals on the right hand side are dominated by the Lebesgue measure $\mathrm{d}\lambda$, we have $P_{(-\rho,\rho)} = P_{[-\rho,\rho]}$, and so the first assertion follows by Lemma 2.4.10.

The $L^2(\mathbb{R})$ convergence now follows from general properties of the projection valued measure, since $P_{(-\rho,\rho)}$ converges to I in the strong operator topology (see [67, Remark after Theorem VIII.5]). ■

The previous corollary will be the germ statement that allows us to derive all required properties of the generalised Fourier transform. Let us start by showing its unitarity.

2.4.12 Lemma. Let $f, g \in C_0^\infty(\mathbb{R})$, and denote by $\tilde{f}, \tilde{g} : \Lambda \to \mathbb{C}$ the transforms of f and g, i.e.

$$\tilde{f}(m) = \mathcal{F}_A f(m) = \int_{\mathbb{R}} f(x)\overline{\Psi}(m,x)\,\mathrm{d}x,$$

and similarly $\tilde{g} = \mathcal{F}_A g$. Then we have Parseval's equality

$$\langle f, g\rangle_{\mathbb{R}} = \langle \tilde{f}, \tilde{g}\rangle_\Lambda,$$

and $\mathcal{F}_A$ can be extended to a unitary isomorphism $\mathcal{F}_A : L^2(\mathbb{R}) \to \mathcal{R}(\mathcal{F}_A)$, where the range $\mathcal{R}(\mathcal{F}_A)$ is understood as a subspace of the Hilbert space $L^2(\Lambda, \mathrm{d}\mu)$. ■

Proof. Let $f \in C_0^\infty(\mathbb{R})$, and let $\tilde{f}(m)$ be defined by the integral above: note that the integral is (point-wise) well-defined, since $\langle f, \Psi^p(\lambda_n, \cdot\,)\rangle_{\mathbb{R}}$ is clearly finite, and that

$$|\tilde{f}^\sigma(\lambda)| = \left| \int_{\mathbb{R}} f(x)\overline{\Psi}^\sigma(\lambda,x)\,\mathrm{d}x \right| \le \|\Psi^\sigma(\lambda,\cdot\,)\|_{L^\infty(\mathbb{R})}\|f\|_{L^1(\mathbb{R})} \le C_1\|f\|_{L^1(\mathbb{R})},$$

by Hölders inequality and since $|\Psi^\sigma(x,\lambda)| < C_1$ by Lemma 2.4.8 for any $\sigma \in \{\pm\}$, $\lambda \in (q_\sigma, \infty)$. Now let $f_\rho := P_{(-\rho,\rho)}f$, that is

$$f_\rho(x) = \sum_{n=1}^N \Psi^p(\lambda_n, x)\tilde{f}^p(\lambda_n) + \frac{1}{2\pi}\sum_{\sigma\in\{\pm\}}\int_{q_\sigma}^{\rho} \Psi^\sigma(\lambda,x)\tilde{f}^\sigma(\lambda)\frac{\mathrm{d}\lambda}{2\sqrt{\lambda - q_\sigma}}$$

Multiplying the last equation by $\overline{f}(x)$, and integrating over $\mathbb{R}$ we obtain

$$\begin{aligned}\langle f_\rho, f\rangle_{\mathbb{R}} &= \sum_{n=1}^N \int_{\mathbb{R}} \overline{f}(x)\Psi^p(\lambda_n,x)\,\mathrm{d}x\ \tilde{f}^p(\lambda_n)\\ &\quad + \frac{1}{2\pi}\sum_{\sigma\in\{\pm\}}\int_{q_\sigma}^{\rho}\int_{\mathbb{R}} \overline{f}(x)\Psi^\sigma(\lambda,x)\,\mathrm{d}x\ \tilde{f}^\sigma(\lambda)\frac{\mathrm{d}\lambda}{2\sqrt{\lambda - q_\sigma}},\end{aligned}$$

where we used that the integrand

$$\overline{f}(x)\Psi_\sigma(\lambda,x)\tilde{f}^\sigma(\lambda)\frac{1}{2\sqrt{\lambda - q_\sigma}}$$

is absolutely integrable on $\mathbb{R} \times \{m \in \Lambda : \hat{\lambda}(m) < \rho\}$, and hence we were able to apply Fubini's theorem. We obtain

$$\langle f_\rho, f\rangle_{\mathbb{R}} = \sum_{n=1}^N |\tilde{f}^p(\lambda_n)|^2 + \frac{1}{2\pi}\sum_{\sigma\in\{\pm\}}\int_{q_\sigma}^{\rho} |\tilde{f}^\sigma(\lambda)|^2\frac{\mathrm{d}\lambda}{2\sqrt{\lambda - q_\sigma}}.$$

Taking the limit $\rho \to \infty$ we obtain by Corollary 2.4.11 that

$$\langle f, f\rangle_{\mathbb{R}} = \int_\Lambda |\tilde{f}(m)|^2\,\mathrm{d}\mu(m).$$

Consequently the map $\mathcal{F}_A : L^2(\mathbb{R}) \to L^2(\Lambda, \mu)$ is an isometry. Similarly, one can prove in the same fashion by considering $\langle g_\rho, f\rangle_{\mathbb{R}}$ with $g_\rho = P_{(-\rho,\rho)}g$ that

$$\langle g, f\rangle_{\mathbb{R}} = \langle \tilde{g}, \tilde{f}\rangle_\Lambda.$$

This finishes the proof. ■

2.4.13 Lemma. Let $f \in C_0^\infty(\mathbb{R})$ and set $\tilde{f} := \mathcal{F}_A f$. Then

$$\mathcal{F}_A(Af)(m) = \hat{\lambda}(m)\tilde{f}(m). \qquad \blacksquare$$

Proof. For $f \in C_0^\infty(\mathbb{R})$, we deduce by integrating by parts two times (the boundary terms vanish, since f has compact support)

$$\begin{aligned}
(\mathcal{F}_A Af)(m) &= \int_{\mathbb{R}} Af(x)\overline{\Psi}(m,x)\,\mathrm{d}x = \int_{\mathbb{R}} (-\Delta + q(x))f(x)\overline{\Psi}(m,x)\,\mathrm{d}x \\
&= \int_{\mathbb{R}} f(x)(-\Delta + q(x))\overline{\Psi}(m,x)\,\mathrm{d}x = \int_{\mathbb{R}} f(x)\hat{\lambda}(m)\overline{\Psi}(m,x)\,\mathrm{d}x \\
&= \hat{\lambda}(m)\tilde{f}(m),
\end{aligned}$$

which finishes the proof. $\blacksquare$

2.4.14 Sweeping up. It is easy to verify the remaining statements of Theorem 2.2.12, up to one fact: we have not shown that $\mathcal{F}_A : L^2(\mathbb{R}) \to L^2(\Lambda, \mathbb{R})$ maps onto $L^2(\Lambda, \mathrm{d}\mu)$, that is, that $\mathcal{F}_A$ is surjective. This follows from the Weyl-Kodeira-Titchmarch theory, but remains unproved here. We cop out and refer to [27]. In any case, it is not of any importance for the remainder of this thesis: one might replace $L^2(\Lambda, \mathrm{d}\mu)$ with the (closed) subspace $\mathcal{R}(\mathcal{F}_A)$ in Theorem 2.2.12, which is sufficient for all following arguments.

2.4.15 On distributions. For the conventional Fourier transform, the set of Schwarz test functions is well-know to allow the extension to arbitrary Schwarz distributions. Can one define a set of distributions adopted to our generalised Fourier transform $\mathcal{F}_A$, to allow its extension to certain distributions? This possible, but in general, not without problems, since in particular the regularity of $q \in L^\infty(\mathbb{R})$ creates some complications. Exactly this is done for a similar problem in Hazard's paper [39].

For more general information on distributions and transforms, we refer to Zayed's book [81], and the functional analysis books by Berezansky, Sheftel and Us [6, 7].

3 Halfspace Problems

3.1 Introduction and References

3.1.1 Introduction. In this chapter we will analyse an explicit solution formula, which will form the core of the method of halfspace matching. Most of the work from Section 3.5 onwards is preparing the central analytical theorems of Chapter 4, and consequently this and the next chapter are closely linked. The reader is invited to check Chapter 4 after reading Sections 3.1 to 3.3, to get an overview over the pupose of this chapter.

We will consider the halfspace

$$\mathbb{R}^2_+ := \{x = (x_1, x_2) \in \mathbb{R}^2 : x_2 > 0\}.$$

Let furthermore A and q be the operator and potential from Section 2.2, defined in Definition and Assumption 2.2.2. We study the problem

$$\begin{cases} \Delta u(x) + (\kappa - q(x_1))u(x) = 0 & \text{for } x \in \mathbb{R}^2_+, \\ u(x_1, 0) = g(x_1) & \text{for } x_1 \in \mathbb{R}, \end{cases} \tag{3.1.1}$$

together with appropriate regularity conditions for u and g. To make this problem well posed, we will generally assume that

$$\kappa \in \mathbb{C} \setminus \mathbb{R},$$

so that Theorem 1.4.3 applies and the problem possesses exactly one solution in $H^1(\mathbb{R}^2_+)$, provided the boundary data fulfils $g \in H^{1/2}(\mathbb{R})$. Note that the assumption for κ can be weakened for example to $\kappa \in \mathbb{C} \setminus [\inf(q), +\infty)$, but we will stay with $\kappa \in \mathbb{C} \setminus \mathbb{R}$ for simplicity.

Our first goal in Section 3.2 is to give an integral representation of the solution u with the help of the generalised Fourier transform associated with A. We will dwell in detail on this representation, and carefully consider its mapping properties.

Afterwards, we will illustrate the representation and the different terms involved in Section 3.3. At this point, we will show a limit-absorption argument, to get closer to the actual (absorption free) problem we are interested in.

Thereafter, we will shortly introduce the *Dirichlet-to-Neumann* operator in Section 3.4. It will play an important role in the numerical formulation of Chapter 5.

The remainder of this chapter will study the *Dirichlet-to-Dirichlet operators* (abbreviated as DtD operators), which will be important in Chapter 4: for $c \in \mathbb{R}$ and $\theta \in (0, \pi)$, the DtD operator D^θ_c is the operator which maps the Dirichlet data g to the trace of the solution u on the line $\Gamma^\theta_c = \{(c + \cos(\theta)z, \sin(\theta)z) : z > 0\}$. Its analysis will be rather involved, since its properties will be crucial for the analysis of halfspace matching in Chapter 4. We point to one aspect that will be critical: the mapping properties of D^θ_c

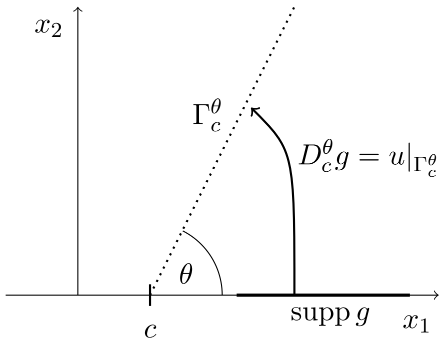

Figure 3.1: Sketch for the DtD operator D_c^θ: it maps the Dirichlet boundary data on $\mathbb{R} \times \{0\}$ to the Dirichlet trace of the solution on the boundary Γ_θ^c.

are dependent on the support of the source $g \in H^{1/2}(\mathbb{R})$; if the support of g and the boundary Γ_c^θ have a contact point, D_c^θ will not be compact. If there is some positive distance between the two sets, D_c^θ will be compact.

To deal with the non-compact part of D_c^θ, we will study an auxiliary problem: the Laplace equation on the halfspace $\mathbb{R}_+^2$. This will be the concern of Section 3.5.

Finally, the works will flow together in Section 3.6, where we will prove the mapping properties of D_c^θ.

3.1.2 References and historical remarks. Halfspace solutions for waveguides can be found for example in [58], and are heavily employed in [10, 9]. The proof of the mapping properties of the DtD operators can be found in [74], which, however, is restricted to the case $\theta = \pi/2$ in the free space. A further paper on this topic by Fliss, Bonnet-Ben Dhia and Tonnoir is being prepared at the moment [75], dealing in more detail with the free space case.

3.1.3 Acknowledgement. This chapter contains some of the core arguments of this thesis, and the author would like to gratefully acknowledge two important hints and contributions for this work. The core step of the proof of Section 3.5 was provided by Antoine Tonnoir to the author. It was expanded and split mainly between the two Lemmata 3.5.6 and 3.5.9. Secondly, the general idea of the splitting in the proofs of the Theorems 3.6.4 and 3.6.6 is due to Sonia Fliss.

3.2 The Solution Operator $\mathcal{S}_{\mathrm{wg}}$

3.2.1 Formal derivation of the solution formula. Let us formally derive an explicit solution formula for (3.1.1). Fix some boundary data $g \in C_0^\infty(\mathbb{R})$ and consider the (unique) solution $u \in H^1(\mathbb{R}_+^2)$ of (3.1.1). The basic idea is to rewrite the Helmholtz operator as

$$\Delta + \kappa - q = \partial_{x_2}^2 - A + \kappa,$$

and to then utilise the diagonalisation of A by $\mathcal{F}_A$. Here A is understood as acting on the x_1-coordinate, that is, $A = -\partial_{x_1}^2 + q$. Hence, let us define the (partial) generalised Fourier transforms for $x_2 > 0$ and $m \in \Lambda$ by

$$\tilde{u}(m, x_2) := [\mathcal{F}_A u(\,\cdot\,, x_2)](m), \quad \tilde{g}(m) := \mathcal{F}_A g(m).$$

So we obtain by Theorem 2.2.12 that

$$\begin{aligned}
&\mathcal{F}_A\left[\Delta u(\,\cdot\,,x_2) - (q(\,\cdot\,)+\kappa)u(\,\cdot\,,x_2)\right](m) \\
&\quad = \mathcal{F}_A\left[\partial_{x_2}^2 u(\,\cdot\,,x_2) - Au(\,\cdot\,,x_2) + \kappa u(\,\cdot\,,x_2)\right](m) \\
&\quad = \partial_{x_2}^2 \tilde{u}(m,x_2) - (\hat{\lambda}(m)-\kappa)\tilde{u}(m,x_2).
\end{aligned}$$

It follows that (3.1.1) is equivalent to

$$\begin{cases} \partial_{x_2}^2 \tilde{u}(m,x_2) - (\hat{\lambda}(m)-\kappa)\tilde{u}(m,x_2) = 0 & \text{for } x_2 > 0,\ m \in \Lambda, \\ \qquad\qquad\qquad\qquad \tilde{u}(m,0) = \tilde{g}(m) & \text{for } m \in \Lambda, \end{cases}$$

together with some appropriate decay condition $u(m,x_2) \to 0$ as $x_2 \to \infty$ to ensure that $u \in H^1(\mathbb{R}^2_+)$. For any fixed $m \in \Lambda$, the latter problem is an ordinary differential equation in x_2, and one can easily compute for $\kappa \in \mathbb{C}\setminus\mathbb{R}$ the solution

$$\tilde{u}(m,x_2) = e^{i\sqrt{\kappa-\hat{\lambda}(m)}\,x_2}\tilde{g}(m).$$

Let us recall the definition of the square root: for $\lambda \in \mathbb{C}$, the square root is chosen such that $\operatorname{Im}(\sqrt{\lambda}) \geq 0$ (see Definition 1.2.1). From $\kappa \in \mathbb{C}\setminus\mathbb{R}$ it follows that $\operatorname{Re}(i(\kappa - \hat{\lambda}(m))^{1/2}) < 0$ for any $m \in \Lambda$, so that $\tilde{u}(m,x_2)$ is exponentially decreasing in x_2. Of course, a second, exponentially increasing solution exists, but since we aim to obtain $u \in H^1(\mathbb{R}^2_+)$, we must drop it. If we now apply the inverse transform, we obtain the following.

3.2.2 The solution formula. Let $\kappa \in \mathbb{C}\setminus\mathbb{R}$. Formally, for any boundary data $g \in C_0^\infty(\mathbb{R})$ the solution u of (3.1.1) is given by

$$u(x) = \mathcal{S}_{\mathrm{wg}}g(x) := \int_\Lambda e^{i\sqrt{\kappa-\hat{\lambda}(m)}\,x_2}\Psi(m,x_1)\tilde{g}(m)\,\mathrm{d}\mu(m), \tag{3.2.1}$$

where $\tilde{g} = \mathcal{F}_A g$ and Λ, Ψ denote the quantities related to the spectral family of A (see Definitions 2.2.5 and 2.2.11 as well as Theorem 2.2.12). Hereby we define the operator $\mathcal{S}_{\mathrm{wg}}$. ∎

The remainder of this chapter will be concerned with proving a number of properties related to $\mathcal{S}_{\mathrm{wg}}$. Particularly, our first goal is to prove that the operator $\mathcal{S}_{\mathrm{wg}}$ indeed gives the same solution as Theorem 1.4.3.

Note that one can make sense of (3.2.1) for $g \in L^2(\mathbb{R})$. In this case, one interprets (3.2.1) for some $x_2 > 0$ as

$$\mathcal{S}_{\mathrm{wg}}g(\,\cdot\,,x_2) = \mathcal{F}_A^{-1}\left[\exp\left(i\sqrt{\kappa-\hat{\lambda}(\,\cdot\,)}\,x_2\right)\mathcal{F}_A g\right].$$

The latter functions and mappings are all defined in L^2: for $g \in L^2(\mathbb{R})$, we have $\mathcal{F}_A g \in L^2(\Lambda, \mathrm{d}\mu)$. The exponential has modulus less or equal than 1, so that we can apply the inverse transform $\mathcal{F}_A^{-1}$ to the product inside the brackets.

To proceed with the analysis, we need an equivalent norm for $H^s(\mathbb{R})$ for $s \in [0,2]$, which is adapted to the transform $\mathcal{F}_A$.

3.2.3 Lemma. Let $s \in [0,2]$. Then for $f : \mathbb{R} \to \mathbb{C}$ the norm

$$\|f\|_{H^s_A(\mathbb{R})} := \int\limits_{\Lambda} (1 + |\lambda(m)|)^s |\mathcal{F}_A f(m)|^2 \,\mathrm{d}\mu(m)$$

is an equivalent norm on $H^s(\mathbb{R})$. ■

Proof. Let us first show that for $f \in H^2(\mathbb{R})$, the norm $(\|f\|^2_{L^2(\mathbb{R})} + \|Af\|^2_{L^2(\mathbb{R})})^{1/2}$ is an equivalent norm on $H^2(\mathbb{R})$. It is well known that $(\|f\|_{L^2(\mathbb{R})} + \|\Delta f\|_{L^2(\mathbb{R})})^{1/2}$ is a norm of $H^2(\mathbb{R})$. We have by the triangle and Hölder's inequality

$$\begin{aligned}\|f\|^2_{\mathbb{R}} + \|Af\|^2_{\mathbb{R}} &= \|f\|^2_{\mathbb{R}} + \|(-\Delta + q)f\|^2_{\mathbb{R}} \\ &\le (1 + 2\|q\|^2_{L^\infty(\mathbb{R})})\|f\|^2_{\mathbb{R}} + 2\|\Delta f\|^2_{\mathbb{R}} \\ &\le (2 + \|q\|^2_{L^\infty(\mathbb{R})}) \left(\|f\|^2_{\mathbb{R}} + \|\Delta f\|^2_{\mathbb{R}}\right).\end{aligned}$$

Recall that we denote $\|\cdot\|_{\mathbb{R}} = \|\cdot\|_{L^2(\mathbb{R})}$ (see Subsection 1.2.2). On the other hand we have

$$\begin{aligned}\|f\|^2_{\mathbb{R}} + \|\Delta f\|^2_{\mathbb{R}} &= \|f\|^2_{\mathbb{R}} + \|(-\Delta + q)f - qf\|^2_{\mathbb{R}} \\ &\le (1 + 2\|q\|^2_{L^\infty(\mathbb{R})})\|f\|^2_{\mathbb{R}} + 2\|Af\|^2_{\mathbb{R}} \\ &\le (2 + 2\|q\|^2_{L^\infty(\mathbb{R})}) \left(\|f\|_{\mathbb{R}} + \|Af\|^2_{\mathbb{R}}\right),\end{aligned}$$

so that the two norms are equivalent. The remainder now follows by a standard interpolation argument, see for example [59, Theorem B.7]. ■

3.2.4 Lemma. Let $\kappa \in \mathbb{C} \setminus \mathbb{R}$. Then there exist constants $c_1, c_2 > 0$ such that

$$c_1 \le \frac{|\lambda - \kappa|}{1 + |\lambda|} \le c_2 \quad \text{for all } \lambda \in \mathbb{R}.$$ ■

Proof. Let $\kappa = \kappa_r + i\kappa_i$ with $\kappa_r \in \mathbb{R}$, $\kappa_i \in \mathbb{R} \setminus \{0\}$. Then

$$|\kappa - \lambda| = \sqrt{(\kappa_r - \lambda)^2 + \kappa_i^2}.$$

The latter term is bounded from below by $|\kappa_i|$, and one easily sees that

$$\frac{|\lambda - \kappa|}{1 + |\lambda|} \longrightarrow 1 \quad \text{as} \quad \lambda \to \pm\infty,$$

so that the boundedness from above and below follows immediately. ■

We will now show that the formal solution formula yields the correct solution.

3.2.5 Lemma. Let $\kappa \in \mathbb{C} \setminus \mathbb{R}$, and let $\mathcal{S}_{\mathrm{wg}}$ be defined by (3.2.1). For given $g \in C_0^\infty(\mathbb{R})$, the function $u = \mathcal{S}_{\mathrm{wg}} g \in H^2(\mathbb{R}^2_+)$ is the unique variational solution given by Theorem 1.4.3. Accordingly, we can continuously extend $S_{\mathrm{wg}} : H^{1/2}(\mathbb{R}) \to H^1(\mathbb{R}^2_+)$. ■

Proof. For $f \in H^2(\mathbb{R}^2_+)$ we have the following equivalent norm on $H^2(\mathbb{R}^2_+)$

$$\|f\|^2_{H^2_A(\mathbb{R}^2_+)} = \int\limits_0^\infty \int\limits_{\Lambda} (1 + |\hat{\lambda}(m)|)^2 |\tilde{f}(m, x_2)|^2 + |\partial^2_{x_2} \tilde{f}(m, x_2)|^2 \,\mathrm{d}\mu(m)\,\mathrm{d}x_2, \tag{3.2.2}$$

where $\tilde{f}(m, x_2) = [\mathcal{F}_A f(\,\cdot\,, x_2)](m)$ denotes the partial Fourier transform of f. This equivalence can be seen as follows. The norm

$$\|f\|^2_{H^2(\mathbb{R}^2_+)} \cong \int_0^\infty \int_{\mathbb{R}} |f(x)|^2 + |\partial^2_{x_1} f(x)|^2 + |\partial^2_{x_2} f(x)|^2 \,\mathrm{d}x_1\,\mathrm{d}x_2,$$

is easily seen to be an equivalent $H^2(\mathbb{R}^2_+)$ norm[1], where we denoted the equivalence in the sense of norms by "$\cong$". We note that

$$\begin{aligned}
\|f\|^2_{H^2(\mathbb{R}^2_+)} &\cong \int_0^\infty \int_{\mathbb{R}} |f(x)|^2 + |\partial^2_{x_1} f(x)|^2 + |\partial^2_{x_2} f(x)|^2 \,\mathrm{d}x_1\,\mathrm{d}x_2 \\
&= \int_0^\infty \|f(\,\cdot\,, x_2)\|^2_{\mathbb{R}} + \|\partial^2_{x_1} f(\,\cdot\,, x_2)\|^2_{\mathbb{R}} + \|\partial^2_{x_2} f(\,\cdot\,, x_2)\|^2_{\mathbb{R}} \,\mathrm{d}x_2 \\
&\cong \int_0^\infty \|f(\,\cdot\,, x_2)\|^2_{H^2(\mathbb{R})} + \|\partial^2_{x_2} f(\,\cdot\,, x_2)\|^2_{\mathbb{R}} \,\mathrm{d}x_2 \\
&\cong \int_0^\infty \|f(\,\cdot\,, x_2)\|^2_{H^2_A(\mathbb{R})} + \|\partial^2_{x_2} f(\,\cdot\,, x_2)\|^2_{\mathbb{R}} \,\mathrm{d}x_2,
\end{aligned}$$

where we used Lemma 3.2.3 for the last equivalence. Rewriting the $H^2_A(\mathbb{R})$-norm by its definition in Lemma 3.2.3 and writing the $L^2(\mathbb{R})$-norm with the help of Parseval's relation (2.2.4), we obtain that the last line of the previous equation is in fact (3.2.2), and thus $\|\cdot\|_{H^2_A(\mathbb{R}^2_+)}$ is an equivalent norm on $H^2(\mathbb{R}^2_+)$.

Let $\mathcal{S}_2 : H^{1/2}(\mathbb{R}) \to H^1(\mathbb{R}^2_+)$ be the (continuous) operator, which maps $g \in H^{1/2}(\mathbb{R})$ to the (unique) solution $v = \mathcal{S}_2 g \in H^1(\mathbb{R}^2_+)$ of (3.1.1). The continuity follows from Theorem 1.4.3. We will show the following: for $g \in C_0^\infty(\mathbb{R})$, the function $u = \mathcal{S}_{\mathrm{wg}} g$ coincides with $v = \mathcal{S}_2 g$, that is, $u \in H^1(\mathbb{R})$ fulfils (3.1.1). Since $C_0^\infty(\mathbb{R})$ is dense in $L^2(\mathbb{R})$, this will imply that the two operators actually agree, i.e. $\mathcal{S}_2 = \mathcal{S}_{\mathrm{wg}} : H^{1/2}(\mathbb{R}) \to H^1(\mathbb{R}^2_+)$.

Let $g \in C_0^\infty(\mathbb{R})$, and let $u = \mathcal{S}_{\mathrm{wg}} g : \mathbb{R}^2_+ \to \mathbb{C}$. Its partial generalised Fourier transform is given by

$$\tilde{u}(m, x_2) = e^{i\sqrt{\kappa - \hat{\lambda}(m)}\,x_2}\,\tilde{g}(m),$$

and we can compute

$$\begin{aligned}
\|u\|^2_{H^2_A(\mathbb{R}^2_+)} = \int_0^\infty \int_\Lambda & (1 + |\hat{\lambda}(m)|)^2 |e^{i\sqrt{\kappa - \hat{\lambda}(m)}\,x_2}\tilde{g}(m)|^2 \\
& + |\partial^2_{x_2} e^{i\sqrt{\kappa - \hat{\lambda}(m)}\,x_2}\tilde{g}(m)|^2 \mathrm{d}\mu(m)\,\mathrm{d}x_2 \\
= \int_\Lambda & \left[(1 + |\hat{\lambda}(m)|)^2 + |\hat{\lambda}(m) - \kappa|^2\right] |\tilde{g}(m)|^2 \int_0^\infty e^{-2\,\mathrm{Im}\sqrt{\kappa - \hat{\lambda}(m)}\,x_2} \mathrm{d}x_2\,\mathrm{d}\mu(m) \\
= \int_\Lambda & \frac{(1 + |\hat{\lambda}(m)|)^2 + |\hat{\kappa} - \lambda(m)|^2}{2\,\mathrm{Im}\sqrt{\kappa - \hat{\lambda}(m)}} |\tilde{g}(m)|^2\,\mathrm{d}\mu(\lambda).
\end{aligned}$$

[1]This norm lies between the two $H^2(\mathbb{R})$ norms $\|f\|^2_{L^2(\mathbb{R}^2_+)} + \|\Delta f\|^2_{L^2(\mathbb{R}^2_+)}$ and the classical $H^2(\mathbb{R}^2_+)$ norm, which involves all partial derivatives up to order two.

Since $\kappa \in \mathbb{C} \setminus \mathbb{R}$, there exists some small $c > 0$ such that $\operatorname{Im}(\kappa - \hat{\lambda}(m))^{1/2} > c > 0$ for any $m \in \Lambda$. This in turn implies that there exists $C > 0$ such that

$$\frac{(1 + |\hat{\lambda}(m)|)^2 + |\kappa - \hat{\lambda}(m)|^2}{2 \operatorname{Im}\sqrt{\kappa - \hat{\lambda}(m)}} < C(1 + |\hat{\lambda}(m)|)^2 \qquad \text{for } m \in \Lambda,$$

so that it follows

$$\|u\|^2_{H^2_A(\mathbb{R}^2_+)} \leq C \int\limits_\Lambda (1 + |\hat{\lambda}(m)|)^2 |\tilde{g}(m)|^2 \,\mathrm{d}\mu(m) = C\|g\|^2_{H^2_A(\mathbb{R})}.$$

Consequently, our solution u is in $H^2(\mathbb{R}^2_+)$. As a result, it is sufficient so show that u fulfils $(\Delta - q + \kappa)u = 0$ in the distributional sense and that $u = g$ on $\mathbb{R} \times \{0\}$. Let $\phi \in C_0^\infty(\mathbb{R}^2_+)$, and consider

$$\begin{aligned}
\langle (\Delta - q + \kappa)u, \phi\rangle_{\mathbb{R}^2_+} &= \langle (-A + \partial^2_{x_2} + \kappa)u, \phi\rangle_{\mathbb{R}^2_+} \\
&= \int\limits_0^\infty \langle (-A + \partial^2_{x_2} + \kappa)u(\,\cdot\,, x_2)\,,\, \phi(\,\cdot\,, x_2)\rangle_{\mathbb{R}} \,\mathrm{d}x_2 \\
&= \int\limits_0^\infty \langle (-\hat{\lambda} + \partial^2_{x_2} + \kappa)\tilde{u}(\,\cdot\,, x_2)\,,\, \tilde{\phi}(\,\cdot\,, x_2)\rangle_{\Lambda} \,\mathrm{d}x_2,
\end{aligned}$$

where $\tilde{\phi}$ again denotes the partial generalised Fourier transform of ϕ. Note that we used that $\partial^2_{x_2}\mathcal{F}_A u(\,\cdot\,, x_2) = \mathcal{F}_A \partial^2_{x_2} u(\,\cdot\,, x_2)$, as can be seen easily to follow from $u \in H^2(\mathbb{R}^2_+)$. We now have for μ-almost all $m \in \Lambda$

$$(-\hat{\lambda}(m) + \partial^2_{x_2} + \kappa)\tilde{u}(m, x_2) = (-\hat{\lambda}(m) + \partial^2_{x_2} + \kappa)e^{i\sqrt{\kappa - \hat{\lambda}(m)}\,x_2}\tilde{g}(m) = 0,$$

so that $\langle (\Delta - q + \kappa)u, \phi\rangle_{\mathbb{R}^2_+} = 0$, and hence u is a solution in the sense of Section 1.4. It remains to show that $u = g$ on $\mathbb{R} \times \{0\}$ in the sense of the trace operator. Since $u \in H^2(\mathbb{R}^2_+)$, u is continuous by the Sobolev-embedding and we have

$$u(x_1, 0) = \int\limits_\Lambda e^{i\sqrt{\kappa - \hat{\lambda}(m)}\,0}\Psi(m, x_1)\tilde{g}(m) \,\mathrm{d}\mu(\lambda) = g(x_1)$$

by the inversion formula of Theorem 2.2.12. Hence, u is the unique solution of Theorem 1.4.3, and thus $\mathcal{S}_{\mathrm{wg}} g = \mathcal{S}_2 g$ for any $g \in C_0^\infty(\mathbb{R})$. In other words, $\mathcal{S}_{\mathrm{wg}}$ agrees with $\mathcal{S}_2$ on a dense subset of $H^{1/2}(\mathbb{R})$, and it can be continuously extended to obtain $\mathcal{S}_2$, finishing the proof. ■

3.2.6 Remark. With the help of the representation formula (3.2.1), the operator $\mathcal{S}_{\mathrm{wg}}$ can be shown to be extendable to different spaces. Let us give a few examples.

(a) Firstly, one can show the continuity of $\mathcal{S}_{\mathrm{wg}}$ without resorting to the Lax–Milgram theorem: utilising that Lemma 3.2.3 actually holds for any $s \in [0, 2]$, it is a rather straightforward calculation with the help of Lemma 3.2.4 to show that $\mathcal{S}_{\mathrm{wg}} : H^{1/2}(\mathbb{R}^2_+) \to H^1(\mathbb{R}^2_+)$ and $\mathcal{S}_{\mathrm{wg}} : H^{3/2}(\mathbb{R}) \to H^2(\mathbb{R}^2_+)$ are continuous.

(b) It is furthermore possible to extend $\mathcal{S}_{\mathrm{wg}}$ to spaces of weaker regularity: one can define the weighted Sobolev space

$$H^1(\mathbb{R}^2_+, x_2\,\mathrm{d}x) := \left\{ f \in \mathcal{D}'(\mathbb{R}^2_+) : \int\limits_{\mathbb{R}^2_+} x_2 \left[|f|^2 + |\nabla f|^2\right] \mathrm{d}x < \infty \right\}.$$

It is then again rather elementary to show that

$$\mathcal{S}_{\mathrm{wg}} : L^2(\mathbb{R}) \to H^1(\mathbb{R}^2_+, x_2\mathrm{d}x)$$

is continuous using the same ingredients and norm representations as in the previous proof. The importance of the space $H^1(\mathbb{R}^2_+, x_2\,\mathrm{d}x)$ lies in the fact that it allows less regularity close to the boundary of $\mathbb{R}^2_+$, so that "more general" traces are allowed. However, there is no proper trace-operator from $H^1(\mathbb{R}^2_+, x_2\,\mathrm{d}x)$ into $L^2(\mathbb{R})$, so that the existence of a trace becomes a more delicate issue. Here, it can be understood in the sense that $u(\,\cdot\,, x_2)$ converges to g in $L^2(\mathbb{R})$ as $x_2 \to 0$.

For some fixed $g \in L^2(\mathbb{R})$ the solution $u = \mathcal{S}_{\mathrm{wg}}g$ will generally not belong to $H^1(\mathbb{R}^2_+)$, and hence it will not be necessarily a weak solution of the Helmholtz equation $\Delta u + (\kappa - q)u = 0$ in $\mathbb{R}^2_+$. However, it can be shown that it is still a distributional solution, again using the same ingredients as in the proof shown above. For more details on those matters, we refer to [56, 55, 12, 53].

We will not use this framework with $L^2(\mathbb{R})$ boundary data any further, but leave it here as a side note.

3.3 The Modal Representation

Our next goal is to give a physical illustration of the expansion we just obtained. In this section we pass to a "proper" scattering problem, that is, to a real $\kappa_0 \in \mathbb{R}$. Let $\kappa = \kappa_0 + i\epsilon$ with $\kappa_0 \in \mathbb{R}$ and $\epsilon > 0$, and let us consider again problem (3.1.1), namely

$$\begin{cases} \Delta u_\epsilon(x) + (\kappa_0 + i\epsilon - q(x_1))u_\epsilon(x) = 0 & \text{for } x \in \mathbb{R}^2_+, \\ \qquad\qquad\qquad u_\epsilon(x_1, 0) = g(x_1) & \text{for } x_1 \in \mathbb{R}. \end{cases} \tag{3.3.1}$$

Our goal is to consider the behaviour of the solution as $\epsilon \to 0$. By Section 3.2.2 and Lemma 3.2.5, the solution is given by

$$u_\epsilon(x) = \mathcal{S}^\epsilon_{\mathrm{wg}}g(x) := \int\limits_\Lambda e^{i\sqrt{\kappa_0 + i\epsilon - \hat\lambda(m)}\,x_2}\,\Psi(m, x_1)\tilde g(m)\,\mathrm{d}\mu(m), \tag{3.3.2}$$

where $\tilde g = \mathcal{F}_A g$. Consider the kernel $e^{i\sqrt{\kappa_0 + i\epsilon - \hat\lambda(m)}\,x_2}\Psi(m, x_1)$ as $\epsilon \to 0+$; it converges pointwise by our choice of the square root. However, its limit is not decreasing any more, implying that the solution u_ϵ will not converge in $H^1(\mathbb{R}^2_+)$. In which sense can one now define a solution to the limit problem? There are several available options, and we will show that u_ϵ converges in a weighted Sobolev space.

3.3.1 Lemma. Let $\mathcal{S}^0_{\text{wg}}$ be defined by (3.3.2) with $\kappa = \kappa_0 + i0 \in \mathbb{R}$, where $\kappa_0 \in \mathbb{R}$. Then for any $s > 1$, the operator $\mathcal{S}^0_{\text{wg}} : H^{1/2}(\mathbb{R}) \to H^1\left(\mathbb{R}^2_+, (1+x_2)^{-s}\mathrm{d}x\right)$ is continuous, and for any $g \in H^{1/2}(\mathbb{R})$

$$\mathcal{S}^\epsilon_{\text{wg}} g \to \mathcal{S}^0_{\text{wg}} g \qquad \text{as } \epsilon \to 0,\ \epsilon > 0,$$

with convergence in $H^1\left(\mathbb{R}^2_+, (1+x_2)^{-s}\mathrm{d}x\right)$. ■

Proof. Let $g \in H^{1/2}(\mathbb{R})$. By Parseval's relation (2.2.4) we have

$$\begin{aligned}&\|(\mathcal{S}^\epsilon_{\text{wg}} - \mathcal{S}^0_{\text{wg}})g\|^2_{L^2\left(\mathbb{R}^2_+,(1+x_2)^{-s}\,\mathrm{d}x\right)}\\ &= \int_0^\infty \int_\Lambda \frac{1}{(1+x_2)^s} \left| e^{i\sqrt{\kappa_0 + i\epsilon - \hat{\lambda}(m)}\,x_2} - e^{i\sqrt{\kappa_0 - \hat{\lambda}(m)}\,x_2} \right|^2 |\tilde{g}(m)|^2 \,\mathrm{d}\mu(m)\,\mathrm{d}x_2\end{aligned}$$

The integrand is bounded by

$$2\frac{1}{(1+x_2)^s}|\tilde{g}(m)|^2,$$

since the modulus of both exponential terms is less or equal one. This term is in $L^1((0,\infty)\times\Lambda, \mathrm{d}x_2 \times \mathrm{d}\mu)$ and accordingly, one can apply the dominated convergence theorem to exchange limit and integral to obtain

$$\lim_{\epsilon\to 0} \|(\mathcal{S}^\epsilon_{\text{wg}} - \mathcal{S}^0_{\text{wg}})g\|^2_{L^2\left(\mathbb{R}^2_+,(1+x_2)^{-s}\,\mathrm{d}x\right)} = 0,$$

and hence $\mathcal{S}^\epsilon_{\text{wg}} g \to \mathcal{S}^0_{\text{wg}} g$ in $L^2\left(\mathbb{R}^2_+, (1+x_2)^{-s}\mathrm{d}x\right)$. To show that convergence is actually in $H^1\left(\mathbb{R}^2_+, (1+x_2)^{-s}\mathrm{d}x\right)$, one repeats the same procedure for the derivatives, exploiting the norms of Lemma 3.2.3.

