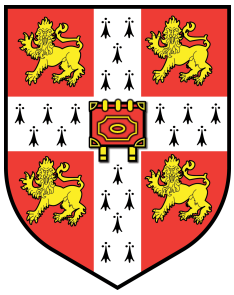
Numerical analysis of the Fokas method in two and three dimensions



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Statement of Originality

I declare that this thesis and the work described in it are my own work; unaided except as may be specified below and by helpful discussions with my supervisor Dr. Anthony Ashton. No part of this thesis has been submitted for another qualification or degree.

The material in Chapters 0 and 1 uses existing material. Most notably, Chapter 1 follows the proof in [FK14] for eigenvalues and eigenfunctions of the Laplacian on a triangle. Other results that are used in these Chapters will be stated.

The results in Chapter 2 up to Section 2.5 are from [Ash13], and also the proposed numerical method in Section 2.6. The proof of spectral convergence is joint work in [AC15], and the remainder of the Chapter with the discussion of this numerical implementation, are new to this thesis.

The results in Chapter 3 are due to the other author in [AC15], and establish that T_β is bounded above and below. The proof of boundedness in Section 3.1.3 is new to this thesis.

The numerical results in Chapters 4 are new to this thesis, and some of them also appear in [AC15]. The proof of convergence in Theorem 4.4.2 is due to the other author.

The derivation of a weak formulation in Chapter 5, and the associated functional analysis is from [Ash14b]. The new weak formulation in Theorem 5.1.4 is new, and is the one studied numerically. The proof of an explicit coercivity bound for a separate weak formulation uses ideas from [Ash14b], but the exact constant is given here for the first time. The remainder of Chapter 5 is new to this thesis.

The weak formulation of Chapter 6 is from [Ash14a] up to Equation (6.0.9), after which the results are new and analogous to the new results presented in Chapter 5 for the Laplace problem.

The numerical results presented in Chapter 7 are entirely new to this thesis.

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Finally I would like to thank my friends in Cambridge, for providing me with such fond memories of this now familiar city. I thank my parents from the bottom of my heart who by raising me; praying for me, and encouraging me constantly have provided a gift I cannot repay. In teaching me to know the Lord they have directed me towards a reason for studying creation; echoed in the words of the world's oldest surviving scientific journal:

> ‘‘To the end, that ... those, addicted to and conversant in such matters, may be invited and encouraged to search, try, and find out new things, impart their knowledge to one another, and contribute what they can to the Grand design of improving Natural knowledge, and perfecting all *Philosophical Arts*, and *Sciences*. All for the Glory of God, the Honour and Advantage of these Kingdoms, and the Universal Good of Mankind.’’[1]

The Heavens declare the glory of God;
the skies proclaim the work of his hands.[2]

Soli Deo Gloria,

[1] *Philosophical Transactions.* **1** (1665), p.2.
[2] *The Holy Bible*, New International Version, Biblica Inc. (2011), Psalm 19:1.

Contents

Summary

This thesis considers the numerical solution to elliptic boundary value problems (BVPs) in convex domains. Specifically we look at the two-dimensional problem in a polygon, and the three dimensional problem in a polyhedron. The nature of elliptic equations means that, knowing the values of a solution on the boundary, one can reconstruct this function inside the domain. This amounts to finding a Dirichlet-to-Neumann (D2N) map, which reconstructs the unknown (Neumann) boundary data from the known (Dirichlet) boundary data. Much is known about the solution to elliptic equations, both theoretically and numerically, but we shall pursue a newer development called the *unified approach* of [Fok08], or "Fokas method". It is hoped that the positive results we present here will motivate further inclusion of the Fokas method in numerical packages.

The combination of a rigorous analysis; the assured stability and convergence rates, as well as MATLAB demonstrations with numerous examples, together form the most interesting and important conclusions of this thesis. Thus the main aims are to demonstrate numerically that which is known analytically: the Fokas method is a viable - and indeed efficient - method for tackling PDEs numerically with controlled convergence. The effectiveness of the Fokas method lies in being able to deal with the D2N map *analytically*, even being able to deform integrals to optimise numerics.

The Fokas method utilises results from complex analysis to provide integral representations for solutions to elliptic and evolution equations; both linear and integrable non-linear. The key equation which allows a given partial differential equation (PDE) to be solved is called the *global relation*. A series of results from [Ash12, Ash13, Ash14a, Ash14b, FP15] have employed techniques from functional analysis to produce a new numerical method to tackle such boundary value problems.

Previous techniques such as finite element methods (FEM) and boundary integral methods (BIM) have both proved successful, yielding stable and very fast convergence. If these techniques exhibit 'spectral' (exponential) convergence rates, they may also be referred to as 'spectral methods'. This thesis fits at the frontier of this development: We introduce the approaches of [Fok08, Ash13, FP15] and provide a numerical implementation of the Fokas method, which is stable and convergent. Furthermore we shall *prove* spectral convergence rates for the two-dimensional problem.

This thesis is divided into two main parts:

- The first four Chapters focus on elliptic BVPs on convex polygons. We show that our method competes well alongside the current state of the art spectral methods, as well as other numerical schemes arising from the Fokas method. Recent successful examples of these include [FFX04, SFFS08, SFPS09, FFSS09, FF11, HFS15].
- The final three Chapters provide the first numerical implementation of the Fokas method in three-dimensional domains. We consider elliptic BVPs on convex polyhedra, which are the natural 3D analogue of polygons. Using results from [Ash14a], we derive numerical examples which break new ground.

Chapter 1 gives an overview of the Fokas method for elliptic problems. A recent paper [FK14] finds explicit eigenvalues and eigenfunctions for the two-dimensional Helmholtz problem in a triangular domain. We discuss in the introduction that tackling this problem via classical analysis is not trivial, and one approach would be to use conformal maps. In contrast, this approach finds analytic solutions using the method of Fokas, and provides a good example to demonstrate the power of this method. We also discuss the Steklov–Poincaré operator S, which is a formal map between the known Dirichlet data and the unknown Neumann data. Indeed, whenever an elliptic BVP is solvable from given (Dirichlet) data, the solution can be used to determine the unknown (Neumann) data. This principle ensures formal existence of this operator S, that maps the Dirichlet data to the (now known) Neumann data.

In Chapter 2, we look at the global relation for the Laplace equation. The global relation leads to a linear operator equation, $T\mathbf{\Phi} = \mathbf{\Psi}$, for the unknown data $\mathbf{\Phi}$, given a function $\mathbf{\Psi}$ which is related to the known Dirichlet data. The chapter begins by setting notation for parameterising the boundary of a polygon, and pullbacks of the functions. Working this way, we can think of the Dirichlet and Neumann data on each edge as functions defined on an interval $[-\sigma, \sigma] \subset \mathbb{R}$. The Fourier transform of such functions lies in the so-called *Paley–Wiener* space. Using specific properties such as analyticity and exponential growth bounds allows an analytical treatment of this operator equation. In particular, the operator T is bounded and coercive on appropriate Banach spaces, and is therefore injective and with closed range. By carefully choosing the spaces on which T is defined, it can be shown that the D2N map admits a unique solution in the relevant Paley–Wiener space. Furthermore, using analyticity of the operator equation, it is sufficient for the global relation to hold on sets with a limit point.

We derive a class of fundamentally *new* variational methods, giving a weak formulation of this global relation. The aforementioned functional properties of T means that the

Lax–Milgram Theorem applies, opening up the possibility for a rigorous numerical treatment. Using Céa's Lemma we prove stability and convergence of our numerical method, and in Section 2.7 we prove *spectral convergence rates* for our method, when the boundary data is infinitely differentiable. We consider existence of a solution to the global relation, and it was shown in [Ash12] that this leads to a solution of the BVP. The uniqueness of this solution follows from injectivity of the operator T, however using Banach's closed range Theorem, we give a second proof of uniqueness by considering properties of the formal adjoint operator, T^*. We prove this result by first considering T as an integral operator with a specific integral kernel, again using strong properties from complex analysis.

Chapter 3 includes the extension of the global relation to more general elliptic equations on convex polygons. Uniqueness is guaranteed up to an additive constant; and whenever Dirichlet data is prescribed on one or more edges, the solution is unique. The Helmholtz and modified-Helmholtz problems are viewed as perturbations of the Laplace equation by a parameter β. Setting $T = T(0)$ and $T_\beta = T(\beta)$ the global relation is written as a linear operator equation $T_\beta \mathbf{\Phi} = \mathbf{\Psi}$. Using results from perturbation theory, the operator T_β is upper semi-Fredholm and is injective for β values away from a discrete set of values. These values are the Dirichlet-eigenvalues of the Laplace operator for a given domain, and away from such points the D2N map has a unique solution. This result follows from [Ash13], and an alternative proof using the representation of T_β^* as an integral operator is suggested.

Using the theory in Chapters 2 and 3, Chapter 4 gives numerical tests for the Helmholtz problem in two test domains, which may be compared with recent alternative collocation-based implementations of the Fokas method [FF11, HFS15]. We observe numerically the exponential convergence rates for our method, as well as relatively low condition numbers for the resulting matrices. Additionally, in Section 4.3 we suggest how these methods may be extended to cases with mixed boundary data in a rigorous way: where each edge of the polygonal domain can be either Dirichlet data or Neumann data. We do this by considering the relevant operator equations, and provide a numerical test for the example considered in [FF11]. For such values of β, a unique solution to the weak problem does not exist, and as a result the matrices for the approximate Galerkin problems are shown to become singular. By plotting the condition numbers of these matrices around known eigenvalues we are able to observe these 'spikes' numerically, as the condition numbers increase by several orders of magnitude.

Finally in Section 4.3.1 we consider four additional test cases for the Helmholtz BVP with Dirichlet data and show how our numerical solutions behave when the exact Neumann data is a-priori unknown. The errors are approximated by comparing the numerical solutions to another one obtained by using a fixed, larger, number of basis

functions. We then proceed to show how the convergence rate for these problems can by approximated, by studying the error plots. The spectral convergence Theorem 2.7.2 guarantees polynomial convergence rates in proportion to the Sobolev regularity of the Neumann data, and thus the convergence is expected to be slower for these problems with less-regular Neumann data. However they still appear to have an exponential decay factor, when we consider the maximum L^2-error over individual faces of the polygonal boundary. Although we cannot expect L^∞-norm convergence from the convergence Theorem, from our numerical tests we see that the first two test cases also exhibit L^∞ norm convergence.

Chapter 5 is similar to Chapter 2: the global relation is constructed for an arbitrary convex polyhedron with prescribed Dirichlet data on each face. Using theoretical results from [Ash14b] we develop a weak formulation of the three-dimensional operator equation $T\mathbf{\Phi} = \mathbf{\Psi}$. Three weak approaches are given: two are from [Ash14b], and for one of these, we prove *explicit* coercivity bounds for the resulting weak problem, and thus obtain exact bounds on the convergence rates for the Galerkin problem. The third approach generalises previous results to give a fundamentally new weak formulation for the global relation. Well-posedness is proven in Sections 5.5-5.6 and Theorem 5.1.4, and it follows that this permits an entirely new Galerkin method which is stable, convergent and practical.