For the mapping properties of $\mathcal{S}^0_{\text{wg}}$, one notices for example for $g \in H^{1/2}(\mathbb{R})$ that

$$\begin{aligned}&\|\mathcal{S}^0_{\text{wg}} g\|^2_{L^2\left(\mathbb{R}^2_+,(1+x_2)^{-s}\,\mathrm{d}x\right)}\\ &= \int_0^\infty \int_\Lambda \frac{1}{(1+x_2)^s} \left| e^{i\sqrt{\kappa_0 - \hat{\lambda}(m)}\,x_2} \right|^2 |\tilde{g}(m)|^2 \mathrm{d}\mu(m)\,\mathrm{d}x_2\\ &\le \int_0^\infty \int_\Lambda \frac{1}{(1+x_2)^s} |\tilde{g}(m)|^2\,\mathrm{d}\mu(m)\,\mathrm{d}x_2\\ &= \int_0^\infty \frac{1}{(1+x_2)^s}\,\mathrm{d}x_2 \int_\Lambda |\tilde{g}(m)|^2 \mathrm{d}\mu(m)\\ &\le C\|g\|^2_{L^2(\mathbb{R})}.\end{aligned}$$

And similarly for the norms of the derivatives (again, take note of Lemma 3.2.3). ■

We have shown here that $\mathcal{S}^\epsilon_{\text{wg}}$ converges in the strong operator topology of operators $H^{1/2}(\mathbb{R}) \to H^1(\mathbb{R}^2_+, (1+x_2)^{-s}\mathrm{d}x)$. In a more classical framework, one usually shows the convergence of $\mathcal{S}^\epsilon_{\text{wg}}$ in the norm topology of (different) weighted spaces. We do not pursue this here since it is non-essential for the remainder of the thesis (for classical scattering, see for example [1], and for the waveguide case [76]).

3.3.2 The modes of the open waveguide. Let us dwell a bit on the previous lemma and explain what we have shown: given any boundary $g \in H^{1/2}(\mathbb{R})$, the *outgoing* solution of (3.3.1) is given by

$$u_0(x) = \int\limits_{\Lambda} e^{i\sqrt{\kappa_0 - \hat{\lambda}(m)}\,x_2} \Psi(m, x_1)\tilde{g}(m)\,\mathrm{d}\mu(m).$$

Note that we have used the notion of *outgoing in the sense of the limit-absorption principle*: that is, a solution u to (3.3.1) with $\epsilon = 0$ is called outgoing, if it is the limit of u_ϵ as $\epsilon > 0$ converges to 0.

Let us have closer look at the representation we have just obtained for this limit-absorption solution. If $\kappa_0 > q_m$ and $\sigma_p(A) \neq \emptyset$ (recall the notation of Definition and Assumption 2.2.2), this solution will not decay any more, but will contain terms constant in modulus as $x_2 \to +\infty$ inside the finite sum over the eigenfunctions. Let us denote

$$U(m; x) := e^{i\sqrt{\kappa_0 - \hat{\lambda}(m)}\,x_2} \Psi(m, x_1),$$

where $m \in \Lambda$. We call $U(m;\,\cdot\,)$ a *(generalised) mode* of the waveguide. Note that any mode fulfils

$$\Delta_x U(m; x) + (\kappa_0 - q(x_1))U(m; x) = 0.$$

As before, we denote $U = (U^p, U^+, U^-)$ to indicate the part of U living on the different parts of Λ. To illustrate the different types of modes, we will now assume that

$$\kappa_0 > q_+ > q_-,$$

which is a non-essential assumption, since the other cases can be discussed in the same fashion. Also note Figure 3.2, where we have plotted a few of these modes.

(a) Guided modes. For $n \in \{1, \ldots, N\}$, we can define the propagation constant $k_2 = \sqrt{\kappa_0 - \lambda_n} > 0$, to rewrite

$$U^p(\lambda_n; x) = e^{ik_2 x_2} \Psi^p(\lambda_n, x_1).$$

This solution of the Helmholtz equation is usually called a *guided mode*: it propagates along the x_2-axis without decay, while it is localized to the waveguide core $\{x \in \mathbb{R}^2 : a < x_1 < b\}$ in the sense that it decays exponentially as $x_1 \to \pm\infty$. In a sense, guided modes represent energy *trapped* inside the waveguide.

(b) Totally reflected, propagative modes. Let us now consider $m = (-, \lambda)$, where $\lambda \in (q_-, q_+)$, so that

$$U^-(\lambda; x) = e^{i\sqrt{\kappa_0 - \lambda}\,x_2} \Psi^-(\lambda, x_1)$$

decays exponentially as $x_1 \to +\infty$, but does not decay as $x_1 \to -\infty$. Defining $k_2^- := \sqrt{\kappa_0 - \lambda}$, and $k_1^- = \sqrt{\lambda - q_-}$, one obtains with the help of the Definition 2.2.11 that we have the following representation for U_λ^- outside of the waveguide core $\{x \in \mathbb{R}^2 : a < x_1 < b\}$:

$$U^-(\lambda; x) = \begin{cases} e^{i(k_1^- x_1 + k_2^- x_2)} + r_\lambda^- e^{i(-k_1^- x_1 + k_2^- x_2)} & \text{for } x_1 < a, \\ t_\lambda^- e^{ik_2 x_2} e^{-\sqrt{q_+ - \lambda}\,x_1} & \text{for } x_1 > b, \end{cases}$$

where r_λ^-, $t_\lambda^- \in \mathbb{C}$ are some coefficients. The last representation now allows a neat physical interpretation: for $x_1 < a$, the solution consists of two plane waves. One that is incident to the waveguide, and a reflected wave. It is a total reflection, since on the other side of the waveguide, U_λ^- decays exponentially.

(c) Partially reflected, propagative modes. Let $m = (-, \lambda)$ with $\lambda \in (q_+, \kappa_0)$. Let us define the two wave vectors for the right and left hand side by $k_2^- = k_2^+ = \sqrt{\kappa_0 - \lambda}$, and set $k_1^+ = \sqrt{\lambda - q_+}$ and $k_1^- = \sqrt{\lambda - q_-}$. In this case, a part of the incident wave is transmitted, and one obtains a plane wave on the right hand side of the waveguide, which reads as follows

$$U^-(\lambda, x) = \begin{cases} e^{i(k_1^- x_1 + k_2^- x_2)} + r_\lambda^- e^{i(-k_1^- x_1 + k_2^- x_2)} & \text{for } x_1 < a, \\ t_\lambda^- e^{i(k_1^+ x_1 + k_2^+ x_2)} & \text{for } x_1 > b. \end{cases}$$

The same discussion can be done for a plane wave incident from the right, which corresponds to $m = (+, \lambda)$ with $\lambda \in (q_+, \kappa_0)$.

(d) Evanescent modes. For $\lambda > \kappa_0$, the exponential $e^{i\sqrt{\kappa_0 - \lambda}\, x_2}$ becomes exponentially decreasing for $x_2 \to +\infty$. These modes oscillate rather quickly along the x_1-axis.

3.3.3 The plane wave representation. Let us, as before in Example 2.2.13, illustrate this expansion theorem for the case of a free halfspace, where no waveguide is present: considering again $q(x) = 0$ and $q_+ = q_- = 0$, we obtain that $\mathcal{F}_A$ is practically the Fourier transform (after some transformation, compare again Example 2.2.13), and the expansion of the solution can be rewritten as follows

$$u_0(x) = \frac{1}{2\pi} \int_{\mathbb{R}} e^{i\sqrt{\kappa_0 - \xi^2}\, x_2 + i\xi x_1} \int_{\mathbb{R}} e^{-i\xi y} g(y)\, \mathrm{d}y\, \mathrm{d}\xi.$$

This is the so-called *plane wave spectrum representation*, which forms the basis for the field of Fourier optics [36]. In this case the types of modes are somewhat reduced. Since $q_m = q_- = q_+ = 0$, the point spectrum of A is empty, and accordingly, there are no guided modes. Also the totally reflected propagating modes are not present, and the partially reflected modes are plane waves (if $|\xi|^2 < \kappa_0$) of the form

$$e^{i\sqrt{\kappa_0 - \xi^2}\, x_2 + i\xi x_1},$$

from which the name of the representation stems from. The exponentially decaying evanescent modes are also present for $|\xi|^2 > \kappa_0$.

3.4 The Dirichlet to Neumann Operator

At a later point in Chapter 5, we will need the so-called *Dirichlet-to-Neumann* operator $\mathcal{N}$ (abbreviated as DtN operator) associated with the halfspace problem (3.1.1). Let us quickly define and show some properties of it.

3.4.1 Definition. For $\kappa \in \mathbb{C}$ and $g \in C_0^\infty(\mathbb{R})$, let $u = \mathcal{S}_{\mathrm{wg}} g$ denote the solution of the halfspace problem (3.1.1). We now define $\mathcal{N}g : \mathbb{R} \to \mathbb{C}$ by

$$\mathcal{N}g(x_1) = \partial_{x_2} u(x_1, 0) \qquad \text{for } x_1 \in \mathbb{R}. \tag{3.4.1}$$

For $\kappa \in \mathbb{R}$, we understand $\mathcal{S}_{\mathrm{wg}}$ in the sense of Lemma 3.3.1. ■

In other words: the Dirichlet to Neumann operator maps the Dirichlet boundary data of u to its Neumann boundary data. Let us also remark that that (3.4.1) has to be

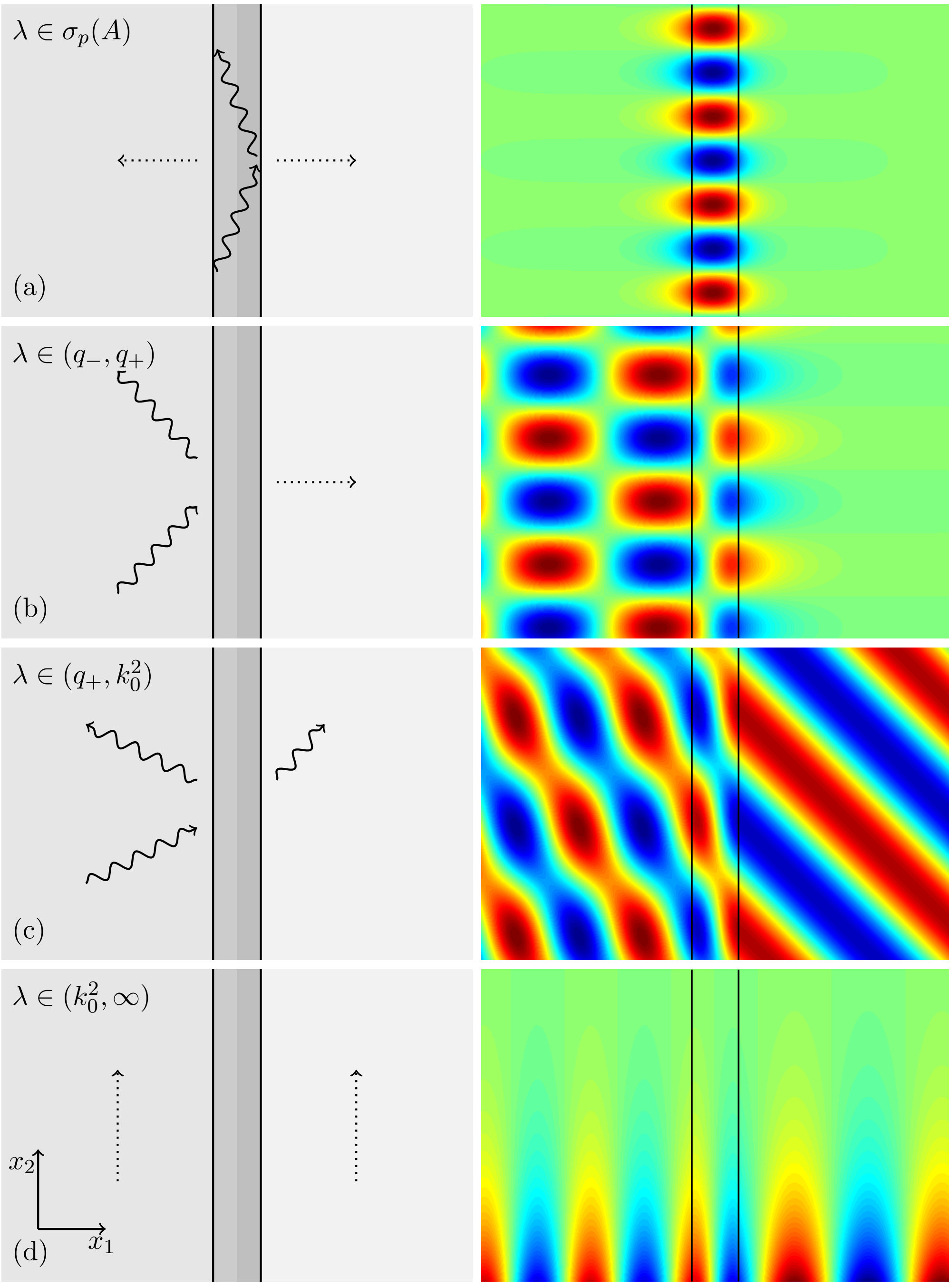

Figure 3.2: Sketches of the different types of modes, as well as (exemplary) plots of their real parts $\operatorname{Re} U(m; x)$. The grey background indicates the function q, with the straight black lines indicating the boundaries of the waveguide (i.e. the sets $\{x = a\}$ and $\{x = b\}$). The curly arrows show the direction of propagation of the plane waves, while dotted arrows indicate an exponential decay of the modes. For (c) note that there is a corresponding mode with a plane wave incident from the right side, which is not shown. Also note that the two wave-vectors in (c) must fulfil Snell's Law.

understood as an equality of functions in $L^2(\mathbb{R})$. Since $q \in L^\infty(\mathbb{R}^2_+)$, the solution u will generally be only in $H^2(\mathbb{R})$, so that its normal derivative is only in $H^{1/2}(\mathbb{R})$, which does not allow point evaluation, even despite the smooth Dirichlet boundary data g.

In most literature, the DtN operators are considered as operators from $H^{1/2}(\mathbb{R})$ into its dual $H^{-1/2}(\mathbb{R})$. However, since we will use an $H^1(\mathbb{R})$ framework for the traces later in Chapter 5, we will use $H^1(\mathbb{R})$ as the domain of $\mathcal{N}$. To implement the DtN operator, we will also need a more explicit representation, which can be given with the help of the spectral family $\mathcal{F}_A$.

3.4.2 Lemma. For $\kappa \in \mathbb{C}$, the DtN operator can be extended to a continuous linear operator $\mathcal{N} : H^1(\mathbb{R}) \to L^2(\mathbb{R})$. For any $g \in H^1(\mathbb{R})$, it holds that

$$\mathcal{N}g = \mathcal{F}_A^{-1}\left(i\sqrt{\kappa - \hat{\lambda}(\,\cdot\,)}\,\mathcal{F}_A g(\,\cdot\,)\right). \qquad ■$$

Proof. We will only show a formal calculation, which can be easily made rigorous if one considers weak derivatives. Let $g \in C_0^\infty(\mathbb{R})$. For $x \in \mathbb{R}^2_+$, we have (formally)

$$\begin{aligned}
\partial_{x_2} u(x) &= \partial_{x_2}(\mathcal{S}_{\mathrm{wg}} g(x)) \\
&= \partial_{x_2} \int_\Lambda e^{i\sqrt{\kappa-\hat{\lambda}(m)}\,x_2}\Psi(m,x_1)\mathcal{F}_A g(m)\,\mathrm{d}\mu(m) \\
&= \int_\Lambda \partial_{x_2} e^{i\sqrt{\kappa-\hat{\lambda}(m)}\,x_2}\Psi(m,x_1)\mathcal{F}_A g(m)\,\mathrm{d}\mu(m) \\
&= \int_\Lambda i\sqrt{\kappa-\hat{\lambda}(m)}e^{i\sqrt{\kappa-\hat{\lambda}(m)}\,x_2}\Psi(m,x_1)\mathcal{F}_A g(m)\,\mathrm{d}\mu(m).
\end{aligned}$$

Setting $x_2 = 0$ yields the desired representation of $\mathcal{N}$. Since $\mathcal{F}_A^{-1} : L^2(\Lambda, \mathrm{d}\mu) \to L^2(\mathbb{R})$ is unitary, we have

$$\begin{aligned}
\|\mathcal{N}g\|_{L^2(R)} &= \left\|\mathcal{F}_A^{-1}\left(i(\kappa-\hat{\lambda})^{1/2}\,\mathcal{F}_A g(\,\cdot\,)\right)\right\|_{\mathbb{R}} \\
&= \|i(\kappa-\hat{\lambda})^{1/2}\,\mathcal{F}_A g\|_{L^2(\Lambda,\mathrm{d}\mu)} \\
&\le C\|(1+|\hat{\lambda}|)^{1/2}\mathcal{F}_A g\|_{L^2(\Lambda,\mathrm{d}\mu)} \\
&= C\|g\|_{H^1_A(\mathbb{R})},
\end{aligned}$$

where we used the equivalent norm from Lemma 3.2.3 in the last step. ■

3.5 A Laplace Problem

3.5.1 Introduction and references. This section will be concerned with an auxiliary problem, which will allow us to study the behaviour of the Diricht-to-Dirichlet operators at the junction point of the source-support and the target boundary. The only statement of relevance for the remainder of this thesis will be Theorem 3.5.10, while the rest will not play a role elsewhere.

The techniques employed in this section are rather classical. Mellin transform arguments have long been used for the study of singularities at corners of the boundary, for example in [53, 81, 66], where also more information on the Fourier–Laplace transform can be found (in [53, 81]).

We also point again to the acknowledgements in Subsection 3.1.3.

3.5.2 The problem of interest. Given $f \in C_0^\infty(\mathbb{R})$, we are going to consider the problem of finding a solution $u \in C^2(\mathbb{R}^2_+) \cap C^0(\overline{\mathbb{R}^2_+})$ to

$$\begin{cases} \Delta u(x) = 0 & \text{for } x \in \mathbb{R}^2_+, \\ u(x_1, 0) = f(x_1) & \text{for } x_1 \in \mathbb{R}, \\ u \text{ bounded} & \text{on } \mathbb{R}^2_+, \end{cases} \tag{3.5.1}$$

as well as certain extensions for boundary data $f \in L^2(\mathbb{R})$ or $f \in H^1(\mathbb{R})$.

3.5.3 Lemma. For any $f \in C_0^\infty(\mathbb{R})$, there exists exactly one solution $u \in C^2(\mathbb{R}^2_+) \cap C^0(\overline{\mathbb{R}^2_+})$ to (3.5.1). ■

Proof. Let us show uniqueness: let u_1, u_2 be two solutions to (3.5.1). Define $w = u_1 - u_2$, so that w fulfils the homogeneous problem, that is, (3.5.1) with $f = 0$. For $x_1 \in \mathbb{R}$, $x_2 > 0$ define $w(x_1, -x_2) := -w(x_1, x_2)$. One easily verifies that w is defined on the whole of $\mathbb{R}^2$, and w as well as its first derivatives are continuous across $\mathbb{R} \times \{0\}$. This implies that $\Delta w(x) = 0$ for any $x \in \mathbb{R}^2$, and accordingly, w is a bounded harmonic function on $\mathbb{R}^2$. From Liouville's Theorem (see [28, Chapter 2, Theorem 8]) we now obtain that w is constant. Since $w(0,0) = 0$, this yields $w = 0$.

To see the existence of a solution, we note that a solution is given by

$$u(x, y) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{i\xi x_1} e^{-|\xi| x_2} \hat{f}(\xi) \,\mathrm{d}\xi, \tag{3.5.2}$$

where $\hat{f}$ denotes the classical Fourier transform of f, that is

$$\hat{f}(\xi) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-i\xi x_1} f(x_1) \,\mathrm{d}x_1.$$

The proof that u is in fact a solution can be performed almost exactly as in Lemma 3.2.5: firstly, one shows that $u \in H^2(\mathbb{R} \times (0,h))$ for any $h > 0$, and then that $\Delta u = 0$. The trace equality is shown exactly the same way as in Lemma 3.2.5, and the boundedness of u can be seen for example by the chain of inequalities

$$|u(x)| \le C \|u(\,\cdot\,, x_2)\|_{H^1(\mathbb{R})} \le C \|f\|_{H^1(\mathbb{R})} \qquad \text{for } x \in \mathbb{R}^2_+,$$

where we employed the Sobolev embedding $H^1(\mathbb{R}) \to C^0(\mathbb{R})$ at the first inequality, and performed a simple estimate with the help of the representation formula of $u(\,\cdot\,, x_2)$ at the second inequality. To see that $u \in C^2(\mathbb{R}^2_+)$ one now employs a standard regularity theorem (see for example [59, Theorem 4.18]). ■

3.5.4 Lemma. Denote by $\mathcal{S}_\Delta f(x) := u(x)$ the solution operator associated with (3.5.1), which maps the boundary data $f \in C_0^\infty(\mathbb{R})$ to the solution $u \in C^2(\mathbb{R}^2_+) \cap C^0(\overline{\mathbb{R}^2_+})$. For any $h > 0$, we can extend $\mathcal{S}_\Delta$ to a continuous operator $\mathcal{S}_\Delta : H^{1/2}(\mathbb{R}) \to H^1(\mathbb{R} \times (0,h))$.

Proof. We have to show that there exists some $C > 0$ such that

$$\|u\|^2_{H^1(\mathbb{R}\times(0,h))} = \|u\|^2_{\mathbb{R}\times(0,h)} + \|\partial_{x_1} u\|^2_{\mathbb{R}\times(0,h)} + \|\partial_{x_2} u\|^2_{\mathbb{R}\times(0,h)} \le C \|f\|_{H^{1/2}(\mathbb{R})},$$

where u is given by (3.5.2). We start by estimating the first and second term of the $H^1(\mathbb{R}\times(0,h))$-norm. It holds that

$$\|u\|^2_{\mathbb{R}\times(0,h)} + \|\partial_{x_1}u\|^2_{\mathbb{R}\times(0,h)} = \int_0^h \|u(\,\cdot\,,x_2)\|^2_{\mathbb{R}} + \|\partial_{x_1}u(\,\cdot\,,x_2)\|^2_{\mathbb{R}}\,\mathrm{d}x_2$$
$$= \int_0^h \|u(\,\cdot\,,x_2)\|^2_{H^1(\mathbb{R})}\,\mathrm{d}x_2 \cong \int_0^h\int_{\mathbb{R}} (1+\xi^2)|\hat{u}(\xi,x_2)|^2\,\mathrm{d}\xi\,\mathrm{d}x_2,$$

where "$\cong$" denotes the equivalence of norms, and $\hat{u}$ denotes the partial Fourier transform of u, that is

$$\hat{u}(\xi,x_2) = \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} e^{-i\xi x_1}u(x_1,x_2)\,\mathrm{d}x_1.$$

From the definition of u one easily obtains $\hat{u}(\xi,x_2) = e^{-|\xi|x_2}\hat{f}(\xi)$, so that

$$\|u\|^2_{\mathbb{R}\times(0,h)} + \|\partial_{x_1}u\|^2_{\mathbb{R}\times(0,h)} \cong \int_0^h\int_{\mathbb{R}} (1+\xi^2)e^{-2|\xi|x_2}|\hat{f}(\xi)|^2\,\mathrm{d}\xi\,\mathrm{d}x_2$$
$$= \int_{\mathbb{R}} \frac{(1+\xi^2)(1-e^{-2|\xi|h})}{2|\xi|}|\hat{f}(\xi)|^2\,\mathrm{d}\xi.$$

It is now elementary to prove that there exists a constant C_1 such that

$$\frac{(1+\xi^2)(1-e^{-2|\xi|h})}{2|\xi|} \le C_1(1+\xi^2)^{1/2} \qquad \text{for all } \xi\in\mathbb{R}.$$

Note in particular that

$$\lim_{\xi\to 0}\frac{1-e^{-2|\xi|h}}{2|\xi|} = h,$$

as can be easily verified by applying L'Hospital's rule. This now yields

$$\|u\|^2_{\mathbb{R}\times(0,h)} + \|\partial_{x_1}u\|^2_{\mathbb{R}\times(0,h)} \cong \int_{\mathbb{R}} \frac{(1+\xi^2)(1-e^{-2|\xi|h})}{2|\xi|}|\hat{f}(\xi)|^2\mathrm{d}\xi$$
$$\le C_1\int_{\mathbb{R}}(1+\xi^2)^{1/2}|\hat{f}(\xi)|^2\mathrm{d}\xi$$
$$= C_1\|f\|^2_{H^{1/2}(\mathbb{R})}.$$

Similarly, one easily calculates

$$\|\partial_{x_2}u\|^2_{\mathbb{R}^2_+} \cong \int_0^h\int_{\mathbb{R}} \left|\partial_{x_2}\left(e^{-|\xi|x_2}\hat{u}(\xi,x_2)\right)\right|^2\,\mathrm{d}\xi\,\mathrm{d}x_2$$
$$\le \int_{\mathbb{R}} \frac{\xi^2(1-e^{-2\xi h})}{2|\xi|}|\hat{f}(\xi)|\,\mathrm{d}\xi$$
$$\le C_2\|f\|^2_{H^{1/2}(\mathbb{R})},$$

finishing the proof. ■

We can now define the Dirichlet-to-Dirichlet operator of (3.5.1). Since our problem is invariant with respect to translations along the x_1-axis, we only consider the target boundary Γ_0^θ.

3.5.5 Definition. Let $\theta \in (0, \pi)$, and let $\mathcal{S}_\Delta : H^{1/2}(\mathbb{R}) \to H^1_{\text{loc}}(\mathbb{R}^2_+)$ denote the solution operator associated with (3.5.1). For $f \in C_0^\infty(0, \infty)$, define the operator D_Δ^θ by

$$D_\Delta^\theta f(z) = (\mathcal{S}_\Delta f)(z\cos(\theta), z\sin(\theta)),$$

where f is extended by zero to be in $C_0^\infty(\mathbb{R})$. ■

Let us reiterate the meaning of D_Δ^θ: for some $f \in C_0^\infty(0, \infty)$, it gives the trace on line $\Gamma_0^\theta = \{(z\cos(\theta), z\sin(\theta))^\top : z > 0\}$ of the solution to

$$\begin{cases} \Delta u = 0 & \text{in } \mathbb{R}^2_+, \\ u(x_1, 0) = f(x_1) & \text{for } x_1 > 0, \\ u(x_1, 0) = 0 & \text{for } x_1 < 0, \\ u \text{ bounded} & \text{on } \mathbb{R}^2_+. \end{cases} \tag{3.5.3}$$

We call D_Δ^θ the *Dirichlet-to-Dirichlet* operator (abbreviated as DtD operator) since it maps the Dirichlet data on $(0, \infty) \times \{0\}$ to the Dirichlet data on Γ. Note that the two sets of interest are touching each other at the origin $(0, 0)$, as shown in Figure 3.3.

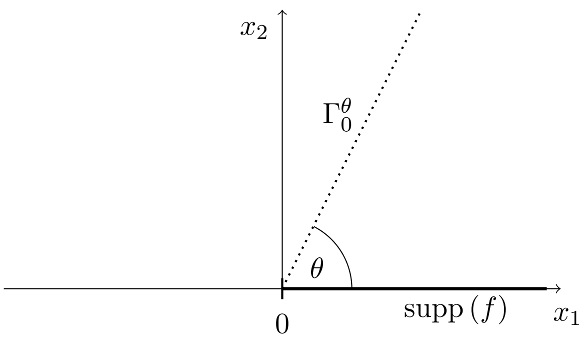

Figure 3.3: Sketch of the geometry behind the problem (3.5.3).

To obtain an explicit estimate of the norm, we transform the Laplace equation into polar coordinates, where the radius is logarithmically scaled.

3.5.6 Lemma. Let $f \in C_0^\infty(0, \infty)$, and let $u = u(r, \theta)$ be the solution to (3.5.3), given in polar coordinates. Define $\tilde{u} : \mathbb{R} \times (0, \pi) \to \mathbb{C}$ and $\tilde{f} : \mathbb{R} \to \mathbb{C}$ by

$$\tilde{u}(\log(r), \theta) = u(r, \theta) \quad \text{and} \quad \tilde{f}(\log(r)) = f(r).$$

Then $\tilde{u}$ fulfils

$$\begin{cases} \partial_\rho^2 \tilde{u}(\rho, \theta) + \partial_\theta^2 \tilde{u}(\rho, \theta) = 0 & \text{for } (\rho, \theta) \in \mathbb{R} \times (0, \pi), \\ \tilde{u}(\rho, 0) = \tilde{f}(\rho) & \text{for } \rho \in \mathbb{R}, \\ \tilde{u}(\rho, \pi) = 0 & \text{for } \rho \in \mathbb{R}, \\ \tilde{u} \text{ bounded}, \end{cases} \tag{3.5.4}$$

and it holds that

$$\begin{aligned}\|g\|^2_{(0,\infty)} &= \int_{\mathbb{R}} |\tilde{g}(\rho)|^2 e^{\rho} \mathrm{d}\rho, \\ \|\partial_r g\|^2_{(0,\infty)} &= \int_{\mathbb{R}} |\partial_\rho \tilde{g}(\rho)|^2 e^{-\rho} \mathrm{d}\rho,\end{aligned} \tag{3.5.5}$$

where $g = u(\,\cdot\,,\theta)$ and $\tilde{g} = \tilde{u}(\,\cdot\,,\theta)$, or similarly $g = f$ and $\tilde{g} = \tilde{f}$. ■

Proof. Let us recall that (see Subsection 1.2.2 to recap the notation)

$$\|g\|^2_{(0,\infty)} = \int_0^\infty |g(x)|^2 \,\mathrm{d}x.$$

We have that

$$\begin{aligned}0 = \Delta_{(r,\theta)} u(r,\theta) &= \left(\partial_r^2 + \frac{1}{r}\partial_r + \frac{1}{r^2}\partial_\theta^2\right) \tilde{u}(\log(r),\theta) \\ &= \partial_\rho^2 \tilde{u}(\log(r),\theta)\frac{1}{r^2} + \frac{1}{r^2}\partial_\theta^2 \tilde{u}(\log(r),\theta).\end{aligned}$$

Multiplying by r^2 yields the Laplace equation for $\tilde{u}$. The equations for the traces are rather clear. For the norm, notice that

$$\begin{aligned}\int_0^\infty |\partial_r u(r,\theta)|^2 \,\mathrm{d}r = \int_0^\infty |\partial_r[\tilde{u}(\log(r),\theta)]|^2 \,\mathrm{d}r &= \int_0^\infty |(\partial_\rho \tilde{u})(\log(r),\theta)\frac{1}{r}|^2 \,\mathrm{d}r \\ &= \int_{\mathbb{R}} |\partial_\rho \tilde{u}(\rho,\theta)|^2 \frac{1}{e^{2\rho}} e^{\rho} \,\mathrm{d}\rho,\end{aligned}$$

where we substituted $\log(r) = \rho$ in the last step. The corresponding statement for $\|u(\,\cdot\,,\theta)\|^2_{(0,\infty)}$ is obtained analogously. ■

We now have to solve (3.5.4) in a representation which gives access to the norms (3.5.5). The usual Fourier transform is not well suited for those spaces, so we will introduce another one.

3.5.7 Definition and Lemma. For $\beta \in \mathbb{R}$ we define the norm

$$\|f\|^2_{L^2(\mathbb{R}, e^{2\beta\rho}\mathrm{d}\rho)} := \int_{\mathbb{R}} |f(\rho)|^2 e^{2\beta\rho} \,\mathrm{d}\rho.$$

We furthermore define the unitary transformation $\mathcal{F}_\beta : L^2(\mathbb{R}, e^{2\beta\rho}\mathrm{d}\rho) \to L^2(\mathbb{R})$ by

$$\mathcal{F}_\beta f(\xi) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-i\xi\rho+\beta\rho} f(\rho) \,\mathrm{d}\rho.$$

Lastly, for f such that $f \in L^2(\mathbb{R}, e^{2\beta\rho}\mathrm{d}\rho)$ and $\partial_\rho f \in L^2(\mathbb{R}, e^{2\beta\rho}\mathrm{d}\rho)$, it holds that

$$[\mathcal{F}_\beta \partial_\rho f](\xi) = (i\xi - \beta)\mathcal{F}_\beta f(\xi). \tag{3.5.6}$$

We call $\mathcal{F}_\beta$ the *β-Fourier–Laplace transform.* ■

Proof. The unitarity can be seen by noting that $\mathcal{F}_\beta f = \mathcal{F}(e^{\beta \cdot} f(\,\cdot\,))$ and exploiting the unitarity of the Fourier transform. The representation for the derivative is easily obtained by partial integration for some $f \in C_0^\infty(\mathbb{R})$. ■

It follows a technical Lemma with a rather long proof, which could be an interesting exercise in an introductory calculus course.

3.5.8 Lemma. Let $\theta \in (0,\pi)$. Then

$$\left|\frac{e^{iz\theta} - e^{i2\pi z}e^{-iz\theta}}{1 - e^{i2\pi z}}\right|^2 \leq \frac{1+\cos(\theta)}{2} \qquad \text{for } z = \pm\frac{1}{2} + i\xi,\ \xi \in \mathbb{R}.$$ ■

Proof. [2] Let $z = a + i\xi$, where $a, \xi \in \mathbb{R}$. We then obtain after a straightforward (but slightly lengthy) calculation

$$\left|\frac{e^{iz\theta} - e^{i2\pi z}e^{-iz\theta}}{1 - e^{i2\pi z}}\right|^2 = \frac{e^{-2\xi\theta} + e^{-2\xi(2\pi-\theta)} - 2e^{-2\xi\pi}\cos(2a(\pi-\theta))}{1 + e^{-4\xi\pi} - 2e^{-2\xi\pi}\cos(2\pi a)}.$$

For $a = \pm\frac{1}{2}$, we obtain $\cos(2\pi a) = -1$, and $\cos(a(2\pi-\theta)) = -\cos(\theta)$, so that

$$\begin{aligned}
\left|\frac{e^{iz\theta} - e^{i2\pi z}e^{-iz\theta}}{1 - e^{i2\pi z}}\right|^2 &= \frac{e^{-2\xi\theta} + e^{-2\xi(2\pi-\theta)} + 2e^{-2\xi\pi}\cos(\theta)}{1 + e^{-4\xi\pi} + 2e^{-2\xi\pi}} \\
&= \frac{e^{2\xi(\pi-\theta)} + e^{-2\xi(\pi-\theta)} + 2\cos(\theta)}{e^{2\xi\pi} + e^{-2\xi\pi} + 2} \\
&= \frac{\cosh(2\xi(\pi-\theta)) + \cos(\theta)}{\cosh(2\pi\xi) + 1} \\
&=: \frac{n(\xi)}{d(\xi)},
\end{aligned}$$

where we abbreviated $n(\xi) = \cosh(2\xi(\pi-\theta)) + \cos(\theta)$ for the numerator and $d(\xi) = \cosh(2\pi\xi) + 1$ for the denominator. Note that both n and d are even functions, so that we can restrict ourselves to considering $\xi \geq 0$. We will now prove that

$$\frac{n(\xi)}{d(\xi)} \leq \frac{n(0)}{d(0)} = \frac{1+\cos(\theta)}{2} \qquad \text{for all } \xi > 0. \tag{3.5.7}$$

We have that

$$\frac{n(\xi)}{d(\xi)} = \frac{n(0)}{d(0)}\,\frac{1 + \frac{n(\xi)-n(0)}{n(0)}}{1 + \frac{d(\xi)-d(0)}{d(0)}},$$

so that (3.5.7) is fulfilled if and only if

$$1 + \frac{n(\xi)-n(0)}{n(0)} \leq 1 + \frac{d(\xi)-d(0)}{d(0)} \qquad \text{for all } \xi > 0,$$

or equivalently (since $d(\xi) - d(0) > 0$, $n(\xi) - n(0) > 0$)

$$\frac{n(\xi)-n(0)}{d(\xi)-d(0)} \leq \frac{n(0)}{d(0)} \qquad \text{for all } \xi > 0. \tag{3.5.8}$$

[2] The Lemma was posed by the author as a "small exercise" to Uwe Zeltmann. The critical idea to use Cauchy's mean value theorem is due to him.

By Cauchy's mean value theorem, for any $\xi > 0$ there exists some $\eta_\xi \in (0, \xi)$ such that

$$\frac{n(\xi) - n(0)}{d(\xi) - d(0)} = \frac{n'(\eta_\xi)}{z'(\eta_\xi)},$$

so that (3.5.8) follows immediately if we can show that

$$\frac{n'(\eta)}{d'(\eta)} \leq \frac{n(0)}{d(0)} \qquad \text{for all } \eta > 0.$$

Hence let us consider

$$f(\eta) := n(0)d'(\eta) - d(0)n'(\eta), \qquad \text{for } \eta > 0.$$

We have to show that $f(\eta) \geq 0$. Explicitly calculating, we obtain

$$f(\eta) = (1 + \cos(\theta))2\pi \sinh(2\pi\eta) - 2(\pi - \theta)\sinh(2(\pi - \theta)\eta).$$

We have $f(0) = 0$, and furthermore, one finds that

$$\begin{aligned} f'(\eta) &= (1 + \cos(\theta))4\pi^2 \cosh(2\pi\eta) - 4(\pi - \theta)^2 \cosh(2(\pi - \theta)\eta) \\ &\geq (1 + \cos(\theta))4\pi^2 \cosh(2\pi\eta) - 4(\pi - \theta)^2 \cosh(2\pi\eta) \\ &= 4(\pi^2(1 + \cos(\theta)) - (\pi - \theta)^2)\cosh(2\pi\eta) \\ &\geq 0, \end{aligned}$$

since both terms on the right hand side are strictly non-negative: this is clear for $\cosh(2\pi\eta)$, and we will consider $(\pi^2(1 + \cos(\theta)) - (\pi - \theta)^2)$ below. Hence it follows that $f'(\eta) \geq 0$ for any $\eta > 0$, and accordingly $f(\eta) \geq f(0) = 0$ for any $\eta > 0$.

Let us pick up the last bit, and consider

$$g(\theta) := (\pi^2(1 + \cos(\theta)) - (\pi - \theta)^2) = \cos(\theta)\pi^2 + (2\pi - \theta)\theta.$$

For $\theta \in (0, \pi/2)$, the cosine is positive, and hence both terms on the right hand side are positive, i.e. $g(\theta) \geq 0$. Let us show that $g(\theta)$ is monotonously decreasing on $(\pi/2, \pi)$. Note that from the convexity of the map $[\pi/2, \pi] \to \mathbb{R}, \theta \mapsto -\sin(\theta)$ one obtains

$$-\sin(\theta) \leq \frac{2}{\pi}(\theta - \pi) \quad \text{for any} \quad \theta \in [\pi/2, \pi],$$

since the right hand side describes the secant through the points $(\pi/2, -\sin(\pi/2))$ and $(\pi, \sin(\pi))$. Hence we obtain for any $\theta \in (\pi/2, \pi)$

$$\begin{aligned} g'(\theta) &= -\sin(\theta)\pi^2 + 2\theta(\pi - \theta) \\ &\leq \pi^2 \frac{2}{\pi}(\theta - \pi) + 2\theta(\pi - \theta) \\ &= 2(\pi - 1)(\theta - \pi) \\ &\leq 0, \end{aligned}$$

and consequently $g(\theta) \geq g(\pi) = 0$ for any $\theta \in (\pi/2, \pi)$, finishing the proof. ■

The proof of the following lemma collects the main ingredients of this section.

3.5.9 Lemma. Let $f \in C_0^\infty(0,\infty)$ and let $u = \mathcal{S}_\Delta f$ be the solution of (3.5.3), in polar coordinates. Then for any $\theta \in (0,\pi)$ it holds that

$$\begin{aligned}\|u(\,\cdot\,,\theta)\|^2_{(0,\infty)} &\le \frac{1+\cos(\theta)}{2}\|f\|^2_{(0,\infty)},\\ \|\partial_r u(\,\cdot\,,\theta)\|^2_{(0,\infty)} &\le \frac{1+\cos(\theta)}{2}\|\partial_r f\|^2_{(0,\infty)}.\end{aligned}$$

■

Proof. Let $f \in C_0^\infty(0,\infty)$, and let $\tilde f : \mathbb{R} \to \mathbb{C}$, $\tilde u : \mathbb{R} \times (0,\pi) \to \mathbb{C}$ be defined as in Lemma 3.5.6. Let us define the partial $\frac{1}{2}$-Fourier–Laplace transform of $\tilde u$ by

$$w(\xi,\theta) = [\mathcal{F}_{1/2}\tilde u(\,\cdot\,,\theta)](\xi) = \frac{1}{\sqrt{2\pi}}\int\limits_{\mathbb{R}} e^{-i\xi\rho+\frac{1}{2}\rho}\tilde u(\rho,\theta)\,\mathrm{d}\rho,$$

and let $h = \mathcal{F}_{1/2}\tilde f$. Then we have by (3.5.5) and the unitarity of $\mathcal{F}_\beta$ (Definition and Lemma 3.5.7) that

$$\|u(\,\cdot\,,\theta)\|^2_{(0,\infty)} = \int\limits_{\mathbb{R}} |\tilde u(\rho,\theta)|^2 e^\rho\,\mathrm{d}\rho = \int\limits_{\mathbb{R}} |w(\xi,\rho)|^2\,\mathrm{d}\xi. \tag{3.5.9}$$

And similarly

$$\|f\|^2_{(0,\infty)} = \|h\|^2_{\mathbb{R}}. \tag{3.5.10}$$

Let us transform the problem for $\tilde u$ by $\mathcal{F}_{1/2}$: from (3.5.4) we obtain with the help of the differentiation rule for $\mathcal{F}_\beta$ (3.5.6) that w fulfils

$$\begin{cases} \left(i\xi - \frac{1}{2}\right)^2 w(\xi,\theta) + \partial_\theta^2 w(\xi,\theta) = 0 & \text{for } \xi \in \mathbb{R},\ \theta \in (0,\pi),\\ w(\xi,0) = h(\xi) & \text{for } \xi \in \mathbb{R},\\ w(\xi,\pi) = 0 & \text{for } \xi \in \mathbb{R}.\end{cases}$$

One easily sees that the solution of this problem is given by (setting $z(\xi) = i\xi - \frac{1}{2}$ for abbreviation)

$$w(\xi,\theta) = h(\xi)\frac{e^{iz(\xi)\theta} - e^{i2\pi z(\xi)}e^{-iz(\xi)\theta}}{1 - e^{i2\pi z(\xi)}},$$

so that we obtain by Lemma 3.5.8

$$|w(\xi,\theta)|^2 = |h(\xi)|^2\left|\frac{e^{iz(\xi)\theta} - e^{i2\pi z}e^{-iz(\xi)\theta}}{1 - e^{i2\pi z(\xi)}}\right|^2 \le \frac{1+\cos(\theta)}{2}|h(\xi)|^2.$$

Integrating ξ over $\mathbb{R}$ we obtain

$$\|w(\,\cdot\,,\theta)\|^2_{\mathbb{R}} \le \frac{1+\cos(\theta)}{2}\|h\|^2_{\mathbb{R}},$$

which by (3.5.9) and (3.5.10) is equivalent to

$$\|u(\,\cdot\,,\theta)\|^2_{(0,\infty)} \le \frac{1+\cos(\theta)}{2}\|f\|^2_{(0,\infty)}.$$

This finishes the proof of the bound for $\|u(\,\cdot\,,\theta)\|_{L^2(0,\infty)}$.

Let us prove the second bound for the $L^2(0,\infty)$ norm of $\partial_r u(\,\cdot\,,\theta)$. We begin by defining the (partial) $-\frac{1}{2}$-Fourier–Laplace transform by

$$v(\xi,\theta) = [\mathcal{F}_{-1/2}\tilde{u}(\,\cdot\,,\theta)](\xi) = \frac{1}{\sqrt{2\pi}} \int\limits_{\mathbb{R}} e^{-i\xi\rho-\frac{1}{2}\rho}\tilde{u}(\rho,\theta)\,\mathrm{d}\rho,$$

and similarly, $k = \mathcal{F}_{-1/2}f$. Then we obtain, as before by (3.5.5) and the unitarity of $\mathcal{F}_{-1/2}$, that

$$\begin{aligned} \|\partial_r f\|^2_{(0,\infty)} &= \int\limits_{\mathbb{R}} |\partial_\rho \tilde{f}(\rho)|^2 e^{-\rho}\mathrm{d}\rho = \int\limits_{\mathbb{R}} \left|[\mathcal{F}_{-1/2}\partial_\rho\tilde{f}](\xi)\right|^2 \mathrm{d}\xi \\ &= \int\limits_{\mathbb{R}} \left|\left(i\xi+\tfrac{1}{2}\right)\mathcal{F}_{-1/2}\tilde{f}(\xi)\right|^2 \mathrm{d}\xi = \left\|\left(i\xi+\tfrac{1}{2}\right)k\right\|^2_{\mathbb{R}}, \end{aligned} \tag{3.5.11}$$

where we used the rule (3.5.6) to calculate the Fourier–Laplace transform of the derivative. Similarly, one obtains that

$$\|\partial_r u(\,\cdot\,,\theta)\|^2_{\mathbb{R}} = \left\|\left(i\xi+\tfrac{1}{2}\right)v(\,\cdot\,,\theta)\right\|^2_{\mathbb{R}}. \tag{3.5.12}$$

By applying the partial $-\frac{1}{2}$-Fourier–Laplace transform to the system (3.5.4), we obtain that v fulfils

$$\begin{cases} \left(i\xi+\frac{1}{2}\right)^2 v(\xi,\theta) + \partial_\theta^2 v(\xi,\theta) = 0 & \text{for } \xi\in\mathbb{R},\ \theta\in(0,\pi), \\ v(\xi,0) = k(\xi) & \text{for } \xi\in\mathbb{R}, \\ v(\xi,\pi) = 0 & \text{for } \xi\in\mathbb{R}, \end{cases}$$

so that (setting $z(\xi) = i\xi+\frac{1}{2}$ for abbreviation)

$$v(\xi,\theta) = k(\xi)\frac{e^{iz(\xi)\theta} - e^{i2\pi z(\xi)}e^{-iz(\xi)\theta}}{1-e^{i2\pi z(\xi)}}.$$

Lemma 3.5.8 yields again that

$$|v(\xi,\theta)|^2 \le \frac{1+\cos(\theta)}{2}|k(\xi)|^2.$$

Multiplying by $|i\xi+1/2|^2$ and integrating ξ over $\mathbb{R}$ yields now

$$\left\|\left(i\xi+\tfrac{1}{2}\right)v(\,\cdot\,,\theta)\right\|^2_{\mathbb{R}} \le \frac{1+\cos(\theta)}{2}\left\|\left(i\xi+\tfrac{1}{2}\right)k\right\|^2_{\mathbb{R}}.$$

Which by (3.5.11) and (3.5.12) actually reads as

$$\|\partial_r u(\,\cdot\,,\theta)\|^2_{\mathbb{R}} \le \frac{1+\cos(\theta)}{2}\|\partial_r f\|^2_{\mathbb{R}},$$

which finishes the proof. ∎

Next we give the main theorem of this section. If the reader is not familiar with the space $H^{1/2}_{00}(0,\infty)$, we refer to the remark after the proof.

3.5.10 Theorem. Let D^θ_Δ be the DtD operator of Definition 3.5.5. If X is one of the spaces $L^2(0,\infty)$, $H^{1/2}_{00}(0,\infty)$ or $H^1_0(0,\infty)$, we have that $D^\theta_\Delta : X \to X$ is continuous and

$$\|D^\theta_\Delta\|_{\mathcal{L}(X,X)} \leq \sqrt{\frac{1+\cos(\theta)}{2}}. \qquad \blacksquare$$

Proof. The statement for $X = L^2(0,\infty)$ and $X = H^1_0(0,\infty)$ follows directly from Lemma 3.5.9 by continuous extension. For $X = H^{1/2}_{00}(0,\infty)$, note that

$$H^{1/2}_{00}(0,\infty) = \big(L^2(0,\infty), H^1_0(0,\infty)\big)_{\frac{1}{2},2},$$

(compare for example [59, Theorem B.9]), where $(X,Y)_{\theta,q}$ denotes the interpolation space between the spaces X and Y. Then it holds (see again [59, Theorem B.2]) that

$$\|D\|_{H^{1/2}_{00}(0,\infty)} \leq \|D\|^{1/2}_{L^2(0,\infty)}\|D\|^{1/2}_{H^1_0(0,\infty)} \leq \left(\sqrt{\frac{1+\cos(\theta)}{2}}\sqrt{\frac{1+\cos(\theta)}{2}}\right)^{\frac{1}{2}},$$

finishing the proof. $\blacksquare$

3.5.11 On the space $H^{1/2}_{00}(0,\infty)$. To obtain a Sobolev space which incorporates zero boundary conditions (in the sense that they can be extended by 0), one often defines for some (sufficiently regular) open set Ω

$$H^s_0(\Omega) := \mathrm{cl}_{H^s(\Omega)} C^\infty_0(\Omega),$$

where cl denotes the closure with respect to the indicated norm. This procedure yields the space of functions which can be extended by 0, *whenever* $s \neq m + 1/2$ *for some* $m \in \mathbb{N} \cup \{0\}$. In this case, $H^s_0(\Omega)$ contains precisely the functions whose normal derivatives up to order $\lfloor s - \frac{1}{2} \rfloor$ vanish on $\partial\Omega$. However, in the case of $s = m + 1/2$ this characterisation fails. For example, if one takes the closure of $C^\infty_0(\Omega)$ in $H^{1/2}(\Omega)$ one obtains the whole space, i.e. (see [59, Theorem 3.40] and Subsection 1.2.2 for more precise references)

$$H^{1/2}(\Omega) = \mathrm{cl}_{H^{1/2}(\Omega)} C^\infty_0(\Omega).$$

On the other hand, if one takes a function from $H^{1/2}(\Omega)$, it generally cannot be extended by zero to obtain an $H^{1/2}(\mathbb{R}^n)$ function. How can one construct a Hilbert space incorporating Dirichlet boundary conditions for this critical exponent? The answer lies in a slightly stronger norm. There are three possible ways to construct a suitable one, which all yield equivalent norms.

(1) Firstly, one can use the construction of the previous theorem and use the fact that it must be the norm obtained by interpolation between H^1_0 and L^2 (see for example [56, 55]).

(2) Secondly, one might extend *before* taking the closure, hence one can define

$$H^{1/2}_{00}(\Omega) := [\mathrm{cl}_{H^{1/2}(\mathbb{R}^n)} C^\infty_0(\Omega)]\Big|_{\Omega},$$

which yields by definition a closed subspace of $H^{1/2}(\mathbb{R}^n)$ with the desired properties. This norm is used in [59].

(3) There are also explicit characterisations with the help of a weighted L^2 norm: for a bounded, sufficiently smooth domain Ω one has the following equivalent norm on $H^{1/2}_{00}(\Omega)$

$$\left(\int\limits_{\Omega} \frac{1}{\operatorname{dist}(x,\partial\Omega)} |f(x)|^2 \,\mathrm{d}x + \|f\|^2_{H^{1/2}(\Omega)}\right)^{\frac{1}{2}},$$

where $\operatorname{dist}(x,\partial\Omega)$ denotes the (Hausdorff) distance between x and the boundary $\partial\Omega$ (see [34, 37, 72]).

3.6 The DtD Operators of $\mathcal{S}_{\mathrm{wg}}$

In this section we will analyse the Dirichlet to Dirichlet operators of $\mathcal{S}_{\mathrm{wg}}$, which we will be employed later in the study of the halfspace matching method.

3.6.1 Definition. Let $c \in \mathbb{R}$, $\theta \in (0,\pi)$. We define $D^\theta_c : H^{1/2}(\mathbb{R}) \to H^{1/2}(0,\infty)$ by

$$D^\theta_c f(z) = \mathcal{S}_{\mathrm{wg}} f(c + \cos(\theta) z, \sin(\theta) z).$$

Furthermore, for some (possibly unbounded) interval $I \subset \mathbb{R}$, the operator $D^\theta_c : H^{1/2}_{00}(I) \to H^{1/2}(0,\infty)$ is defined the same way, that is, for $f \in H^{1/2}_{00}(I)$, denote its extension by 0 by $\tilde{f} \in H^{1/2}(\mathbb{R})$, and let $D^\theta_c f := D^\theta_c \tilde{f}$. ■

Later on, we will study for $d \in \mathbb{R}$ the mapping properties of $D^\theta_c : H^{1/2}_{00}(d,+\infty) \to H^{1/2}(0,\infty)$. The parameter d describes the domain of D^θ_c, and the mapping properties will depend on it. The reader is advised to carefully take note of this.

We proceed by preparing with two auxiliary lemmata.

3.6.2 Lemma. Let $(X_1, \mathrm{d}\nu_1)$ and $(X_2, \mathrm{d}\nu_2)$ be two measure spaces, and let $K : L^2(X_1, \mathrm{d}\nu_1) \to L^2(X_2, \mathrm{d}\nu_2)$ be defined by

$$(Kf)(m_2) = \int\limits_{X_1} k(m_2, m_1) f(m_1) \,\mathrm{d}\nu(m_1) \qquad \text{for almost all } m_2 \in X_2,$$

with a kernel $k : X_2 \times X_1 \to \mathbb{C}$ such that

$$\int\limits_{X_1}\int\limits_{X_2} |k(m_2,m_1)|^2 \,\mathrm{d}\nu_2(m_2)\,\mathrm{d}\nu_1(m_1) < \infty.$$

Then $K : L^2(X_1, \mathrm{d}\nu_1) \to L^2(X_2, \mathrm{d}\nu_2)$ is compact. We call K a *Hilbert–Schmidt operator*. ■

Proof. This Lemma is contained in [47, Section IV.11.2]. ■

3.6.3 Lemma. Let $(X, \mathrm{d}\nu)$ be some measure space, and let the integral operator $K : L^2(X, \mathrm{d}\mu) \to H^1(h,+\infty)$ be defined by

$$Kf(z) := \int\limits_X k(z,m) f(m) \,\mathrm{d}\nu(m) \qquad \text{for } z > h,$$

with a kernel $k : (h, \infty) \times X \to \mathbb{C}$ such that

$$\int\limits_X \int\limits_h^{+\infty} |k(z,m)|^2 \,\mathrm{d}z \,\mathrm{d}\nu(m) < \infty \quad \text{and} \quad \int\limits_X \int\limits_h^{+\infty} |\partial_z k(z,m)|^2 \,\mathrm{d}z \,\mathrm{d}\nu(m) < \infty.$$

Then K is compact. ■

Proof. From the first assumption it follows easily that $K : L^2(X, \mathrm{d}\nu) \to L^2(h, +\infty)$ is a compact operator by Lemma 3.6.2, and similarly the second bound implies that $K' : L^2(X, \mathrm{d}\nu) \to L^2(\mathbb{R}),\ f \mapsto \partial_z K f$ is compact. Let us show that those two imply that K is compact as an operator into $H^1(h, \infty)$. Let $(v_n)_{n\in\mathbb{N}} \subset L^2(X, \mathrm{d}\nu)$ be a bounded sequence. Then, since $K : L^2(X, \mathrm{d}\nu) \to L^2(h, \infty)$ is compact, there is some subsequence $(v_n)_{n\in I}$ such that $(Kv_n)_{n\in I}$ converges strongly in $L^2(h, \infty)$. This sequence is still bounded, and hence by the compactness of K', there exists a second subsequence $(v_n)_{n\in\hat{I}}$ of $(v_n)_{n\in I}$ such that $(K'v_n)_{n\in\hat{I}}$ converges in $L^2(h, \infty)$. Since $\partial_z K v_n = K' v_n$, this implies that our second subsequence $(Kv_n)_{n\in\hat{I}}$ converges in $H^1(h, \infty)$. Hence any bounded sequence in $L^2(X, \mathrm{d}\nu)$ has a subsequence such that its image under K converges strongly in $H^1(h, \infty)$, finishing the proof. ■

The following theorem considers the "nice" DtD operators: if the support has a positive distance to the target boundary, the DtD operator is compact.

3.6.4 Theorem. Let $c < d$. Then $D_c^\theta : H_{00}^{1/2}(d, \infty) \to H_{00}^{1/2}(0, \infty)$ is compact. ■

Proof. Let $\phi : (0, \infty) \to [0, 1]$ be such that $\phi \in \mathbb{C}^\infty(0, \infty)$ and

$$\phi(z) = \begin{cases} 1 & \text{for } z \in [0,1], \\ 0 & \text{for } z \in [2, \infty). \end{cases}$$

Define the two operators $D_1, D_2 : H_{00}^{1/2}(d, \infty) \to H_{00}^{1/2}(0, \infty)$ by

$$D_1 f(z) = \phi(z) D_c^\theta f(z) \quad \text{and} \quad D_2 f(z) = (1 - \phi(z)) D_c^\theta f(z).$$

So that

$$D_c^\theta = D_1 + D_2.$$

For $h_1 < h_2$, let us furthermore introduce $\Gamma(h_1, h_2) := \{(c + \cos(\theta) z, \sin(\theta) z)^\top : z \in [h_1, h_2]\}$, so that $D_c^\theta f = \gamma_{\Gamma(0,\infty)} \mathcal{S}_{\mathrm{wg}} f$, where $\gamma_{\Gamma(0,\infty)}$ denotes the Dirichlet trace on $\Gamma(0, \infty)$.

(a) Let us show that D_1 is compact: denote $u = \mathcal{S}_{wg} f$. We will apply the boundary regularity Theorem 4.18 from [59], with the domains $\Omega_1 \subset \Omega_2$ as sketched in Figure 3.4. Since the trace on $\Gamma_2 = \Omega_2 \cap \{(x_1, 0) : x_1 \in \mathbb{R}\}$ is equal to 0, we obtain that $u \in \hat{H}_0^2(\Omega_1) = \{\psi \in H^2(\Omega_1) : \psi|_{\Gamma_1} = 0\}$, so that $u \in \hat{H}_0^1(\Omega_1) = \{f \in H^1(\Omega_1) : f|_{\Gamma_1} = 0\}$. Here we denoted $\Gamma_1 = \Omega_1 \cap \{(x_1, 0) : x_1 \in \mathbb{R}\}$. Now let us apply the trace theorem [59, Theorem 3.37] to the (partial) Lipschitz boundary

$$B := ([c - 1, c] \times \{0\}) \cup \Gamma(0, 2),$$

which is also sketched in Figure 3.4. Since the B is $C^{0,1}$-smooth, we obtain that $\gamma_B u \in H^{1/2}(B)$. Furthermore, since $\gamma_B u = 0$ on $[c - 1, c] \times \{0\}$, we obtain that

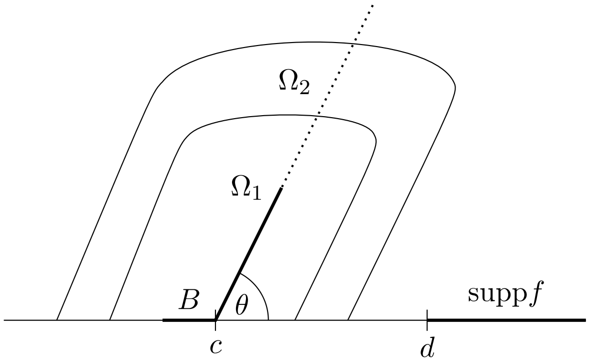

Figure 3.4: Sketch of the domains involved in the application of Theorem 4.18. in [59].

$\gamma_{\Gamma(0,2)}u \in \hat{H}^{1/2}_{00}(0,2)$, where we denote by $\hat{H}^{1/2}_{00}(0,2)$ the subspace of $H^{1/2}(0,2)$ of functions which can be extended by 0 for $x<0$. Hence we obtain that D_1 is factored as follows

$$D_1 : H^{1/2}_{00}(d,\infty) \xrightarrow{\mathcal{S}_{\mathrm{wg}}} \hat{H}^2_0(\Omega_1) \xrightarrow{I} \hat{H}^1_0(\Omega_1) \xrightarrow{\gamma_{\Gamma(0,2)}} \hat{H}^{1/2}_{00}(0,2) \xrightarrow{\phi\,\cdot} H^{1/2}_{00}(0,\infty),$$

where $\phi\,\cdot$ denotes the operator of multiplication by ϕ and extension by zero to obtain a function on $(0,\infty)$. All operators in the chain are bounded, and the embedding $I : \hat{H}^2_0(\Omega_1) \to \hat{H}^1_0(\Omega_1)$ is compact by the Sobolev embedding theorem [59, Theorem 3.27]. This implies that $D_1 = (\phi\,\cdot\,) \circ \gamma_{\Gamma(0,2)} \circ I \circ \mathcal{S}_{wg}$ is compact.

(b) Let us now consider $D_2 : H^{1/2}_{00}(d,\infty) \to H^{1/2}_{00}(0,\infty)$. Due to the multiplier $(1-\phi)$, which vanishes on $[0,1]$, it is sufficient to show that D^θ_c is compact as an operator between $L^2(\mathbb{R}) \to H^1(1,\infty)$. Note that we significantly increased the domain of definition from $H^{1/2}_{00}(d,\infty)$ to $L^2(\mathbb{R})$, while we reduced the image space to $H^1(1,\infty)$.

Let us show that $D^\theta_c : L^2(\mathbb{R}) \to H^1(1,\infty)$ is compact, and define the operator $K : L^2(\Lambda, \mathrm{d}\mu) \to H^1(1,\infty)$ by

$$Kg(z) = \int\limits_\Lambda k(z,m)g(m)\,\mathrm{d}\mu(m) \qquad \text{for } z>1,$$

where

$$k(z,m) = e^{i\sqrt{\kappa-\hat{\lambda}(m)}\sin(\theta)z}\Psi(m, d+\cos(\theta)z) \qquad \text{for } m \in \Lambda, z>1.$$

From the representation formula (3.2.1) we obtain

$$D^\theta_c = K \circ \mathcal{F}_A.$$

Since $\mathcal{F}_A : L^2(\mathbb{R}) \to L^2(\Lambda,\mathrm{d}\mu)$ is bounded, it is sufficient to show that $K : L^2(\Lambda,\mathrm{d}\mu) \to H^1(1,\infty)$ is compact. We will apply Lemma 3.6.3 and show that K is a Hilbert–

Schmidt operator. We have

$$\begin{aligned}
&\int\limits_{\Lambda}\int\limits_{1}^{\infty} |k(z,m)|^2 \,\mathrm{d}z\,\mathrm{d}\mu(m) \\
&\quad = \int\limits_{\Lambda}\int\limits_{1}^{\infty} e^{-2\operatorname{Im}\left(\sqrt{\kappa-\hat{\lambda}(m)}\right)\sin(\theta)z} |\Psi(m, d+\cos(\theta)z)|^2 \,\mathrm{d}z\,\mathrm{d}\mu(m) \\
&\quad \le C_1^2 \int\limits_{\Lambda}\int\limits_{1}^{\infty} e^{-2\operatorname{Im}\left(\sqrt{\kappa-\hat{\lambda}(m)}\right)\sin(\theta)z} \,\mathrm{d}z\,\mathrm{d}\mu(m) \\
&\quad = C_1^2 \int\limits_{\Lambda} \underbrace{\frac{\exp\left(-2\operatorname{Im}\left(\sqrt{\kappa-\hat{\lambda}(m)}\right)\sin(\theta)\right)}{2\operatorname{Im}\left(\sqrt{\kappa-\hat{\lambda}(m)}\right)\sin(\theta)}}_{=:\varphi(\hat{\lambda}(m))} \,\mathrm{d}\mu(m),
\end{aligned}$$

where C_1 is the constant from Lemma 2.4.8, that is, the L^∞-bound for Ψ. We now have to check that this integral is bounded, and recall the definition of the spectral integral (see Definition 2.2.5)

$$\int\limits_{\Lambda} \varphi(\hat{\lambda}(m))\mathrm{d}\mu(m) = \sum_{n=1}^{N} \varphi(\lambda_n) + \int\limits_{q_+}^{\infty} \frac{\varphi(\lambda)}{2\sqrt{\lambda-q_+}}\mathrm{d}\lambda + \int\limits_{q_-}^{\infty} \frac{\varphi(\lambda)}{2\sqrt{\lambda-q_-}}\mathrm{d}\lambda. \tag{3.6.1}$$

Note that since $\operatorname{Im}(\kappa) \neq 0$, we obtain that $\operatorname{Im}\left(\sqrt{\kappa-\lambda}\right)$ does not vanish for any $\lambda \in \mathbb{R}$. Accordingly, the finite sum in (3.6.1) is well defined. Let us consider the first integral: note that φ is continuous on $\mathbb{R}$. It is straightforward to show that for $\lambda \in (q_+, \infty)$ we have

$$\operatorname{Im}\left(\sqrt{\kappa-\lambda}\right) = \sqrt{1+|\lambda|} + \mathcal{O}(1) \qquad \text{as } \lambda \to \infty,$$

where $\mathcal{O}$ denotes the Landau symbol. So we obtain

$$\varphi(\lambda) = \frac{\exp\left(-2\sqrt{1+|\lambda|}\sin(\theta)\right)}{2\sqrt{1+|\lambda|}\sin(\theta)}(1+\mathcal{O}(1)) \qquad \text{as } \lambda \to \infty.$$

The continuity at q_+ as well as the (almost exponential) decrease for $\lambda \to \infty$ now implies that

$$\int\limits_{q_+}^{\infty} \frac{\varphi(\lambda)}{2\sqrt{\lambda-q_+}}\,\mathrm{d}\lambda < \infty,$$

since the only singularity of the integrand at zero is integrable. The same argument holds true for the second integral from q_- to ∞, showing that the kernel k is square integrable.

It remains to show that $\partial_z k$ is also square integrable. We start by calculating

$$\begin{aligned}
|\partial_z k(z,m)|^2 &= \left|\partial_z \left[e^{i\sqrt{\kappa-\hat\lambda(m)}\sin(\theta)z}\Psi(m,d+\cos(\theta)z)\right]\right|^2 \\
&= e^{-2\operatorname{Im}\left(\sqrt{\kappa-\hat\lambda(m)}\right)\sin(\theta)z}\Big|i\sqrt{\kappa-\hat\lambda(m)}\sin(\theta)\Psi(m,d+\cos(\theta)z) \\
&\qquad\qquad + \partial_x\Psi(m,d+\cos(\theta)z)\cos(\theta)\Big|^2 \\
&\leq e^{-2\operatorname{Im}\left(\sqrt{\kappa-\hat\lambda(m)}\right)\sin(\theta)z}2\Big(|\kappa-\hat\lambda(m)|C_1^2\sin^2(\theta) \\
&\qquad\qquad + (1+|\hat\lambda(m)|)C_2^2\cos^2(\theta)\Big) \\
&\leq C\exp\left(-2\operatorname{Im}\left(\sqrt{\kappa-\hat\lambda(m)}\right)\sin(\theta)z\right)(1+|\hat\lambda(m)|),
\end{aligned}$$

as one easily obtains by Lemma 2.4.8, which gives the constants C_1 and C_2 to estimate both Ψ and $\partial_x\Psi$. This now implies that

$$\begin{aligned}
&\int_\Lambda\int_1^\infty |\partial_z k(z,m)|^2 \,\mathrm{d}z\,\mathrm{d}\mu(m) \\
&\leq C\int_\Lambda\int_1^\infty \exp\left(-2\operatorname{Im}\left(\sqrt{\kappa-\hat\lambda(m)}\right)\sin(\theta)z\right)(1+|\hat\lambda(m)|)\,\mathrm{d}z\,\mathrm{d}\mu(m) \\
&= C\int_\Lambda \underbrace{\frac{\exp\left(-2\operatorname{Im}\left(\sqrt{\kappa-\hat\lambda(m)}\right)\sin(\theta)z\right)}{2\operatorname{Im}\left(\sqrt{\kappa-\hat\lambda(m)}\right)\sin(\theta)}(1+|\hat\lambda(m)|)}_{=:\tilde\varphi(\hat\lambda(m))}\,\mathrm{d}\mu(m).
\end{aligned}$$

By the very same arguments as before, one now sees that this integral is finite: $\tilde\varphi$ is still continuous and $\tilde\varphi(\lambda)$ decreases almost exponentially as $\lambda\to\infty$. Hence it follows that

$$\int_\Lambda\int_1^\infty |\partial_z k(z,m)|^2\,\mathrm{d}z\,\mathrm{d}\mu(m) \leq C\int_\Lambda \tilde\varphi(\hat\lambda(m))\,\mathrm{d}\mu(m) < \infty.$$

This now shows by Lemma 3.6.3 that $K : L^2(\Lambda,\mathrm{d}\mu)\to H^1(1,\infty)$ is compact, and hence $D_c^\theta = K\circ\mathcal{F}_A : H_{00}^{1/2}(d,\infty)\to H^1(1,\infty)$ is compact. This implies that $D_2 = (1-\phi)\circ D_c^\theta : H_{00}^{1/2}(d,\infty)\to H_0^1(0,\infty)$ is also compact, which in turn yields by the continuity of the embedding $H_0^1(0,\infty)\to H_{00}^{1/2}(0,\infty)$ that this proof is at its end.

■

3.6.5 Corollary. For $c > d$, the operator $D_c^\theta : H_{00}^{1/2}(-\infty,d)\to H_{00}^{1/2}(0,\infty)$ is compact. ■

Proof. This follows from the previous theorem by mirroring along the axis $\{x_1 = 0\}$. ■

The last theorem deals with the mapping properties of the DtD operator when the two boundaries touch. In this case, compactness cannot be retained, however the non-compact part can be shown to be bounded and sufficiently small.

3.6.6 Theorem. Let $c = d \in \mathbb{R}$, $\theta \in (0, \pi)$. Then $D_c^\theta : H_{00}^{1/2}(d, \infty) \to H_{00}^{1/2}(0, \infty)$ can be split into two parts,

$$D_c^\theta = D_C + D_B,$$

where $D_C : H_{00}^{1/2}(d, \infty) \to H_{00}^{1/2}(0, \infty)$ is compact, and $D_B : H_{00}^{1/2}(d, \infty) \to H_{00}^{1/2}(0, \infty)$ is bounded with $\|D_B\| < 1$. ■

Proof. Without loss of generality, we assume $d = 0$, so that $D_c^\theta = D_0^\theta$: else, one can redefine the parameters a, b, q to translate the solution operator to obtain $c = 0$. Let $\phi : (0, \infty) \to [0, 1]$ be some $C^\infty(0, \infty)$-function such that

$$\phi(z) = \begin{cases} 1 & \text{for } z \in [0, 1], \\ 0 & \text{for } z \in [2, \infty). \end{cases}$$

We now split D_0^θ into three parts, namely

$$D_0^\theta f(z) = \phi(z) D_\Delta^\theta f(z) + \phi(z)(D_0^\theta - D_\Delta^\theta) f(z) + (1 - \phi(z)) D_0^\theta f(z),$$

where D_Δ^θ denotes the DtD operator of the Laplacian as defined in Definition 3.5.5. Let us consider each of the three operators in the previous splitting.

Firstly, the operator $D_B := \phi D_\Delta^\theta : H_{00}^{1/2}(0, \infty) \to H_{00}^{1/2}(0, \infty)$ is bounded with

$$\|D_B\| < \sqrt{\frac{\cos(\theta) + 1}{2}} < 1$$

by Theorem 3.5.10.

Secondly, the operator $(1 - \phi) D_0^\theta : H_{00}^{1/2}(0, \infty) \to H_{00}^{1/2}(0, \infty)$ can be shown to be compact as in the second part of the proof of Theorem 3.6.4, analogous to the operator D_2 therein.

Hence we only have to consider

$$\phi(D_0^\theta - D_\Delta^\theta) : H_{00}^{1/2}(0, \infty) \to H_{00}^{1/2}(0, \infty).$$

To see that this operator is compact, let $f \in H_{00}^{1/2}(0, \infty)$, denote $u = \mathcal{S}_{\mathrm{wg}} f$ and $v = \mathcal{S}_\Delta f$. By Lemma 3.2.5 we have $u \in H^1(\mathbb{R}_+^2)$, while by Lemma 3.5.4 we have $v \in H^1(\mathbb{R} \times (0, h))$ for any $h > 0$. Furthermore, the two functions are solutions of

$$\begin{cases} \Delta u + (\kappa - q) u = 0 & \text{in } \mathbb{R}^2, \\ u(x_1, 0) = f(x_1) & \text{for } x_1 > 0, \\ u(x_1, 0) = 0 & \text{for } x_1 < 0, \end{cases}$$

and

$$\begin{cases} \Delta v = 0 & \text{in } \mathbb{R}^2, \\ v(x_1, 0) = f(x_1) & \text{for } x_1 > 0, \\ v(x_1, 0) = 0 & \text{for } x_1 < 0. \end{cases}$$

Accordingly, their difference $w = v - u \in H^1(\mathbb{R} \times (0,h))$ solves (in a variational sense)

$$\begin{cases} \Delta w = (\kappa - q)u & \text{in } \mathbb{R}^2, \\ \quad w = 0 & \text{on } \mathbb{R} \times \{0\}. \end{cases}$$

As in part (a) of the proof of Theorem 3.6.4, we can now apply the regularity Theorem 4.18 in [59] to obtain that $w \in \hat{H}^2(\Omega_1)$, and by again considering the traces on B, we obtain that $\gamma_{\Gamma(0,2)} w \in \hat{H}^{1/2}_{00}(0,2)$ (for the definitions of $\hat{H}^2_0(\Omega_1)$, Ω_1, $\Gamma(0,1)$, B and $\hat{H}^{1/2}_{00}(0,2)$ we refer to the proof of Theorem 3.6.4). Hence, as before, we can factorise $\phi(D^\theta_0 - D^\theta_\Delta)$ as follows

$$\begin{aligned} &\phi(D^\theta_0 - D^\theta_\Delta) = (\phi\,\cdot\,) \circ \gamma_{\Gamma(0,2)} \circ I \circ (\mathcal{S}_\Delta - \mathcal{S}_{\mathrm{wg}}) : \\ &H^{1/2}_{00}(d,\infty) \xrightarrow{\mathcal{S}_\Delta - \mathcal{S}_{\mathrm{wg}}} \hat{H}^2_0(\Omega_1) \xrightarrow{I} \hat{H}^1_0(\Omega_1) \xrightarrow{\gamma_{\Gamma(0,2)}} \hat{H}^{1/2}_{00}(0,2) \xrightarrow{\phi\,\cdot} H^{1/2}_{00}(0,\infty), \end{aligned}$$

and due to the compactness of the embedding $I : \hat{H}^1_0(0,2) \to \hat{H}^{1/2}_{00}(0,2)$ the composition of all operators becomes compact. ■

3.6.7 Corollary. For $c = d$, the operator $D^\theta_c : H^{1/2}_{00}(-\infty,d) \to H^{1/2}_{00}(0,\infty)$ can be split into two parts.

$$D^\theta_c = D_C + D_B,$$

where $D_C : H^{1/2}_{00}(-\infty,d) \to H^{1/2}_{00}(0,\infty)$ is compact and $D_B : H^{1/2}_{00}(-\infty,d) \to H^{1/2}_{00}(0,\infty)$ is bounded with $\|D_B\| < 1$. ■

Proof. This follows from the previous theorem by mirroring along the axis $\{x_1 = 0\}$. ■

3.6.8 Remark. The mapping properties of the DtD as given in Theorems 3.6.4 and 3.6.6 can be shown with the space $H^{1/2}_{00}$ replaced by L^2 or H^1_0. For the L^2 case, some additional arguments are required, to adapt to the lower regularity of the boundary data (compare Remark 3.2.6), since we cannot use the classical trace theorems. The H^1_0 case can be studied with the same arguments as already presented. We have decided to use the $H^{1/2}_{00}$ framework, since it seems the canonical choice in the context of variational problems and allows us to use the classical trace and embedding theorems.