An additional challenge for the three-dimensional problem is to choose a basis that represents functions on a given face of the polygon. In two-dimensions there are good choices for basis functions on a line segment, and which have an explicit Fourier transform [FIS15], whereas for two-dimensional convex polygonal faces, such a choice is less clear. For each face Q_j of the polyhedron, we choose to use a polynomial basis which must be orthogonalised over Q_j. Because the Gram–Schmidt algorithm is in general unstable (due to propagation of numerical errors), in Section 5.3.1 we carry out an *exact* Gram–Schmidt orthogonalisation where the relevant inner products are given precisely in terms of the geometry of the polyhedra. These functions are analytic with sufficient decay, but they have removable singularities along rays in $\mathbb{C}^2$, so the implementation of such functions in MATLAB is briefly discussed. A new integral representation is obtained which gives rise to a practical weak formulation of the global relation. Because of the additional complexities of higher-dimensional integration, we mention briefly how a statistical (Monte–Carlo) integration may aid with future numerics. The implementation provided later (Chapter 7) gives a proof of concept of this approach, and is the first numerical implementation of these BVPs via the Fokas method.

Chapter 6 extends the theory given in Chapter 5 to the Helmholtz and modified-Helmholtz equations. Given the theoretical considerations of Chapters 2, 3 and 5, this is provided as a brief summary, and it is observed that any elliptic equation with

constant coefficients can be reduced to one of these equations by a change of variables and substitution. We propose a new variational method for these BVPs, and prove that this yields a convergent numerical method. Furthermore because of symmetries in the Galerkin matrix components, we are able to reduce the number of a-priori integrations required; and this aids numerical efficiency. In particular, by choosing the linear forms to omit a symmetric set around the origin, the integrals may be performed over a sub-region of $\mathbb{R}^2$.

Finally in Chapter 7, we provide numerical implementation for the three-dimensional Laplace, Helmholtz and modified-Helmholtz problems as a proof of concept for our weak formulation of the global relation. As test cases, we consider two domains: a cube and a pyramid, and a known solution, u, to the respective BVPs. The numerical results obtained corroborate the analytical framework of Chapters 6 and 7, and demonstrate that the Galerkin problem is numerically tractable. This chapter (combined with the appendix) includes suggestions for a future improvement, which incorporates a compatibility criterion - that the integral of the Neumann data over the boundary must be zero - into the choice of our subspaces for the Galerkin problem.

The theory applied in this thesis may be extended to smooth domains and curvilinear domains by artificially segmenting the boundary Γ in to various components $\{\Gamma_j\}_{j=1}^n$, and would require a modified Fourier-like transform over a curve. The approach studied here and in [Ash12, Ash13] for convex polygons, will be extended to curvilinear domains using these modified transforms in [Roc16]. It is expected that good numerical results like those we present here for polygons and polyhedra, may also be observed for these cases.

Introduction

With the layout of this thesis given, let us proceed with a classical example of solving the Laplace equation analytically in a square. We wish to highlight two points in this example: First, how easily an exact solution may be given for some examples, but secondly how such an approach is limited to specific polygonal domains. This approach is valid for a square, but not for a general triangular domain (though it could be used for a right isosceles triangle). The Fokas method by contrast is not as sensitive, and we will show how numerical solutions to the global relation may be obtained for any convex polygonal domain. When considering existence and regularity results, such domains fall in to the category of 'curvilinear polygons' [Gri85, HW08, Dau88].

Consider the Laplace equation with Dirichlet boundary values in a unit square $\Omega := \{(x, y) : 0 \leq x, y \leq 1\} \subset \mathbb{R}^2$:

$$\begin{aligned} u_{xx} + u_{yy} &= 0 \text{ on } \Omega \\ u(x, 0) = u(0, y) = u(x, 1) &= 0 \\ u(1, y) &= f(y), \end{aligned} \tag{0.0.1}$$

where we suppose that $f \in C_0^0([0, 1])$, where $C_0^0([a, b])$ is the space of continuous functions which are zero at both the points a and b. Then the data around the entire boundary is continuous. By considering a general separable solution $u(x, y) = F(x)G(y)$ for some unknown functions F and G we find that, for (0.0.1) to be satisfied, these unknown functions must satisfy a second order linear PDE. Using this separation of variables method, we find that

$$u(x, y) = \sum_{n=1}^{\infty} A_n \sinh(n\pi x) \sin(n\pi y) \tag{0.0.2}$$

for constants $\{A_n\}_{n\geq 1}$ to be determined from the boundary data. The function f can be written as a convergent Fourier series

$$f(y) = \sum_{n=1}^{\infty} 2b_n \sin(n\pi y),$$

where $\{b_n\}_{n\geq 1} \subset \mathbb{R}$ are known. The series consists only of sine terms because $f(0) = f(1) =$

0. By comparison with (0.0.2) we have the relation $b_n = A_n \sinh(n\pi)$, and therefore u is given by a sum of exponential terms

$$\begin{aligned} u(x,y) &= \sum_{n=1}^{\infty} \frac{b_n}{\sinh(n\pi)} \sinh(n\pi x)\sin(n\pi y) \\ &= \sum_{n=1}^{\infty} \frac{b_n}{4\mathrm{i}\sinh(n\pi)} \left(e^{n\pi x} - e^{-n\pi x}\right)\left(e^{\mathrm{i}n\pi y} - e^{-\mathrm{i}n\pi y}\right) \\ &= \sum_{n=1}^{\infty} \frac{b_n}{4\mathrm{i}\sinh(n\pi)} \left(e^{n\pi(x+\mathrm{i}y)} - e^{n\pi(x-\mathrm{i}y)} - e^{-n\pi(x+\mathrm{i}y)} + e^{-n\pi(x-\mathrm{i}y)}\right). \end{aligned} \tag{0.0.3}$$

Let us consider the set $Z_P := \{(\lambda_1, \lambda_2) : \lambda_1^2 + \lambda_2^2 = 0\} \subset \mathbb{C}^2$. And let $Z_1 \subset Z_P$ be given by

$$Z_1 := \{(\lambda_1, \lambda_2) : \lambda_1 = -\mathrm{i}n\pi, \lambda_2 = n\pi, n \geq 1\}.$$

Also, for a set $A \subseteq \mathbb{C}$, let μ_A denote the Dirac measure on A. Finally we define a corresponding function $c_1(\boldsymbol{\lambda})$ which takes the values

$$c_1(\boldsymbol{\lambda}_n) = \frac{b_n}{4\mathrm{i}\sinh(n\pi)}, \quad \text{for every } \boldsymbol{\lambda}_n = (-\mathrm{i}n\pi, n\pi) \in Z_1,\ n \geq 1.$$

Then we may rewrite the sum (0.0.3) as an integral over this set $Z_1 \subset Z_P$. The first of four terms is

$$\int_{Z_1} e^{\mathrm{i}(\lambda_1 x + \lambda_2 y)} c_1(\lambda_1, \lambda_2)\, \mathrm{d}\mu_{Z_1}(\lambda). \tag{0.0.4}$$

Similarly the other terms may be written in integral form, for sets $Z_i \subset Z_P$, $i = 1, 2, 3, 4$, so that

$$u(x,y) = \sum_{i=1}^{4} \int_{Z_i} e^{\mathrm{i}(\lambda_1 x + \lambda_2 y)} c_i(\lambda_1, \lambda_2)\, \mathrm{d}\mu_{Z_i}(\lambda). \tag{0.0.5}$$

For any fixed $(x, y) \in \mathbb{R}^2$ this integral is finite because of the $\sinh(n\pi)$ decay in each $c_i(\boldsymbol{\lambda})$; and also as $f \in C_0^0([0,1])$, the constants $b_n \to 0$ as $n \to \infty$.

The representation (0.0.5) is a special case of a more general result in [Ehr70, Pal70], which states that the solution to any linear PDE with constant coefficients can be written in the form

$$u(\boldsymbol{x}) = \int_{Z_P} e^{\mathrm{i}\boldsymbol{\lambda}\cdot\boldsymbol{x}} c(\boldsymbol{\lambda}, \boldsymbol{x})\, \mathrm{d}\mu_{Z_P}(\boldsymbol{\lambda}), \quad \boldsymbol{x} \in \Omega \tag{0.0.6}$$

where Z_P is the algebraic variety described by the zero set of the characteristic polynomial, P, for the PDE; $c(\boldsymbol{\lambda}, \boldsymbol{x})$ is a polynomial in $\boldsymbol{x}$, and μ_{Z_P} is a complex measure supported on Z_P. This result forms the basis for our analysis of the Fokas method, so in the next section we provide a review of this Theorem. It should be noted that this result is highly abstract and non-constructive, though in special cases (such as the one we have presented above) an explicit solution may be given. With this view, the Fokas method yields a concrete

realisation of the representation result (0.0.6). Before we proceed, let us look back on the result we have derived:

Looking at the calculations above, one might ask why further methods are required? If the Laplace equation can be solved using Fourier series so easily, are the problems not already solved? Indeed it is true that the solution to (0.0.1) can be extended to arbitrary non-zero data (continuous at the vertices) around the square:

Suppose the boundary data is such that on each vertex $(x_1, y_1), \dots, (x_4, y_4)$, it takes the values $a_1, \dots, a_4$ respectively. Then by Lagrange interpolation, we can find a complex polynomial p (of degree at most 3) such that $p(x_j + \mathrm{i}y_j) = a_j$ for every $j = 1, \dots, 4$. Since the real part of a polynomial is harmonic, we may solve the related problem for $w(x, y) := u(x, y) - \Re p(x + \mathrm{i}y)$, where w has continuous boundary data that vanishes at the vertices. Now solving (0.0.1) for data on each edge $j = 1, \dots, 4$ respectively (and zero boundary data on the other edges), we find solutions w_j. Then $w = w_1 + w_2 + w_3 + w_4$ solves the general boundary value problem.

However, this relatively straightforward calculation cannot even be extended to triangular domains. Even for (0.0.2), we are unable to find the constants unless the boundaries lie parallel to the coordinate choice. For a right-angled triangle with vertices at $(0, 0), (1, 0)$ and $(1, 1)$ with boundary data specified on the edge $u(1, y) = f(y) \in C_0^0([0, 1])$, the equations only reduce to

$$\begin{aligned} u(x, 0) = 0 \quad &\implies \quad G(0) = 0 \\ u(1, y) = f(y) \quad &\implies \quad F(1)G(y) = f(y) \\ u(x, 1 - x) = 0 \quad &\implies \quad F(x)G(1 - x) = 0, \end{aligned}$$

which cannot in general be simplified (although the Laplace eigenvalues for the specific case of an equilateral triangle were identified in [Lam33]).

Remark 0.0.1. *There are solutions to this, such as finding conformal maps between the triangle and a rectangle. Or even in general a polygon can be mapped to a circle, where the Laplace equation can be solved. Here we are highlighting only that the method has no direct generalisation to even relatively simple domains. This permits us to expect (and hope for) further transform techniques to solve such problems.*

We shall see that the Fokas method is indeed a generalisation of the Fourier transform, and the resulting functions share similar analytic properties. As we would expect given the examples above, the nature of this transform depends heavily on the domain geometry. Before introducing this approach, we begin with a related abstract approach of Ehrenpreis and Palamodov. This existence Theorem states that such a solution to linear PDE can be expected, though the proof is non-constructive. The Fokas method for elliptic PDEs can be viewed as a realisation of their result.