4 Halfspace Matching

4.1 Introduction and References

4.1.1 Introduction. In this chapter, we will introduce the method of *halfspace matching* for a rather simple model problem: it will allow us to reduce the 2D Helmholtz problem in the exterior of a triangle to a set of equations for the traces on certain boundaries, reducing the overall dimension by 1.

The resulting set of equations, called *compatibility equations* in the following, will be shown to be Fredholm and uniquely solvable, which in turn will yield the equivalence of the exterior Helmholtz problem with the compatibility equations.

A small warning: this Chapter requires some rather ghastly notation describing the geometry and the DtD operators. The author tried to reduce complications by drawing some pictures illustrating the geometrical notations.

This chapter mostly collects arguments from the previous chapter to show the well-posedness. The result itself will not be relevant for the following chapters, and serves mainly as a validation that this reformulation works. We note, however, that the notation introduced in Section 4.2 will be relevant for the following chapters, while the remainder can be skipped at first reading.

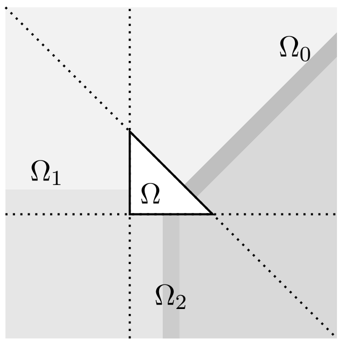

Figure 4.1: Sample geometry as considered in this chapter. The grey areas indicate the value of q (dark grey corresponds to low $q(x)$).

4.1.2 References. The basic structure of this proof is not new, it can found in Tonnoir's thesis [74] for the free space, and a second publication is being prepared right now [75]. Compared to [74], our work is mostly analogous, with a few differences in the details, since we use a slightly different functional framework, and study the case of a triangle instead of a rectangular domain.

4.2 The Problem of Interest and Notations

4.2.1 The problem of interest. Let $\kappa \in \mathbb{C}\backslash\mathbb{R}$ and $\Omega \subset \mathbb{R}^2$ be some arbitrary triangle. Furthermore, let g be some boundary data in $H^{1/2}(\partial\Omega)$. We assume that $q : \mathbb{R}^2 \to \mathbb{R}$ fulfils Definition and Assumption 2.2.2 *in each halfspace associated with* Ω. Below we will define accurately what this means. Consider the problem of finding $U \in H^1(\mathbb{R}^2 \setminus \overline{\Omega})$

such that

$$\begin{cases} \Delta U + (\kappa - q)U = 0 & \text{in } \Omega, \\ U = g & \text{on } \partial\Omega. \end{cases} \tag{4.2.1}$$

This problem is uniquely solvable by Theorem 1.4.3.

Before going on, let us give a very rough description of the assumption for q: the "halfspaces associated with Ω", denoted by $\Omega_0, \Omega_1, \Omega_2$, can be found by extending the sides of the triangle, and taking the halfspace on other side of the resulting line (see Figure 4.2). Note that the halfspaces overlap at infinite cones originating from the edges of the triangle.

In particular, we will allow for q to describe waveguides which extend perpendicular from the sides of the triangle to infinity. An example configuration is shown in Figure 4.1.

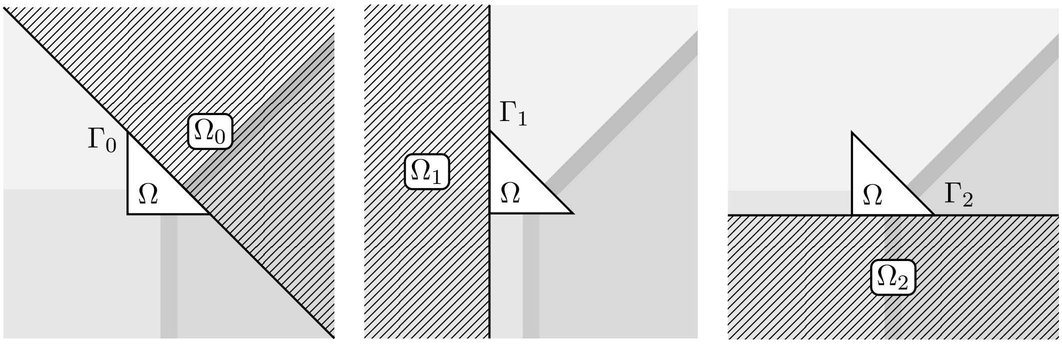

Figure 4.2: Sketch of the three exterior halfspaces associated with the triangle Ω.

4.2.2 Notation of geometry. Let us introduce a number of notations describing the geometry. In advance we point to Figure 4.3, where the following quantities are illustrated.

- The sign-variable $\sigma \in \{\pm\}$ is used more freely here: in equations, we identify it with (the real numbers) $+1 \mathrel{\widehat{=}}$ "+" and $-1 \mathrel{\widehat{=}}$ "−".

- Since the three halfspaces are ordered in a periodical sense, we generally consider the halfspace index $n \in \{0, 1, 2\}$ as an element of

$$n \in \mathbb{Z}/3\mathbb{Z},$$

  so that for example $\Omega_{2+1} = \Omega_0$. We will write $n \in \mathbb{Z}/3\mathbb{Z}$ only when the corresponding relation actually uses this convention.

- Let Γ_0^0, Γ_1^0, Γ_2^0 denote the sides of the triangle, ordered in a counter clockwise sense.

- For $n \in \{0, 1, 2\}$, let $\eta^{(n)} \in \mathbb{R}^2$ denote the exterior unit normal of each side of Ω, and let

$$\xi^{(n)} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \eta^{(n)} \in \mathbb{R}^2$$

  denote (the clockwise oriented) tangent vectors to the three sides.

- For $n \in \{0,1,2\}$, define $h_n \in \mathbb{R}$ and $c_n^- < c_n^+$ by
$$\Gamma_n^0 = \{x \in \mathbb{R}^2 : \eta^{(n)} \cdot x = h_n,\ c_n^- \leq \xi^{(n)} \cdot x \leq c_n^+\},$$
so that in the coordinate system $(\xi^{(n)}, \eta^{(n)})$, the boundary Γ_n^0 is given by $[c_n^-, c_n^+] \times \{h_n\}$. In particular, the side of the triangle Γ_n^0 has the (signed) distance h_n from the origin.

- For $n \in \{0,1,2\},\ \sigma \in \{\pm\}$, define the semi-infinite lines Γ_n^σ by
$$\Gamma_n^\sigma = \left\{ h_n \eta^{(n)} + c_n^\sigma \xi^{(n)} + \sigma t \xi^{(n)} : t \geq 0 \right\}.$$
Note that we have a small collision of notation here: the boundary Γ_n^σ should not be confused with the boundary Γ_c^θ from Chapter 3.

- For $n \in \{0,1,2\}$, define the halfspace $\Omega_n \subset \mathbb{R}^2$ by
$$\Omega_n = \{x \in \mathbb{R}^2 : x \cdot \eta^{(n)} > h_n\},$$
which has the boundary
$$\Gamma_n := \partial\Omega_n = \Gamma_n^+ \cup \Gamma_n^0 \cup \Gamma_n^-.$$

- For $n \in \mathbb{Z}/3\mathbb{Z},\ \sigma \in \{\pm\}$, let $\theta_n^\sigma \in (0, \pi)$ denote the angle between
$$\xi^{(n)} \text{ and } \sigma\xi^{(n-\sigma)}.$$

- To simplify notation, we will use a number of canonical isomorphisms: for any $n \in \{0,1,2\}$, a function $f \in H^{1/2}(\mathbb{R})$ is identified with a function $\hat{f} \in H^{1/2}(\Gamma_n)$ by
$$f(\xi) = \hat{f}(\xi\,\xi^{(n)} + h_n\,\eta^{(n)}) \qquad \text{for } \xi \in \mathbb{R}. \tag{4.2.2}$$
Similarly, one obtains canonical isomorphism $H_{00}^{1/2}(\Gamma_n^+) \cong H_{00}^{1/2}(c_n^+, \infty)$, $H_{00}^{1/2}(\Gamma_n^-) \cong H_{00}^{1/2}(-\infty, c_n^-)$, $H_{00}^{1/2}(\Gamma_n^0) \cong H_{00}^{1/2}(c_n^-, c_n^+)$, and similarly for other spaces on the same boundaries. The same way we identify $f \in H^1(\Omega_n)$ with $\hat{f} \in H^1(\mathbb{R}_+^2)$ by
$$f(\xi\,\xi^{(n)} + (\eta + h_n)\,\eta^{(n)}) = \hat{f}(\xi, \eta) \qquad \text{for } \xi \in \mathbb{R},\ \eta > 0. \tag{4.2.3}$$

We can now make our assumption for q more accurate.

4.2.3 Definition and Assumption. We assume that on each halfspace Ω_n, the potential q only depends on the $\xi^{(n)}$ coordinate, that is, there exist three functions $q^{(n)} : \mathbb{R} \to \mathbb{R}$, $n \in \{0,1,2\}$, each fulfilling Definition and Assumption 2.2.2, such that
$$q(\xi\,\xi^{(n)} + (\eta + h_n)\,\eta^{(n)}) = q^{(n)}(\xi) \qquad \text{for all } \xi \in \mathbb{R},\ \eta > 0.$$
We denote by $A_n = -\Delta + q^{(n)}$ the associated operator, and $\mathcal{S}_n$ the corresponding halfspace solution operators (see Section 3.2.2). ■

Note that these assumptions pose rather strong restrictions, which are not necessarily obvious in all cases: for example, if Γ_n^0 and Γ_{n+1}^0 are two sides which join at an obtuse angle, this implies that $q|_{\Omega_n} = \text{const} = q|_{\Omega_{n+1}}$. Compare also Subsection 5.1.3 in Chapter 5 below.

To simplify notation, we need a number of DtD operators, which take the coordinate systems of the different halfspaces into account.

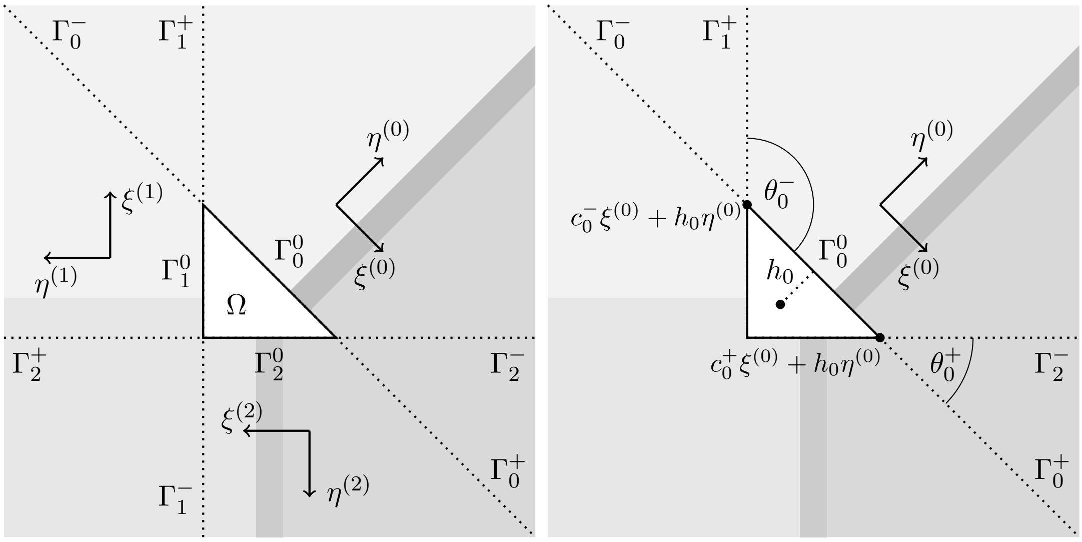

Figure 4.3: Sketch and illustration of the geometrical notation.

4.2.4 Definition. Let $n \in \{0,1,2\}$. For $c \in \mathbb{R}$ and $\theta \in (0,\pi)$, let D_c^θ denote the Dirichlet to Dirichlet operator associated with Ω_n. For $f \in H^{1/2}(\Gamma_n)$, we define the operators $\mathcal{D}_n^+$, $\mathcal{D}_n^-$ by

$$\mathcal{D}_n^+ f(\xi) = \begin{cases} D_{c_n^-}^{\theta_n^-} f(\xi - c_{n+1}^+) & \text{for } \xi > c_{n+1}^+, \\ 0 & \text{for } \xi < c_{n+1}^+, \end{cases}$$

and

$$\mathcal{D}_n^- f(\xi) = \begin{cases} D_{c_n^+}^{\theta_n^+} f(c_{n-1}^- - \xi) & \text{for } \xi < c_{n-1}^-, \\ 0 & \text{for } \xi > c_{n-1}^-. \end{cases}$$

■

What is the purpose of these operators? They take the trace on Γ_n and calculate the corresponding trace on $\Gamma_{n\pm1}^\pm$ in the coordinate system associated with $\Gamma_{n\pm1}$.

4.2.5 The compatibility equations. Consider a solution U of (4.2.1). For $n \in \mathbb{Z}/3\mathbb{Z}$, let us denote the traces on the boundaries of the halfspaces by

$$u_n := U|_{\Gamma_n}.$$

Since $U|_{\Omega_n}$ fulfils a halfspace problem of the type (3.1.1), we obtain (by exploiting the canonical identifications (4.2.2) and (4.2.3)) that

$$U|_{\Omega_n} = \mathcal{S}_n u_n.$$

In particular, by taking the trace of $U|_{\Omega_n}$ on the boundary Γ_{n+1}^+, which is contained in Ω_n, we obtain (recall that we interpret n as an element of $\mathbb{Z}/3\mathbb{Z}$)

$$U|_{\Gamma_{n+1}^+} = [\mathcal{S}_n u_n]|_{\Gamma_{n+1}^+}.$$

The left hand side can be identified with u_{n+1} on the interval (c_{n+1}^+, ∞). Denoting the Dirichlet-to-Dirichlet operator of the halfspace Ω_n by D_c^θ, the right hand side can be rewritten to obtain

$$[\mathcal{S}_n u_n]|_{\Gamma_{n+1}^+}(\xi) = D_{c_n^-}^{\theta_n^-} u_n(\xi - c_{n+1}^+) = \mathcal{D}_n^+ u_n(\xi) \qquad \text{for } \xi > c_{n+1}^+,$$

where we applied Definition 4.2.4. Accordingly, we obtain that

$$u_{n+1}(\xi) = \mathcal{D}_n^+ u_n(\xi) \qquad \text{for } \xi > c_{n+1}^+. \tag{4.2.4}$$

Similarly, one obtains by considering the trace of $U|_{\Omega_n}$ on the boundary Γ_{n-1}^- (which is also contained in Ω_n) that

$$u_{n-1}(\xi) = \mathcal{D}_n^- u_n(\xi) \qquad \text{for } \xi < c_{n-1}^-. \tag{4.2.5}$$

The last two equations (4.2.4) and (4.2.5) are called *compatibility equations*, and are the key equations which have to be solved for the method of halfspace matching. Let us bring them into a (preliminary) operator equation.

4.2.6 The preliminary operator equation. Let us define for $n \in \{0, 1, 2\}$ and $\sigma \in \{-, +, 0\}$

$$u_n^\sigma := U|_{\Gamma_n^\sigma}. \tag{4.2.6}$$

We furthermore extend each function by 0 to get a function on the whole boundary Γ_n, so we can write

$$u_n = u_n^+ + u_n^0 + u_n^-.$$

This helps us to rewrite (4.2.4) as

$$u_{n+1}^+ = \mathcal{D}_n^+(u_n^+ + u_n^0 + u_n^-),$$

while (4.2.5) becomes

$$u_{n-1}^- = \mathcal{D}_n^-(u_n^+ + u_n^0 + u_n^-),$$

which can be rewritten together as

$$u_{n+\sigma}^\sigma - \mathcal{D}_n^\sigma(u_n^+ + u_n^-) = \mathcal{D}_n^\sigma u_n^0, \qquad \text{for } \sigma \in \{\pm\},\ n \in \mathbb{Z}/3\mathbb{Z}. \tag{4.2.7}$$

This is (almost) the equation we will study.

Let us have a look at the original problem in the exterior (4.2.1). Since we aim to find $U \in H^1(\mathbb{R}^2 \setminus \overline{\Omega})$, given the boundary data $g \in H^{1/2}(\partial\Omega)$, we already know $u_n^0 = g|_{\Gamma_n^0}$. Hence we consider the right hand side of (4.2.7) as known, while the remainder of functions are unknowns.

Our goal is to define and study a functional setting, in which the compatibility equations (4.2.7) are well posed.

4.3 Fredholmness for the Exterior of a Triangle

Let us first define a space which contains all unknown traces, and define the *total DtD operator* which acts on this space.

4.3.1 Definition. We define the Hilbert space $\mathcal{V}$ by

$$\mathcal{V} := H^{1/2}_{00}(-\infty, c_0^-) \times H^{1/2}_{00}(c_0^+, +\infty) \times \ldots \times H^{1/2}_{00}(c_2^+, +\infty).$$

We furthermore define the continuous operator $\mathcal{D} : \mathcal{V} \to \mathcal{V}$ as follows: for given $u = (u_0^-, u_0^+, \ldots, u_2^+) \in \mathcal{V}$, let $\mathcal{D}u := v = (v_0^-, v_0^+, \ldots, v_2^+) \in \mathcal{V}$ be given by

$$v^\sigma_{n+\sigma} = \mathcal{D}^\sigma_n (u_n^+ + u_n^-), \qquad \text{for } \sigma \in \{\pm\},\ n \in \mathbb{Z}/3\mathbb{Z}. \qquad \blacksquare$$

We can now rewrite (4.2.7) with the help of $\mathcal{D}$ in the form

$$(I - \mathcal{D})u = F,$$

where F is some right hand side. Note also equation (4.3.1) below, where we have written this equation as an operator matrix.

This definition actually contains an assertion: that $\mathcal{D}$ is well-defined and bounded from $\mathcal{V}$ into $\mathcal{V}$. This, of course, has to be proved, which we will do in a side remark in the proof of Theorem 4.3.3.

Let us also point to a second peculiarity of this definition. If we consider the solution U of (4.2.1), and define u_n^σ via (4.2.6), the vector $u = (u_0^-, \ldots, u_2^+)$ will not be contained in $\mathcal{V}$: there is no reason for u_0^- to vanish at c_0^- to be in $H^{1/2}_{00}(-\infty, c_0^-)$. However, the system of equations for u can be recast into an equivalent system with unknowns in $\mathcal{V}$.

4.3.2 The operator equation in $\mathcal{V}$. Let U be a solution to (4.2.1) with some fixed boundary data $g \in H^{1/2}(\partial\Omega)$. We define $w_n^0 \in H^{1/2}(\mathbb{R})$ (utilising again the canonical identifications (4.2.2)) by

$$w_n^0 = g|_{\Gamma_n^0} \qquad \text{for } n \in \{0, 1, 2\},$$

with some (arbitrary) extension to the whole of Γ such that $w_n^0 \in H^{1/2}(\Gamma)$. Let us now define w_n^+ and w_n^- by

$$w_n^+ = \begin{cases} U|_{\Gamma_n^+} - w_n^0 & \text{on } (c_n^+, \infty), \\ 0 & \text{else,} \end{cases} \quad \text{and} \quad w_n^- = \begin{cases} U|_{\Gamma_n^-} - w_n^0 & \text{on } (-\infty, c_n^-), \\ 0 & \text{else.} \end{cases}$$

One now easily sees that $w_n^- \in H^{1/2}_{00}(-\infty, c_n^-)$, $w_n^+ \in H^{1/2}_{00}(c_n^+, \infty)$ and that $U|_{\Gamma_n} = w_n^- + w_n^0 + w_n^+$. We now rewrite (4.2.4) as

$$w_{n+1}^+ + w_{n+1}^0 = \mathcal{D}_n^+ (w_n^- + w_n^0 + w_n^+) \qquad \text{on } (c_{n+1}^+, \infty),$$

which can be reformulated as

$$w_{n+1}^+ - \mathcal{D}_n^+(w_n^- + w_n^+) = -w_{n+1}^0 + \mathcal{D}_n^+ w_n^0 \qquad \text{on } (c_{n+1}^+, \infty).$$

It is now easy to verify that $-w_{n+1}^0 + \mathcal{D}_n^+ w_n^0 \in H^{1/2}_{00}(c_{n+1}^+, \infty)$. This yields that $w = (w_0^-, w_0^+, \ldots, w_2^+)$ solves the equation

$$(I - \mathcal{D})w = f,$$

where the source term $f = (f_0^-, f_0^+, \ldots, f_2^+) \in \mathcal{V}$ is given by

$$f^\sigma_{n+\sigma} = -w^0_{n+\sigma} + \mathcal{D}^\sigma_n w^0_n \qquad \text{for } n \in \mathbb{Z}/3\mathbb{Z},\ \sigma \in \{\pm\}.$$

We can now finally prove the analytical main theorem of this thesis: the Fredholm property for the compatibility equations. The proof will be rather short, since most of the work has already been done in Chapter 3.

4.3.3 Theorem. $\mathcal{D}:\mathcal{V}\to\mathcal{V}$ is bounded, and the operator $I-\mathcal{D}:\mathcal{V}\to\mathcal{V}$ is Fredholm of index 0, that is, there exist two operators $\mathcal{B},\mathcal{C}:\mathcal{V}\to\mathcal{V}$ such that

$$I-\mathcal{D}=\mathcal{B}+\mathcal{C},$$

where $\mathcal{B}$ is bounded and boundedly invertible and $\mathcal{C}$ is compact. ∎

Proof. For $u=(u_0^+,u_0^-,\dots,u_2^+)^\top$ and $v=(v_0^-,v_0^+,\dots,v_2^+)^\top$, let us write $(I-\mathcal{D})u=v$ in an operator matrix notation. We have

$$\left[I-\begin{pmatrix} & & \mathcal{D}_1^- & \mathcal{D}_1^- & & \\ & & & & \mathcal{D}_2^+ & \mathcal{D}_2^+ \\ & & & & \mathcal{D}_2^- & \mathcal{D}_2^- \\ \mathcal{D}_0^+ & \mathcal{D}_0^+ & & & & \\ \mathcal{D}_0^- & \mathcal{D}_0^- & & & & \\ & & \mathcal{D}_1^+ & \mathcal{D}_1^+ & & \end{pmatrix}\right]\begin{pmatrix}u_0^-\\u_0^+\\u_1^-\\u_1^+\\u_2^-\\u_2^+\end{pmatrix}=\begin{pmatrix}v_0^-\\v_0^+\\v_1^-\\v_1^+\\v_2^-\\v_2^+\end{pmatrix}. \tag{4.3.1}$$

Consider the first line of this equation: it is

$$v_0^-=u_0^--\mathcal{D}_1^-u_1^--\mathcal{D}_1^-u_1^+.$$

The mapping properties of the identity part are clear, and we only have to consider how $\mathcal{D}_1^-$ acts on u_1^- and u_1^+. For clarification, we have sketched the supports of the source and targets of $\mathcal{D}_1^-$ in Figure 4.4. By definition of $\mathcal{D}_1^-$, we have that

$$[\mathcal{D}_1^-u_1^-](\xi)=[D_{c_1^+}^{\theta_1^+}u_1^+](c_0^--\xi),\qquad \text{for } \xi<c_0^-.$$

Recall that by definition $u_1^-\in H_{00}^{1/2}(-\infty,c_1^-)$. Since $c_1^-<c_1^+$, we obtain from Corollary 3.6.5 that $D_{c_1^+}^{\theta_1^+}:H_{00}^{1/2}(-\infty,c_1^-)\to H_{00}^{1/2}(0,+\infty)$ is compact. $\mathcal{D}_1^-$ is the composition of this operator with a translation/mirroring operator; keeping this in mind, we obtain that $\mathcal{D}_1^-:H_{00}^{1/2}(-\infty,c_1^-)\to H_{00}^{1/2}(-\infty,c_0^-)$ is also compact.

Let us now consider how $\mathcal{D}_1^-$ acts on u_1^+, that is, let us consider the mapping properties of $\mathcal{D}_1^-:H_{00}^{1/2}(c_1^+,\infty)\to H_{00}^{1/2}(-\infty,c_0^-)$. In this case, we can apply Corollary 3.6.7 to obtain that $D_{c_1^+}^{\theta_1^+}:H_{00}^{1/2}(c_1^+,\infty)\to H_{00}^{1/2}(0,+\infty)$ can be split into two operators

$$D_{c_1^+}^{\theta_1^+}=B+C,$$

where $\|B\|<1$ and C is compact. Since again $\mathcal{D}_1^-$ is the composition of $D_{c_1^+}^{\theta_1^+}$ with a mirroring/translation operator, we obtain the same splitting for $\mathcal{D}_1^-$, i.e. there exist operators $\mathcal{B}_1^-,\mathcal{C}_1^-:H_{00}^{1/2}(c_1^+,\infty)\to H_{00}^{1/2}(-\infty,c_0^-)$ such that

$$\mathcal{D}_1^-=\mathcal{B}_1^-+\mathcal{C}_1^-,$$

where $\|\mathcal{B}_1^-\|<1$, and $\mathcal{C}_1^-$ is compact. Similarly, one proceeds for all other lines of the operator matrix: whenever the sign in the operator agrees with the sign of the function upon which it acts, the operator is compact, i.e. $\mathcal{D}_n^\sigma$ in the pairing $\mathcal{D}_n^\sigma u_n^\sigma$ is compact (by Theorem 3.6.4 or Corollary 3.6.5). If the signs differ (i.e. in the pairing $\mathcal{D}_n^\sigma u_n^{-\sigma}$), the corresponding operator can be split into a bounded and a compact part by Theorem

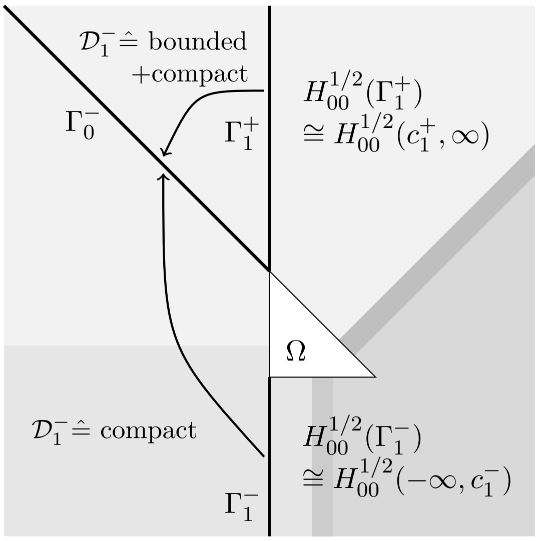

Figure 4.4: Sketch of the supports of the domains of $\mathcal{D}_0^-$, as considered in the proof of Theorem 4.3.3. Depending on the domain of $\mathcal{D}_0^-$, it is either compact or the sum of a compact and a bounded operator.

3.6.6 or Corollary 3.6.7. This way, we can split the operator matrix $I - \mathcal{D}$ into a bounded and a compact operator,

$$I - \mathcal{D} = (I - \mathcal{B}) + \mathcal{C},$$

where the compact part is given by

$$\mathcal{C} = \begin{pmatrix} & & \mathcal{D}_1^- & \mathcal{C}_1^- & & \\ & & & & \mathcal{C}_2^+ & \mathcal{D}_2^+ \\ & & & & \mathcal{D}_2^- & \mathcal{C}_2^- \\ \mathcal{C}_0^+ & \mathcal{D}_0^+ & & & & \\ \mathcal{D}_0^- & \mathcal{C}_0^- & & & & \\ & & \mathcal{C}_1^+ & \mathcal{D}_1^+ & & \end{pmatrix},$$

while the bounded part is given by

$$I - \mathcal{B} = \begin{pmatrix} & & & \mathcal{B}_1^- & & \\ & & & & \mathcal{B}_2^+ & \\ & & & & & \mathcal{B}_2^- \\ \mathcal{B}_0^+ & & & & & \\ & \mathcal{B}_0^- & & & & \\ & & \mathcal{B}_1^+ & & & \end{pmatrix}.$$

We claim that $I - \mathcal{B}$ is bounded and boundedly invertible: in fact, this follows since each line and each row of the matrix $\mathcal{B}$ contains exactly one operator, so that

$$\|\mathcal{B}\| = \max_{\substack{n \in \{0,1,2\} \\ \sigma \in \{\pm\}}} \|\mathcal{B}_n^\sigma\| < 1,$$

since $\|\mathcal{B}_n^\sigma\| < 1$ for any $n \in \{0, 1, 2\}$ and $\sigma \in \{\pm\}$. Using a Neumann series argument one obtains the bounded invertibility of $I - \mathcal{B}$, finishing the proof. ■

Having the Fredholm alternative at hand (see for example [59, Theorem 2.27]), uniqueness and existence are equivalent. In fact, we can show that uniqueness holds, and obtain the following theorem.

4.3.4 Theorem. $I - \mathcal{D} : \mathcal{V} \to \mathcal{V}$ is boundedly invertible, that is, for any $f \in \mathcal{V}$ there exists exactly one solution $u \in \mathcal{V}$ of

$$(I - \mathcal{D})u = f. \qquad \blacksquare$$

Proof. By Theorem 4.3.3, $I - \mathcal{D} : \mathcal{V} \to \mathcal{V}$ is Fredholm, and as a consequence of the Fredholm alternative, it is boundedly invertible if and only if

$$(I - \mathcal{D})u = 0$$

possesses only the trivial solution $u = 0$. Hence, let $u = (u_0^-, u_0^+, \dots, u_2^+) \in \mathcal{V}$ be such that $(I - \mathcal{D})u = 0$. For $n \in \{0, 1, 2\}$, define $u_n \in H^{1/2}(\Gamma_n)$ by

$$u_n(x) = \begin{cases} u_n^-(x) & \text{for } x \in \Gamma_n^-, \\ 0 & \text{for } x \in \Gamma_n^0, \\ u_n^+(x) & \text{for } x \in \Gamma_n^+. \end{cases}$$

Note that since $u_n^- \in H_{00}^{1/2}(-\infty, c_n^-)$ and $u_n^+ \in H_{00}^{1/2}(c_n^+, \infty)$, the extension u_n by 0 in between yields a function in $H^{1/2}(\Gamma_n)$. Let us now define $U_n \in H^1(\Omega_n)$ by

$$U_n := \mathcal{S}_n u_n.$$

By definition, U_n fulfils $(\Delta + \kappa - q)U_n = 0$ in Ω_n, together with the boundary condition $U_n = u_n$ on Γ_n. We now claim that for any $n \in \mathbb{Z}/3\mathbb{Z}$ it holds that

$$U_n = U_{n+1} \qquad \text{in } \Omega_n \cap \Omega_{n+1}.$$

Since $U_n, U_{n+1} \in H^1(\Omega_n \cap \Omega_{n+1})$ are solutions to the homogeneous Helmholtz equation on this domain, it is sufficient (due to the uniqueness of Theorem 1.4.3) to prove their traces agree on $\partial(\Omega_n \cap \Omega_{n+1}) = \Gamma_n^- \cap \Gamma_{n+1}^+$. We have by definition of $\mathcal{S}_n$ that

$$U_n|_{\Gamma_n^-} = u_n^-,$$

as well as

$$U_n|_{\Gamma_{n+1}^+} = \mathcal{D}_n^+(u_n^+ + u_n^-).$$

From $(I - \mathcal{D})u = 0$, one obtains from the line corresponding to u_{n+1}^+ that

$$u_{n+1}^+ - \mathcal{D}_n^+ u_n^+ - \mathcal{D}_n^+ u_n^- = 0.$$

The last two equations imply that

$$U_n|_{\Gamma_{n+1}^+} = u_{n+1}^+.$$

Analogously, one can now show that we have $U_{n+1}|_{\Gamma_{n+1}^+} = u_{n+1}^+$ and $U_{n+1}|_{\Gamma_n^-} = u_n^-$, so that the Dirichlet traces of U_n and U_{n+1} agree on $\partial(\Omega_n \cap \Omega_{n+1})$.

Hence we have shown that $U_n = U_{n+1}$ on the intersection of their domains $\Omega_n \cap \Omega_{n+1}$, and we can define $U \in H^1(\mathbb{R}^2 \setminus \overline{\Omega})$ by

$$U(x) = U_n(x) \qquad \text{for } x \in \Omega_n.$$

U fulfils $(\Delta + \kappa - q)U = 0$ in $\mathbb{R}^2 \setminus \Omega$ and $U = 0$ on $\partial\Omega$, since we have set $u_n^0 = 0$ in the beginning. By Theorem 1.4.3, this implies $U = 0$ and finishes the proof. $\blacksquare$

4.3.5 Equivalence of the problems. Let $g \in H^{1/2}(\partial\Omega)$ be given with the corresponding solution U to (4.2.1), and let the source $f \in \mathcal{V}$ and $w \in \mathcal{V}$ be constructed as in Subsection 4.3.2. Then w and f solve

$$(I - \mathcal{D})w = f,$$

that is, from a solution to the Helmhotz equation we can obtain a solution to the compatibility equations.

Conversely, if one takes some $g \in H^{1/2}(\partial\Omega)$ and constructs f as in Subsection 4.3.2, we obtain the existence of exactly one solution $w \in \mathcal{V}$ of

$$(I - \mathcal{D})w = f.$$

From w, we can reconstruct the solution U on the exterior by setting

$$u_n = w_n^+ + w_n^- + w_n^0,$$

and then using $\mathcal{S}_n$ to extend it to the halfspace Ω_n. Following the proof of the previous theorem, one can than again show that this gives a (well-defined) solution U to (4.2.1). That is, from a solution to the compatibilty equations we can reconstruct the solution of (4.2.1).

In other words: $(I - \mathcal{D})w = f$ and (4.2.1) are equivalent.

4.3.6 Other functional frameworks. In [74, Chapter 6], other functional frameworks are proposed for halfspace matching. Most notably, by introducing an overlap between the interior triangle Ω and the halfspaces Ω_n, $n \in \{0, 1, 2\}$, it is possible to derive a Fredholm property for the problem on the full space, that is, for example for the problem: for given $f \in L^2(\Omega)$, find some $u \in H^1(\mathbb{R}^2)$ such that

$$\Delta u(x) + \kappa u(x) = f(x) \qquad \text{for } x \in \mathbb{R}^2.$$

An example for the domain splitting is shown in Figure 4.5. While being more complicated on first sight, the analysis turns out to be simplified by the inclusion of the triangle Ω with overlap. This stems from the fact that the behaviour of the Dirichlet-to-Dirichlet operators at the edges is not of relevance. Again, we refer to [74, Chapter 6] for more details.

It should pose no problem to translate this analysis to the case with waveguides. We did not include this here, mostly for the reason that this functional framework is farther from the numerical implementation in the following chapter, where we did not implement an overlap with the interior domain.

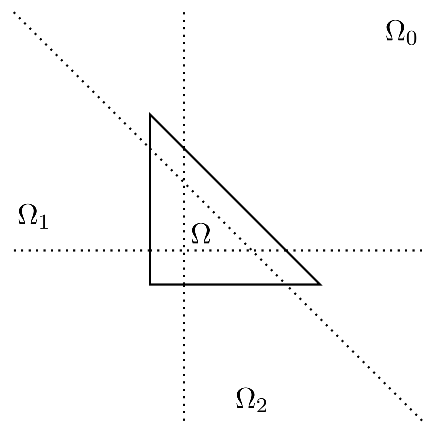

Figure 4.5: An exemplary splitting into an interior domain, which overlaps with the exterior halfspaces Ω_0, Ω_1, Ω_2.

5 Implementation for the Full Space

5.1 Introduction

5.1.1 Introduction. In this chapter we will describe a weak formulation for Helmholtz problems in $\mathbb{R}^2$, which utilises the compatibility equations (4.2.7) to treat the exterior domain. We only introduce and describe the method, any numerical analysis is far outside the scope of this work. Accordingly, we will mostly do some formal calculations, followed by a description of the discretisation used. Let us give a quick overview.

We start in Section 5.2 to derive a weak formulation for Helmholtz problems of the type

$$\Delta u + (\kappa - q)u = f \qquad \text{in } \mathbb{R}^2,$$

where $\kappa \in \mathbb{C} \setminus \mathbb{R}$, that is, we consider again only the absorptive case. Here, we can still apply Theorem 1.4.3 to obtain well-posedness in $H^1(\mathbb{R}^2)$, and accordingly, the functional framework can be chosen in a rather simple fashion.

Afterwards, we will continue to the interesting case and consider (for certain incident fields u_i) the problem of finding $u \in H^2_{\mathrm{loc}}(\mathbb{R}^2)$ such that

$$\begin{cases} \Delta u + (\kappa_0 - q)u = 0 & \text{in } \mathbb{R}^2, \\ \qquad\qquad u - u_\mathrm{i} & \text{outgoing}, \end{cases}$$

where $\kappa_0 \in \mathbb{R}$ is a properly real wavenumber. At this point, a number of complications arise, which we will deal with in a rather formal way. We need to define the notion of an "outgoing wave". Motivated from Section 3.3, we will use our halfspace solution expansion to define a radiation condition for each halfspace. This will allow us to derive a (distributional) weak formulation, utilising again the compatibility equations.

The discretisation we used for creating numerical examples will be shown in Section 5.4. We describe how the involved matrices can be numerically computed, and will show a few convergence results afterwards.

5.1.2 Assumption. Let $q : \mathbb{R}^2 \to \mathbb{R}$ be some real-valued $L^\infty(\mathbb{R}^2)$ function such that there exists a triangular (or rectangular) domain Ω such that $q|_{\mathbb{R}^2\setminus\Omega}$ fulfils Definition and Assumption 4.2.3. We denote by $\boldsymbol{m}$ the number of sides of Ω. Furthermore, we assume that in each halfspace $n \in \{0, \dots, \boldsymbol{m} - 1\}$, the potential $q^{(n)} : \mathbb{R} \to \mathbb{R}$ is of Pekeris type (compare Section 2.3). That is, there exist three constants $q_-^{(n)}$, $q_+^{(n)}$, $q_m^{(n)} \in \mathbb{R}$ and $a^{(n)} < b^{(n)}$ such that

$$q^{(n)}(\xi) = \begin{cases} q_-^{(n)} & \text{for } \xi < a^{(n)}, \\ q_m^{(n)} & \text{for } a^{(n)} \le \xi \le b^{(n)}, \\ q_+^{(n)} & \text{for } b^{(n)} < \xi. \end{cases}$$

■

We restrict ourselves to potentials of Pekeris type, since for those we can explicitly calculate the generalised Fourier transform as shown in Section 2.3. One might consider more general potentials as in Definition and Assumption 2.2.2, but to realise this, one needs to determine the spectral family Ψ by some numerical method.

Let us also recall the notation of Subsection 4.2.2, which will be exploited heavily in this chapter. Since we now allow for either a triangular or rectangular interior domain Ω, we might have $\boldsymbol{m} \in \{3, 4\}$ overlapping halfspaces Ω_n with boundaries $\Gamma_n = \Gamma_n^+ \cup \Gamma_n^0 \cup \Gamma_n^-$, $n \in \{0, \dots, \boldsymbol{m} - 1\}$.

5.1.3 Allowed geometrical configurations. Before going on, let us discuss shortly the geometrical restrictions that follow from Definition and Assumption 4.2.3 and the previous assumptions. Note that "rectangular" means that we have a quadrangle with right angles at every corner. We restrict ourselves to this situation here. However, it is also possible to allow for splittings of the exterior where more than two halfspace overlap (see Figure 5.1). This can be also treated with our method, but we omit a detailed discussion of this situation here.

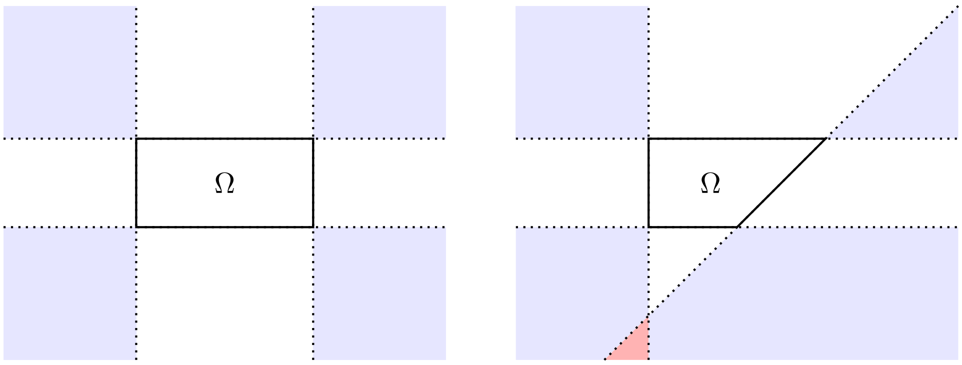

Figure 5.1: Sketch of the overlap areas for two quadrangular interior domains. The light blue areas indicate where two halfspaces overlap. For the right hand example, there is a small, red area, where three halfspaces overlap.

Note that for rectangular Ω, every halfspace can contain a waveguide. This is not necessarily the case for triangles, since one cannot fulfil Definition and Assumption 4.2.3, if there is a waveguide adjacent to an obtuse angle (see Figure 5.2).

5.2 The Sesquilinear Form of the Problem

We aim to derive a sesquilinear form which admits the numerical treatment of the following problem.

5.2.1 Problem of interest. For given $\kappa \in \mathbb{C} \setminus \mathbb{R}$ and $f \in L^2(\mathbb{R}^2)$ with $\operatorname{supp}(f) \subset \Omega$, we consider the problem of finding $u \in H^1(\mathbb{R}^2)$ such that

$$\Delta u + (\kappa - q)u = f \qquad \text{in } \mathbb{R}^2.$$

Note that Theorem 1.4.3 gives existence and uniqueness for this problem.

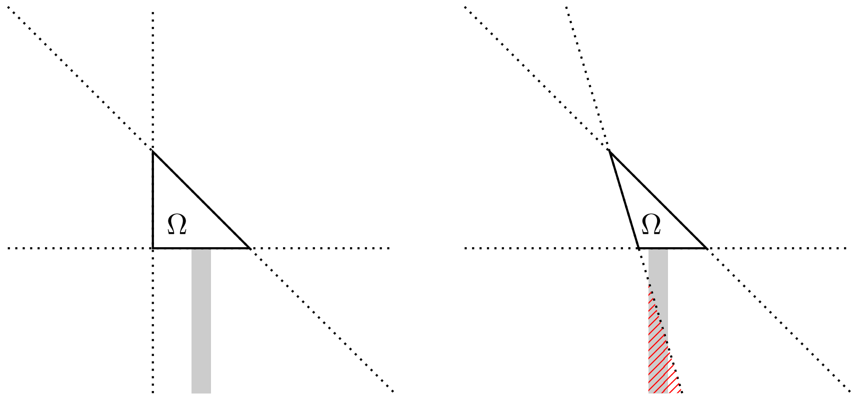

Figure 5.2: Two triangles with a waveguide extending perpendicularly from one side. The left geometry is allowed, while the right one is not admissible, since in the hatched area, Definition and Assumption 4.2.3 cannot be fulfilled by any $q^{(n)}$ for the left hand side halfspace.

5.2.2 The weak formulation. To make the problem suitable for halfspace matching, we will split the domain into an exterior and interior part, and define $u_\mathrm{e} := u|_{\mathbb{R}^2\setminus\overline{\Omega}}$ and $u_\Omega = u|_\Omega$, so that $u_\mathrm{e} \in H^1(\mathbb{R}^2 \setminus \overline{\Omega})$ and $u_\Omega \in H^1(\Omega)$ fulfil

$$\begin{cases} \Delta u_\mathrm{e} + (\kappa - q)u_\mathrm{e} = 0 & \text{in } \mathbb{R}^2 \setminus \overline{\Omega}, \\ u_\mathrm{e} - u_\Omega = 0 & \text{on } \partial\Omega, \\ \partial_\nu u_\Omega - \partial_\nu u_\mathrm{e} = 0 & \text{on } \partial\Omega, \\ \Delta u_\Omega + (\kappa - q)u_\Omega = f & \text{in } \Omega. \end{cases} \tag{5.2.1}$$

Here ∂_ν denotes the derivative in direction of the exterior normal on Ω. We note that u_e fulfils an exterior problem as considered in Chapter 4 (see Subsection 4.2.1), and accordingly, it solves the corresponding compatibility equations. To write them down, let us introduce the trace unknowns

$$u_n = u_\mathrm{e}|_{\Gamma_n} \qquad \text{for } n \in \{0, \dots, \boldsymbol{m} - 1\}.$$

As in Subsection 4.2.5 we can derive that the traces must fulfil the compatibility equations

$$u_{n+\sigma} - \mathcal{D}_n^\sigma u_n = 0 \qquad \text{on } \Gamma_n^\sigma,\ \sigma \in \{\pm\},\ n \in \mathbb{Z}/\boldsymbol{m}\mathbb{Z}.$$

To realise the coupling of the Neumann traces in (5.2.1), we recall the DtN operators from Section 3.4, which are defined by

$$\mathcal{N}_n f(x) := \partial_\nu \mathcal{S}_n f(x) \qquad \text{for } x \in \Gamma_n^0,\ n \in \{0, \dots, \boldsymbol{m} - 1\},$$

where ν denotes the inward normal of Ω_n, that is, the outward normal on Ω. Hence we arrive at the following problem equivalent to (5.2.1), which contains the new unknowns, the traces $(u_0, \dots, u_{\boldsymbol{m}-1})$ and u_Ω

$$\begin{cases} u_{n+\sigma} - \mathcal{D}_n^\sigma u_n = 0 & \text{on } \Gamma_{n+\sigma}^\sigma,\ \sigma \in \{\pm\},\ n \in \mathbb{Z}/\boldsymbol{m}\mathbb{Z}, \\ u_n - u_\Omega = 0 & \text{on } \Gamma_n^0,\ n \in \{0, \dots, \boldsymbol{m} - 1\}, \\ \mathcal{N}_n u_n - \partial_\nu u_\Omega = 0 & \text{on } \Gamma_n^0,\ n \in \{0, \dots, \boldsymbol{m} - 1\}, \\ \Delta u_\Omega + (\kappa - q)u_\Omega = f & \text{in } \Omega. \end{cases} \tag{5.2.2}$$

Let us recast this problem into a weak formulation. For this aim, define the space

$$\mathcal{V} := \Big\{ (u_\Omega, u_0, \ldots, u_{\boldsymbol{m}-1}) \in H^1(\Omega) \times \prod_{n=0}^{\boldsymbol{m}-1} H^1(\Gamma_n) : \\ u_\Omega = u_n \text{ on } \Gamma_n^0,\ n \in \{0, \ldots, \boldsymbol{m}-1\} \Big\}.$$

The equality of the Dirichlet traces of (5.2.2) is already incorporated by definition of our space $\mathcal{V}$. Note that this space is somewhat ill-balanced: one would naturally demand the traces to be only $H^{1/2}$ on the boundary. We reiterate that this functional frame is most likely ill-suited for proper numerical analysis.

Let $u = (u_\Omega, u_1, \ldots, u_{\boldsymbol{m}-1}) \in \mathcal{V}$ be a solution of (5.2.2), and let $v = (v_\Omega, v_1, \ldots, v_{\boldsymbol{m}-1}) \in \mathcal{V}$ be some test function. Consider the solution in the interior u_Ω: by multiplying the Helmholtz equation in Ω with $\overline{v}_\Omega$ and integrating over Ω, we obtain by partial integration that

$$\int_\Omega \nabla u_\Omega \cdot \nabla \overline{v}_\Omega - (\kappa - q) u_\Omega \overline{v}_\Omega \,\mathrm{d}x - \int_{\partial\Omega} (\partial_\nu u_\Omega) \overline{v}_\Omega \,\mathrm{d}s = - \int_\Omega f \overline{v}_\Omega \,\mathrm{d}x,$$

The volume integral on the left side will be the first part of our sesquilinear form, so we define

$$b_\Omega(u, v) := \int_\Omega \nabla u_\Omega \cdot \nabla \overline{v}_\Omega - (\kappa - q) u_\Omega \overline{v}_\Omega \,\mathrm{d}x. \tag{5.2.3}$$

Let us now consider the boundary integral. From $\partial\Omega = \bigcup_{n=0}^{\boldsymbol{m}-1} \Gamma_n^0$, we obtain

$$- \int_{\partial\Omega} (\partial_\nu u_\Omega) \overline{v}_\Omega \,\mathrm{d}s = - \sum_{n=0}^{\boldsymbol{m}-1} \int_{\Gamma_n^0} (\partial_\nu u_\Omega) \overline{v}_\Omega \,\mathrm{d}s = - \sum_{n=0}^{\boldsymbol{m}-1} \int_{\Gamma_n^0} (\mathcal{N}_n u_n) \overline{v}_n \,\mathrm{d}s,$$

where we used the continuity of the Dirichlet trace of $v \in \mathcal{V}$ as well as the continuity of the Neumann trace from (5.2.2). This motivates the definition of the second part of the sesquilinear form, namely

$$b_n^{\mathcal{N}}(u, v) := - \int_{\Gamma_n^0} (\mathcal{N}_n u_n) \overline{v}_n \,\mathrm{d}s. \tag{5.2.4}$$

It remains to realise the compatibility equations in (5.2.2). To do this, we simply fix $\sigma \in \{\pm\}$, $n \in \mathbb{Z}/\boldsymbol{m}\mathbb{Z}$, multiply the corresponding compatibility equation by $\overline{v}_{n+\sigma}$ and integrate over $\Gamma_{n+\sigma}^\sigma$. We obtain that the following sesquilinear form must be always equal to 0:

$$b_n^\sigma(u, v) = \int_{\Gamma_{n+\sigma}^\sigma} (u_{n+\sigma} - \mathcal{D}_n^\sigma u_n) \overline{v}_{n+\sigma} \,\mathrm{d}s. \tag{5.2.5}$$

Lastly, we denote the sum of all previously defined sesquilinear forms by

$$b(u, v) = b_\Omega(u, v) + \sum_{n=1}^{\boldsymbol{m}-1} b_n^{\mathcal{N}}(u, v) + \sum_{n=1}^{\boldsymbol{m}-1} \sum_{\sigma \in \{\pm\}} b_n^\sigma(u, v). \tag{5.2.6}$$

Summarily, we obtain that solution of (5.2.2) fulfils the following problem.

5.2.3 Weak problem. For given $f \in L^2(\mathbb{R}^2)$ such that $\operatorname{supp}(f) \subset \Omega$, find a solution $u \in \mathcal{V}$ such that

$$b(u, v) = -\int_{\Omega} f \overline{v}_{\Omega} \, \mathrm{d}x \qquad \text{for all } v \in \mathcal{V},$$

where b is defined by (5.2.6) (which involves the sesquilinear forms (5.2.5), (5.2.4), (5.2.3)). ■

We will later discretise this variational problem by using a Galerkin method. Note that the sesquilinear form is bounded on $\mathcal{V}$, as can be easily seen by standard arguments (for b_Ω) or using the already shown mapping properties: for $b_n^{\mathcal{N}}$ check Lemma 3.4.2. To show that b_n^σ is bounded, one simply applies the trace theorem for one of the halfspace problems.

Let us remark here that the choice of our space and sesquilinear form merely allows us to write down a variational problem. Note that they are also somewhat ill adapted to each other, since we use H^1-unknowns for the semi-infinite lines, while we use an L^2-scalar product to realise the compatibility equations. Consequently, it seems questionable whether one can use this framework for numerical analysis.

5.3 The Non-absorptive Case, Incident Waves

5.3.1 Introduction. In this section, we aim to consider for

$$\kappa_0 \in \mathbb{R},$$

the Helmholtz equation without absorption, that is

$$\Delta u + (\kappa_0 - q)u = 0 \qquad \text{in } \mathbb{R}^2.$$

With this choice, the classical problems associated with the mathematical theory of scattering problems arises: we will need a radiation condition, which ensures the well-posedness of the problem, and corresponding to this we need a functional analytic framework. This is no easy task, and we discuss it only in a formal fashion.

To have a starting point, we will define an (not explicitly specified) trace space $V_?$, that fulfils certain properties, allowing us to define the "outward propagation radiation condition". This will then allow us to write down a distributional formulation of our scattering problem, utilising the sesquilinear form b from the previous section for special test functions.

Another important topic of this section is the realisation of incident waves in the weak formulation, which will first be illustrated for a simple, unperturbed waveguide, and then incorporated in the general weak formulation.

We begin by specifying the properties we will require from our mystery trace space $V_?$.

5.3.2 Definition and Assumption. Consider again the halfspace $\mathbb{R}^+_2$. Let $\kappa_0 \in \mathbb{R}$, and let $q : \mathbb{R}^2 \to \mathbb{R}$ fulfil Definition and Assumption 2.2.2. We now assume that

$$V_? \subset \{f : \mathbb{R} \to \mathbb{C}\}$$

is some function space such that:

(a) The associated solution operator $\mathcal{S} : H^{1/2}(\mathbb{R}) \to H^1(\mathbb{R}^2_+, (1+x_2)^{-s}\,\mathrm{d}x)$ (see Lemma 3.3.1) can be extended to a continuous operator

$$\mathcal{S} : V_? \to H^1_{\mathrm{loc}}(\mathbb{R}^2_+).$$

Furthermore $\mathcal{S}f|_{\{0\}\times\mathbb{R}} = f$ in $H^{1/2}_{\mathrm{loc}}(\mathbb{R})$ for any $f \in V_?$.

(b) The associated DtN operator $\mathcal{N} : H^1(\mathbb{R}) \to L^2(\mathbb{R})$ can be extended to a continuous operator

$$\mathcal{N} : V_? \to L^2_{\mathrm{loc}}(\mathbb{R}).$$

(c) It contains at least the functions $e^{ik\,\cdot}$ for $k \in \mathbb{R}$. ■

Let us comment a bit on this space, and what might be possible candidates. Note that (b) implies that functions in $V_?$ should be at least in $H^1_{\mathrm{loc}}(\mathbb{R})$, since otherwise the regularity of the Neumann trace cannot be realised. On the other hand, assumption (c) requires that this space should be rather large. We conjecture that the choice

$$V_? = H^1_{\mathrm{loc}}(\mathbb{R}) \cap L^\infty(\mathbb{R}),$$

might fulfil these assumptions. Why? The first critical point is the extension of the solution operator $\mathcal{S}$. Let us sketch how this might be possible. Let $f \in C_0^\infty(\mathbb{R})$. Then we have by Fubini's theorem

$$\begin{aligned}
\mathcal{S}f(x) &= \int_\Lambda e^{i\sqrt{\kappa-\hat\lambda(m)}\,x_2}\,\Psi(m,x_1) \int_{\mathbb{R}} \overline{\Psi}(m,y) f(y)\,\mathrm{d}y\,\mathrm{d}\mu(m) \\
&= \int_{\mathbb{R}} f(y) \int_\Lambda e^{i\sqrt{\kappa-\hat\lambda(m)}\,x_2}\,\Psi(m,x_1)\overline{\Psi}(m,y)\,\mathrm{d}\mu(m)\,\mathrm{d}y \\
&= \int_{\mathbb{R}} f(y)\Phi(x,y)\,\mathrm{d}y,
\end{aligned}$$

where we defined for $x \in \mathbb{R}^2_+$ and $y \in \mathbb{R}$ the function

$$\Phi(x,y) := \int_\Lambda e^{i\sqrt{\kappa-\hat\lambda(m)}\,x_2}\,\Psi(m,x_1)\overline{\Psi}(m,y)\,\mathrm{d}\mu(m).$$

It is now easy to see that the integral on the right hand side is well-defined. Furthermore, we conjecture that with the help of integration by parts and the stationary phase method (see [21, Section 2.7]) one can show that for fixed $x \in \mathbb{R}^2_+$

$$|\Phi(x,y)| = c(x)\frac{1}{|y|^{3/2}}\left(1 + \mathcal{O}\left(|y|^{-1}\right)\right) \qquad \text{as } |y| \to \infty.$$

This would imply that the integral

$$Sf(x) = \int_{\mathbb{R}} f(y)\Phi(x,y)\,\mathrm{d}y$$

is well defined for any $f \in L^\infty(\mathbb{R})$, since $\Psi(x,\,\cdot\,) \in L^1(\mathbb{R})$ for any $x \in \mathbb{R}^2_+$. Hence, one can extend $\mathcal{S}$ to $L^\infty(\mathbb{R})$, which together with the additional regularity assumptions should be able to yield the desired properties.

Let us remark that the previous approach of defining an extension to $\mathcal{S}$ is rather well known for the case of a free halfspace in the context of the upward propagation radiation condition. We refer to the references after Definition 5.3.4.

Let us also mention that in [74, Section 4.4], it is suggested that the space

$$V_{\kappa_0} = \{f : \mathbb{R} \to \mathbb{C} : |\kappa_0 - \hat{\lambda}|^{1/4} \mathcal{F}_A f \in L^2(\Lambda, \mathrm{d}\mu)\}$$

might be a suitable choice. Therein, however, lie a few complications. Firstly, it is necessary to properly define the generalised Fouriertransform on $\mathcal{F}_A$ on V_{κ_0}, since V_{κ_0} is *not* contained in $L^2(\mathbb{R})$, due to the zero of the weight $|\kappa_0 - \hat{\lambda}|^{1/4}$. Hence it is necessary to define appropriate distributions adapted to $\mathcal{F}_A$ and extend the transform accordingly. Luckily, at least this problem has been overcome and has been discussed in [10] and [39]. Secondly, this space is not large enough for our purpose. Definition and Assumption 5.3.2 (c) is violated, which prohibits us from considering Example 5.3.5 below.

One might also ask the following question: assume $L^\infty(\mathbb{R}) \cap H^1_{\mathrm{loc}}(\mathbb{R})$ (or something similar) is a suitable choice for $V_?$. Might it be possible to reproduce the analysis of Chapter 3 and 4, to obtain a similar Fredholm alternative? The answer is, most likely, negative. One can show that on the free halfspace the condition $f \in L^\infty(\mathbb{R})$ is not sufficient to ensure that $\mathcal{S}f$ is in $L^\infty(\mathbb{R}^2_+)$ (see [13]). This, however, should be the case to guarantee $D^\theta_c f \in L^\infty(0,\infty)$ for some Dirichtlet-to-Dirichlet operator D^θ_c. At least in the authors opinion, this question does not allow an obvious answer.

We can now define the spaces which will be involved in our absorption free problem.

5.3.3 Definition. Define

$$\mathcal{V}_? := \Bigg\{ (u_\Omega, u_0, \ldots, u_{\boldsymbol{m}-1}) \in H^1(\Omega) \times \prod_{n=0}^{\boldsymbol{m}-1} V_?(\Gamma_n) : \\ u_\Omega = u_n \text{ on } \Gamma^0_n \text{ for } n \in \{0, \ldots, \boldsymbol{m}-1\} \Bigg\}.$$

We furthermore define the following space of test functions

$$\mathcal{V}^*_? := \Bigg\{ (u_\Omega, u_0, \ldots, u_{\boldsymbol{m}-1}) \in H^1(\Omega) \times \prod_{n=0}^{\boldsymbol{m}-1} L^2(\Gamma_n) : \\ \operatorname{supp}(u_n) \text{ is compact for } n \in \{0, \ldots, \boldsymbol{m}-1\} \Bigg\}.$$

■

We will use a different test space in the variational formulation, since our assumptions for $V_?$ do not ensure that the Dirichlet-to-Dirichlet operators $\mathcal{D}^\sigma_n$ stay bounded (for $n \in \{0, \ldots, \boldsymbol{m}-1\}$, $\sigma \in \{\pm\}$). Consequently, the sesquilinear form b^σ_n will generally be unbounded on $\mathcal{V}_? \times \mathcal{V}_?$, so we restrict ourselves to $\mathcal{V}_? \times \mathcal{V}^*_?$, switching effectively to a distributional formulation.

5.3.4 Definition. Let $\hat{\Omega}$ be some halfspace, $\kappa_0 \in \mathbb{R}$, and let $u \in H^2_{\mathrm{loc}}(\mathbb{R})$ be a solution to the Helmholtz equation

$$\Delta u + (\kappa_0 - q) u = 0 \qquad \text{in } \hat{\Omega}.$$

We say that u fulfils the *outward propagation radiation condition* (OPRC) in $\hat{\Omega}$, if $u|_{\partial\hat{\Omega}} \in V_?(\partial\hat{\Omega})$, and

$$u = \mathcal{S}[u|_{\partial\hat{\Omega}}].$$

■

We motivated this radiation condition in Section 3.3, where we deduced that the limit-absorption solution on a halfspace must fulfil this condition, provided that $u|_{\partial\hat{\Omega}} \in H^{1/2}(\partial\hat{\Omega})$. For the free space, this radiation condition has been thoroughly analysed and is called the "upward propagation radiation condition", for example by Chandler-Wilde and others (see for example [2, 14, 15] and references therein) in the context of rough layer scattering.

For waveguides, the same radiation condition has already been applied, most notably by Bonnet-ben Dhia, Hazard and others. Certain well-posedness results can be found for special geometries (see [9, 10]). Note however, that these results are restricted to the case of parallel waveguides, and do not consider overlapping domains in the exterior. There are no results for non-parallel waveguides to the author's knowledge.

5.3.5 Example. Let us illustrate at a simple example how this radiation condition can be applied. We will also introduce a certain splitting in incident and outgoing parts for a solution, which might seem arbitrary at first sight, but will be used for different scattering problems, where this particular splitting is of importance. Let $h > b > 0$, $q_0 < 0$, $\kappa_0 > 0$ and define for $x_1 \in \mathbb{R}$

$$q(x_1) = \begin{cases} 0 & \text{for } |x_1| > b, \\ q_0 & \text{for } |x_1| \leq b. \end{cases}$$

Let $A = -\partial_{x_1}^2 + q$ be the associated operator, and let $\psi \in H^2(\mathbb{R})$ be the first eigenfunction of A corresponding to the eigenvalue $\lambda_1 \in (q_0, 0)$. It has a representation of the form

$$\psi(x_1) = \begin{cases} ce^{-\sqrt{|\lambda_1|}\,x_1} & \text{for } x_1 > h, \\ ce^{\sqrt{|\lambda_1|}\,x_1} & \text{for } x_1 < -h. \end{cases}$$

Let us now consider the function

$$u(x) = e^{-i\sqrt{\kappa_0-\lambda_1}\,x_2}\psi(x_1) \qquad \text{for } x \in \mathbb{R}^2,$$

which is a solution to the Helmholtz equation

$$\Delta u(x) + (\kappa_0 - q(x_1))u(x) = 0 \qquad \text{for } x \in \mathbb{R}^2.$$

We will now write $u : \mathbb{R}^2 \to \mathbb{C}$ as the solution to a very particular scattering problem with the help of the halfspace representations. We define the square

$$\Omega = \{x \in \mathbb{R}^2 : |x_1| < h, |x_2| < h\},$$

as well as the four halfspaces (which are subset of $\mathbb{R}^2$)

$$\Omega_0 = \{x_1 < -h\},\ \Omega_1 = \{x_2 < -h\},\ \Omega_2 = \{x_1 > h\},\ \Omega_3 = \{x_2 > h\},$$

and the boundaries $\Gamma_n := \partial\Omega_n$, $n \in \{0, 1, 2, 3\}$. As before, let us denote the traces by $u_n = u|_{\Gamma_n}$, $n \in \{0, \ldots, 3\}$. In which halfspaces can u be considered outgoing?

(0) On the halfspace Ω_0 the function q is constantly equal to 0. Hence we can write down the solution operator $\mathcal{S}_0$ for $g \in H^{1/2}(\mathbb{R})$ by

$$\mathcal{S}_0 g(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-i\sqrt{\kappa_0-\xi^2}\,(h-x_1)} e^{i\xi x_2} \hat{g}(\xi)\, \mathrm{d}\xi,$$

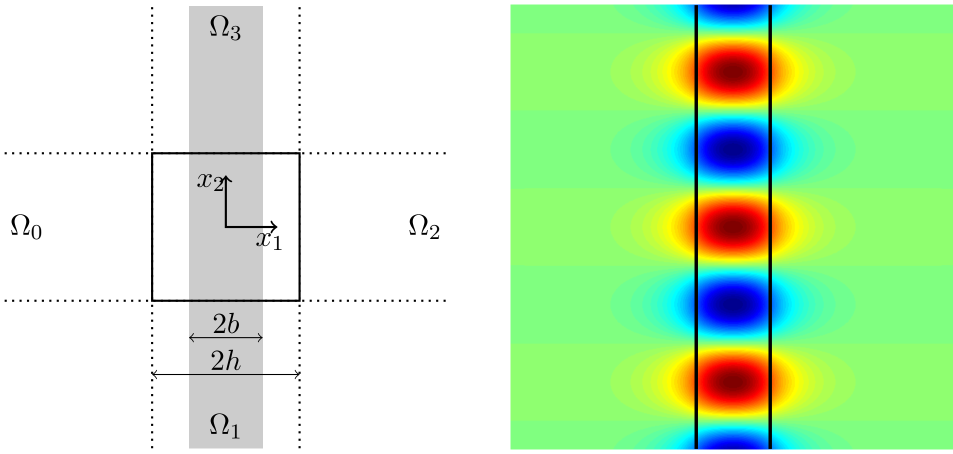

Figure 5.3: Sketch of the geometrical notation (left) and the real part of the solution for Example 5.3.5. The solution on the right hand side can be considered as propagating downwards.

where $\hat{g}$ denotes the 1D Fourier transform of g. The trace on $\Gamma_0 = \{x \in \mathbb{R}^2 : x_1 = -h\}$ is given by

$$u_0(x_2) = \psi(-h)\exp(-i\sqrt{\kappa_0 - \lambda_1}\, x_2).$$

We can now formally apply the Fourier transform (in the sense of distributions) to obtain

$$\hat{u}_0(\xi) = \psi(-h)\delta(\xi - \sqrt{\kappa_0 - \lambda_1}),$$

where δ denotes the δ-distribution. Interpreting the inverse Fourier transform in the sense of distribution, we obtain that

$$\mathcal{S}_0 u_0(x) = \psi(-h)e^{-i\sqrt{\kappa_0-(\kappa_0-\lambda_1)}\,(h+x_1)}e^{-i\sqrt{\kappa_0-\lambda_1}\,x_2}.$$

Keeping the branch cut of the square root in mind and using the representation for ψ, one easily sees that the right hand side is equal to u, so that we obtain

$$u(x) = S_0 u_0(x) \qquad \text{on } \Omega_0,$$

that is, u is outgoing on Ω_0.

(1) On Γ_1 we have that

$$u_1(x_1) = \psi(x_1)e^{i\sqrt{\kappa_0-\lambda_1}\,h}.$$

This function is clearly in $H^2(\mathbb{R})$, and we can employ $\mathcal{F}_A$ in the classical sense. One easily obtains

$$(\mathcal{F}_A u_1)^p(\lambda_1) = e^{i\sqrt{\kappa_0-\lambda_1}\,h} \qquad \text{and} \qquad \mathcal{F}_A u_1(m) = 0 \qquad \text{for } m \in \Lambda \setminus \{(p,\lambda_1)\}.$$

Employing the inverse transform, this in turn gives

$$\mathcal{S}_1 u_1(x) = e^{-i\sqrt{\kappa_0-\lambda_1}(x_2+h)}e^{+i\sqrt{\kappa_0-\lambda_1}\,h}\psi(x_1) = u(x),$$

showing that u can be considered outgoing in Ω_1.

(2) On Ω_2 the same discussion as for Ω_0 yields that u is outgoing here, too.

(3) For the last halfspace, we obtain that

$$u_3(x_1) = \psi(x_1) e^{-i\sqrt{\kappa_0 - \lambda_1}\, h}.$$

Plugging this boundary data into the solution operator now yields

$$\mathcal{S}_3 u_3(x) = \psi(x_1) e^{-i\sqrt{\kappa_0 - \lambda_1}\, h} e^{i\sqrt{\kappa_0 - \lambda_1}\,(x_2 - h)},$$

which clearly is different from u, so that u is not outgoing in Ω_3. However, if we define the incident and scattered field on Ω_3 by $u_\mathrm{i} := u$ and $u_\mathrm{s} := u - u_\mathrm{i}$, we obtain that

$$u = u_\mathrm{i} + \mathcal{S}_3(u_\mathrm{s}|_{\Gamma_3}) = u_\mathrm{i} + \mathcal{S}_3(u_3 - u_\mathrm{i}|_{\Gamma_3}),$$

so we can represent the total field u as a superposition of incident and outgoing field.

Summarily, we see that u fulfils

$$\begin{cases} \quad u = \mathcal{S}_n u_n & \text{on } \Omega_n,\ n \in \{0,1,2\}, \\ \quad u = \mathcal{S}_3(u_3 - u_\mathrm{i}|_{\Gamma_3}) + u_\mathrm{i} & \text{on } \Omega_3, \\ \Delta u + (\kappa_0 - q) u = 0 & \text{on } \mathbb{R}^2, \end{cases}$$

which can be read as a scattering problem: find a solution u to the Helmholtz equation, such that u is outgoing on $\Omega_0, \Omega_1, \Omega_2$, while $u - u_\mathrm{i}$ is outgoing on Ω_3. This is the type of problem for which we now want to derive a weak formulation.

5.3.6 Weak formulation of scattering problems. Let $q \in L^\infty(\mathbb{R}^2)$ fulfil Assumption 5.1.2, $\kappa_0 \in \mathbb{R}$ and let $u_\mathrm{i} \in H^2_{\mathrm{loc}}(\Omega_0)$ be an incident field, such that there exist functions $w_1 \in V_?(\Gamma_1)$ and $w_{\boldsymbol{m}-1} \in V_?(\Gamma_{\boldsymbol{m}-1})$ such that

$$u_\mathrm{i} = \mathcal{S}_1 w_1 \quad \text{on } \Omega_0 \cap \Omega_1, \qquad u_\mathrm{i} = \mathcal{S}_{\boldsymbol{m}-1} w_{\boldsymbol{m}-1} \quad \text{on } \Omega_{\boldsymbol{m}-1} \cap \Omega_0.$$

The last statement formulates that we can consider u_i as outgoing on the two halfspaces Ω_1 and $\Omega_{\boldsymbol{m}-1}$, where it is partially defined. Let $u \in H^2_{\mathrm{loc}}(\mathbb{R}^2)$ be a solution of

$$\begin{cases} \Delta u + (\kappa_0 - q) u = 0 & \text{in } \mathbb{R}^2, \\ \qquad\qquad u - u_\mathrm{i} & \text{OPRC in } \Omega_0, \\ \qquad\qquad\quad u & \text{OPRC in } \Omega_n,\ n \in \{1, \dots, \boldsymbol{m}-1\}. \end{cases} \tag{5.3.1}$$

Let us reformulate this problem by utilising the compatibility equations. Define again

$$u_n = u|_{\Gamma_n} \qquad n \in \{0, \dots, \boldsymbol{m}-1\}.$$

Then we have by considering the solution on Ω_n, $n \in \{1, \dots, \boldsymbol{m}-1\}$, that

$$u_{n\pm\sigma} = [\mathcal{S}_n u_n]|_{\Gamma^\sigma_{n+\sigma}} = \mathcal{D}^\sigma_n u_n \qquad \text{on } \Gamma^\sigma_{n+\sigma},\ \sigma \in \{\pm\},\ n \in \mathbb{Z}/3\boldsymbol{m}\mathbb{Z} \setminus \{0\}.$$

This is just the same set of compatibility equations as before. For those halfspaces, the DtN part also takes the same form as previously.

Let us now consider the halfspace Ω_0, where our incident wave is defined. Denoting $u_{\mathrm{i},0} := u_{\mathrm{i}}|_{\Gamma_0}$, we have

$$u = \mathcal{S}_0(u_0 - u_{\mathrm{i},0}) + u_{\mathrm{i}} = \mathcal{S}_0 u_0 + (u_{\mathrm{i}} - \mathcal{S}_0 u_{\mathrm{i},0}) \qquad \text{on } \Omega_0,$$

which translates by taking the trace on Γ_σ^σ to

$$u_\sigma = \mathcal{D}_0^\sigma u_0 + (u_{\mathrm{i}}|_{\Gamma_\sigma^\sigma} - \mathcal{D}_0^\sigma u_{\mathrm{i},0}) \qquad \text{on } \Gamma_\sigma^\sigma,\ \sigma \in \{\pm\}.$$

Similarly, for the DtN part we obtain that

$$\partial_\nu u = \partial_\nu(\mathcal{S}(u_0 - u_{\mathrm{i},0})|_{\Gamma_0^0} + u_{\mathrm{i}}) = \mathcal{N}_0 u_0 + [\partial_\nu \mathcal{S}_0 u_{\mathrm{i},0} - \partial_\nu u_{\mathrm{i}}] \qquad \text{on } \Gamma_0^0.$$

We obtain that our solution variables $(u_\Omega, u_0, \dots, u_{\boldsymbol{m}-1})$ fulfil

$$\begin{cases} u_\sigma - \mathcal{D}_0^\sigma u_0 = \mathcal{D}_0^\sigma u_{\mathrm{i},0} - u_{\mathrm{i}} & \text{on } \Gamma_{0+\sigma}^\sigma,\ \sigma \in \{\pm\}, \\ u_{n+\sigma} - \mathcal{D}_n^\sigma u_n = 0 & \text{on } \Gamma_{n+\sigma}^\sigma,\ \sigma \in \{\pm\},\ n \in (\mathbb{Z}/\boldsymbol{m}\mathbb{Z}) \setminus \{0\}, \\ u_n - u_\Omega = 0 & \text{on } \Gamma_n^0,\ n \in \{0, \dots, \boldsymbol{m}-1\}, \\ \mathcal{N}_0 u_0 - \partial_\nu u_\Omega = \partial_\nu u_{\mathrm{i}} - \partial_\nu \mathcal{S}_0 u_{\mathrm{i},0} & \text{on } \Gamma_0^0, \\ \mathcal{N}_n u_n - \partial_\nu u_\Omega = 0 & \text{on } \Gamma_n^0,\ n \in \{1, \dots, \boldsymbol{m}-1\}, \\ \Delta u_\Omega + (\kappa - q) u_\Omega = 0 & \text{in } \Omega. \end{cases}$$

Which yields, by the same discussion as before, the following weak formulation.

5.3.7 Weak problem. In the notation of the previous section, the weak formulation of (5.3.1) is given as follows: find $u \in \mathcal{V}_?$ such that

$$b(u, \psi) = f(\psi) \qquad \text{for all } \psi \in \mathcal{V}_?^*,$$

where the right hand side is given by

$$f(\psi) := \sum_{\sigma \in \{\pm\}} \int_{\Gamma_\sigma^\sigma} (\mathcal{S}_0 u_{\mathrm{i},0} - u_{\mathrm{i}}) \overline{\psi}_\sigma \,\mathrm{d}s + \int_{\Gamma_0^0} (\partial_\nu u_{\mathrm{i}} - \partial_\nu \mathcal{S}_0 u_{\mathrm{i},0}) \overline{\psi}_0 \,\mathrm{d}s. \qquad \blacksquare$$

Note that by Definition and Assumption 5.3.2, all terms of the sesquilinear form are well-defined for any $u \in \mathcal{V}_?$ and $\psi \in \mathcal{V}_?^*$.

5.4 Discretisation

In this section we will describe different discretisations for the weak problems of the previous two sections. Note that here we do not differentiate between the two cases, so that we use the same discretisation independent of κ. In essence, we will describe a Galerkin ansatz space $\mathcal{V}^h$ fulfilling

$$\mathcal{V}^h \subset \mathcal{V} \subset \mathcal{V}_?$$

and show how the different terms of the sesquilinear forms b can be computed.

Let us remark that so far, we have not shown the (analytical) well-posedness of the sesquilinear form in the absorptive case, so it is not obvious how to proceed with the numerical analysis. For the absoprtion free case, note that with our conjectured choice $V_? = L^\infty(R) \cap H^1_{\mathrm{loc}}(\mathbb{R})$, it is not trivial to choose a Galerkin ansatz space which approximates $L^\infty(R) \cap H^1_{\mathrm{loc}}(\mathbb{R})$, since, for example, the functions with compact support are not dense in $L^\infty(\mathbb{R})$.

Let us recall that geometrically, we have to discretise the interior domain Ω and the semi-infinite lines $\Gamma_n^\sigma,\ n \in \{0, \dots, \boldsymbol{m}-1\},\ \sigma \in \{\pm\}$.