0.1 A representation Theorem by Ehrenpreis and Palamodov

Suppose $\alpha = (\alpha_1, \ldots, \alpha_n)$ are multi-indices, and $(P_\alpha)_{|\alpha|\leq N}$ are constants. Then these define a linear homogeneous partial differential equation with constant coefficients, as

$$P(D)u \equiv \sum_{|\alpha|\leq N} P_\alpha D^\alpha(u) = 0, \quad \text{with} \quad D^\alpha = \mathrm{i}^{|\alpha|} \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \ldots \partial x_n^{\alpha_n}}, \tag{0.1.1}$$

which has order at most N. The function $P(\lambda) := \sum_{|\alpha|\leq N} P_\alpha \lambda^\alpha$ defines a map from $\mathbb{R}^n \to \mathbb{R}$; and whenever $P(\lambda) = 0$, the function $e_\lambda(x) := e^{\mathrm{i}\lambda\cdot x}$ is a solution of (0.1.1). Let $(\lambda_J)_{J\in Z_P}$ be the set of such values, for some set $Z_P \subset \mathbb{C}^n$. Any $L^2(\mathbb{R}^n)$ function can be written as a superposition of $e_\lambda(x)$ by the inverse Fourier transform:[1] For $f \in L^1(\mathbb{R}^n) \cap L^2(\mathbb{R}^n)$, and $\hat{f}$ its Fourier transform,

$$f(x) = \int_{\mathbb{R}^n} \hat{f}(\lambda) e_\lambda(x)\, \mathrm{d}\lambda. \tag{0.1.2}$$

If we can find values λ_J, such that $e_{\lambda_J}(x)$ solve the PDE (0.1.1), then we may expect that a general solution can be obtained as a *superposition* of these exponential solutions, $e_{\lambda_J}(x)$. This is a deep result, proven by Ehrenpreis [Ehr70, Chap. VII] and Palamodov [Pal70, Chap. VI] concurrently. That this result holds is not clear from our intuition, and the proof itself is non-constructive. The respective Theorems state that any solution to (0.1.1) takes the form

$$u(x) = \int_{Z_P} e^{\mathrm{i}\lambda\cdot x} c(\lambda, x) d\mu(\lambda), \tag{0.1.3}$$

where $c(\lambda, x)$ are polynomials, and the measure $\mu(\lambda)$ has support contained inside the algebraic variety

$$Z_P := \{\lambda \in \mathbb{C}^n : P(\lambda) = 0\}.$$

The approach taken in the introduction of [Pal70] is very instructive, and relates closely to our use of special spaces called *Paley–Wiener* spaces, which we will use later on. First note that our set Z_P, being the level set of a smooth function, will at general points be locally $n-1$ dimensional. In the case of one complex coordinate, e.g. $P(D) = \partial_x^2$,

$$P(\lambda) = -\lambda^2$$

and the zeroes will be isolated; whereas for the 2-dimensional Laplacian: $P(D) = \partial_{x_1}^2 + \partial_{x_2}^2$, we have

$$P(\lambda) = -\lambda_1^2 - \lambda_2^2,$$

which has zeroes along characteristics parameterised by $(\lambda, \pm\mathrm{i}\lambda)$, $\lambda \in \mathbb{C}$.

[1] For $f \in L^2(\mathbb{R}^n)$, the Fourier transform is considered to be the formal extension of the Fourier transform operator on $L^1(\mathbb{R}^n) \cap L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$, and the integral representation (0.1.2) holds in a limit over balls B_R, of radius R, as $R \to \infty$.

0.1.1 One-dimension: a motivational example

Taking firstly the case of one-dimension, a general polynomial has the form

$$P(\lambda) = \alpha_n \prod_{j=1}^{n} (\lambda - \lambda_j)^{m_j} \equiv \alpha_0 + \alpha_1 \lambda + \cdots + \alpha_n \lambda^n, \tag{0.1.4}$$

where n is the number of distinct roots $(\lambda_j)_{j=1}^n$ of $P(\lambda)$. Then $P(D)e_\lambda(x) = 0$ if and only if $\lambda = \lambda_j$ for some $j = 1, \ldots, n$. Letting Z_P denote the algebraic variety described by the zero set of the polynomial $P(\lambda)$, we see that $e_\lambda(x)$ solves the PDE (0.1.1) for every $\lambda \in Z_P$, and for no other λ.

The natural question to ask then is whether it is possible to find other solutions. Consider the function $xe_\lambda(x)$. Applying the operator $P(D)$ we find

$$\begin{aligned} P(D)\left(xe_\lambda(x)\right) &= xP(D)e_\lambda(x) + (-\mathrm{i}\partial_x x)\left[\alpha_1 + 2\alpha_2(-\mathrm{i}\partial_x) + \cdots + n\alpha_n((-\mathrm{i})^{n-1}\partial_x^{n-1})\right] e_\lambda(x) \\ &= e_\lambda(x)\left[xP(\lambda) + P'(\lambda)\right]. \end{aligned}$$

For each $\lambda \in Z_P$, $P(\lambda) = 0$ and so the term in square brackets is precisely $P'(\lambda)$. Recalling the product representation for $P(\lambda)$ in (0.1.4), the roots of $P'(\lambda)$ are those λ_j with $m_j > 1$. That is,

$$P(D)\left(xe_\lambda(x)\right) = 0 \quad \iff \quad \lambda \in \{\lambda_j : m_j > 1 \text{ for } j = 1, \ldots, n\}.$$

In general then, as Palamodov notes, for $f(z)$ an arbitrary polynomial of order $A \leq m_1 + \cdots + m_n$,

$$P(D)\left(f(x)e_\lambda(x)\right) = \sum_{|\beta| \leq A} D_x^\beta f(x) P^{(\beta)}(\lambda) e_\lambda(x), \tag{0.1.5}$$

which follows from the Leibniz formula and our discussion above, where we have let $P^{(\beta)}(\lambda) := D_\lambda^\beta P(\lambda)$ denotes the β-th derivative of $P(\lambda)$. For our one-dimensional case, β is a scalar, but this can be replaced by a multi-index.

Again, we observe that the roots of $P^{(\beta)}(\lambda)$ are precisely those λ_j for which $m_j > |\beta|$. Thus any exponential of the form

$$x^\beta e_{\lambda_j}(x), \quad \beta = 0, \ldots, m_j - 1;\ j = 1, \ldots, n \tag{0.1.6}$$

solves (0.1.1). Looking more closely at (0.1.5), we see that this can only equal zero for all $x \in \mathbb{R}$ if each individual term $D_x^\beta f(x) P^{(\beta)}(\lambda) = 0$, for which we certainly require (at least)

$$f(x)P(\lambda) = 0 \quad \iff \quad \lambda \in Z_P.$$

The question remains, are all solutions of this exponential type (0.1.6)? In one-dimension this is indeed true, and was known to Euler.

Proposition 0.1.1 ([Pal70]). *Let Ω be a convex domain*[2]*, then any distributional solution to the PDE (0.1.1) is a classical solution, and is a linear combination of*

$$x^k e_{\lambda_j}(x), \quad k = 0, \dots, m_j - 1, \quad j = 1 \dots, n.$$

And the converse holds trivially by the above discussion. Indeed this solution is given by

$$u(x) = \sum_{j=1,\dots,n} \sum_{|\beta| \leq m_j - 1} a_{j,\beta} x^\beta e_{\lambda_j}(x),$$

for some coefficients $a_{j,\beta} \in \mathbb{C}$.

0.1.2 The case for higher dimensional PDEs

Now we let $P(D)$ be a multi-dimensional differential operator of order M. Leibniz's formula [Pal70, p. 3] again gives us that for f a polynomial of order A and $x \in \mathbb{R}^n$

$$P(D) f(x) e_\lambda(x) = \sum_{|\beta| \leq A} D^\beta f(x) P^{(\beta)}(\lambda) e_\lambda(x).$$

$f(x)e_\lambda(x)$ is a solution to (0.1.1) provided the derivatives $P^{(\beta)}(\lambda) := D^\beta_\lambda P(\lambda)$ all vanish at a given root $\lambda = \lambda_J$ in the algebraic variety $Z_P := \{\lambda = (\lambda_1, \dots, \lambda_n) \in \mathbb{C}^n : P(\lambda_1, \dots, \lambda_n) = 0\}$. As we saw above for the two-dimensional Laplacian: $P(\lambda) = -\lambda_1^2 - \lambda_2^2$, and the algebraic variety Z_P can be parameterised by the curves $\{(\lambda, \pm \mathrm{i}\lambda) \in \mathbb{C}^2 : \lambda \in \mathbb{C}\}$.

Remark 0.1.2. *One part of Z_P contains the points $\delta(\lambda) = (\lambda, \mathrm{i}\lambda)$. For our analysis, it will be sufficient to consider relations* only *on this curve. That is, if a relation holds on $\delta(\lambda)$, then it will necessarily hold on the remainder of Z_P. We shall remark on this during the derivation of the global relation, but this fact essentially follows from symmetry properties of the Paley–Wiener space. Indeed, in this case although the measure $\mu(\lambda)$ in (0.1.3) is supported on Z_P, the contribution from $(\lambda, -\mathrm{i}\lambda)$ can be written in terms of that from $\delta(\lambda)$. And a similar result holds for the Helmholtz problems.*

0.1.3 A concrete Ehrenpreis-type representation

Owing to work in [Fok01, Fok08, FP15], solutions to the Laplace and Helmholtz equations may be given precisely in the Ehrenpreis representation (0.1.3) above. For the two-dimensional Laplace equation on a polygon, it is shown that[3]

$$\frac{\partial q}{\partial z}(z, \bar{z}) = \frac{1}{2\pi} \sum_{k=1}^{n} \int_{l_k} e^{\mathrm{i}\lambda z} \rho_k(\lambda) \, \mathrm{d}\lambda, \tag{0.1.7}$$

[2] In 1D, this is equivalent to the set being connected. For higher dimensional domains, convexity is required. We will comment on this at the end of Section 2.2, once the global relation has been constructed.

[3] As noted in [FK03], we can reconstruct the function q, by $q = 2\Re \int_{z_0}^{z} q_z \, \mathrm{d}z + \text{const}$.

where $\rho_k(\lambda)$ is known in terms of the boundary values of q. The rays l_k lie in the complex plane and are determined from the edge angles at the k-th vertex. For any $\lambda \in l_k$, the exponential may be rewritten as

$$e^{\mathrm{i}\lambda z} = e^{\mathrm{i}(\lambda,\mathrm{i}\lambda)\cdot(x,y)},$$

and so the integral is indeed over the algebraic variety $Z_P = \{\boldsymbol{\lambda} = (\lambda_1, \lambda_2) : \lambda_1^2 + \lambda_2^2 = 0\}$, as stated in the Ehrenpreis representation (0.1.3). Similarly for the two-dimensional Helmholtz equation (3.0.1), it is shown in [Fok08] that

$$q(z,\bar{z}) = \frac{1}{4\pi\mathrm{i}} \sum_{k=1}^{n} \int_{l_k} e^{\mathrm{i}\lambda z - \mathrm{i}\beta^2 \bar{z}/\lambda} \rho_k(\lambda) \frac{\mathrm{d}\lambda}{\lambda}.$$

Similarly for $\lambda \in l_k$, the exponential term can be written as

$$e^{\mathrm{i}\lambda z - \mathrm{i}\beta^2 \bar{z}/\lambda} = e^{\mathrm{i}\boldsymbol{\lambda}\cdot(x,y)},$$

where for $\lambda \in \mathbb{C}$, the vector $\boldsymbol{\lambda} = \left(\lambda - \frac{\beta^2}{\lambda}, \mathrm{i}\left(\lambda + \frac{\beta^2}{\lambda}\right)\right)$ lies in the zero set, Z_P, of the polynomial $P(\lambda) = \lambda^2 - 4\beta^2$ for the Helmholtz problem:

$$Z_P := \{\boldsymbol{\lambda} \in \mathbb{C}^2 : \lambda_1^2 + \lambda_2^2 + 4\beta^2 = 0\}.$$

The same is true for the three-dimensional Laplace problem, where it is shown in [Ash14b] that for $\boldsymbol{x} \in \Omega \subset \mathbb{R}^3$,

$$q(\boldsymbol{x}) = \frac{1}{8\pi^2} \sum_{k=1}^{n} \int_{Z_k} e^{\mathrm{i}\boldsymbol{\lambda}\cdot\boldsymbol{x}} \rho_k(\boldsymbol{\lambda})\, \mathrm{d}\nu_k(\boldsymbol{\lambda}).$$

These sets Z_k are subsets of $Z_P = \{\boldsymbol{\lambda} \in \mathbb{C}^3 : \lambda_1^2 + \lambda_2^2 + \lambda_3^2 = 0\}$ associated to the PDE, and $\mathrm{d}\nu_k(\boldsymbol{\lambda})$ is a complex Radon measure with support contained inside Z_k. In each of these cases, the Fokas method provides a *concrete realisation* of the Ehrenpreis representation. In the subsequent chapters, we will examine these functions $\rho_k(\boldsymbol{\lambda})$, which couple the Dirichlet and the Neumann data. These functions satisfy an equation, called the global relation, which is analytic in $\mathbb{C}$ for Laplace, and holomorphic away from 0 for Helmholtz. Inverting this relation gives a solution for the Neumann data from the Dirichlet data, and in this sense is called the Dirichlet-to-Neumann (D2N) map. Before we begin, let us recall the classical theory of boundary integral methods: similarly to the Fokas method, these yield a solution $u(x)$ as an integral over the boundary, which likewise involves the Dirichlet and Neumann values for u. Providing the unknown Neumann values amounts to solving an integral operator equation, in much the same way as the Fokas method requires a solution to the global relation.

0.2 A review of some existing methods

In this thesis, we will introduce the Fokas method from [Fok01, FK03] as a viable way of solving the Dirichlet BVP for the Laplace, Helmholtz and modified-Helmholtz PDEs numerically. Let us first give an overview of some alternative methods for solving these problems, which combine theoretical results as well as requiring numerical methods to solve.

We will first discuss conformal mappings, as these are a way to generate solutions to the Laplace problem, by finding a transformation from a given domain to one in which a solution may already be known. This is especially of interest, because we will be considering the Laplace BVP on polygonal domains, and there are a class of conformal maps called the Schwartz-Christoffel transformations which map the unit disk on to any given polygon. To solve the Laplace BVP the inverse of this map can be calculated numerically, for example in [Tre80].

Secondly in Sections 0.2.2-0.2.3 we will discuss boundary integral methods using layer potentials. Analogously to the approach implemented in this thesis, the result of the boundary integral method is to reduce the problem to one of inverting a linear operator equation. This can be challenging due to singularities in the integrands to be computed.

Finally in Sections 0.2.4-0.2.5 we discuss the formal Steklov-Poincaré map, between the known and unknown boundary data for the Laplace BVP. Since we will be considering polygonal domains, we discuss the classical existence result for Lipschitz domains, and also compatibility restrictions on the boundary data at the vertices. We will do this by considering trace spaces for polygons and obtaining sufficient conditions such that the boundary data will ensure a solution. Indeed, it is sufficient that the Dirichlet data lies in an H^1 Sobolev space, and are continuous across the vertices. This will ensure that a solution does exist to to the BVP we consider in (2.1.1).

0.2.1 Conformal mappings

One method for solving Laplace's equation in 2D domains is by a conformal mapping. A conformal map $\phi : D \to U$ is a holomorphic map, such that the boundaries map on to each other, $\phi(\partial D) = \partial U$, and $\phi'(z) \neq 0$ for every $z \in D$. The idea is that if a solution exists in some domain (such as a circle) and a conformal map exists between this domain and another, then we can generate a solution to the Laplace problem in the second domain too.

To see this, let $U, D \subset \mathbb{C}$ be two simply-connected domains, and $\phi : D \to U$ a conformal map between them. If $q(z) : D \to \mathbb{C}$ is holomorphic, then $q \circ \phi^{-1} : U \to \mathbb{C}$ is also holomorphic. Since the real part of a holomorphic function is analytic, this provides a way to generate analytic functions on a new domain U, given a harmonic function on D. Indeed, any harmonic function u on D is the real part of some holomorphic function f, which is

seen by constructing the *harmonic conjugate*: Let u_x, u_y be the partial derivatives of u with respect to x and y, then by the Cauchy–Riemann equations the function $g(x+\mathrm{i}y) := u_x(x,y) - \mathrm{i}u_y(x,y)$ is holomorphic in D. The function, f, such that $g = f'$, exists since the domain is simply-connected by defining f pointwise as the path integral

$$f(z) := \int_{C_{z_0,z}} g(w)\,\mathrm{d}w,$$

for some fixed $z_0 \in D$. By the Cauchy–Riemann equations the function $v(x,y) = \Im f(x\mathrm{i}y)$ is the harmonic conjugate to u, and $u(x,y) = \Re f(x+\mathrm{i}y)$.

Suppose now that in a unit disk $D \subset \mathbb{C}$ with boundary $\partial D = S$, we can solve the Laplace problem:

$$\begin{aligned} \Delta u &= 0 \quad \text{in } D \\ u &= f \in H^1(S) \quad \text{on } S. \end{aligned} \tag{0.2.1}$$

Then we can generate a solution to Laplace's equation in U as follows:

1. Given u, construct a holomorphic function $g : D \to \mathbb{C}$ such that $\Re g = u$.
2. The function $h := g \circ \phi^{-1} : U \to \mathbb{C}$ is holomorphic.
3. The function $\tilde{u} := \Re h : U \to \mathbb{R}$ is harmonic and

$$\tilde{u}(x,y) = \Re\left(g \circ \phi(x+\mathrm{i}y)\right), \quad x, y \in \partial U.$$

Then given any domain U, and a conformal map $\phi : D \to U$, the function $\tilde{u}(z) := u \circ \phi^{-1}(z)$ is holomorphic, and $\Re\tilde{u}$ is a harmonic function, with the boundary values $\tilde{f} = \phi(f)$ on ∂U. Thus, by an inversion of a conformal map, one may construct solutions to the Laplace problem in a greater variety of domains.

One important class of conformal maps are called the Schwartz–Christoffel transformations (see e.g. [AF03]), which yield a conformal mapping ϕ between the disk D, and the interior of any polygon. An explicit Green's function exists for D, so the Laplace equation can be solved. By numerically inverting the Schwartz–Christoffel transformation ϕ, solutions for the Laplace equation can be obtained in polygons via this method. We shall see later that for the Fokas method, the analogous step is to invert a matrix equation, where the entries consist of numerical integrals.

0.2.2 The boundary integral technique

Boundary integral methods are an established method for solving the classes of linear elliptic PDEs considered in this thesis. These methods yield the unknown Neumann data as the solution of an integral operator equation between functions defined in the physical

domain. In [McL87, Fol95, McL00] it is shown that the form of these equations involve *weakly singular* integrals: as a result, efficient numerical integrators are required to compute these terms. In contrast, our analysis of the global relation will be in *spectral* space, so we may use powerful results from complex analysis. In our case, the relevant functions are holomorphic, square-integrable and free from singularities and highly oscillatory terms.

We present here a brief overview of the boundary integral technique for the analysis and solution of the Laplace equation. We follow the presentation in [Fol95, pp. 116–141] for bounded domains Ω with a C^2 boundary S (see also [Eva10]). This approach leads to a solution $u(x)$ of the Laplace equation in terms of an integral over S. In a similar way the Fokas method will also involve an integral relation over the boundary, however the analysis is done in spectral space i.e. using the Fourier transforms of known functions. Since the Fourier transform of any compactly supported function is *analytic*, many of the issues below relating to spatial singularities for boundary integral methods *do not* appear in the Fokas method.

To provide the best picture with which to compare the Fokas method, we consider a simple case where Ω is a simply-connected domain. We are primarily interested in solutions to the Laplace equation in polygonal and polyhedral domains, and indeed much of the Layer Potential theory here extends to Lipschitz domains [Ver84].

Given a PDE $P(D)u = 0$, the *fundamental solution* is defined to be the distribution N which solves the equation

$$P(D)N = \delta_0.$$

For the Laplacian on $\mathbb{R}^n$, N is given as a function with a singularity at zero

$$N(x) = \begin{cases} \frac{1}{2\pi} \log |x|, & n = 2 \\ \frac{|x|^{2-n}}{(2-n)\omega_n}, & n \geq 3, \end{cases} \qquad N(x,y) := N(x-y) \tag{0.2.2}$$

where ω_n is the surface area of the $(n-1)$-sphere, for example $\omega_3 = 4\pi$. Suppose that

$$u(x) = \int_\Omega u(y)\delta(x-y)\,\mathrm{d}y,$$

is a $C^1(\bar{\Omega})$ solution to Laplace's equation. Using Green's second identity and that S is a C^2 boundary, it is shown in [Fol95, p. 86] by a limiting process in place of $\delta(x-y)$, that u must satisfy the integral relation

$$u(x) = \int_S \left(u(y)\partial_{\nu_y} N(x,y) - \partial_\nu u(y) N(x,y) \right), \quad x \in \Omega. \tag{0.2.3}$$

This relation is incredibly useful, but also deceptive. To see this, consider the well-posedness statement for the Laplace equation:

Given Dirichlet data $f \in H^1(S)$, the Laplace equation has a unique solution u.

That is to say, specifying f is sufficient to generate a solution u. And given a solution u, the Neumann data g can be calculated. But since all u, f and g exist, (0.2.3) holds. This argument shows that the relation is overdetermined (in the sense that any f will prescribe the unique g such that the relation holds).