5.4.1 Description of the discretisation subspace. Let $B_\Omega = \{\psi_m \in H^1(\Omega),\ m \in \{1,\dots,M_\Omega\}\}$ be a first order Galerkin basis of the domain Ω. We define a corresponding subset of $\mathcal{V}$ by

$$\begin{aligned}\mathcal{V}_\Omega^h = \operatorname{span}\big\{&(\psi_{m,\Omega},\ \psi_{m,0},\dots,\psi_{m,\boldsymbol{m}-1}) \in \mathcal{V} : \psi_{m,\Omega} = \psi_m,\\ &\psi_{m,n} = \psi_m|_{\Gamma_n},\ n \in \{0,\dots,\boldsymbol{m}-1\},\ m \in \{1,\dots,M_\Omega\}\big\}.\end{aligned}$$

A special case has to be made for the elements on the corners of Ω. Let $\psi_m \in H^1(\Omega)$ be such that $\psi_m(x) \neq 0$, where $x \in \partial\Omega$ is one of the corners of Ω. In this case, at least one of the traces

$$\psi_m|_{\Gamma_n},\ n \in \{0,\dots,\boldsymbol{m}-1\}$$

will not be contained in $H^1(\Gamma_n)$. For these interior elements, we define $\psi_{m,n} \in H^1(\Gamma_n)$ as an $H^1(\Gamma_n)$ extension of

$$\psi_{m,n} := \psi_m|_{\Gamma_n^0}.$$

So that we actually obtain a subspace of $\mathcal{V}$.

To discretise the boundaries, namely Γ_n^σ, $n \in \{0,\dots\boldsymbol{m}-1\}$, $\sigma \in \{\pm\}$, let us denote by $B_{\text{ife}} = \{\phi_m \in H_0^1(0,\infty) : m \in \{1,\ \dots, M_{\text{ife}}\}\}$ a basis of functions living on the positive real line, which will serve (after transformation) as a basis for the different semi-infinite lines. For this aim, let us define for $m \in \{1,\dots,M_{\text{ife}}\}$, $n \in \{0,\dots,\boldsymbol{m}-1\}$ and $\sigma \in \{\pm\}$ the transformed basis function $\psi_{m,n}^\sigma \in \mathcal{V}$ as follows. On Γ_n^σ, $\psi_{m,n}^\sigma$ is given by

$$\psi_{m,n}^\sigma(\sigma z + c_n^\sigma) = \phi_n(z) \qquad \text{for } z > 0,$$

where we used the canonical identification (4.2.2). Elsewhere, we set $\psi_{m,n}^\sigma = 0$ (that is, in the interior of Ω and on the remaining semi-infinite lines). So we define for $n \in \{0,\dots,\boldsymbol{m}-1\}$, $\sigma \in \{\pm\}$ the finite element ansatz space for Γ_n^σ by

$$\mathcal{V}_{\Gamma_n^\sigma}^h := \operatorname{span}\left\{\psi_{m,n}^\sigma : m \in \{1,\dots,M_{\text{ife}}\}\right\}.$$

So that our full ansatz space will be

$$\mathcal{V}^h = \mathcal{V}_\Omega^h \oplus \bigoplus_{\substack{\sigma\in\{\pm\}\\ n\in\{0,\dots,\boldsymbol{m}-1\}}} \mathcal{V}_{\Gamma_n^\sigma}^h.$$

In Subsection 5.4.5, we will give explicit formulae for the basis B_{ife}.

5.4.2 Assembly of the matrices. Let us note that for $\psi, \phi \in \mathcal{V}^h$ the matrices associated with the volume part of the sesquilinear form $b_\Omega(\psi,\phi)$ can be computed by standard techniques. Accordingly, we will only describe how the matrices of the sesquilinear forms $b_n^{\mathcal{N}}$ and b_n^σ will be computed.

We fix some $n \in \{0,\dots,\boldsymbol{m}-1\}$, that is, we operate in the halfspace Ω_n. Let A be the associated operator with the generalised Fourier transform $\mathcal{F}_A$, and also recall the spectral space $L^2(\Lambda, \mathrm{d}\mu)$ with the corresponding family of (generalised) eigenfunctions $\Psi : \Lambda \times \mathbb{R} \to \mathbb{C}$ (compare Chapter 2).

(a) DtN part $b_n^{\mathcal{N}}$. Let $\psi_{\mathrm{s}},\ \psi_{\mathrm{t}} \in \mathcal{V}^h$ be two basis functions. We assume that $\psi_{\mathrm{s}}|_{\Gamma_n}$ and $\psi_{\mathrm{t}}|_{\Gamma_n^0}$ do not vanish, since elsewise $b_n^{\mathcal{N}}(\psi_{\mathrm{s}},\psi_{\mathrm{t}}) = 0$. Let now $\phi_{\mathrm{s}} := \psi_{\mathrm{s}}|_{\Gamma_n}$ and $\phi_{\mathrm{t}} := \psi_{\mathrm{t}}|_{\Gamma_n^0}$. Utilising the canonical identification (4.2.2), we have to compute

$$b_n^{\mathcal{N}}(\psi_s,\psi_t) = -\int_{\Gamma_n^0} (\mathcal{N}\phi_{\mathrm{s}})\overline{\phi}_{\mathrm{t}}\,\mathrm{d}s = -\int_{\mathbb{R}} (\mathcal{N}\phi_{\mathrm{s}})(x_1)\overline{\phi}_{\mathrm{t}}(x_1)\,\mathrm{d}x_1.$$

Denoting $\tilde{\phi}_\mathrm{s} := \mathcal{F}_A\phi_s$ and $\tilde{\phi}_\mathrm{t} = \mathcal{F}_A\tilde{\phi}_\mathrm{t}$, we obtain by applying Lemma 3.4.2 to express $\mathcal{N}$, and by Fubini's theorem

$$\begin{aligned}
-b_n^{\mathcal{N}}(\psi_s,\psi_t) &= \int\limits_{\mathbb{R}} \Psi(m,x_1) \int\limits_{\Lambda} i\sqrt{\kappa-\hat{\lambda}(m)}\,\tilde{\phi}_\mathrm{s}(m)\,\mathrm{d}\mu(m)\,\overline{\phi}_\mathrm{t}(x_1)\,\mathrm{d}x_1 \\
&= \int\limits_{\Lambda} i\sqrt{\kappa-\hat{\lambda}(m)}\,\tilde{\phi}_\mathrm{s}(m) \int\limits_{\mathbb{R}} \Psi(m,x_1)\overline{\phi}_\mathrm{t}(x_1)\,\mathrm{d}x_1\,\mathrm{d}\mu(m) \\
&= \int\limits_{\Lambda} i\sqrt{\kappa-\hat{\lambda}(m)}\,\tilde{\phi}_\mathrm{s}(m)\overline{\tilde{\phi}_\mathrm{t}(m)}\,\mathrm{d}\mu(m).
\end{aligned}$$

This formula helps us to reduce the problem of computing $b_n^{\mathcal{N}}(\psi_s,\psi_t)$ to two smaller sub-problems:

(i) We have to calculate the transforms $\tilde{\phi}_\mathrm{s} = \mathcal{F}_A\phi_\mathrm{s}$, $\tilde{\phi}_\mathrm{t} = \mathcal{F}_A\phi_\mathrm{t}$. Later in Subsection 5.4.4, we will present explicit but somewhat complicated formulae for those quantities.

(ii) We have to evaluate the integrals over the spectral space Λ, that is, we have to give some quadrature for the integral

$$\int\limits_{\Lambda} f(m)\,\mathrm{d}\mu(m)$$

for an explicitly known function f. This will be the topic of Subsection 5.4.3.

(b) DtD part of b_n^σ: Fix $\sigma \in \{\pm\}$. Note that we can write

$$b_n^\sigma(\psi_\mathrm{s},\psi_\mathrm{t}) = \int\limits_{\Gamma_{n+1}^\sigma} [(I-\mathcal{D}_n^+)\psi_s]\overline{\psi}_t\,\mathrm{d}s = \int\limits_{\Gamma_{n+1}^\sigma} \psi_s\overline{\psi}_t\,\mathrm{d}s - \int\limits_{\Gamma_{n+1}^\sigma} [\mathcal{D}_n^+\psi_s]\overline{\psi}_t\,\mathrm{d}s$$

We discuss the two integrals on the right hand side separately. First consider the part involving the DtD operator $\mathcal{D}_n^\sigma$. Let $\psi_\mathrm{s},\ \psi_\mathrm{t} \in \mathcal{V}^h$ be such that $\psi_\mathrm{s}|_{\Gamma_n}$ and $\psi_\mathrm{s}|_{\Gamma_{n+\sigma}^\sigma}$ do not vanish, since otherwise the corresponding integral would be zero. Let $\phi_\mathrm{s} = \psi_\mathrm{s}|_{\Gamma_n}$. We have to express $\psi_\mathrm{t}|_{\Gamma_{n+\sigma}^\sigma}$ in the coordinate system of the halfspace Ω_n. For this purpose, let us define

$$\phi_\mathrm{t}(z) := \psi_\mathrm{t}(c_{n+\sigma}^\sigma + \sigma z) \qquad \text{for } z > 0.$$

Furthermore, let us introduce the vector

$$d = \begin{pmatrix} d_1 \\ d_2 \end{pmatrix} := \begin{pmatrix} \cos(\theta_n^{-\sigma}) \\ \sin(\theta_n^{-\sigma}) \end{pmatrix},$$

where we refer again to Subsection 4.2.2, where we defined the angles θ_n^σ. This now allows us to write (denoting $\tilde{\phi}_{\mathrm{s}} = \mathcal{F}_A \phi_{\mathrm{s}}$)

$$\begin{aligned}
&\int\limits_{\Gamma^\sigma_{n+1}} (\mathcal{D}_n^+ \psi_s)\overline{\psi}_t \,\mathrm{d}s \\
&= \int\limits_0^\infty \int\limits_\Lambda e^{i\sqrt{\kappa-\hat{\lambda}(m)}\, d_2 z} \Psi(m, c_n^{-\sigma} + d_1 z)\tilde{\phi}_{\mathrm{s}}(m)\,\mathrm{d}\mu(m)\,\overline{\phi}_{\mathrm{t}}(z)\,\mathrm{d}z \\
&= \int\limits_\Lambda \tilde{\phi}_{\mathrm{s}}(m) \int\limits_0^\infty e^{i\sqrt{\kappa-\hat{\lambda}(m)}\, d_2 z} \Psi(m, c_n^{-\sigma} + d_1 z)\overline{\phi}_{\mathrm{t}}(z)\,\mathrm{d}z\,\mathrm{d}\mu(m).
\end{aligned}$$

This leaves us with another sub-problem: we have to compute the integral

$$\tilde{\phi}_{\mathrm{t}}(z) := \int\limits_0^\infty e^{i\sqrt{\kappa-\hat{\lambda}(m)}\, d_2 z} \Psi(m, c_n^{-\sigma} + d_1 z)\overline{\phi}_{\mathrm{t}}(z)\,\mathrm{d}z \tag{5.4.1}$$

explicitly. This will be dealt with in Subsection 5.4.4.

(c) Identity part of b_n^σ: If ψ_{s} and ψ_{t} both have parts which are supported on $\Gamma^\sigma_{n+\sigma}$, we have to compute the integral

$$\int\limits_{\Gamma^\sigma_{n+1}} \psi_s \overline{\psi}_t \,\mathrm{d}s.$$

This will be done explicitly when we describe our bases in Subsection 5.4.5.

5.4.3 The quadrature of the spectral space. Let $f : \Lambda \to \mathbb{C}$ be some function, $f = (f^p, f^+, f^-)$. We approximate the integral

$$\int\limits_\Lambda f(m)\,\mathrm{d}\mu(m) = \sum_{n=1}^N f^p(\lambda_n) + \frac{1}{2\pi} \sum_{\sigma\in\{\pm\}} \int\limits_{q_\sigma}^\infty f^\sigma(\lambda) \frac{\mathrm{d}\lambda}{2\sqrt{\lambda - q_\sigma}}$$

as follows. The computation of the finite sum is clear. For $\sigma \in \{\pm\}$, we obtain by substituting $\lambda = \xi^2 + q_\sigma$

$$\frac{1}{2\pi} \int\limits_{q_\sigma}^\infty f^\sigma(\lambda) \frac{\mathrm{d}\lambda}{2\sqrt{\lambda - q_\sigma}} = \frac{1}{2\pi} \int\limits_0^\infty f^\sigma(q_\sigma + \xi^2)\,\mathrm{d}\xi.$$

This integral is now approximated as follows: we truncate the integral at some maximal value $T_\xi > 0$, and divide the interval $(0, T_\xi)$ into a number of subintervals. For each subinterval, we apply Gauss quadrature weights and knots. Since the integrands (as functions of λ) will depend on $\sqrt{\kappa - \lambda}$, $\sqrt{\lambda - q_-}$, $\sqrt{\lambda - q_+}$, which are not differentiable at certain points, we will choose the subintervals so that the discontinuities are boundary points of the subintervals. The critical points are given by

$$\xi \in \left\{ \sqrt{\kappa - q_\sigma}, \sqrt{q_+ - q_\sigma}, \sqrt{q_- - q_\sigma} \right\}.$$

5.4.4 Explicit formulae for transforms. To keep the presentation somewhat contained, we will only consider the integral from (5.4.1) here. The other integrals (in particular the transforms of the basis functions) can be calculated analogously. Let $\theta \in (0, \pi)$, $c \in \mathbb{R}$, $d = (\cos(\theta), \sin(\theta))$, and let us consider

$$I(m) := \int_0^\infty e^{i\sqrt{\kappa - \hat{\lambda}(m)}\, d_2 z} \Psi(m, c + d_1 z) \overline{\phi}_{\mathrm{t}}(z)\, \mathrm{d}z.$$

Let us make a few additional assumptions to avoid a tedious case-by-case analysis. Let $a < b$ be the quantities from the definition of q (the potential of A, see Section 2.3). We now assume that $d_1 < 0$ and that $c < a$. This implies that $c + d_1 z < a$ for all $z > 0$, so that $\Psi(m, c + d_1 z)$ is given by a closed representation for any $z > 0$. Otherwise, the different cases of (2.3.1) have to be considered separately. Under these assumptions, we now have that

$$\begin{aligned} \Psi(m, c + d_2 z) = {} & \alpha_1(m) e^{i\sqrt{\lambda - q_-}(c + d_1 z - a)} \\ & + \alpha_2(m) e^{-i\sqrt{\lambda - q_-}(c + d_1 z - a)} \qquad \text{for } z > 0, \end{aligned}$$

where $\alpha_1,\ \alpha_2 : \Lambda \to \mathbb{C}$ are explicitly known functions (see Section 2.3). If we now introduce for $k \in \mathbb{C},\ \mathrm{Re}(k) \leq 0$, the function

$$E(k) := \int_0^\infty e^{kz} \overline{\phi}_{\mathrm{t}}(z)\, \mathrm{d}z,$$

we can easily compute

$$\begin{aligned} I(m) = {} & \alpha_1(m) e^{i\sqrt{\hat{\lambda}(m) - q_-}(c-a)} E\left(i\sqrt{\kappa - \hat{\lambda}(m)}\, d_2 + i\sqrt{\hat{\lambda}(m) - q_-}\, d_1 \right) \\ & + \alpha_1(m) e^{-i\sqrt{\hat{\lambda}(m) - q_-}(c-a)} E\left(i\sqrt{\kappa - \hat{\lambda}(m)}\, d_2 - i\sqrt{\hat{\lambda}(m) - q_-}\, d_1 \right). \end{aligned}$$

We will compute the function E explicitly for the different types of basis functions in the following Subsection 5.4.5.

5.4.5 Infinite element discretisation. We will define a few discretisations for the semi-infinite lines, and compute the required terms of the previous section. In effect, we only need to specify a basis B_{ife}, whose span is a sufficiently large subspace of $H_0^1(0, \infty)$. We will give two different choices in the following for the basis $B_{\mathrm{ife}} = \{\phi_m \in H_0^1(0, \infty) : m \in \{1, \ldots, M_{\mathrm{ife}}\}\}$.

FE-IFE. Our first basis is taken from [74], where it has been used in the very same context. We can truncate the semi-infinite line and discretise the functions on the bounded interval by first order finite elements. Let $h > 0$, then we choose for $m \in \{1, \ldots, M_{\mathrm{ife}}\}$ the basis functions

$$\phi_m(z) = \begin{cases} \frac{x - (m-1)h}{h} & \text{for } z \in ((m-1)h, mh), \\ \frac{(m+1)h - x}{h} & \text{for } z \in (mh, (m+1)h), \\ 0 & \text{for } z \in (0, (m-1)h) \cup ((m+1)h, \infty). \end{cases}$$

From this, one easily computes

$$E_m(k) = \int_{\mathbb{R}} e^{kz}\overline{\phi}_m(z)\,\mathrm{d}z = \frac{4}{k^2h}\sinh(\tfrac{kh}{2})e^{mkh} \qquad \text{for } k \in \mathbb{C},$$

as well as for $m, m' \in \{1, \dots, M_{\text{ife}}\}$

$$\int_0^\infty \phi_m(z)\overline{\phi}_{m'}(z)\,\mathrm{d}z = \begin{cases} \frac{2}{3}h & \text{for } m = m', \\ \frac{1}{6}h & \text{for } |m - m'| = 1, \\ 0 & \text{else.} \end{cases}$$

FT-IFE. We propose a type of Fourier–Laplace infinite elements. Let $\gamma > 0$ and $\delta > 0$ be two arbitrary tuning parameters. We now choose for $m \in \{1, \dots, M_{\text{ife}}\}$

$$\phi_m(z) = e^{-\gamma z}\sin(m\delta z).$$

Let us comment further on those two parameters: $\gamma > 0$ assures the finiteness of the integrals we will compute later. The parameter δ describes how fine we discretise in the “Fourier domain”. Again, one easily calculates for $m, m' \in \{1, \dots, M_{\text{ife}}\}$ and $k \in \mathbb{C}$ with $\mathrm{Re}(k) < \gamma$

$$E_m(k) = \frac{\delta m}{(k-\gamma)^2 + \delta^2 m^2},$$

$$\int_0^\infty \phi_m(z)\overline{\phi}_{m'}(z)\,\mathrm{d}z = \frac{\gamma}{\delta^2(m-m')^2 + 4\gamma^2} - \frac{\gamma}{\delta^2(m+m')^2 + 4\gamma^2}.$$

5.4.6 Extension of corner elements. As mentioned in Subsection 5.4.1, we have to extend the interior elements living on the corners of $\partial\Omega$ to the adjacent semi-infinite lines Γ_n^σ. This will be done by an additional function $\phi_0 : [0, \infty) \to \mathbb{C}$, which fulfils $\phi_0(0) = 1$. We will choose this function corresponding to the rest of the IFE basis, and have to compute the corresponding integrals.

FE-IFE. In this case we choose

$$\phi_0(z) = \begin{cases} \frac{h-z}{h} & \text{for } z \in (0, h), \\ 0 & \text{else.} \end{cases}$$

Again, one easily computes

$$E_0(k) = \frac{1}{k^2h}(e^{kh} - 1 - kh)$$

and for $m \in \{0, \dots, M_{\text{ife}}\}$

$$\int_0^\infty \phi_0(z)\overline{\phi}_m(z)\,\mathrm{d}z = \begin{cases} \frac{1}{3}h & \text{for } m = 0, \\ \frac{1}{6}h & \text{for } m = 1, \\ 0 & \text{else.} \end{cases}$$

FT-IFE. Here we set

$$\phi_0(z) = e^{-\gamma z} \qquad \text{for } z > 0.$$

Then

$$E_0(k) = \frac{1}{k+\gamma},$$

$$\int_0^\infty \phi_0(z)\overline{\phi}_m(z)\,\mathrm{d}z = \begin{cases} \frac{1}{2\gamma} & \text{for } m = 0, \\ \frac{\delta m}{2^2\gamma^2+\delta^2 m^2} & \text{for } m \geq 1. \end{cases}$$

5.4.7 Implementation and convergence tests. The method we just described was implemented with first order elements for the interior in MATLAB, and it turned out that this restriction to first order elements was a rather bad choice, since it significantly inhibits convergence. Nonetheless we will show a few results, but keep this section very brief, and restrict ourselves to the non-absorptive case including incident waves. For a more detailed study of the numerical convergence in the case of an unperturbed free space, we refer to Tonnoir's PhD thesis [74].

We will test the two different discretisations FT-IFE and FE-IFE on two examples of scattering problems of the type of Section 5.3. For these examples we know the exact solution, and will try to reconstruct it by our method. The first benchmark is the same problem as sketched in Example 5.3.5: a mode propagating in a simple open waveguide. The solution we expect to obtain is exactly the mode without any disturbance. The second benchmark situation is a homogeneous space, with a plane wave incident on a triangular finite element domain. Again, we expect the plane wave to propagate through our domain, which will be our reference solution.

The error we show is the relative L^2-error on a square $\hat{\Omega}$, which contains the finite element domain Ω as well as parts of the surrounding halfspaces. Outside of the finite element domain, we used the solution operators $\mathcal{S}_n$ to compute the solution.

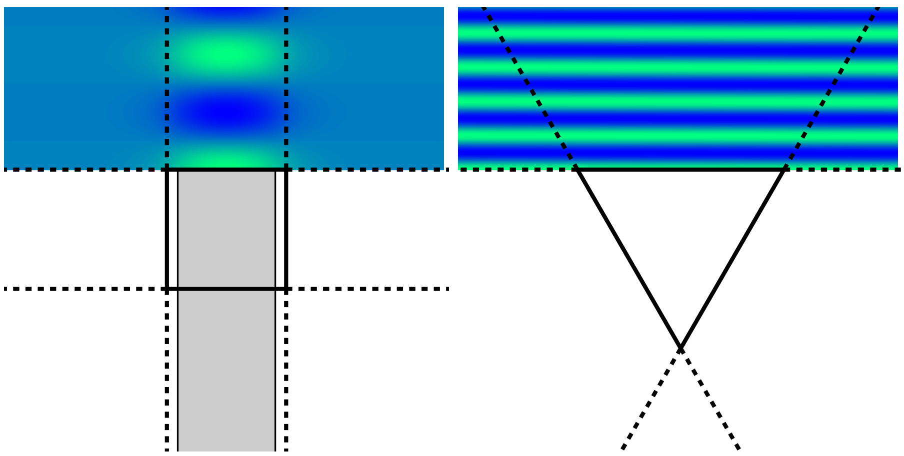

Figure 5.4: The two test situations for the convergence test. The coloured field shows the real part of the incident field, which is only supported on the top halfspace. They are straightforwardly extendable to the whole $\mathbb{R}^2$, which serves as the reference solution. As before, the grey area indicates the waveguide.

FE-IFE. There are five parameters that influence the convergence:

(1) the mesh size of the finite element discretisation in the interior,

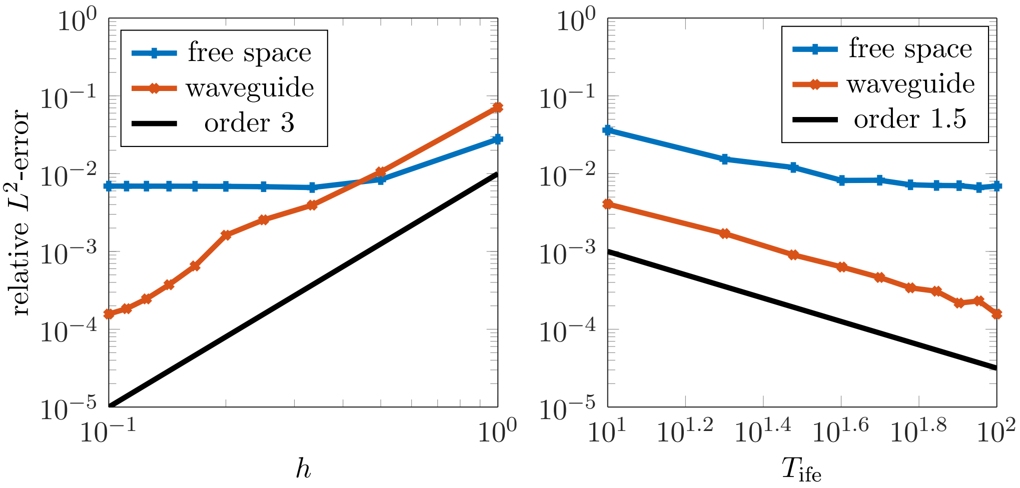

Figure 5.5: Convergence for the FE-IFE. The black lines are guides for the eye, to give orientation of the order of convergence. Note that in particular for the free space case, there is no proper convergence.

(2) the truncation of the integration interval for the quadrature of the spectral integrals (see Subsection 5.4.3),

(3) the order and number of subintervals for the quadrature,

(4) the mesh size h of discretisation of the infinite elements,

(5) the truncation of the semi-infinite lines, which is given by

$$T_{\text{ife}} = M_{\text{ife}} h,$$

where we recall that M_{ife} is the number of infinite elements.

This is a rather large parameter space we should cover, but for the sake of brevity we will restrict ourselves to showing some results regarding point (4) and (5), while we will deal with (1) to (3) just in a few remarks.

The convergence with respect of the mesh-size in the interior is well-analysed, and we omit any analysis here. For the integration parameters, one needs to choose the truncation distance T_ξ larger than

$$T_\xi > \sqrt{\|\kappa_0 - q\|_{L^\infty}}.$$

[74] found that the error depends exponentially on $T_\xi - \sqrt{\|\kappa_0 - q\|_{L^\infty}}$, which we can confirm. The number of subintervals was chosen as 500, each one integrated by a (Gauss) quadrature of order 5. Increasing the order did not significantly reduce the number of function evaluations necessary. We suspect, however, that in particular the resolution close to the critical points of discontinuity (see Subsection 5.4.3) is of importance. The convergence with respect to the remaining two parameters is shown in Figure 5.5. One notes that the convergence for the free space plane wave is particularly bad, which is actually not very surprising, since each of the traces we try to retrieve is not decaying at all. For the waveguide case, we see a reasonable polynomial convergence with respect to both the truncation and the mesh size.

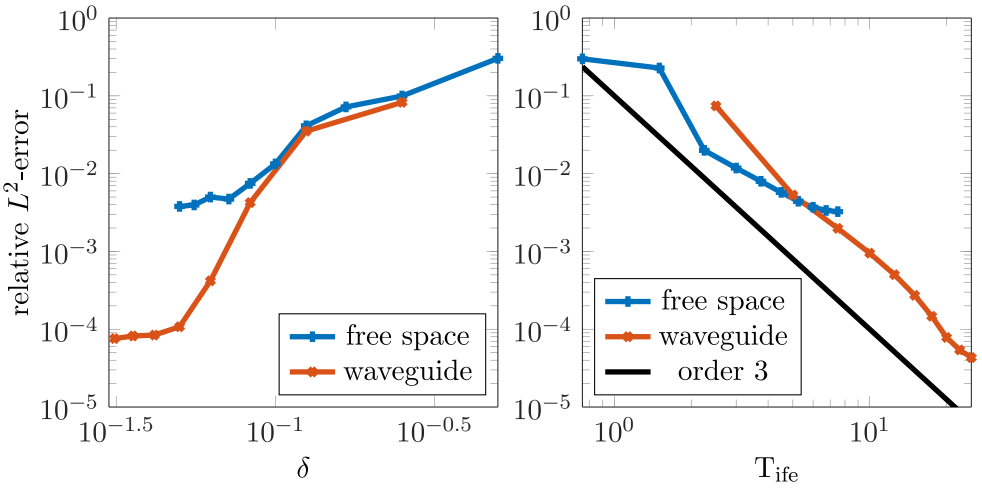

Figure 5.6: Convergence for the FT-IFE discretisation of the semi-infinite lines. The convergence seems to be faster than the FE-IFE. In particular the convergence with respect to δ seems to be exponential, but flattens out due to residual error from the finite elements in the interior.

FE-IFE. Let us quickly have a look at the second type of discretisation, the Fourier–Laplace infinite elements. Here, the parameters (4) and (5) from the previous list are replaced by

(4) the mesh-size in the Fourier domain δ,

(5) the truncation in Fourier domain,

$$T = M_{\text{ife}}\delta.$$

We omitted the parameter γ, which was chosen as 0.1 for the examples shown.

The corresponding convergence results are shown in Figure 5.6. Let us point here to the fact that these infinite elements seem to provide a higher order of convergence, which is not easy to quantify. One main reason is the limiting influence of the finite elements in the interior, which proved to be a bottleneck for this type of discretisation (for the waveguide case).

5.4.8 Comparison to other transparent boundary conditions. During the introduction in Subsection 1.1.3, we mentioned two other methods which in principle allow dealing with the same problem as ours: the perfectly matched layer (PML) and the Hardy space infinite elements (HSIE). How do these three methods compare?

In the authors opinion, our method is at a clear disadvantage, due to a number of reasons.

- Halfspace matching is much more complicated in terms of implementation than the other two methods. It requires the explicit availability of the generalised Fourier transform, which is only given for very particular cases. Furthermore, the assembly of the different types of matrices is rather complicated.

- Related to this is the second, severe drawback: each matrix entry is computed by the numerical evaluation of an integral. For a fine discretisation of the semi-infinite lines (i.e. for small δ or h), one needs to carefully increase the accuracy of the quadrature, additionally increasing the cost of the matrix assembly, making it very costly compared to the other methods.
- A third disadvantage is the lower rate of convergence we obtain. For PML and HSIE, the convergence in the non-absorptive case is effectively exponential [63] with respect to the number of exterior degrees of freedom. As seen above, this kind of convergence is only partly shared by our method, and due to the high number of discretisation parameters, there is some balancing required to obtain good results.
- Lastly, our method imposes a number of additional restrictions on the geometrical arrangements of the waveguides in the exterior, which is not shared by either PML or HSIE.

However, it should be mentioned, that our method also has a few advantages.

- For incident waves, our problem formulation allows for very close cropping of the interior domain (see Figure 5.4). Since the mode far outside the interior is incorporated, one can practically cut directly at the waveguide. This is not shared for other methods, since the in-coupling of the incident mode is usually done by a Dirichlet and Neumann jump.
- Our method gives easy access to the solution outside of the interior domain.
- The additional degrees of freedom introduced by our method do not depend on the size of the interior domain, but only on the number of corners. For PML and HSIE, the number of degrees of freedom to realise the transparent boundary condition is rougly proportional to the circumference of the interior domain.

6 Optimisation of Waveguide Junctions

6.1 Introduction

In this chapter we want to illustrate the physical background behind the method developed in the last chapters. To do this, we will study scattering problems at waveguide junctions, and try to manipulate them to create a special scattering behaviour. To be able to introduce the calculus required for the optimisation, we will again make a detour into the absorptive world, so the outline of this chapter is as follows.

We will start by introducing a formulation for incident waves in the absorptive case, to get an analogous problem to the non-absorptive problem from Section 5.3. This will allow us to study the differentiability properties of the solution as a function of the potential q, and gives rise to an interesting property of waveguide junctions. If we try to optimise the transmission into a particular mode, the resulting adjoint state will take a very peculiar form: it is again a guided incident mode.

The required derivatives will be introduced in Section 6.3, where we will keep up with a rigorous mathematical definition-lemma style. This will end with the next section, where we will switch back to the non-absorptive case and formal calculations. To give a proper meaning to the *energy flow* associated with some mode, we will derive an energy conservation relation for junctions of open waveguides in Section 6.4. In Section 6.5, we will describe the optimisation algorithm we will use in the examples afterwards.

Let us again clarify the scope of this chapter: it is not to give a thorough analysis of the optimisation algorithms or an extensive testing thereof, but rather to illustrate the physics of our problem.

6.1.1 References. Shape, material, and topology optimisation are a large field, and we will give only a few general references. The general method we use originates from Bendsøe and Kikuchi's papar [3]. A large number of examples and a general introduction into topology/material optimisation can be found in Bendsøe's and Sigmund's book [4] and the references therein, which is, however, more application oriented. The notation and approach here is more heavily influenced by shape optimisation, for which we reference [26], as well as by inverse problem scattering, for which we reference to [41, 50].

6.2 Incident Fields in the Absorptive Case

To give a more precise treatment of the shape calculus and the adjoint states, we will switch back to a scattering problem with absorption, that is, we choose again

$$\kappa \in \mathbb{C} \setminus \mathbb{R}$$

and let $q \in L^\infty(\mathbb{R}^2)$ be some arbitrary real-valued potential. We start with an incident field u_i that solves

$$\Delta u_\mathrm{i} + (\kappa - q)u_\mathrm{i} = 0 \qquad \text{in } \Omega_0,$$

where Ω_0 is a halfspace. We furthermore assume that $u_\mathrm{i}|_{\Gamma_0} \in H^{1/2}(\Gamma_0)$, where $\Gamma_0 = \partial\Omega_0$ as before. These assumptions are already rather restrictive for u_i. However, for example a guided mode of the form

$$u_\mathrm{i}(x) = e^{-i\sqrt{\kappa-\lambda_n}\,x_2}\Psi^p(\lambda_n, x_1)$$

fulfils these conditions on $\Omega_0 := \{x \in \mathbb{R}^2 : x_2 < 0\}$, provided q is chosen appropriately. Note that u_i is exponentially increasing as $x_2 \to -\infty$.

One can easily repeat the following procedure solely under the condition that u_i fulfils the Helmholtz equation in the proximity of Γ_0, so that sources contained in Ω_0 can be incorporated in u_i as well.

We aim to give meaning to the problem

$$\begin{cases} \Delta u + (\kappa - q)u = 0 & \text{in } \mathbb{R}^2, \\ u - u_\mathrm{i} & \text{outgoing in } \mathbb{R}^2, \end{cases} \tag{6.2.1}$$

in a variational setting. We start by slightly redefining our incident field as $\tilde{u}_\mathrm{i} := u_\mathrm{i} - w$, where $w \in H^1(\Omega_0)$ solves

$$\begin{cases} \Delta w + (\kappa - q)w = 0 & \text{in } \Omega_0, \\ w = u_\mathrm{i} & \text{on } \Gamma_0, \end{cases}$$

in the variational sense. w exists and is unique by Theorem 1.4.3. The new incident field $\tilde{u}_\mathrm{i}$ has the advantage that it vanishes on Γ_0, so that we expect that the scattered field, defined by

$$u_\mathrm{s} := \begin{cases} u - \tilde{u}_\mathrm{i} & \text{in } \Omega_0, \\ u & \text{in } \mathbb{R}^2 \setminus \overline{\Omega}_0, \end{cases}$$

will be in $H^1(\mathbb{R}^2)$: we choose to demand that $u_\mathrm{s} \in H^1(\Omega_0)$ as well as $u_\mathrm{s} \in H^1(\mathbb{R}^2 \setminus \overline{\Omega}_0)$, since this has turned out to give a notion of "outgoing" in the absorptive case. Furthermore, since $\tilde{u}_i$ vanishes on Γ_0, we obtain that the left-sided and right-sided traces on Γ_0 of u_s agree, which implies that u_s is in $H^1(\mathbb{R}^2)$.

Let us derive a variational formulation for u_s. Since $u \in H^2_\mathrm{loc}(\mathbb{R}^2)$, we can multiply the Helmholtz equation (6.2.1) by some $\psi \in C_0^\infty(\mathbb{R}^2)$, and integrate over $\operatorname{supp}(\psi)$ to obtain by partial integration

$$\begin{aligned} 0 &= \int_D -\nabla u \cdot \nabla\overline{\psi} + (\kappa - q)u\overline{\psi}\,\mathrm{d}x \\ &= \int_{\Omega_0 \cap D} -\nabla(u_\mathrm{s} + \tilde{u}_\mathrm{i}) \cdot \nabla\overline{\psi} + (\kappa - q)(u_\mathrm{s} + \tilde{u}_\mathrm{i})\overline{\psi}\,\mathrm{d}x \\ &\quad + \int_{(\mathbb{R}^2 \setminus \Omega_0) \cap D} -\nabla u_\mathrm{s} \cdot \nabla\overline{\psi} + (\kappa - q)u_\mathrm{s}\overline{\psi}\,\mathrm{d}x, \end{aligned}$$

which can be rearranged to get

$$\int_{\mathbb{R}^2} \nabla u_s \cdot \nabla\overline{\psi} - (\kappa - q)u\overline{\psi}\,\mathrm{d}x = \int_{\Omega_0\cap D} -\nabla\tilde{u}_\mathrm{i} \cdot \nabla\psi + (\kappa - q)\tilde{u}_\mathrm{i}\overline{\psi}\,\mathrm{d}x$$
$$= \int_{\Gamma_0} (\partial_\nu \tilde{u}_\mathrm{i})\overline{\psi}\,\mathrm{d}s,$$

where we used that u_i solves the Helmholtz equation in the last step. Let us reformulate (6.2.1) with a sesquilinear form.

6.2.1 Weak problem. Let $\tilde{u}_\mathrm{i} \in H^2_\mathrm{loc}(\Omega_0)$ be some incident field such that $\tilde{u}_\mathrm{i}|_{\Gamma_0} = 0$. We say that u is a variational solution to (6.2.1), if

$$u = \begin{cases} u_\mathrm{s} + \tilde{u}_\mathrm{i} & \text{on } \Omega_0, \\ u_\mathrm{s} & \text{on } \mathbb{R}^2 \setminus \overline{\Omega}_0, \end{cases}$$

where $u_\mathrm{s} \in H^1(\mathbb{R}^2)$ is the unique solution of

$$\int_{\mathbb{R}^2} \nabla u_\mathrm{s} \cdot \nabla\overline{\psi} - (\kappa - q)u_\mathrm{s}\overline{\psi}\,\mathrm{d}x = \int_{\Gamma_0} (\partial_\nu \tilde{u}_\mathrm{i})\overline{\psi}\,\mathrm{d}s \qquad \text{for all } \psi \in H^1(\mathbb{R}^2).$$ ■

This variational problem can be shown to be uniquely solvable by the Lax–Milgram theorem, as in the proof of Theorem 1.4.3, since the right hand side is a bounded conjugate linear functional on $H^1(\mathbb{R}^2)$ by the trace theorem.

Let us also comment on the meaning of the problem we just derived: essentially, we implemented an incident wave by a Neumann jump of the scattered field u_s. Let us now formulate the underlying conjecture, which will allow us to translate the result to the absorption free case, i.e. $\kappa_0 \in \mathbb{R}$.