One solution is to search for a related function $G : \Omega \times \overline{\Omega} \to \mathbb{R}$, called the *Green's function* for Ω, which must satisfy the following two properties:

- $G(x, \cdot) - N(x, \cdot)$ is harmonic on Ω and continuous on $\overline{\Omega}$
- $G(x, y) = 0$ for every $x \in \Omega$ and $y \in S$.

For such functions G, solutions to the Laplace equation are given as [Fol95, p. 87]

$$u(x) = \int_S f(y) \partial_{\nu_y} G(x, y) \, \mathrm{d}\sigma(y).$$

However in many cases it is difficult to find this function G explicitly. Consider instead a modified integral expression

$$v(x) := \int_S f(y) \partial_{\nu_y} N(x, y) \, \mathrm{d}\sigma(y).$$

By construction of N and differentiating inside the integral, we see that v is harmonic. The function v does not equal f on the boundary S, however it differs from f by a linear compact operator T:

$$v|_S = \frac{1}{2} f + Tf.$$

In particular, if we can find a function ϕ such that $(\frac{I}{2} + T)\phi = f$, then

$$v(x) := \int_S \phi(y) \partial_{\nu_y} N(x, y) \, \mathrm{d}\sigma(y) \tag{0.2.4}$$

solves the Dirichlet problem, with $v|_S = f$. That is, $u = v$ is our required solution. It remains then to solve this linear problem for ϕ given f. Equivalently, we must analyse the range of the operator $(\frac{I}{2} + T)$.

Remark 0.2.1. *The integral expression* (0.2.4) *is called the* double layer potential with moment ϕ. *A similar expression called the* single layer potential with moment ϕ *is given by*

$$v(x) := \int_S \phi(y) N(x, y) \, \mathrm{d}\sigma(y). \tag{0.2.5}$$

The motivation for these names comes from electrostatics: Suppose a unit charge Q is placed at a point $\mathbf{y} \in \mathbb{R}^3$, then the resulting electric field E and potential V due to Q at a point $\mathbf{x} \in \mathbb{R}^3$ is

$$E(\mathbf{x}) = \frac{\mathbf{x} - \mathbf{y}}{|\mathbf{x} - \mathbf{y}|^3} \quad \text{and} \quad V(\mathbf{x}) = \frac{1}{|\mathbf{x} - \mathbf{y}|}.$$

Replacing Q by a charge density $\phi(\mathbf{y})$ over a surface S, the resulting potential is given by integrating the density

$$\int_S \phi(\mathbf{y}) \frac{1}{|\mathbf{x}-\mathbf{y}|} \, \mathrm{d}\sigma(\mathbf{y}) = -4\pi \int_S \phi(\mathbf{y}) N(\mathbf{x},\mathbf{y}) \, \mathrm{d}\sigma(\mathbf{y}).$$

Up to a constant then, (0.2.5) is seen to be the potential due to a charge density ϕ on S. Similarly by considering $\partial_{\nu_y} N(x,y)$ as a limit of difference quotients

$$\partial_{\nu_y} N(x,y) = \lim_{t\to 0} \frac{N(\mathbf{x},\mathbf{y}+t\boldsymbol{\nu}(\mathbf{y})) - N(\mathbf{x},\mathbf{y})}{t},$$

the double-layer potential (0.2.4) can be thought of as the potential due to surfaces S and $S_{t\nu_y} := \{\mathbf{y}+t\boldsymbol{\nu}(\mathbf{y}) : \mathbf{y} \in S\}$ with opposite charges $\pm\frac{\phi(\mathbf{y})}{t}$.

0.2.3 Solution via layer potentials

Let us give an overview of how these layer potentials yield existence and uniqueness for the Dirichlet Laplace problem, which is achieved by forming an operator equation in physical space for the unknown Neumann data. By comparison, our work is the Fourier analogue of this approach, where the global relation is an operator equation to be solved in spectral space instead. We emphasise that this approach *does not* rely on these classical results: Instead, existence and uniqueness results will be obtained independently via the Fokas method for Dirichlet data in $H^1(\partial\Omega)$, which is continuous across the vertices. Recall that for illustration of the layer potential method, we are following the approach of [Fol95], which considers domains with a C^2 boundary.

First, notice that (0.2.4) involves the outward normal derivative of N, $\partial_{\nu_y} N(x,y)$, for $x \in \Omega$. Let us denote this term by

$$K(x,y) := \partial_{\nu_y} N(x,y), \quad x,y \in S;$$

then $K(x,y)$ is continuous on $\{(x,y) \in S \times S : x \neq y\}$ and lies in the class of continuous kernels of order $(n-2)$. The associated integral operators to such kernels have important properties when defined on L^p spaces.

Proposition 0.2.2 ([Fol95])**.** *Given K, introduce the operator $T_K : L^2 \to L^2$ as*

$$T_K f(x) := \int_S K(x,y) f(y) \, \mathrm{d}\sigma(y).$$

- *T_K is a bounded and compact linear map*
- *For any bounded function f, $(T_K f)(x)$ is continuous.*
- *If $(I+T_K)f$ is continuous, then f is continuous.*

We are ready to consider boundary values of the solution. For this, consider the functions

$$u_t(x) := u(x + t\nu(x)).$$

Fix $x \in S$. Then the inner and outer boundary values are defined as

$$u_-(x) := \lim_{\substack{t\to 0\\ t<0}} u_t(x), \quad u_+(x) := \lim_{\substack{t\to 0\\ t>0}} u_t(x)$$

Theorem 0.2.3 ([Fol95]). *Suppose that u is a double layer potential with moment ϕ from (0.2.4). If $\phi \in C(S)$ then*

$$u_- = \left(\frac{1}{2}I + T_K\right)\phi, \quad u_+ = \left(-\frac{1}{2}I + T_K\right)\phi, \tag{0.2.6}$$

and so $\phi = u_+ + u_-$.

In a similar way, for the single layer potential, the normal derivative of u is given by

$$\partial_{\nu_x} u(x) = \int_S \partial_{\nu_x} N(x,y)\phi(y)\,\mathrm{d}\sigma(y), \quad x \in V \setminus S$$

where the change is ∂_{ν_x} instead of ∂_{ν_y}. Note that V is a tubular neighbourhood of S. For intuition, we think of this set as containing points on the inward normal $-\nu(x)$ and the outward normal $\nu(x)$ for each point $x \in S$. Then setting $K^*(x,y) := K(y,x)$, this integral is precisely $(T_{K^*}\phi)(x)$. For functions where the following limit exists, we can define the normal derivatives of u on an infinitesimally parallel surface as

$$\partial_{\nu_-} u(x) := \lim_{\substack{t\to 0\\ t<0}} \nu(x)\cdot\nabla u(x + t\nu(x)), \quad \partial_{\nu_+} u(x) := \lim_{\substack{t\to 0\\ t>0}} \nu(x)\cdot\nabla u(x + t\nu(x)),$$

then a similar result to Theorem 0.2.3 holds for these derivatives.

Theorem 0.2.4 ([Fol95]). *Suppose that u is a single layer potential with moment ϕ from (0.2.4). If $\phi \in C(S)$ then the limits $\partial_{\nu_\pm} u(x)$ exist for $x \in S$ and*

$$\partial_{\nu_-} u = \left(-\frac{1}{2}I + T_{K^*}\right)\phi, \quad \partial_{\nu_+} u = \left(\frac{1}{2}I + T_{K^*}\right)\phi,$$

and so $\phi = \partial_{\nu_+} u - \partial_{\nu_-} u$.

With this notation set, we are looking at the operators $T_K \pm \frac{1}{2}I$ and $T_{K^*} \pm \frac{1}{2}I$. It is convenient to consider the null spaces of these operators (see [Fol95, p.134]), and as such we obtain a decomposition result for the ranges, of these operators, and one such result is

that $L^2(S)$ can be decomposed as [4]:

$$L^2(S) = \text{Range}\left(\frac{1}{2}I + T_K\right).$$

Then given any Dirichlet data $f \in L^2(S)$, it must equal $(\frac{1}{2}I + T_K)\phi$ for some $\phi \in L^2(S)$. Thus

$$u(x) = \int_S \phi(y)\partial_{\nu_y} N(x,y)\,\mathrm{d}\sigma(y)$$

defines a harmonic function u with $u|_S = f$, as required.

Remark 0.2.5. *To solve the Laplace equation numerically, algorithms are required which can invert the operator $\frac{1}{2}I + T_K$. For the Fokas method we will show that we must also solve an operator equation of the form*

$$T\mathbf{\Phi} = \mathbf{\Psi},$$

where $\mathbf{\Psi}$ is a known function, and $T = I + K$ is similarly a compact perturbation of the identity. However while $N(x,y)$ has singularities as x approaches y in S, we will show that such singularities do not occur for the Fokas method.

0.2.4 The Steklov–Poincaré operator

For Lipschitz domains Ω and $u|_{\partial\Omega} \in C^1(\partial\Omega)$, the solution to the Laplace equation is determined uniquely from the Dirichlet data. For the Laplace problem it is usual to work with the derivative, q_z, of the solution q. For this, it was shown in [Fok08] that

$$q_z(z) = \frac{1}{2\pi}\sum_{k=1}^{n}\int_{l_k} e^{\mathrm{i}\lambda z}\rho_k(\lambda)\,\mathrm{d}\lambda,$$

and for the Helmholtz equation in (1.2.3). In either case, this formal integral representation involves both the values of q at the boundary, and its outward derivative; that is, both the Dirichlet and the Neumann data. The global relation seen above, is an equation relating the known boundary values to the unknown data. In view of these integral representations, this yields a solution to the PDE. Given Dirichlet data, D, a solution to the global relation means we have a formal map, S, which will reconstruct the Neumann data, N (and there is an inverse modulo Neumann data that differs by a constant)

$$S : D \mapsto N.$$

[4] In [Fol95] this is done in more generality, where Ω consists of an arbitrary number of disconnected regions, potentially with 'holes'.

The map S is a special case of the Steklov–Poincaré operator, which is a map between two forms of boundary data. In our case, we intend to solve for the Fourier transform $\hat{D}$ and $\hat{N}$ of the Dirichlet and Neumann data respectively. Given the one-to-one correspondence between square-integrable functions and their Fourier transform, this map S induces a map $\hat{S}$ between the Fourier transform, $\hat{D}$, of the Dirichlet data and the Fourier transform, $\hat{N}$, of the Neumann data:

$$\hat{S} : \hat{D} \mapsto \hat{N}.$$

This map will be realised as the solution to an operator equation $T\mathbf{\Phi}^{\mathrm{Ne}} = \mathbf{\Psi}$, where $\mathbf{\Phi}^{\mathrm{Ne}}$ consists of the Fourier transform of the unknown Neumann data, and $\mathbf{\Psi}$ can be determined precisely from the Fourier transform, $\mathbf{\Sigma}^d$, of the known Dirichlet data. Fixing $\mathbf{\Psi} \in \mathrm{Ran}(T)$, the Steklov–Poincaré operator is the map $\hat{S} : \mathbf{\Sigma}^d \mapsto \mathbf{\Phi}^{\mathrm{Ne}}$. Furthermore, since $\mathcal{F}S\mathcal{F}^{-1}(\mathcal{F}D) = \mathcal{F}N$, then to compare this new method with the Steklov–Poincaré operator S, one may compare eigenvalues.

Solution in Lipschitz domains

Before introducing the Fokas method as a new way to solve the Laplace BVP, we would like to remark on classical existence and uniqueness results for the Laplace equation. This will give us confidence that the domains used later are the natural spaces in which to look for solutions to the global relation. For simplicity, let us start with the following existence results for elliptic equations in a domain $\Omega \subset \mathbb{R}^2$ with a Lipschitz boundary. Consider the following Dirichlet BVP:

$$\begin{aligned} -\Delta u - \epsilon u = 0 \quad & \text{in } \Omega \\ u = f \quad & \text{on } \partial\Omega, \end{aligned} \tag{0.2.7}$$

which is the Helmholtz equation for $\epsilon > 0$, and the modified-Helmholtz equation for $\epsilon < 0$. Then the following classical existence theorem holds.

Theorem 0.2.6 ([GT01, Theorems 8.3, 8.6])**.** *For any function $\phi \in H^1(\Omega)$, the equation (0.2.7) with $f := \phi|_{\partial\Omega}$ has a unique solution, provided $\epsilon \leq 0$. If $\epsilon > 0$, there is a discrete set $\Sigma \subseteq \mathbb{R}_{>0}$ such that for $\epsilon \notin \Sigma$, the problem has a unique solution.*

In this Theorem, the boundary data is taken as $u = \phi$ on $\partial\Omega$, where both $u, \phi \in H^1(\Omega)$ are functions defined on the whole of Ω. So for this existence Theorem, f must be the boundary value of some such function ϕ. We will use standard properties of Sobolev spaces, which are helpfully introduced in [Eva10, Gri85, HW08]. It is known for example, that whenever functions are in $H^1(\Omega)$ their boundary values can be compared as L^2 functions (equivalently we require $u - \phi \in H^1_0(\Omega)$, which is the closure of test functions $D(\Omega)$ with respect to H^1 - see [Gri85, p.17]). Boundary values of such functions are known as *traces*,

and the trace γ is a map between a function defined on the domain Ω and a new function defined on the boundary $\partial\Omega$.

This Theorem tells us that whenever a function f defined on $\partial\Omega$ can be defined as the trace of a H^1 function on Ω, (0.2.7) has a unique solution, away from the Laplace eigenvalues.

An overview of the Steklov–Poincaré operator

We take these simplified results from more general ones given in [McL00, pp. 145-156]. Whenever the PDE (0.2.7) with $f = 0$ has a unique solution, we can define a solution operator of the Dirichlet problem as the map

$$\mathcal{U} : f \mapsto u.$$

The inverse of this map is called the trace operator, and the following Theorem indicates that we expect loss of $1/2$ Sobolev regularity. Indeed, this map is surjective and therefore optimal.

Theorem 0.2.7 (Trace Theorem [McL00, 3.37-38])**.** *Let Ω be a Lipschitz domain, then the trace operator may be defined on continuous functions as*

$$\begin{aligned} \gamma : C(\bar{\Omega}) &\to C(\partial\Omega) \\ u &\mapsto u|_{\partial\Omega}. \end{aligned} \tag{0.2.8}$$

This map γ has a unique extension as a bounded operator

$$\gamma : H^s(\Omega) \to H^{s-1/2}(\partial\Omega), \text{ for } s \in \left(\frac{1}{2}, \frac{3}{2}\right),$$

which has a continuous right-inverse.

Setting $s = 1$, and since γ is surjective, $\mathcal{U}f$ exists for any $f \in H^{\frac{1}{2}}(\partial\Omega)$ by Theorem 0.2.6. So the solution operator is defined as a map

$$\mathcal{U} : H^{\frac{1}{2}}(\partial\Omega) \to H^1(\Omega).$$

Since then this solution operator exists, the following Theorem permits a bounded extension of the conormal trace map. Indeed, it follows directly from this Theorem that for any Dirichlet data $\phi^{\mathrm{Di}} \in H^1(\partial\Omega)$, the Neumann data ϕ^{Ne} exists as an L^2 function.

Theorem 0.2.8 ([McL00, 4.25])**.** *Let Ω be a Lipschitz domain. Define the Steklov–Poincaré operator*

$$S : f \mapsto \mathcal{U}f \mapsto \gamma\partial_\nu\left(\mathcal{U}f\right).$$

If the solution operator exists for $f \in H^{\frac{1}{2}}(\partial\Omega)$, then S satisfies

$$\begin{aligned} S : H^1(\partial\Omega) &\to L^2(\partial\Omega) \\ f \mapsto \mathcal{U}f = u &\mapsto \gamma\partial_\nu u. \end{aligned} \tag{0.2.9}$$

Remark 0.2.9. *In the general setting, the Steklov–Poincaré operator corresponding to this is a map*

$$\begin{aligned} \mathcal{B}_\nu\mathcal{U} : H^{1/2}(\partial\Omega) &\to H^{-1/2}(\partial\Omega) \\ g \mapsto \mathcal{U}g = u &\mapsto \mathcal{B}_\nu u, \end{aligned} \tag{0.2.10}$$

where $\mathcal{B}_\nu u$ is the conormal derivative *which one can define (e.g. in Lipschitz domains) as*

$$\mathcal{B}_\nu u = \sum_j \nu_j \gamma(\mathcal{B}_j u),$$

with $\mathcal{B}_j u$ forming the principal part of the PDE in divergence form: $\mathcal{P}_0 u = -\sum_j \partial_j \mathcal{B}_j u$. In our case the elements $\mathcal{B}_j u = \partial_j u$, so that the conormal derivative is simply the outward normal in a trace sense. Thus the above equation for the conormal derivative can be realised as the (trace γ of) the normal derivative. In our specific case, this operator maps the Dirichlet *data f to the* Neumann data *$\mathcal{B}_\nu\mathcal{U}f$.*

In this discussion, we have assumed use of Sobolev spaces defined on the boundary. However for the polygon, we would like to consider functions defined on each edge. For $f \in H^1(\partial\Omega)$, it is necessary that for each edge Γ_j, $f_j := f|_{\Gamma_j} \in H^1(\Gamma_j)$, however we must also ask: is this sufficient? Since H^1 functions are continuous on line segments, we will see that a necessary and sufficient constraint is for the individual functions f_j to be continuous across the vertices (in lower regularity Sobolev spaces, this condition should be replaced by an integral constraint).

0.2.5 Trace spaces for the polygon

In this thesis we will be solving the Laplace and Helmholtz problems on polygons, and so it is necessary to understand the trace spaces corresponding to these domains. In our case, we begin with the Dirichlet data ϕ^{Di} on $\partial\Omega$ and, to use Theorem 0.2.6, we must find ϕ such that its trace is equal to ϕ^{Di}. We have seen that classically, having Dirichlet data in $H^{1/2}$ is sufficient for a solution. Practically, we will consider data in $\phi^{\mathrm{Di}} \in H^1(\partial\Omega)$, because we require the derivatives to be in $L^2(\partial\Omega)$ for our functionals to be bounded. Furthermore by Morrey's inequality, on each edge Γ_j we have the continuous embedding

$$H^1(\Gamma_j) \hookrightarrow C^{0,\frac{1}{2}}(\Gamma_j),$$

so that ϕ^{Di} is indeed Hölder continuous on each edge. This will make the compatibility criteria on each edge easier to deal with. We note here that these are classical results, which *are not* required for the Fokas method. Instead, the Fokas method provides an alternative proof of existence via the Ehrenpreis-type integral representations. In this sense, the classical results are *not* assumed in this thesis; they do however provide motivation for working in spaces with Dirichlet data in $H^1(\partial\Omega)$. In this thesis, through an integration by parts, the conditions for regularity are obtained independently, and will be presented for two-dimensional and three-dimensional problems in Sections 2.9 and 5.5. By way of comparison, we shall present some selected (weaker than optimal) classical results, from which the following result is deduced.

Theorem 0.2.10 (Existence for the Helmholtz Dirichlet problem)**.** *Let Ω be a polygonal domain with boundary $\partial\Omega = \cup_{j=1}^{n}\Gamma_j$, where each Γ_j is an edge of the polygon. Further, let $f_j \in H^1(\Gamma_j)$ for each $j = 1, \ldots, n$. Set $\Gamma_0 := \Gamma_n$ and suppose further that these functions are continuous across the vertices:*

$$f_j(z_j) = f_{j-1}(z_j) \quad \text{at the vertex} \quad \{z_j\} = \Gamma_{j-1} \cap \Gamma_j, \quad \text{for } j = 1, \ldots, n.$$

Define $f \in L^2(\partial\Omega)$ by $f|_{\Gamma_j} := f_j$.

Then there exists $\tilde{f} \in H^1(\Omega)$ such that $\gamma\tilde{f} = f$ on $\partial\Omega$, and thus a unique solution to the Dirichlet problem (0.2.7) away from eigenvalues.

This result means that the Steklov–Poincaré map defined above exists; that the Dirichlet–Neumann map we consider later is well-defined (we will provide a second proof of this), and that the Paley–Wiener space we choose for our analysis is valid for finding solutions to (0.2.7).

Finally, before introducing the global relation, it remains to consider the trace Theorems for polygonal domains. In Theorem 0.2.7 we have assumed use of the Sobolev spaces $H^{1/2}(\partial\Omega)$. The difficulty in our case is that the boundary is not smooth, so firstly we emphasise some characteristics of Sobolev spaces defined on polygons.