6.2.2 Conjecture. Let $q : \mathbb{R}^2 \to \mathbb{R}$ fulfil Assumption 5.1.2, and let Ω_0 contain a waveguide. Consider the incident field

$$\tilde{u}_\mathrm{i}(\xi\,\xi^{(0)} + \eta\,\eta^{(0)}) = \left(e^{-i\sqrt{\kappa-\lambda_l}\,\eta} - e^{i\sqrt{\kappa-\lambda_l}\,\eta}\right)\Psi^{(p)}(\lambda_l, \xi) \qquad \xi \in \mathbb{R},\ \eta > 0,$$

where λ_l and $\Psi^{(p)}$ denotes an eigenvalue and eigenfunction of the operator A associated with Ω_0 (also note that we heavily employ the notation of Subsection 4.2.2), which fulfils the requirement of the previous subsection. Fix now $\kappa_0 \in \mathbb{R}$, and let $\epsilon > 0$ and set

$$\kappa = \kappa_0 + i\epsilon.$$

Denote by u_ϵ the solution of

$$\begin{cases} \Delta u_\epsilon + (\kappa_0 + i\epsilon - q)u_\epsilon = 0 & \text{in } \mathbb{R}^2, \\ u_\epsilon - u_\mathrm{i} & \text{is outgoing,} \end{cases}$$

which has to be understood in the variational sense. Let furthermore u_0 denote the solution of the last problem for $\epsilon = 0$, which is understood in the sense of Subsection 5.3.6. We now conjecture that

$$u_\epsilon \to u_0 \qquad \text{as } \epsilon \to 0,\ \epsilon > 0 \text{ in } H^2_\mathrm{loc}(\mathbb{R}^2).$$ ■

Let us point again to the references at the end of Section 1.3, where we already discussed the limit-absorption principle in open waveguides. Note however, that with the somewhat unsure formulation we use in our non-absorptive framework, there are still large gaps to be filled.

Note that this assumption holds for the scattering problem of a straight mode (see Example 5.3.5).

For the remainder of this chapter we will proceed as follows: we will develop material optimisation on the level of the absorptive, variational problem, and in the end pull all results over to the non-absorptive case in a rotating-arm argument[1].

6.3 The Fréchet Derivative

In this section we will consider the dependence of the solution on the potential q. To reflect the change of scope, we will introduce a bit of notation.

6.3.1 Definition. Let us define the space

$$H^1(\mathbb{R}^2)^* := \{F : H^1(\mathbb{R}^2) \to \mathbb{C} : F \text{ conjugate linear and continuous}\},$$

which we equip with the norm

$$\|F\|_{H^1(\mathbb{R}^2)^*} := \sup_{u \in H^1(\mathbb{R}^2)} |F(u)|.$$

Furthermore we denote by

$$L^\infty(\mathbb{R}^2, \mathbb{R}) = \{f : \mathbb{R}^2 \to \mathbb{R} : \|f\|_{L^\infty(\mathbb{R}^2)} < \infty\},$$

the space of real-valued L^∞-functions on $\mathbb{R}^2$. For $q \in L^\infty(\mathbb{R}^2, \mathbb{R})$, we define the sesquilinear form $b_q : H^1(\mathbb{R}^2) \times H^1(\mathbb{R}^2) \to \mathbb{C}$ by

$$b_q(u, v) := \int_{\mathbb{R}^2} \nabla u \cdot \nabla \overline{\psi} - (\kappa - q) u \overline{\psi} \, \mathrm{d}x. \qquad \blacksquare$$

We recall a few facts, which fall out of the proof of Theorem 1.4.3, and give the following corollary.

6.3.2 Corollary. Let $\kappa \in \mathbb{C} \setminus \mathbb{R}$, $q \in L^\infty(\mathbb{R}^2, \mathbb{R})$. Then there exist constants $0 < c_1 = c_1(\|q\|_{L^\infty(\mathbb{R})}, \kappa)$ and $0 < c_2 = c_2(\|q\|_{L^\infty(\mathbb{R})}, \kappa)$, which only depend on $\|q\|_{L^\infty(\mathbb{R})}$ and κ, such that

$$\begin{aligned} |b_q(u, v)| &\leq c_1 \|u\|_{H^1(\mathbb{R}^2)} \|v\|_{H^1(\mathbb{R}^2)} && \text{for all } u, v \in H^1(\mathbb{R}^2), \\ |b_q(u, u)| &\geq c_2 \|u\|^2_{H^1(\mathbb{R}^2)} && \text{for all } u \in H^1(\mathbb{R}^2). \end{aligned}$$

For any $F_\mathrm{s} \in H^1(\mathbb{R}^2)^*$, there exists exactly one solution u_q of

$$b_q(u, \psi) = F_\mathrm{s}(\psi) \qquad \text{for all } \psi \in H^1(\mathbb{R}^2),$$

[1] In physics, a "hand-waving proof" is an argument, which seems somewhat plausible, but is actually build on very shaky assumptions. A "very hand-waving" argument is sometimes raised to be a "rotating-arm" argument for obvious reasons. Whether another comparative to rotating-arm exists is not known to the author.

and it holds that

$$\|u_q\|_{H^1(\mathbb{R}^2)} \leq \frac{1}{c_2}\|F_\mathrm{s}\|_{H^1(\mathbb{R}^2)^*}. \tag{6.3.1}$$

■

Proof. Rechecking the proof of Theorem 1.4.3, the bounds are easily obtained. The existence of the solution for any functional follows by the Lax–Milgram lemma, and the bound for the $H^1(\mathbb{R}^2)$ norm follows by exploiting the coerciveness of b_q. ■

6.3.3 Definition. Fix $\kappa \in \mathbb{C}\backslash\mathbb{R}$ and $F_\mathrm{s} \in H^1(\mathbb{R}^2)^*$. We define the potential-to-solution operator

$$\mathcal{L} : L^\infty(\mathbb{R}^2, \mathbb{R}) \to H^1(\mathbb{R}^2), \qquad \mathcal{L}(q) := u_q,$$

where $u_q \in H^1(\mathbb{R}^2)$ is the solution of

$$b_q(u, \psi) = F_\mathrm{s}(\psi) \qquad \text{for all } \psi \in H^1(\mathbb{R}^2).$$ ■

We now aim to take the Fréchet-derivative of the operator $\mathcal{L}$. It will be denoted by $d\mathcal{L} : L^\infty(\mathbb{R}^2, \mathbb{R}) \times L^\infty(\mathbb{R}^2, \mathbb{R}) \to H^1(\mathbb{R}^2)$. Since it is non-linear in the first and linear in the second argument, we choose the notation

$$d\mathcal{L}(q)p \in H^1(\mathbb{R}^2)$$

for the derivative at q in direction p.

6.3.4 Lemma. Fix $\kappa \in \mathbb{C} \setminus \mathbb{R}$, $F_\mathrm{s} \in H^1(\mathbb{R}^2)^*$. Then the Fréchet-derivative of $\mathcal{L}$ at $q \in L^\infty(\mathbb{R}^2, \mathbb{R})$, denoted by $d\mathcal{L}(q) : L^\infty(\mathbb{R}^2, \mathbb{R}) \to H^1(\mathbb{R}^2)$, is given by

$$d\mathcal{L}(q)p = u'_p,$$

where $u'_p \in H^1(\mathbb{R}^2)$ is the solution of

$$b_q(u'_p, \psi) = -\int\limits_{\mathbb{R}^2} p u_q \overline{\psi}\,\mathrm{d}x \qquad \text{for all } \psi \in H^1(\mathbb{R}^2),$$

where $u_q = \mathcal{L}(q)$. ■

Proof. Let $q \in L^\infty(\mathbb{R}^2, \mathbb{R})$ be fixed for the following, and let us define the ball with radius 1 around 0 by

$$B_1 := \left\{\tilde{p} \in L^\infty(\mathbb{R}^2, \mathbb{R}) : \|\tilde{p}\|_{L^\infty(\mathbb{R}^2)} < 1\right\}.$$

First note that u'_p depends linearly and continuously on p, which are the usual properties of the derivative. To prove differentiability, we will show that there exists a constant $C > 0$ such that

$$\|u_{q+p} - u_q - u'_p\|_{H^1(\mathbb{R}^2)} < C\|p\|^2_{L^\infty(\mathbb{R}^2)} \qquad \text{for all } p \in B_1 \setminus \{0\},$$

where $u_{p+q} = \mathcal{L}(p + q)$. Let us define $C_2 > 0$ by

$$C_2 := \inf\left\{c_2(\|q + \tilde{p}\|_{L^\infty(\mathbb{R}^2)}, \kappa) : \tilde{p} \in B_1\right\},$$

where $c_2(\|q+\tilde{p}\|_{L^\infty(\mathbb{R}^2)}, \kappa)$ is the constant from Corollary 6.3.2. One now easily obtains by the definition of b_q that

$$b_q(u_{q+p} - u_q, \psi) = -\int\limits_{\mathbb{R}^2} p\, u_{q+p}\overline{\psi}\,\mathrm{d}x.$$

Setting $\psi = u_{q+p} - u_q$ in the last equation and exploiting (6.3.1) as well as the Cauchy–Schwarz inequality now yields

$$\begin{aligned}
\|u_{q+p} - u_q\|_{H^1}^2 &\leq \frac{1}{C_2}\left|\int\limits_{\mathbb{R}^2} p u_{q+p}(u_{q+p} - u_q)\,\mathrm{d}x\right| \\
&\leq \frac{1}{C_2}\|p\|_{L^\infty}\|u_{p+q}\|_{H^1}\|u_{q+p} - u_q\|_{H^1} \\
&\leq \frac{\|F\|_{H^1(\mathbb{R}^2)^*}}{C_2^2}\|p\|_{L^\infty}\|u_{q+p} - u_q\|_{H^1},
\end{aligned}$$

where we omitted the domain of the spaces (which is always $\mathbb{R}^2$) for better readability. Dividing by the norm of $u_{q+p} - u_q$ yields

$$\|u_{q+p} - u_q\|_{H^1} \leq \frac{\|F\|_{H^1(\mathbb{R}^2)^*}}{C_2^2}\|q\|_{L^\infty}. \tag{6.3.2}$$

Let $\psi \in H^1(\mathbb{R}^2)$, then we obtain by the definitions of $u_{q+p},\ u_q$ and u_p'

$$\begin{aligned}
&b_q(u_{q+p} - u_q - u_p', \psi) \\
&\quad = b_{q+p}(u_{q+p}, \psi) - \int\limits_{\mathbb{R}^2} p\, u_{q+p}\overline{\psi}\,\mathrm{d}x - b_q(u_q, \psi) - b_q(u_p', \psi) \\
&\quad = F(\psi) - \int\limits_{\mathbb{R}^2} p\, u_{q+p}\overline{\psi}\,\mathrm{d}x - F(\psi) + \int\limits_{\mathbb{R}^2} p\, u_q\overline{\psi}\,\mathrm{d}x \\
&\quad = -\int\limits_{\mathbb{R}^2} p(u_{q+p} - u_q)\overline{\psi}\,\mathrm{d}x.
\end{aligned}$$

Setting $\psi = u_{q+p} - u_q - u_p'$, we obtain by (6.3.2), (6.3.1), and the Cauchy–Schwarz inequality

$$\begin{aligned}
\|u_{q+p} - u_q - u_p'\|_{H^1}^2 &\leq \frac{1}{C_2}\left|b_q(u_{q+p} - u_q - u_p', u_{q+p} - u_q - u_p')\right| \\
&\leq \frac{1}{C_2}\left|\int\limits_{\mathbb{R}^2} p(u_{q+p} - u_q)(u_{q+p} - u_q - u_p')\,\mathrm{d}x\right| \\
&\leq \frac{1}{C_2}\|p\|_{L^\infty}\|u_{q+p} - u_q\|_{H^1}\|u_{q+p} - u_q - u_p'\|_{H^1} \\
&\leq \frac{\|F_{\mathrm{s}}\|_{H^1(\mathbb{R}^2)^*}}{C_2^3}\|p\|_{L^\infty}^2\|u_{q+p} - u_q - u_p'\|_{H^1}.
\end{aligned}$$

Dividing the last equation by the H^1-norm of $u_{q+p} - u_q - u_p'$ now gives the estimate we set out to prove in the beginning, finishing the proof. ■

In order to optimise, we need a figure of merit (abbreviated as FOM). Let us define the class of functionals we will consider.

6.3.5 Definition and Lemma. Let $F_{\mathrm{t}} \in H^1(\mathbb{R}^2)^*$. We will consider figures of merit $J : H^1(\mathbb{R}) \to \mathbb{R}$, given by

$$J(u) := |F_{\mathrm{t}}(u)|^2.$$

It holds in the sense of Fréchet derivatives for $u, v \in H^1(\mathbb{R}^2)$

$$dJ(u)v = 2\,\mathrm{Re}\left(F_{\mathrm{t}}(u)\overline{F_{\mathrm{t}}(v)}\right). \qquad \blacksquare$$

Proof. Note that J is not complex-differentiable, and hence one has to interpret previous derivative as a real derivative, that is, one has to identify $H^1(\mathbb{R}^2, \mathbb{C}) \cong H^1(\mathbb{R}^2, \mathbb{R}^2)$ and take the real linear structure of the latter space. The proof gets rather trivial by writing $J(u) = [\mathrm{Im}(F_{\mathrm{t}}(u))]^2 + [\mathrm{Re}(F_{\mathrm{t}}(u))]^2$, noting that the two functionals $\mathrm{Im}(F_{\mathrm{t}}(u))$ and $\mathrm{Re}(F_{\mathrm{t}}(u))$ are real-linear and real-differentiable. $\blacksquare$

Our goal is to determine the Fréchet-derivative of the potential-to-FOM function

$$\mathcal{J} : L^\infty(\mathbb{R}^2, \mathbb{R}) \to \mathbb{R}, \qquad \mathcal{J}(q) := J(\mathcal{L}(q)).$$

By the chain rule, one obtains

$$\begin{aligned} d\mathcal{J}(q)p &= d(J \circ \mathcal{L})(q)p = dJ(\mathcal{L}(q))\, d\mathcal{L}(q)\, p \\ &= 2\,\mathrm{Re}\left(F_{\mathrm{t}}(u_q)\overline{F_{\mathrm{t}}(u'_p)}\right), \end{aligned} \tag{6.3.3}$$

where we used the previous Definition and Lemma 6.3.5 as well as Lemma 6.3.4. Let us now consider that we want to calculate the derivative of $\mathcal{J}$ with respect to a number of directions $p_1, \dots, p_N \in L^\infty(\mathbb{R}^2, \mathbb{R})$: for each p_n, we have to calculate u'_{p_n}, that is, we have to solve a large linear system of equations. To compute all derivatives, one needs to solve in total $N + 1$ large systems. With the help of the adjoint state, this can be reduced to solving two systems.

6.3.6 Definition. Fix $\kappa \in \mathbb{C} \setminus \mathbb{R}$, $F_{\mathrm{s}},\ F_{\mathrm{t}} \in H^1(\mathbb{R}^2)^*$, and let $q \in L^\infty(\mathbb{R}^2, \mathbb{R})$. Denote $u_q = \mathcal{L}(q)$. We now define the adjoint state w_q by

$$b_q(w_q, \psi) = 2F_{\mathrm{t}}(u_q)\overline{F_{\mathrm{t}}(\overline{\psi})} \qquad \text{for all } \psi \in H^1(\mathbb{R}^2). \qquad \blacksquare$$

Note that due to the double conjugation, the right hand side is still conjugate linear in ψ.

6.3.7 Lemma. Let $\kappa \in \mathbb{C}\setminus\mathbb{R}$, $F_{\mathrm{s}},\ F_{\mathrm{t}} \in H^1(\mathbb{R}^2)^*$. Then we have for all $q, p \in L^\infty(\mathbb{R}^2, \mathbb{R})$

$$d\mathcal{J}(q)p = -\int_{\mathbb{R}^2} p\,\mathrm{Re}\,(u_q w_q)\ \mathrm{d}x,$$

where $u_q = \mathcal{L}(q)$ and w_q is the adjoint state at q. $\blacksquare$

Proof. Let us start by noting the following symmetry relation for b_q. We have

$$b_q(u, v) = b_q(\overline{v}, \overline{u}) \qquad \text{for } u, v \in H^1(\mathbb{R}^2).$$

Let $u_p' = d\mathcal{L}(q)p$ be the derivative of $\mathcal{L}$ in direction of p. Setting $\psi = \overline{u}_p'$ in the sesquilinear form for w_q we obtain

$$2F_{\mathrm{t}}(u_q)\overline{F_{\mathrm{t}}(u_p')} = b_q(w_q, \overline{u}_p') = b_q(u_p', \overline{w}_q) = -\int\limits_{\mathbb{R}^2} p\, u_q w_q \,\mathrm{d}x,$$

where we used the definition the sesquilinear form for u_p' (see Lemma 6.3.4) at the last step. Taking the real part yields by (6.3.3) that

$$d\mathcal{J}(q)p = -2\,\mathrm{Re}\left(F_{\mathrm{t}}(u_q)\overline{F_{\mathrm{t}}(u_p')}\right) = -\mathrm{Re}\left(\int\limits_{\mathbb{R}^2} p\, u_q w_q \,\mathrm{d}x\right),$$

finishing the proof. ■

Let us also state (without proof) the second derivative, which we later use to determine the step width in iterative optimisation schemes.

6.3.8 Lemma. Let $\kappa \in \mathbb{C} \setminus \mathbb{R}$, F_{s}, $F_{\mathrm{t}} \in H^1(\mathbb{R}^2)^*$ and $q, p_1, p_2 \in L^\infty(\mathbb{R}^2, \mathbb{R})$. Then the second Fréchet derivative $d^2\mathcal{J}(q) : L^\infty(\mathbb{R}^2,\mathbb{R}) \times L^\infty(\mathbb{R}^2,\mathbb{R}) \to \mathbb{R}$ is given by

$$d^2\mathcal{J}(q)[p_1,p_2] = 2\,\mathrm{Re}\left(F_{\mathrm{t}}(u''_{p_1,p_2})\overline{F_{\mathrm{t}}(u_q)}\right) + 2\,\mathrm{Re}\left(F_{\mathrm{t}}(u'_{p_1})\overline{F_{\mathrm{t}}(u'_{p_2})}\right),$$

where $u''_{p_1,p_2} \in H^1(\mathbb{R}^2)$ is the unique solution of

$$b_q(u''_{p_1,p_2}, \psi) = -\int\limits_{\mathbb{R}^2} p_1 u'_{p_2}\overline{\psi}\,\mathrm{d}x - \int\limits_{\mathbb{R}^2} p_2 u'_{p_1}\overline{\psi}\,\mathrm{d}x \qquad \text{for all } \psi \in H^1(\mathbb{R}^2),$$

where $u'_{p_1} = d\mathcal{L}(q)p_1$, $u'_{p_2} = d\mathcal{L}(q)p_2$. ■

Proof. We omit the proof here, but remark that not many additional arguments compared to the proof of the first derivative are necessary. ■

6.4 Energy Conservation

We now pass back to a more specific example of waveguide junctions.

6.4.1 Setting. Let us fix $\kappa \in \mathbb{C}\setminus\mathbb{R}$, and let q fulfil Definition and Assumption 5.1.2. Let Ω denote the corresponding interior domain, and let $\Omega_0, \dots, \Omega_{\boldsymbol{m}-1}$ be the overlapping exterior halfspaces. For $n \in \{0, \dots, \boldsymbol{m}-1\}$, $k \in \{1, \dots N_n\}$, we denote by $\lambda_k^{(n)}$ the kth eigenvalue of $A_n = -\Delta + q_n$, with the eigenfunction $\Psi_n^p(\lambda_k^{(n)}, \cdot)$.

6.4.2 Definition. For $n \in \{0, \dots, \boldsymbol{m}-1\}$ and $k \in \{1, \dots, N_n\}$, we define the amplitude functional $F_{n,k} \in H^1(\mathbb{R}^2)^*$ by

$$F_{n,k}(\psi) = \int\limits_{\Gamma_n} \Psi_n^p(\lambda_k^{(n)}, \cdot\,)\,\overline{\psi}\,\mathrm{d}s. \qquad ■$$

We name it amplitude functional, since it yields the amplitude of the kth guided mode in the field on the halfspace Ω_n: if one unwraps the definition of the solution operator $\mathcal{S}_n$, including the different coordinate systems, one obtains that the sum over the eigenmodes reads as follows

$$\begin{aligned}
&\mathcal{S}_n^{\text{guided}} g(\xi\,\xi^{(n)} + (\eta + h_n)\eta^{(n)}) \\
&\quad = \sum_{k=1}^{N_n} e^{i\sqrt{\kappa-\lambda_k^{(n)}}\,\eta}\,\Psi_n^p(\lambda_k^{(n)},\xi) \int\limits_{\Gamma_n} \Psi_k^p(\lambda_k^{(n)},\,\cdot\,) g\,\mathrm{d}s \\
&\quad = \sum_{k=1}^{N_n} e^{i\sqrt{\kappa-\lambda_k^{(n)}}\,\eta}\,\Psi_n^p(\lambda_k^{(n)},\xi)\overline{F_{n,k}(g)},
\end{aligned}$$

where $\eta > 0,\ \xi \in \mathbb{R}$. These functionals will come in handy later.

6.4.3 Lemma. For $n \in \{0, \dots, \boldsymbol{m} - 1\}$ and $k \in \{1, \dots, N_n\}$ let $\tilde{u}_{\mathrm{i}}$ be the incident field corresponding to the kth incident mode on Ω_n with amplitude 1 at Γ_n, that is

$$\tilde{u}_{\mathrm{i}}(\xi\,\xi^{(n)} + (\eta + h_n)\eta^{(n)}) = \left(e^{-i\sqrt{\kappa-\lambda_k^{(n)}}\ \eta} - e^{i\sqrt{\kappa-\lambda_k^{(n)}}\ \eta}\right)\Psi_n^p(\lambda_k^{(n)},\xi)$$

for $\xi \in \mathbb{R},\ \eta > 0$. Then the corresponding source functional in the sense of the weak problem 6.2.1 is given by

$$F_{n,k}^{\text{inc}}(\psi) := \int\limits_{\Gamma_n} (\partial_\nu \tilde{u}_{\mathrm{i}})\overline{\psi}\,\mathrm{d}s = 2i\sqrt{\kappa - \lambda_k^{(n)}}\,F_{n,k}(\psi). \qquad \blacksquare$$

Proof. This follows immediately by noting that that $\partial_\nu = \partial_\eta$ in the corresponding coordinate system. ■

Let us now define the functional we will optimise: the energy contained in an outgoing mode.

6.4.4 Definition. Let $n \in \{0, \dots, \boldsymbol{m} - 1\},\ k \in \{1, \dots, N_n\}$. We define the energy functional $J_{n,k} : H^1(\mathbb{R}^2) \to \mathbb{R}$ by

$$J_{n,k}(u) := \left|\sqrt{\kappa - \lambda_k^{(n)}}\right|\,|F_{n,k}(u)|^2. \qquad \blacksquare$$

It will become clearer later on, why this functional represents the energy flow. Let us now derive the corresponding adjoint state representation of the derivative.

6.4.5 Lemma. Let $\kappa \in \mathbb{C} \setminus \mathbb{R}$, $F_{\mathrm{s}} \in H^1(\mathbb{R}^2)^*$, and let $q \in L^\infty(\mathbb{R}^2, \mathbb{R})$ fulfil Assumption 5.1.2. Let $\mathcal{L} : L^\infty(\mathbb{R}^2, \mathbb{R}) \to H^1(\mathbb{R}^2)$ be the potential-to-solution operator (Definition 6.3.3). Let $n \in \{0, \dots, \boldsymbol{m} - 1\},\ k \in \{1, \dots, N_n\}$. Then we have for any $p, q \in L^\infty(\mathbb{R}^2)$

$$d(J_{n,k} \circ \mathcal{L})(q)p = -\int\limits_{\mathbb{R}^2} p\,\mathrm{Re}\,(u_q w_q)\,\mathrm{d}x,$$

where $u_q = \mathcal{L}(q)$ and $w_q \in H^1(\mathbb{R}^2)$ is the solution of

$$b_q(w_q, \psi) = -i\frac{\left|\sqrt{\kappa - \lambda_k^{(n)}}\right|}{\sqrt{\kappa - \lambda_k^{(n)}}}\,F_{n,k}(u_q)F_{n,k}^{\text{inc}}(\psi) \qquad \text{for all } \psi \in H^1(\mathbb{R}^2). \qquad \blacksquare$$

Proof. Up to a real constant of $|\kappa - \lambda_k^{(n)}|^{1/2}$, the energy functional is exactly of the same type as considered in Definition and Lemma 6.3.5: accordingly, we obtain by Lemma 6.3.7 that the adjoint state is given by

$$\begin{aligned}
b_q(w_q, \psi) &= 2\left|\sqrt{\kappa - \lambda_k^{(n)}}\right| F_{n,k}(u_q)\overline{F_{n,k}(\overline{\psi})} \\
&= 2\left|\sqrt{\kappa - \lambda_k^{(n)}}\right| F_{n,k}(u_q)\overline{\int_{\Gamma_n} \Psi_n^p(\lambda_k^{(n)}, \,\cdot\,)\, \psi \,\mathrm{d}s} \\
&= 2\frac{\left|\sqrt{\kappa - \lambda_k^{(n)}}\right|}{2i\sqrt{\kappa - \lambda_k^{(n)}}} F_{n,k}(u_q)\, 2i\sqrt{\kappa - \lambda_k^{(n)}} \int_{\Gamma_n} \Psi_n^p(\lambda_k^{(n)}, \,\cdot\,)\, \overline{\psi} \,\mathrm{d}s \\
&= -i\frac{\left|\sqrt{\kappa - \lambda_k^{(n)}}\right|}{\sqrt{\kappa - \lambda_k^{(n)}}}\, F_{n,k}(u_q) F_{n,k}^{\mathrm{inc}}(\psi),
\end{aligned}$$

where we used that $\Psi_n^p(\lambda_k^{(n)}, \,\cdot\,)$ is real-valued and the definition of $F_{n,k}^{\mathrm{inc}}$ (see Lemma 6.4.3). ■

The last lemma tells us that the adjoint state of the energy functional is nothing but a rescaled incident guided mode. This will become important later on in the optimisation section.

6.4.6 Back to the absorption free case. To justify the notion of energy functional, let us now go back to the absorption free case, that is, let now

$$\kappa_0 \in \mathbb{R}$$

be properly real. For $n \in \{0, \dots, \boldsymbol{m}-1\}$, let $u_{\mathrm{i}}^{(n)} \in H^2_{\mathrm{loc}}(\Omega_n)$ be a superposition of guided modes, that is, there exists coefficients $\alpha_k^{(n)} \in \mathbb{C}$ for $n \in \{0, \dots, \boldsymbol{m}-1\},\ k \in \{1, \dots, N_n\}$, such that on Ω_n we have

$$u_{\mathrm{i}}^{(n)}(\xi\, \xi^{(n)} + (\eta + h_n)\eta^{(n)}) = \sum_{k=1}^{N_n} \alpha_k^{(n)} e^{-i\sqrt{\kappa_0 - \lambda_l^{(n)}}\,\eta} \psi_n^p(\lambda_p^{(n)}, \xi).$$

For this particular incident field let us now consider the solution of

$$\begin{cases} \Delta u + (\kappa_0 - q)u = 0 & \text{in } \mathbb{R}^2, \\ \qquad\quad u - u_{\mathrm{i}}^{(n)} & \text{OPRC in } \Omega_n,\ n \in \{0, \dots, \boldsymbol{m}-1\}, \end{cases} \tag{6.4.1}$$

which has to be understood in the sense of Section 5.3. Our goal is to formally derive an energy conservation property for this solution.

6.4.7 The energy flow. Take a solution u of (6.4.1). By multiplying the Helmholtz equation by $\overline{u}$, integrating over some bounded domain $D \subset \mathbb{R}^2$ and applying integration by parts we obtain

$$0 = \underbrace{\mathrm{Im} \int_D |\nabla u|^2 - (\kappa - q)|u|^2 \,\mathrm{d}x}_{=0} - \int_{\partial D} \mathrm{Im}[(\partial_\nu u)\overline{u}] \,\mathrm{d}s,$$

that is, we have obtained the energy conservation relation

$$0 = \int\limits_{\partial D} \operatorname{Im}[(\partial_\nu u)\overline{u}]\,\mathrm{d}s. \tag{6.4.2}$$

We interpret this equation as the conservation of the energy-flow, which is defined as the real valued vector field

$$\operatorname{Im}[(\nabla u)\overline{u}],$$

so that the boundary integral over ∂D gives the energy flow through the closed surface ∂D.

6.4.8 The energy flow of a halfspace. We now aim to calculate the energy-flow of our solution u across the boundary of some halfspace. Hence, let us fix again $n \in \{0, \dots, m-1\}$. To simplify the calculation, we will transform into the coordinate system of Ω_n. Let us denote

$$\begin{aligned} \hat{u}(x) &:= u(x_1\xi^{(n)} + (x_2 + h_n)\eta^{(n)}) \qquad \text{for all } x \in \mathbb{R}^2_+, \\ \hat{u}_\mathrm{i}(x) &:= u_\mathrm{i}^{(n)}(x_1\xi^{(n)} + (x_2 + h_n)\eta^{(n)}) \qquad \text{for all } x \in \mathbb{R}^2_+. \end{aligned}$$

Let us furthermore denote the traces

$$g_\mathrm{i}(x_1) := \hat{u}_\mathrm{i}^{(n)}(x_1, 0), \qquad g_\mathrm{s}(x_1) := \hat{u}(x_1, 0) - \hat{u}_\mathrm{i}(x_1, 0), \qquad \text{for } x_1 \in \mathbb{R}.$$

By definition, we have for $x \in \mathbb{R}^2_+$

$$\hat{u}(x) = \mathcal{S}_n g_s(x) + \hat{u}_\mathrm{i}(x) = \mathcal{F}_A^{-1}\left[e^{i\sqrt{\kappa_0 - \lambda(\,\cdot\,)}\,x_2}\mathcal{F}_A g_\mathrm{s}\right](x_1) + u_\mathrm{i}(x),$$

and note furthermore that similarly

$$\hat{u}_\mathrm{i}(x) = \mathcal{F}_A^{-1}\left[e^{-i\sqrt{\kappa_0 - \lambda(\,\cdot\,)}\,x_2}\mathcal{F}_A g_\mathrm{i}\right](x_1).$$

We can now calculate with the help of Parseval's equality (see Theorem 2.2.12)

$$\begin{aligned} \operatorname{Im}\int\limits_{\Gamma_n} (\partial_\nu u)\overline{u}\,\mathrm{d}s &= \operatorname{Im}\int\limits_{\mathbb{R}} (\partial_{x_2}\hat{u})(x_1)\overline{u}(x_1)\,\mathrm{d}x_1 \\ &= \operatorname{Im}\int\limits_{\mathbb{R}} \mathcal{F}_A^{-1}\left[i\sqrt{\kappa_0 - \hat{\lambda}(\,\cdot\,)}\mathcal{F}_A g_\mathrm{s} - i\sqrt{\kappa_0 - \hat{\lambda}(\,\cdot\,)}\mathcal{F}_A g_\mathrm{i}\right](\overline{g}_\mathrm{s} + \overline{g}_\mathrm{i})\,\mathrm{d}x \\ &= \operatorname{Im}\int\limits_{\Lambda} i\sqrt{\kappa_0 - \hat{\lambda}(\,\cdot\,)}\,(\mathcal{F}_A g_\mathrm{s} - \mathcal{F}_A g_\mathrm{i})\left(\overline{\mathcal{F}_A g_\mathrm{s}} + \overline{\mathcal{F}_A g_\mathrm{i}}\right)\mathrm{d}\mu \\ &= \int\limits_{\Lambda} \operatorname{Re}\left(\sqrt{\kappa_0 - \hat{\lambda}(\,\cdot\,)}\right)|F_A g_\mathrm{s}|^2\,\mathrm{d}\mu - \int\limits_{\Lambda} \operatorname{Re}\left(\sqrt{\kappa_0 - \hat{\lambda}(\,\cdot\,)}\right)|F_A g_\mathrm{i}|^2\,\mathrm{d}\mu. \end{aligned}$$

Let us now assume that $\kappa_0 > q_-$, so that $\sqrt{\kappa_0 - \lambda_k^{(n)}} \in \mathbb{R}$ for all $k \in \{1, \dots, N_n\}$. One now easily obtains that

$$\int\limits_{\Lambda} \operatorname{Re}\left(\sqrt{\kappa_0 - \hat{\lambda}(\,\cdot\,)}\right)|F_A g_\mathrm{i}|^2\,\mathrm{d}\mu = \sum_{k=1}^{N_s} \sqrt{\kappa_0 - \lambda_k^{(n)}}\,|\alpha_k^{(n)}|^2.$$

Furthermore, by definition of $\mathcal{F}_A$ we have

$$\beta_k^{(n)} := (\mathcal{F}_A g_\mathrm{s})^p(\lambda_k^{(p)}) = \int_{\mathbb{R}} \Psi_n^p(\lambda_k^{(n)}, x_1) g_\mathrm{s}(x_1)\,\mathrm{d}x_1.$$

Note that we defined $\beta_k^{(n)}$ here. This in turn implies that

$$\begin{aligned}
&\int_\Lambda \mathrm{Re}\left(\sqrt{\kappa_0 - \lambda(\,\cdot\,)}\right) |F_A g_\mathrm{s}|^2 \,\mathrm{d}\mu \\
&= \sum_{k=1}^{N_n} \sqrt{\kappa_0 - \lambda_k^{(n)}}\, |\beta_k^{(n)}|^2 + \sum_{\sigma\in\{\pm\}} \int_{q_\sigma}^{\kappa_0} \sqrt{\kappa - \lambda} |(F_A g_\mathrm{s})^\sigma(\lambda)|^2 \frac{\mathrm{d}\lambda}{2\sqrt{\lambda - q_\sigma}} \\
&= \sum_{k=1}^{N_n} \sqrt{\kappa_0 - \lambda_k^{(n)}}\, |\beta_k^{(n)}|^2 + E_\mathrm{free}(u_\mathrm{s}),
\end{aligned}$$

where we defined the scattered energy $E_\mathrm{free}(u_\mathrm{s})$ in the last equation. Now, let us note the meaning of the energy functional $J_{n,k}(u)$: we have

$$\begin{aligned}
J_{n,k}(u - u_\mathrm{i}) &= \sqrt{\kappa_0 - \lambda_k^{(n)}} \left| \int_{\Gamma_n} \Psi_n^p(\hat{\lambda}_k^{(n)}, \,\cdot\,)\overline{(u - u_\mathrm{i})}\,\mathrm{d}s \right|^2 \\
&= \sqrt{\kappa_0 - \lambda_k^{(n)}}\, |\beta_k^{(n)}|^2,
\end{aligned}$$

so that $J_{n,k}(u - u_\mathrm{i}^{(n)})$ yields the energy contained in the kth outgoing mode of the waveguide in Ω_n. Similarly, we can also deduce that

$$J_{n,k}(u_\mathrm{i}^{(n)}) = \sqrt{\kappa_0 - \lambda_k^{(n)}}\, |\alpha_k^{(n)}|^2$$

To sum up, we have obtained the following expression for the energy flow

$$\begin{aligned}
\int_{\Gamma_n} \mathrm{Im}[(\partial_\nu u)\overline{u}]\,\mathrm{d}s = &-\left(\sum_{k=1}^{N_n} J_{n,k}(u_\mathrm{i}^{(n)})\right) \\
&+ \left(\sum_{k=1}^{N_n} J_{n,k}(u - u_\mathrm{i}^{(n)}) + E_\mathrm{free}(u - u_\mathrm{i}^{(n)})\right).
\end{aligned} \tag{6.4.3}$$

6.4.9 Energy conservation for the halfspace flows. Let us, again in a rather hand-waving fashion, derive an energy conservation equality. First note that carefully checking the calculation of the last section, we see that the energy flow of a halfspace does not change if we take a surface parallel to Γ_n, that is

$$\int_{\Gamma_n} \mathrm{Im}[(\partial_\nu u)\overline{u}]\,\mathrm{d}s = \int_{\Gamma_n^R} \mathrm{Im}[(\partial_\nu u)\overline{u}]\,\mathrm{d}s,$$

where $\Gamma_n^R := \{\xi\,\xi^{(n)} + (h_n + R)\,\eta^{(n)} : \xi \in \mathbb{R}\}$. This now motivates the following discussion. Assume that $0 \in \Omega$. Denote the stretched version of Ω by

$$\Omega_R = (1 + R)\Omega = \{(1 + R)x : x \in \Omega\}.$$

We get by the energy conservation relation (6.4.2) that

$$0 = \int_{\partial\Omega_R} \operatorname{Im}[(\partial_\nu u)\overline{u}] \, \mathrm{d}s = \sum_{n=0}^{\boldsymbol{m}-1} \int_{\Gamma_n^{(1+R)h_n} \cap \partial\Omega_R} \operatorname{Im}[(\partial_\nu u)\overline{u}] \, \mathrm{d}s$$
$$\longrightarrow \sum_{n=0}^{\boldsymbol{m}-1} \int_{\Gamma_n} \operatorname{Im}[(\partial_\nu u)\overline{u}] \, \mathrm{d}s \qquad \text{as } R \to \infty.$$

Applying now (6.4.3) to rewrite the expression after the limit, we obtain that

$$\sum_{n=1}^{\boldsymbol{m}-1} \sum_{k=1}^{N_n} J_{n,k}(u_{\mathrm{i}}^{(n)}) = \sum_{n=1}^{\boldsymbol{m}-1} \left(E_{\mathrm{free}}(u - u_{\mathrm{i}}^{(n)}) + \sum_{k=1}^{N_n} J_{n,k}(u - u_{\mathrm{i}}^{(n)}) \right). \tag{6.4.4}$$

6.5 Optimisation

6.5.1 The generic setting. Let $\kappa_0 \in \mathbb{R}$, and let $q_{\mathrm{e}} \in L^\infty(\mathbb{R}^2 \setminus \overline{\Omega})$ fulfil Definition and Assumption 5.1.2. In the following, we will consider a few optimisation examples of the following type: let $U_{\mathrm{i}} = (u_{\mathrm{i}}^{(0)}, \dots, u_{\mathrm{i}}^{(\boldsymbol{m}-1)})$ be some incident field consisting of guided modes. Let furthermore

$$J(u) := J_{n_t,k_t}(u)$$

be the energy contained in the k_tth outgoing mode in Ω_{n_t}. Let $q_{\min} < q_{\max}$ be two fixed constants. We define the design space of admissible potentials by

$$\mathcal{D} := \{q \in L^\infty(\Omega, \mathbb{R}) : q_{\min} \le q(x) \le q_{\max} \text{ for almost all } x \in \Omega\}.$$

Now consider the following optimisation problem

$$\left| \begin{array}{l} \text{Maximise } J(u_q) \text{ for } q \in \mathcal{D}, \text{ where } u_q \text{ solves} \\ \begin{cases} \Delta u_q + (\kappa_0 - q) u_q = 0 & \text{in } \mathbb{R}^2, \\ \qquad\qquad u_q - u_{\mathrm{i}}^{(n)} & \text{OPRC in } \Omega_n, \ n \in \{0, \dots, \boldsymbol{m}-1\}, \end{cases} \\ \text{where } q \text{ is extended by } q_{\mathrm{e}} \text{ outside of } \Omega. \end{array} \right.$$

We interpret this problem as follows: given an exterior potential q_{e} as well as an incident field, we try to construct a structure contained in Ω, which allows us to transmit the incident energy into the k_tth outgoing mode of the waveguide in Ω_n.

Recall that we defined $\mathcal{J} : L^\infty(\Omega, \mathbb{R}) \to \mathbb{R}$ by

$$\mathcal{J}(q) := J(u_q).$$

6.5.2 An iterative optimisation algorithm. To solve this problem numerically, let us give a rough iterative algorithm yielding such structures. Start by choosing two tuning parameters, the maximal step size $h_{\max} > 0$ and a regularisation parameter $\alpha \in (0, 1]$. Begin with some starting guess $q_1 \in \mathcal{D}$, and construct the next iteration by the following algorithm in the lth iteration, $l \in \mathbb{N}$.

(a) Compute the forward solution $u_l = u_{q_l}$.

(b) Compute the adjoint state w_l as the solution to

$$\begin{cases} \Delta w_l + (k_0 - q_l) w_l = 0 & \text{in } \mathbb{R}^2, \\ w_l - w_{\mathrm{i}}^{(n)} & \text{OPRC in } \Omega_n,\ n \in \{0, \dots, \boldsymbol{m} - 1\}, \end{cases}$$

where the incident field is given on Ω_{n_t} by

$$w_{\mathrm{i}}^{(n_t)}(\xi \xi^{(n)} + (\eta + h_n)\eta^{(n)}) = -i F_{n_t,k_t}(u_l) e^{-i\sqrt{k_0 - \lambda_{k_t}^{(n_t)}}\,\eta} \Psi_{n_t}^{p}(\lambda_{k_t}^{(n_t)} \xi),$$

for $\xi \in \mathbb{R},\ \eta > 0$, and by $w_{\mathrm{i}}^{(n)} = 0$ on the other halfspaces $\Omega_n,\ n \neq n_t$.

(c) Define the gradient $g_l \in L^\infty(\Omega, \mathbb{R})$ by

$$g_l(x) := -\mathrm{Re}(u_l(x) w_l(x)) \qquad \text{for } x \in \Omega.$$

Note that the gradient is the L^2-gradient of $d\mathcal{J}(q_l) : L^\infty(\mathbb{R}^2, \mathbb{R}) \to \mathbb{R}$, that is, the unique element $q_l \in L^2(\Omega)$ such that

$$\int_\Omega g_l p \,\mathrm{d}x = d\mathcal{J}(q_l) p = \int_\Omega -\mathrm{Re}(u_l w_l) p \,\mathrm{d}x \qquad \text{for all } p \in L^2(\Omega),$$

where we used Lemma 6.4.5 to obtain the representation of the derivative. To be able to use this representation, we invoke again the limit-absorption principle of Conjecture 6.2.2.

(d) Based on the already computed gradients $g_0, \dots, g_l$, choose some preliminary ascent direction $\tilde{d}_l \in L^\infty(\Omega, \mathbb{R})$. We will use a non-linear conjugate gradient method with the Polak-Ribière update formula [29].

(e) Project the descent direction, so that it points into $\mathcal{D}$: that is, define

$$d_l(x) := \begin{cases} 0 & \text{if } q_l(x) = q_{\max} \text{ and } d_l(x) > 0, \\ 0 & \text{if } q_l(x) = q_{\min} \text{ and } d_l(x) < 0, \\ \tilde{d}_l(x) & \text{else.} \end{cases}$$

(f) To calculate a step size h_l, we use utilise the second derivative, so we calculate the first material derivative u_l' in direction d_l, which is the solution of

$$\begin{cases} \Delta u_l' + (\kappa_0 - q_l) u_l' = -d_l u_l & \text{in } \mathbb{R}^2, \\ u_l' & \text{OPRC in } \Omega_n,\ n \in \{0, \dots, \boldsymbol{m} - 1\}, \end{cases}$$

as well as the second derivative u_l'' in direction d_l, which solves

$$\begin{cases} \Delta u_l'' + (\kappa_0 - q_l) u_l'' = -2 d_l u_l' & \text{in } \mathbb{R}^2, \\ u_l'' & \text{OPRC in } \Omega_n,\ n \in \{0, \dots, \boldsymbol{m} - 1\}, \end{cases}$$

Now the first and second derivative of $\mathcal{J}$ in direction d_l are given by

$$\begin{aligned} \delta_1 &:= d\mathcal{J}(q_l) d_l = \sqrt{\kappa_0 - \lambda_{k_t}^{(n_t)}}\, 2\,\mathrm{Re}\left(F_{n_t,k_t}(u_l) \overline{F_{n_t,k_t}(u_l')}\right) \\ \delta_2 &:= d^2\mathcal{J}(q_l)[d_l, d_l] = \sqrt{\kappa_0 - \lambda_{k_t}^{(n_t)}} \Bigg(2\,\mathrm{Re}\left(F_{n_t,k_t}(u_l'') \overline{F_{n_t,k_t}(u_l)}\right) \\ &\qquad\qquad + 2\,\mathrm{Re}\left(F_{n_t,k_t}(u_l') \overline{F_{n_t,k_t}(u_l')}\right) \Bigg), \end{aligned}$$

where we employed Lemmata 6.3.4, 6.3.8 and Definition and Lemma 6.3.5. We also used the limit-absorption principle of Conjecture 6.2.2 again. Now we choose the step size as follows

$$h_l = \begin{cases} \min\left\{h_{\max}\|d_l\|^{-1}_{L^\infty(\Omega)}, -\alpha\frac{\delta_1}{\delta_2}\right\} & \text{if } \delta_2 < 0, \\ h_{\max}\|d_l\|^{-1}_{L^\infty(\Omega)} & \text{else.} \end{cases}$$

Let us quickly explain the purpose of this step size: if $\mathcal{J}$ is negatively curved along the direction d_l, that is, if $\delta_2 < 0$, we have a maximum and choose the step size to step onto this maximum (of the second order Taylor expansion). The parameter α serves as a security value to avoid overstepping.

On the other hand, if $\delta_2 > 0$, we choose the pre-defined maximal step distance $h_{\max}$.

(g) Calculate the preliminary update by

$$\tilde{q}_{l+1} = q_l + h_l d_l,$$

and project back into the set of admissible designs $\mathcal{D}$, that is define

$$q_{l+1}(x) = \begin{cases} q_{\max} & \text{if } \tilde{q}_l(x) > q_{\max}, \\ q_{\min} & \text{if } \tilde{q}_l(x) < q_{\min}, \\ \tilde{q}_{l+1}(x) & \text{else.} \end{cases}$$

With the new iterate q_{l+1}, restart the process at step (a).

6.6 Examples

In this section, we will consider different examples of waveguide scattering problems and study equations of the form

$$\Delta u(x) + p(x)u(x) = 0 \qquad \text{for } x \in \mathbb{R}^2, \tag{6.6.1}$$

with real-valued $p : \mathbb{R}^2 \to \mathbb{R}$. From p, one easily finds suitable q and $\kappa_0 \in \mathbb{R}$ to get back to our conventional setting by setting $\kappa_0 = 0$ and $q = -p$. The situations we consider are motivated from design problems surrounding optical waveguides, which have been studied in the physical literature to a large extend. For more information, we refer to [31, 33, 32, 69].

6.6.1 A bend of a waveguide. Let us start with the first example of a bent waveguide, which turns by 90 degrees, with a first mode incident from one side to the bend. An example solution is shown in Figure 6.1 together with the basic geometry of the computational domain: note that the waveguide bend forms a quarter circle, with an inner radius r_i and an outer radius r_o. Since the waveguide has a width of h, we have that $r_o = r_i + h$.

For many applications it is of relevance to construct bends with minimal loss. The first, somewhat intuitive idea is to increase the radius of curvature. How does the transmission of energy change for bends of different radius? Figure 6.2 shows the dependence of the transmission on the radius of curvature. The transmission is defined by

$$\tau := \frac{J_{1,1}(u - u_{\mathrm{i}})}{J_{0,1}(u_{\mathrm{i}})},$$

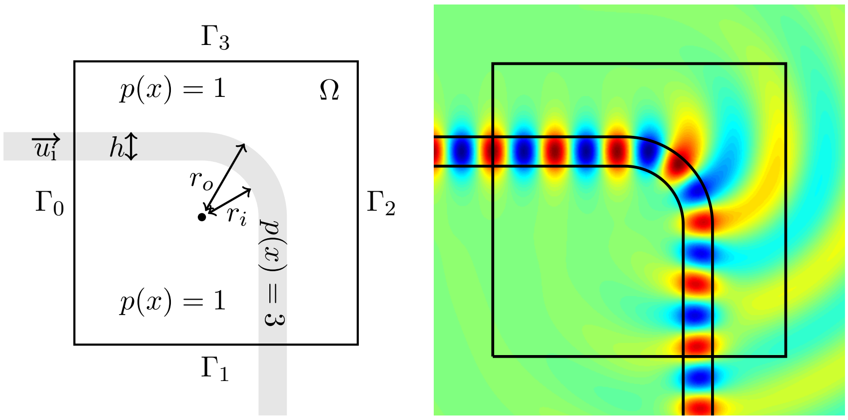

Figure 6.1: Sketch of the geometrical situation for the bent waveguide (left) and the real part of the solution for a bend radius of $r_0 = 6$ (right).

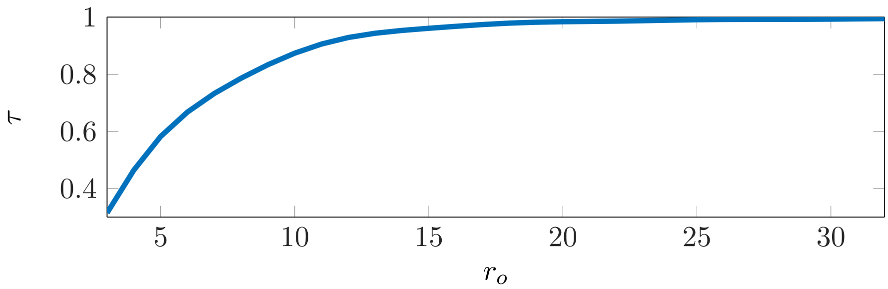

Figure 6.2: Transmission of energy for different radii of curvature.

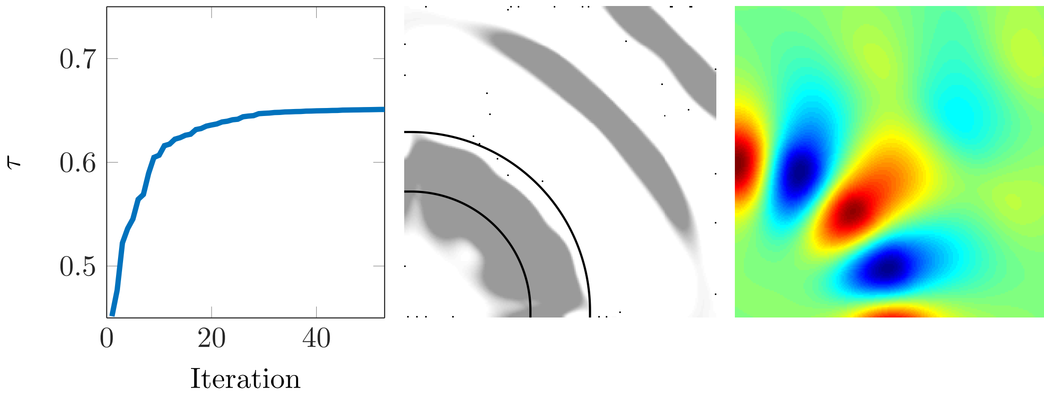

Figure 6.3: Optimisation of a waveguide bend. On the left, the transmission as a function of the number of iterations is shown. The middle shows the structure after the optimisation. Dark grey corresponds to to $p(x) = 3$, while white corresponds to $p(x) = 1$. On the right the real part of the solution after optimisation is shown. Note that the transmission was increased from 45.1% to 65.1% without increasing the effective curvature of the waveguide. The initial curvature corresponds to $r_o = 6$, which is the same as in Figure 6.1.

that is, as the energy contained in the first mode in Ω_1 of the scattered field, divided by the energy contained in the first mode of the incident field on Ω_0, which is the only part of the incident field. From (6.4.4), we obtain that

$$J_{0,1}(u_{\mathrm{i}}^{(n)}) = \sum_{n=1}^{\boldsymbol{m}-1} \left(E_{\mathrm{free}}(u - u_{\mathrm{i}}^{(n)}) + \sum_{k=1}^{N_n} J_{n,k}(u - u_{\mathrm{i}}^{(n)}) \right) \geq J_{1,1}(u - u_{\mathrm{i}}^{(n)}),$$

which in turn implies

$$\tau \leq 1,$$

which is why we consider $\tau = 1$ a *perfectly lossless* transmission.

We have now applied the optimisation algorithm from subsection 6.5.2 to this problem, to find a structure which allows a waveguide bend with low losses, without effectively increasing the "curvature" of the bend (in the sense that input and output waveguide stay at the same place). A reasonable increase of transmission from 45% to 65% was obtained (see Figure 6.3).

6.6.2 A mode splitter. As a second example, we want to construct a junction, which splits a single mode into two. For this aim, let again u_{i} denote the first incident mode in the top waveguide in Ω_0, as sketched in Figure 6.4. We demand again that $J_{0,1}(u_{\mathrm{i}}) = 1$.

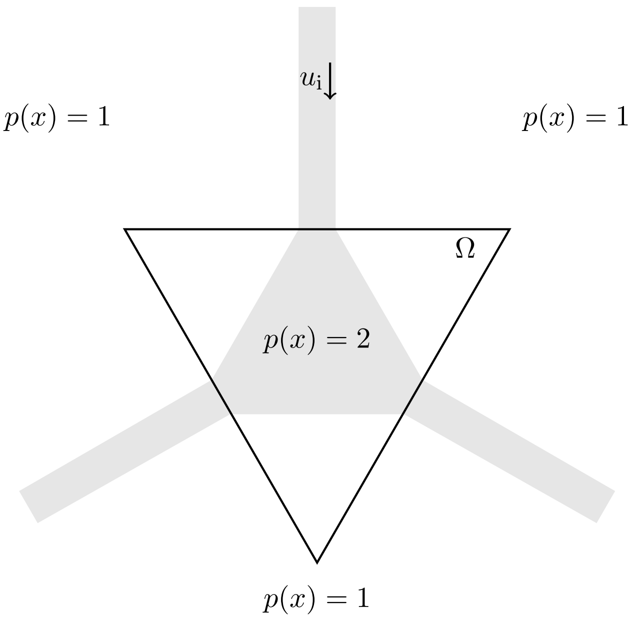

Figure 6.4: Sketch of the waveguide splitter.

Note that we used a triangular interior domain. Our goal is now to construct a junction, which evenly splits the mode in the top waveguide into the two bottom waveguides. We model this with help of the following optimisation problem:

> Find some $p \in \{\tilde{p} \in L^\infty(\mathbb{R}^2, \mathbb{R}) : 1 \leq \tilde{p}(x) \leq 2 \text{ for all } x \in \Omega\}$ such that the functional
>
> $$J(u) = J_{1,1}(u - u_{\mathrm{i}}) J_{2,1}(u - u_{\mathrm{i}})$$
>
> gets maximal. Here u is the outgoing solutions to (6.6.1) with incident fields u_{i}.

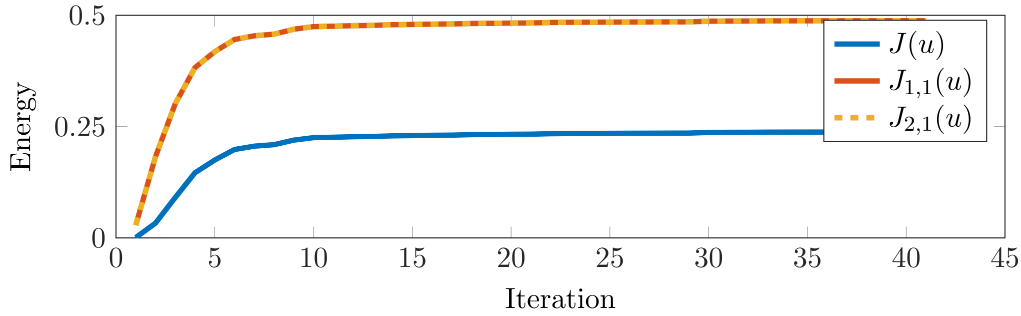

Figure 6.5: Evolution of the FOM during the optimisation. Note that we reach almost 50% transmission for each of the two waveguides.

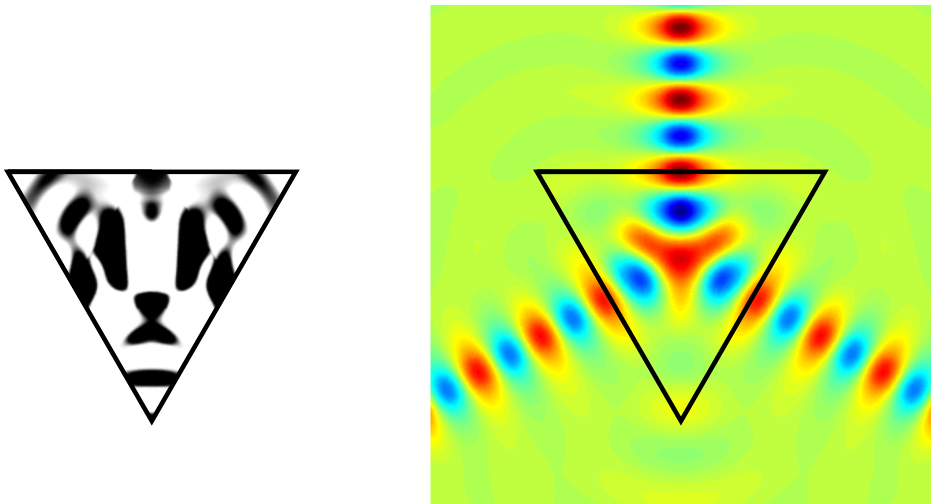

Figure 6.6: Resulting structure and real part of the solution after the optimisation.

Note that we chose the product of the two energies as the figure of merit. By the energy conservation relation we have

$$1 = J_{0,1}(u_{\mathrm{i}}) \geq J_{1,1}(u - u_{\mathrm{i}}) + J_{2,1}(u - u_{\mathrm{i}}).$$

Assuming that no energy is lost due to some scattered part, that is, if equality holds in the last inequality, i.e. if

$$J_{1,1}(u - u_{\mathrm{i}}) + J_{2,1}(\tilde{u} - \tilde{u}_{\mathrm{i}}) = 1,$$

one easily sees that J gets maximal if and only if

$$J_{1,1}(u - u_{\mathrm{i}}) = J_{2,1}(\tilde{u} - \tilde{u}_{\mathrm{i}}),$$

that is, if the energy is evenly distributed between the two lower waveguides. In this case, half the energy would be transmitted into each of the waveguides, and we would obtain

$$J(u) = \frac{1}{2}\frac{1}{2} = \frac{1}{4}.$$

So that our choice J ensures that a optimal solution will both ensure a low scattering loss of energy, while evenly balancing out the energy between the two output waveguides. We note that this optimisation problem does not fall in the scheme we studied in the previous section. A straightforward, but somewhat technical discussion, which we omit for brevity, yields that the adjoint state of 6.5.2(b) can be computed as the solution of

$$\begin{cases} \Delta w_l + (k_0 - q_l) w_l = 0 & \text{in } \mathbb{R}^2, \\ \qquad\qquad w_l - w_{\mathrm{i}}^{(n)} & \text{OPRC in } \Omega_n,\ n \in \{0, \dots, \boldsymbol{m}-1\}, \end{cases}$$

where the incident field is given (in a slightly sloppy notation) by

$$w_{\mathrm{i}}(x) = \begin{cases} 0 & \text{on } \Omega_0, \\ -iJ_{2,1}(u_l) F_{1,1}(u_l) e^{-i\sqrt{k_0 - \lambda_1^{(1)}}\,\eta} \Psi_1^p(\lambda_1^{(1)}\xi) & \text{on } \Omega_1, \\ -iJ_{1,1}(u_l) F_{2,1}(u_l) e^{-i\sqrt{k_0 - \lambda_1^{(2)}}\,\eta} \Psi_2^p(\lambda_1^{(2)}\xi) & \text{on } \Omega_2. \end{cases}$$

for $\xi \in \mathbb{R},\ \eta > 0$. Similarly, δ_1 and δ_2 in 6.5.2(f) have to be replaced by slightly bulky expressions

$$\begin{aligned} \delta_1 = & \sqrt{\kappa_0 - \lambda_1^{(2)}} \sqrt{\kappa_0 - \lambda_1^{(1)}} \\ & \cdot \Big(2\operatorname{Re}\big(F_{1,1}(u_l)\overline{F_{1,1}(u_l')}\big) |F_{1,1}(u_l)|^2 \\ & \quad + 2\operatorname{Re}\big(F_{2,1}(u_l) F_{2,1}(u_l')\big) |F_{2,1}(u_l)|^2 \Big), \\ \delta_2 = & \sqrt{\kappa_0 - \lambda_1^{(2)}} \sqrt{\kappa_0 - \lambda_1^{(1)}} \\ & \cdot \Big(2\operatorname{Re}\big(F_{1,1}(u_l)\overline{F_{1,1}(u_l'')}\big) |F_{2,1}(u_l)|^2 \\ & \quad + 2\operatorname{Re}\big(F_{2,1}(u_l)\overline{F_{2,1}(u_l'')}\big) |F_{1,1}(u_l)|^2 \\ & \quad + 2\,|F_{1,1}(u_l')|^2 |F_{2,1}(u_l)|^2 + 2\,|F_{2,1}(u_l')|^2 |F_{1,1}(u_l)|^2 \\ & \quad + 8\operatorname{Re}\big(F_{1,1}(u_l)\overline{F_{1,1}(u_l')}\big) \operatorname{Re}\big(F_{2,1}(u_l)\overline{F_{2,1}(u_l')}\big) \Big). \end{aligned}$$

With those modifications, we can now optimise the waveguide splitter to obtain a better splitting. The results can be seen in Figures 6.5 and 6.6.

6.6.3 A mode flipper. For the next example, we aim to construct a waveguide which optimises two scattering problems at the same time. Consider a straight waveguide, as shown in Figure 6.7. This waveguide has two guided modes, and we can sent in both as incident fields on Ω_0. Let u_{i} be the first incident mode, and let $\tilde{u}_{\mathrm{i}}$ be the second, which are normalised so that

$$J_{0,1}(u_{\mathrm{i}}) = 1 \quad \text{and} \quad J_{0,2}(\tilde{u}_{\mathrm{i}}) = 1,$$

that is, they both contain the same energy. In the sketched configuration, both modes will simply propagate through the domain without changing their shape.

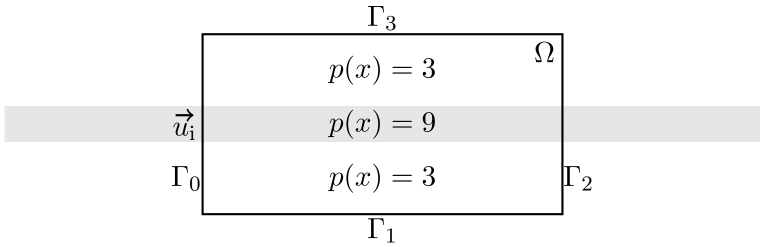

Figure 6.7: Geometry of the mode flipping problem: the modes are incident in the straight waveguide from the left, and we try to manipulate the output on the right.

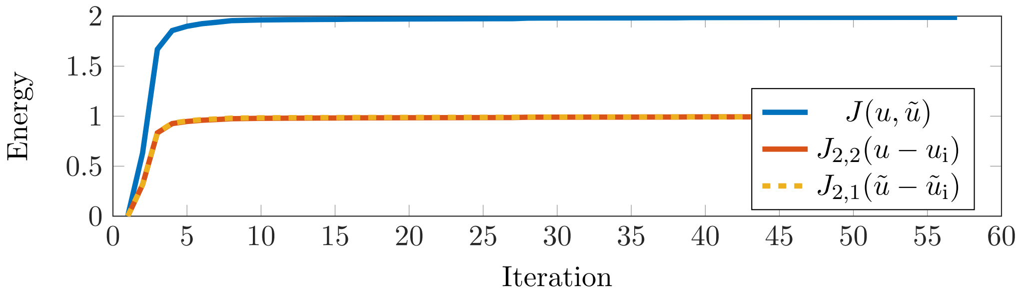

Figure 6.8: Evolution of the figure of merit for the waveguide flipping during the optimisation. Note that we get a total figure of merit of up to 1.988, which is rather close to the optimal value of 2.

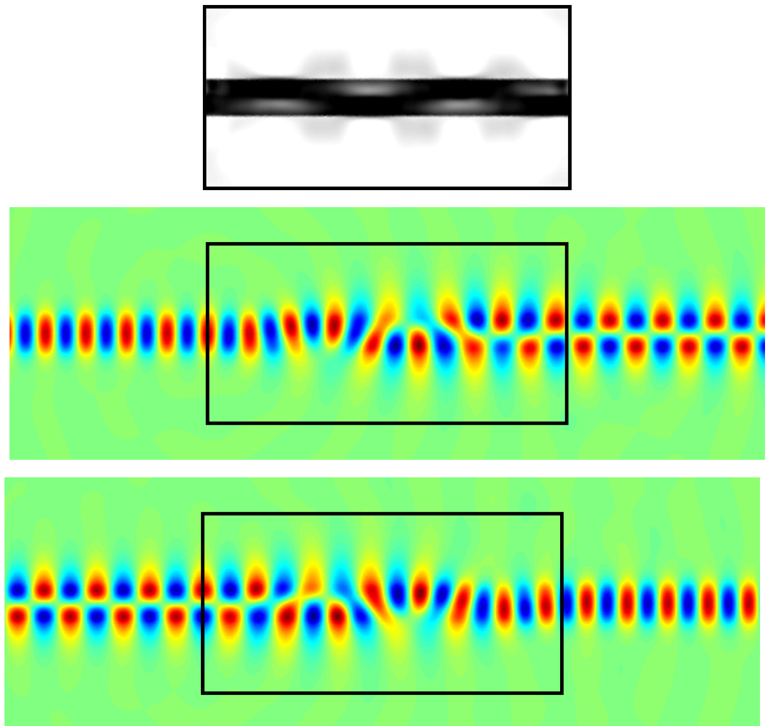

Figure 6.9: Optimised material configuration (top) and corresponding real part of the total field u (middle) and $\tilde{u}$ (bottom). Note that all figures are almost point symmetrical to the origin.

We can now ask the following question: can we perturb the waveguide in such way that the modes are *flipped* at the end of the finite element domain Ω? That is, so that u_i produces a second outgoing mode on the right, while $\tilde{u}_\mathrm{i}$ produces a first outgoing mode? We can reformulate this problem in the following (simultaneous) optimisation problem:

> Find some $p \in \{\tilde{p} \in L^\infty(\Omega, \mathbb{R}) : 3 \leq \tilde{p}(x) \leq 9 \text{ for all } x \in \Omega\}$ such that the functional
> $$J(u, \tilde{u}) = J_{2,2}(u - u_\mathrm{i}) + J_{2,1}(\tilde{u} - \tilde{u}_\mathrm{i})$$
> gets maximal. Here u and $\tilde{u}$ are the outgoing solutions to (6.6.1) with incident fields u_i and $\tilde{u}_\mathrm{i}$.

In other words: we aim to maximise the sum of two energies: the energy produced by the first incident mode in the second outgoing mode, and the energy produced by the second incident mode in the first outgoing mode. Note that we obtain that by (6.4.4)

$$J(u, \tilde{u}) = J_{2,2}(u - u_\mathrm{i}) + J_{2,1}(\tilde{u} - \tilde{u}_\mathrm{i}) \leq J_{0,1}(u_\mathrm{i}) + J_{0,2}(\tilde{u}_\mathrm{i}) = 2,$$

so that we can consider $J(u, \tilde{u}) = 2$ as a perfect flipping of the modes. Note that in Figures 6.8 and 6.9, we almost achieve this perfect flipping (we obtain $J(u, \tilde{u}) = 1.988$). This is a somewhat simpler version of a mode converter (see [49, 44]).

6.6.4 A mode multiplexer. The last example we want to study is a *mode multiplexer*: assume we have a junction of three waveguides as shown in Figure 6.10. Note the width of the waveguides: the two *output waveguides* on the right and top have a smaller width, while the input waveguide in Ω_0 has a larger width. This causes it to have two guided modes, while the output waveguides each have one guided mode. Note that we put this arrangement of waveguides on top of a substrate, whose material parameter $p_\mathrm{subs} = 6$ is between the free space $p_\mathrm{free} = 3$ and the waveguide $p_\mathrm{wg} = 9$. We now aim to construct

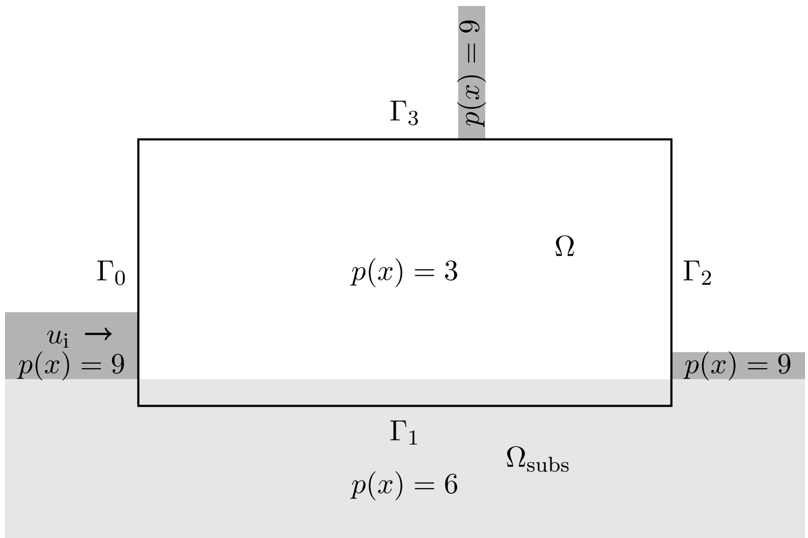

Figure 6.10: Sketch of the geometry of the waveguide multiplexer.

a junction which transmits the first mode incident in the left waveguide into the right hand waveguide, while the second incident mode is transmitted into the top waveguide. Let again u_i be the first incident mode on Ω_0, and let $\tilde{u}_\mathrm{i}$ be the second mode on Ω_0,

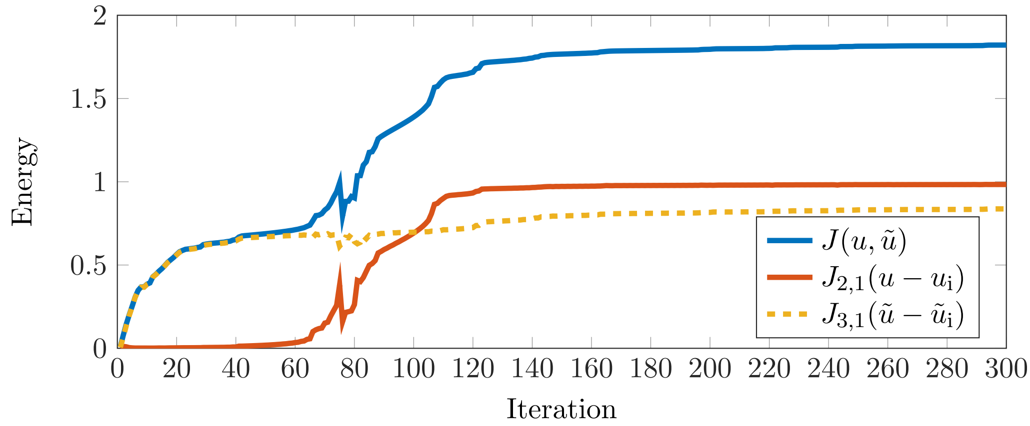

Figure 6.11: Evolution of the figure of merit for the waveguide multiplexer. Note that around iteration 75, the algorithm oversteps and actually reduces the figure of merit. Note that at the final shape, around 2% of the energy in the first mode is not transmitted to right. The second mode has a higher loss of around 16%.

which are normalised so that

$$J_{0,1}(u_{\mathrm{i}}) = 1 \quad \text{and} \quad J_{0,2}(\tilde{u}_{\mathrm{i}}) = 1.$$

To add an additional restriction, we consider the substrate as fixed, that is, we cannot change the coefficient p on the domain Ω_{subs}, which is the light grey area in Figure 6.10. Let us now reformulate the multiplexer problem as the following optimisation problem:

> Find some $p \in \{\tilde{p} \in L^\infty(\Omega,\mathbb{R}) : 3 \leq \tilde{p}(x) \leq 9$ for all $x \in \Omega,\ q(x) = 6$ for $x \in \Omega_{\mathrm{subs}}\}$ such that the functional
>
> $$J(u,\tilde{u}) = J_{2,1}(u-u_{\mathrm{i}}) + J_{3,1}(\tilde{u}-\tilde{u}_{\mathrm{i}})$$
>
> gets maximal. Here u and $\tilde{u}$ are the outgoing solutions to (6.6.1) with incident fields u_{i} and $\tilde{u}_{\mathrm{i}}$.

This problem has been considered recently in the context of nanophotonics, see for example [69, 32]. Conventional mode multiplexers require relatively much space, and do not allow the integration in a small, compact device, so it seems a rather interesting prospect to integrate them on a smaller scale.

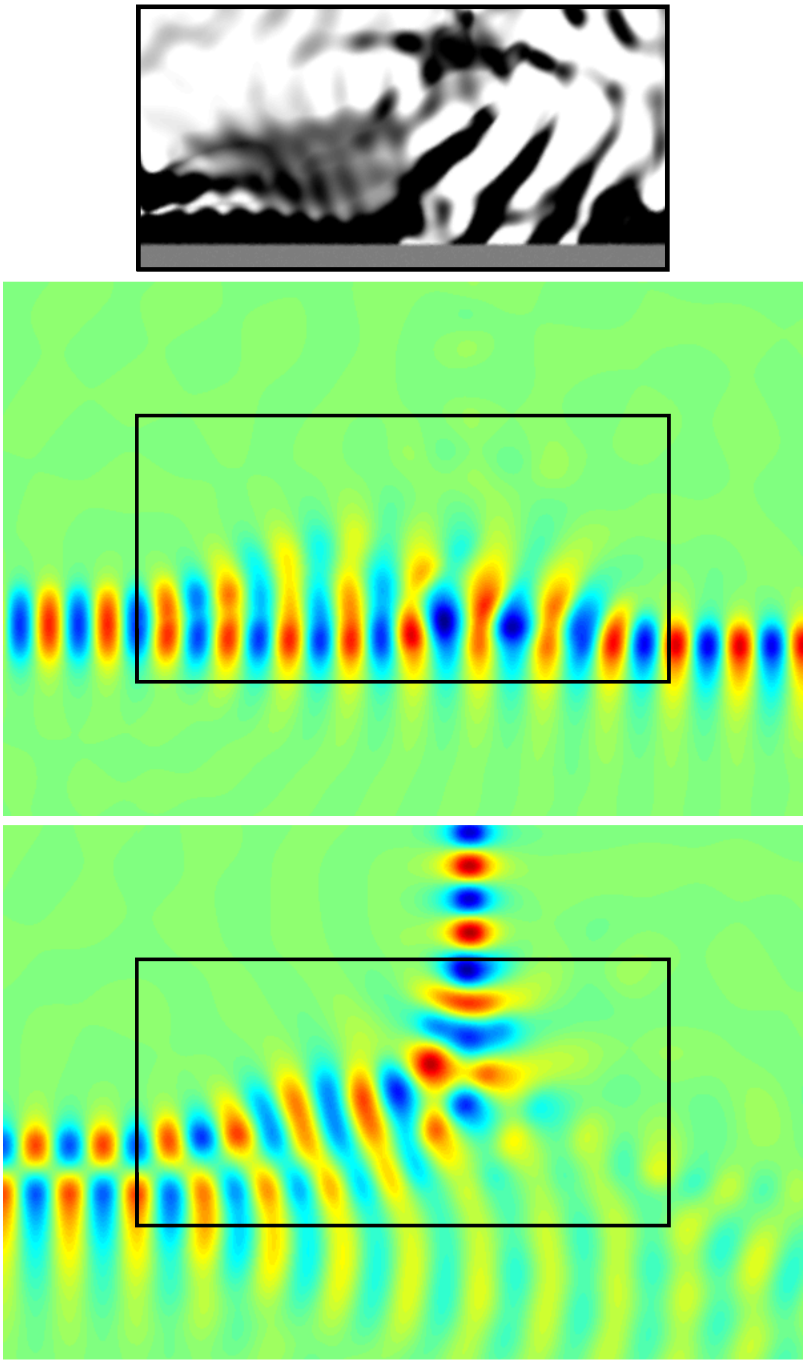

Figure 6.12: Result of the optimisation process for the waveguide multiplexer. At the top one can see the resulting material distribution in the computational domain, while the real parts of the two solutions u and $\tilde{u}$ are shown below.

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