Consider two line segments $\Gamma_1 = (-1, 0)$ and $\Gamma_2 = (0, 1)$. Is it sufficient to say that $H^1((-1, 1)) \cong H^1(\Gamma_1) \times H^1(\Gamma_2)$? Is a general H^1 function simply a concatenation of any two H^1 functions on the individual segments? Indeed, for $s > n/2$ it is known that functions in $H^s(\mathbb{R}^n)$ have a continuous representative. In particular for a one-dimensional line segment $H^1(\partial\Omega)$ functions are continuous[5]. But in general two functions in $H^1(\Gamma_1)$ and $H^1(\Gamma_2)$ will not respect this condition. There must be an additional *compatibility requirement*. For our example here, the compatibility requirement is clear: it is necessary and sufficient for the two functions to agree at 0 (recall these individual functions are

[5]to avoid burdensome discussion, if a member of an equivalence class has a special property (such as continuity), we shall speak of the equivalence class in terms of this function. So we say for example that H^1 functions *are continuous* on line segments.

continuous). That is,

$$H^1(-1,1) = \{u : (-1,1) \to \mathbb{R} : u_j := u|_{\Gamma_j} \in H^1(\Gamma_j),\ j = 1,2 \text{ and } \gamma u_1|_{x=0} = \gamma u_2|_{x=0}\}.$$

We now extend the definition of Sobolev spaces defined on open sets to a closed polygonal boundary. We follow the approach of [Gri85] and rephrased in [HW08]. These results can be extended to more general (curvilinear) domains; more general Sobolev spaces for $p \neq 2$, and general manifolds. But let us follow a coordinate-based parameterisation approach to aid intuition:

Definition 0.2.11. *Given an open bounded set $\Omega \subset \mathbb{R}^n$, the Sobolev space $H^m(\Omega)$ for $m \in \mathbb{Z}_{\geq 0}$ is defined as the completion of $C^m(\Omega)$ with respect to the norm*

$$\|u\|_{H^m(\Omega)} := \left(\sum_{|\alpha| \leq m} \|D^\alpha u\|_{L^2(\Omega)} \right)^{1/2}.$$

For $0 < s \in \mathbb{R} \setminus \mathbb{Z}$, write $s = m + \sigma$ for $\sigma \in (0,1)$. Then $H^s(\Omega)$ is the completion of $C^m(\Omega)$ with respect to the norm

$$\|u\|_{H^s(\Omega)} := \left(\|u\|_{H^m(\Omega)} + \sum_{|\alpha|=m} \iint_{\Omega \times \Omega} \frac{|D^\alpha u(x) - D^\alpha u(y)|^2}{|x-y|^{n+2\sigma}} \,\mathrm{d}x \,\mathrm{d}y \right)^{1/2}.$$

Definition 0.2.12. *Given a curve segment Γ_j defined by the map $\gamma_j : [a_j, b_j] \to \mathbb{R}$, the Sobolev space is defined using the definition above for $H^s(a,b)$:*

$$H^s(\Gamma_j) := \{u : \Gamma_j \to \mathbb{R} : u|_{\Gamma_j}(\gamma_j(\cdot)) \in H^s(a_j, b_j)\}.$$

For a general polygonal boundary $\partial\Omega = \bigcup_{j=1}^n \Gamma_j$ with smooth components, we would like to think of the analogue of the trace at the boundary. This involves firstly the boundary spaces, T, which enforce Sobolev regularity on each edge Γ_j; and secondly the necessary compatibility conditions. These results can be extended for *mixed* Dirichlet and Neumann data, however it is sufficient for our needs here to consider Dirichlet data only.

Definition 0.2.13 ([HW08, p.186])**.** *Define the boundary space to be a product of the admissible functions over each segment of the boundary*[6]*:*

$$T^1(\partial\Omega) = \prod_{j=1}^n H^1(\Gamma_j).$$

As we have discussed, some compatibility conditions at the vertices are required, and

[6] Similar definitions yield fractional spaces $T^{k+1/2}(\partial\Omega)$, for $k \in \mathbb{N}$.

these are given in [HW08, p.187] and [Gri85, p.50]. For our Dirichlet problem, these reduce to the following:

Definition 0.2.14 (Compatibility conditions)**.** *The compatibility conditions at the vertex* $z_j \in \Gamma_j \cap \Gamma_{j-1}$ *are:*

$$f_j(z_j) = f_{j-1}(z_j), \quad \text{for } \sigma > 0 \tag{0.2.11}$$

Remark 0.2.15. *In [Gri85], (0.2.11) is replaced by an integral relation. This is not required in our case, because we shall only consider* more regular *boundary data* $\phi^{\mathrm{Di}} \in T^1(\partial\Omega)$*, i.e. on each edge,* $\phi^{\mathrm{Di}}|_{\Gamma_j} \in H^1(\Gamma_j) \subset H^{1/2}(\Gamma_j)$*. As remarked in [Gri85, p.44], the integral condition reduces to (0.2.11) (and indeed whenever the given function is Hölder continuous). Thus the compatibility conditions are satisfied if, and only if, the functions are continuous across the vertices.*

Finally then, let us define the subspaces, P, of T to be those satisfying the compatibility conditions

$$P^1(\partial\Omega) := \{f \in T^1(\partial\Omega) : f_j := f|_{\Gamma_j} \text{ satisfy conditions (0.2.11)}\}.$$

Then the following trace Theorem is a restatement of Theorem 0.2.7 in this new notation.

Theorem 0.2.16 (Trace Theorem [Gri85, HW08])**.** *The mapping*

$$u \mapsto \gamma u$$

is a linear and surjective mapping from $H^1(\Omega)$ *onto* $P^{\frac{1}{2}}(\partial\Omega) \supset P^1(\partial\Omega)$*. In particular, for any* $f \in P^1(\partial\Omega)$ *there exists a function* $\tilde{f}$ *in* $H^1(\Omega)$ *such that* $\gamma\tilde{f} = f$*.*

Remark 0.2.17. *Similar to the trace Theorems for smooth domains, we observe loss of* $1/2$ *derivatives in the Sobolev sense. The additional requirement here is the compatibility conditions.*

We may now prove the existence Theorem 0.2.10 in this new notation. This is the key theorem that justifies our choice of spaces in the following chapters. This states that provided the Dirichlet data is in H^1 on each edge, then we need only impose continuity at the vertices to obtain existence and uniqueness to the Dirichlet problem (away from eigenvalues). Thus in the following chapters we will choose spaces that respect this condition.

Theorem 0.2.18 (Existence for the Helmholtz Dirichlet problem on a polygon)**.** *Let* $f \in H^1(\Gamma_j)$*, and satisfying (0.2.11). Then the Dirichlet problem (0.2.7) has a unique solution* $u \in H^1(\Omega)$ *away from the Dirichlet eigenvalues.*

Proof. The boundary data lies in $P^{1/2}(\partial\Omega)$. By Theorem 0.2.16, there exists a function f, such that $f \in H^1(\Omega)$ and $\gamma f|_{\Gamma_j} = f_j$. By the existence Theorem 0.2.6, there exists a unique solution $u \in H^1(\Omega)$ to the Dirichlet problem. □

Remark 0.2.19. *In the mixed boundary data case, we require additional regularity on the Dirichlet components, so that the Dirichlet data f_j on edge Γ_j with $j \in \mathcal{D}$ is in $H^{3/2}(\Gamma_j)$, and the Neumann data for $j \in \mathcal{N}$ we have $f_j \in H^{1/2}(\Gamma_j)$. Furthermore the compatibility criteria are more complicated due to the interaction between Dirichlet and Neumann data over the boundary. Since the Dirichlet data is now more regular, there is a stronger result in [Gri85, Theorem 5.1.2.4] which guarantees existence of a solution $u \in H^2(\Omega)$.*

To conclude this overview, it is worth remarking that a separate approach in literature is to consider the inhomogeneous Dirichlet Laplace problem

$$\begin{aligned} -\Delta w &= g \text{ in } L^2(\Omega) \\ w &= 0 \text{ on } \partial\Omega. \end{aligned}$$

Supposing this can be solved and in view of the trace Theorems, our Dirichlet problem (0.2.7) may be reduced to this case as follows:

1. Let $f \in H^{\frac{3}{2}}(\partial\Omega)$.
2. There exists $\tilde{f} \in H^2(\Omega)$ such that $\gamma\tilde{f} = f$.
3. Solve the inhomogeneous Dirichlet problem with $g = \Delta\tilde{f} \in L^2(\Omega)$.
4. The solution $u = w + \tilde{f} \in H^1(\Omega)$ solves (0.2.7).

This naive approach does require additional Dirichlet regularity, and is therefore non-optimal, but provides a good bridge between the related Theorems. Indeed, whenever the proof involves a weak formulation, w and g are only required to be in $H^1(\Omega)$, or even $H^{-1}(\Omega)$, and the regularity of f may be reduced.

CHAPTER 1

Introduction to the Fokas method

In this Chapter we present the Fokas method for the Helmholtz equation in an equilateral triangle, following the theory introduced in [Fok01, Fok08] and developed in [FK14]. We will see the first example of the global relation which, given an elliptic PDE, is an equation relating the known boundary data to the unknown boundary data. Solving this equation is equivalent to solving the PDE in the following sense: if at every point on the boundary of a domain both the Dirichlet and Neumann data is known, then the solution is given as an integral involving these (known) functions. This follows from Green's integral representation for the solution to a PDE [FS12]: For $4\beta^2 \in \mathbb{R}$, whenever we have a fundamental solution, $E(\boldsymbol{\xi}, \boldsymbol{x})$, which is a function satisfying

$$\left(-\Delta + 4\beta^2\right) E(\boldsymbol{\xi}, \boldsymbol{x}) = \delta(\boldsymbol{\xi} - \boldsymbol{x}), \quad \boldsymbol{\xi} \in \mathbb{R}^2,$$

then a solution to $-\Delta u + 4\beta^2 u = 0$ is given as an integral of the Dirichlet, Neumann and Green's function:

$$u(\boldsymbol{x}) = \int_{\partial\Omega} \left(E(\boldsymbol{\xi}, \boldsymbol{x})\partial_{\boldsymbol{\nu}} u(\boldsymbol{\xi}) - u(\boldsymbol{\xi})\partial_{\boldsymbol{\nu}} E(\boldsymbol{\xi}, \boldsymbol{x})\right) \mathrm{d}S(\boldsymbol{\xi}), \quad \boldsymbol{x} \in \Omega.$$

Such an integral representation over the boundary may also be obtained by Green's Theorem. We will be using similar results throughout, so we present here the equivalence between the "complex" Green's Theorem and the real Green's Theorem. This follows through a change of coordinates and differing notation for integrals of complex differential forms, and real integrals. As a result, it is hopefully helpful to remark on some of the conventions here; so the reader may compare more easily the different approaches.

1.1 Green's Theorem, real and complex

Recall that Green's Theorem for real-valued functions P, Q depending on two variables x, y is given for a region Ω with a boundary Γ as

$$\int_\Gamma P(x,y)\,\mathrm{d}x + Q(x,y)\,\mathrm{d}y = \iint_\Omega \left(Q_x(x,y) - P_y(x,y)\right)\mathrm{d}x\,\mathrm{d}y,$$

where for a given line segment $(x,y)(t) = (f(t), g(t))$, the left-hand integral uses precisely that $\mathrm{d}x = f'(t)\,\mathrm{d}t$, and similarly for $\mathrm{d}y$. However for complex functions, we wish to apply a similar trick on a differential form $W(z,\bar{z})$. Suppose now that $W(z,\bar{z}) = F(z,\bar{z})\,\mathrm{d}z - G(z,\bar{z})\,\mathrm{d}\bar{z}$. Then

$$\mathrm{d}W = -\left(F_{\bar{z}} + G_z\right)\mathrm{d}z \wedge \mathrm{d}\bar{z}.$$

Stoke's Theorem would give us

$$\iint_\Omega \mathrm{d}W = \int_\Gamma W.$$

We can recover Stoke's Theorem from Green's Theorem by setting $W = (F-G)\,\mathrm{d}x + \mathrm{i}(F+G)\,\mathrm{d}y$ using $\mathrm{d}z = \mathrm{d}x + \mathrm{i}\,\mathrm{d}y$ and $\mathrm{d}\bar{z} = \mathrm{d}x - \mathrm{i}\,\mathrm{d}y$. By Green's Theorem, we obtain

$$\begin{aligned}\int_\Gamma (F-G)\,\mathrm{d}x + \mathrm{i}(F+G)\,\mathrm{d}y &= \iint_\Omega \left(\mathrm{i}(F+G)_x - (F-G)_y\right)\mathrm{d}x\,\mathrm{d}y \\ &= \iint_\Omega \left((\mathrm{i}F_x - F_y) + (\mathrm{i}G_x + G_y)\right)\mathrm{d}x\,\mathrm{d}y.\end{aligned} \tag{1.1.1}$$

The left-hand side is $\int_\Gamma W$. We can check that this is precisely Stokes' Theorem, by using the substitutions

$$\mathrm{d}x = \frac{1}{2}(dz + d\bar{z}), \quad \mathrm{d}y = \frac{1}{2\mathrm{i}}(dz - d\bar{z}),$$

so $\mathrm{d}x\,\mathrm{d}y = \frac{-1}{2\mathrm{i}}\,\mathrm{d}z \wedge \mathrm{d}\bar{z}$. Using standard differentiation identities (see also (2.1.2)),

$$\mathrm{d}W = -(F_{\bar{z}} + G_z)\,\mathrm{d}z \wedge \mathrm{d}\bar{z} = \frac{-1}{2}\left(F_x + \mathrm{i}F_y + G_x - \mathrm{i}G_y\right)(-2\mathrm{i}\,\mathrm{d}x \wedge \mathrm{d}y),$$

which is precisely equal to the right-hand side of (1.1.1).

1.2 Helmholtz problem

To introduce the Fokas method, let us follow the approach of [FK14], which solves the Dirichlet eigenvalue problem for the Laplacian in an equilateral triangle. Setting the do-

main Ω to be the equilateral triangle with vertices at

$$z_1 = \frac{2}{\sqrt{3}} e^{-\mathrm{i}\pi/3}, \quad z_2 = \frac{2}{\sqrt{3}} e^{\mathrm{i}\pi/3}, \quad z_3 = \frac{-2}{\sqrt{3}},$$

the modified Helmholtz equation ($\beta^2 > 0$) in our triangle is $\Delta q - 4\beta^2 q = 0$, with zero Dirichlet data. We have seen this is equivalent to the complex form

$$q_{z\bar{z}} - \beta^2 q = 0.$$

A quick calculation shows that the following differential forms are closed ($\mathrm{d}W = 0$):

$$W_1 = \left(e^{-\mathrm{i}kz + \mathrm{i}\beta^2/k} \left(q_z + \mathrm{i}kq \right) \right) \mathrm{d}z - \left(e^{-\mathrm{i}kz + \mathrm{i}\beta^2/k} \left(q_{\bar{z}} + \frac{\beta^2}{\mathrm{i}k} q \right) \right) \mathrm{d}\bar{z}$$
$$W_2 = \left(e^{-\mathrm{i}\beta^2(kz - \bar{z}/k)} \left(q_z + \mathrm{i}k\beta^2 q \right) \right) \mathrm{d}z - \left(e^{-\mathrm{i}\beta^2(kz - \bar{z}/k)} \left(q_{\bar{z}} + \frac{\beta^2}{\mathrm{i}k} q \right) \right) \mathrm{d}\bar{z}$$

The latter equation yields more symmetric functions in $k - 1/k$, but any resulting equations are 'effectively' equivalent - insomuch as solving the global relation is equivalent to solving the PDE. The former equation will be used in our analysis, as it permits us to treat large k behavior of the Helmholtz as perturbations of the Laplace problem (for $\beta^2 = 0$). Specifically, any path deformations valid for $\beta^2 = 0$ are also valid for $\beta^2 \neq 0$. We shall pursue this in later chapters. For now, we show how the method in [FK14] uses the Fokas method to give *precise* eigenvalues for the Laplacian.

It is convenient to consider the parameterisation of each edge in terms of $z_j(s)$. By symmetry of the problem, we can set $w = e^{2\pi \mathrm{i}/3}$ and

$$z_1(s) = \frac{1}{\sqrt{3}} + \mathrm{i}s, \quad z_2(s) = w z_1(s), \quad z_3(s) = w^2 z_1(s) \equiv \overline{w} z_1(s).$$

Since $W := W_1$ is closed, we have the global relation

$$\int_{\partial\Omega} W = 0, \tag{1.2.1}$$

that the sum of the integrals over each edge is 0. Considering the first edge, we can equally think of the parameterisation as $z_1(s) = m_1 + s e^{\mathrm{i}\alpha_1}$, for m_1 the midpoint and α_1 the angle of the edge. Then a substitution into the global relation (1.2.1) gives a contribution from the first edge of

$$\int_{-1}^{1} e^{-\mathrm{i}k(m_1 + s e^{\mathrm{i}\alpha_1}) + \mathrm{i}\frac{\beta^2}{k}(\overline{m_1} + s e^{-\mathrm{i}\alpha_1})} \left(\frac{e^{-\mathrm{i}\alpha_1}}{2} (q_\tau^{(1)} + \mathrm{i} q_N^{(1)}) + \mathrm{i}k q^{(1)} \right) e^{\mathrm{i}\alpha_1} \, \mathrm{d}s$$
$$- e^{-\mathrm{i}k(m_1 + s e^{\mathrm{i}\alpha_1}) + \mathrm{i}\frac{\beta^2}{k}(\overline{m_1} + s e^{-\mathrm{i}\alpha_1})} \left(\frac{e^{\mathrm{i}\alpha_1}}{2} (q_\tau - \mathrm{i} q_N) - \mathrm{i}\frac{\beta^2}{k} q \right) e^{-\mathrm{i}\alpha_1} \, \mathrm{d}s$$

$$= e^{-\mathrm{i}km_1+\mathrm{i}\frac{\beta^2}{k}\overline{m_1}}\int_{-1}^{1} e^{-\mathrm{i}kse^{\mathrm{i}\alpha_1}+\mathrm{i}\frac{\beta^2}{k}se^{-\mathrm{i}\alpha_1}}\left(\mathrm{i}q_N^{(1)}+(\mathrm{i}ke^{\mathrm{i}\alpha_1}+\mathrm{i}\frac{\beta^2}{k}e^{-\mathrm{i}\alpha_1})q^{(1)}\right)\mathrm{d}s.$$

Here, the functions $q^{(j)}(s) := q(z_j(s))$ and $q_\tau^{(j)}(s), q_N^{(j)}(s)$ are the pullback of the function q and its tangential and normal derivatives on the edge j - see also Section 2.1.1. In our particular case however, $\alpha_1 = \pi/2$ so the expression simplifies to

$$\hat{q}_j(k) := e^{-\mathrm{i}km_1+\mathrm{i}\frac{\beta^2}{k}\overline{m_1}}\int_{-1}^{1} e^{(k+\frac{\beta^2}{k})s}\left(\mathrm{i}q_N^{(j)}-\left(k-\frac{\beta^2}{k}\right)q^{(j)}\right)\mathrm{d}s, \quad \text{for } j=1,$$

meaning that the data $q_N^{(1)}, q^{(1)}$ is taken on the first edge.

By symmetry of the problem, it was shown that $m_2 = wm_1, \overline{m_2} = \overline{m_1}/w$ and $e^{\mathrm{i}\alpha_2} = we^{\mathrm{i}\alpha_1}$, so the resulting expression on the second edge is

$$e^{-\mathrm{i}(wk)m_1+\mathrm{i}\frac{\beta^2}{(wk)}\overline{m_1}}\int_{-1}^{1} e^{((wk)+\frac{\beta^2}{k})s}\left(\mathrm{i}q_N^{(2)}-\left((wk)-\frac{\beta^2}{(wk)}\right)q^{(2)}\right)\mathrm{d}s = \hat{q}_2(wk).$$

Thus the global relation can be written, symmetrically and succinctly in [FK14] as

$$\sum_{j=1}^{3}\hat{q}_j(w^{j-1}k) = 0. \tag{1.2.2}$$

The solution to the Helmholtz equation is given by[1]

$$q(z,\bar{z}) = \frac{1}{4\pi\mathrm{i}}\sum_{j=1}^{3}\int_{l_j} e^{\mathrm{i}kz-\mathrm{i}\frac{\beta^2}{k}\bar{z}}\hat{q}_j(w^{j-1}k)\frac{\mathrm{d}k}{k} \tag{1.2.3}$$

where l_j are the rays of argument $-\arg(z_{j+1}-z_j)$, i.e. $-\pi/2, 5\pi/6, \pi/6$ respectively [2]. Most importantly, these contours are free to be deformed *inside* the regions where the exponent is bounded, and this idea will be crucial throughout.

For the purposes of simplifying our equation, we may use the functions

$$N_j(k) = \int_{-1}^{1} e^{\left(k+\frac{\beta^2}{k}\right)s}q_N^{(j)}(s)\,\mathrm{d}s, \quad E(k) := e^{\left(k+\frac{\beta^2}{k}\right)\frac{1}{\sqrt{3}}}.$$

Then the resulting global relation is

$$E(-\mathrm{i}k)N_1(k)+E(-\mathrm{i}wk)N_2(wk)+E(-\mathrm{i}w^2k)N_3(w^2k) = 0.$$

The Dirichlet problem for the modified-Helmholtz equation is for zero boundary data, $q^{(j)}(s) = 0$ for $j = 1,2,3$. The values $4\beta^2$ which admit a non-zero solution are called the

[1] Compare with (0.1.7).

[2] The contours for Helmholtz are slightly different than these for modified-Helmholtz (see [Fok01]), and arise because of the algebraic variety Z_P.

eigenvalues for the Laplacian. Importantly, using the Fokas method, the corresponding eigenfunctions may be derived *analytically* for the equilateral triangle.

Proposition 1.2.1 ([FK14]Proposition 2.1)**.** *There exists solutions*

$$q_N^{(j)}(s) = \sum_{l=1}^{3} \alpha_l^{(j)} e^{ia_l^{(j)} s},$$

for every eigenvalue $4\beta^2 = -4(m^2 + mn + n^2)\pi^2/9$ *with* $n, m \in {}^{\mathbb{Z}}$*. The constants* $a_l^{(j)}$ *are given precisely in terms of* n, m*, and the coefficients* $\alpha_l^{(j)}$ *as constant multiples of* $\alpha_1^{(1)}$*, i.e. the eigenfunctions are defined up to a rescaling.*

In [FFX04, SFFS08, SSF10, FF11, Dav08, FIS15] a number of approaches have been given for solving the D2N map numerically, and these are discussed and compared also in [FP15, 6.1.10]. In these approaches the D2N map has been inverted numerically via a collocation method, such that the relation is enforced to hold on a number of points in the plane. By choosing these points well, and using a suitable basis to reconstruct, good results of convergence have been obtained. We shall later be comparing convergence results with [FF11] who choose 'Halton nodes' as the collocation points, and use a polynomial basis of Legendre polynomials, for which the Fourier transform of the basis is given analytically. As such, this will be a convenient basis for us to use here. Furthermore, numerical experiments show exponential convergence rates for this approach, but a rigorous proof of convergence is not given. In contrast, the numerical approach presented in this thesis yields a proof of spectral convergence rates for the two-dimensional Laplace problem with C^∞ boundary data, where the Legendre polynomial basis is used. This will be presented in Theorem 2.7.2.

CHAPTER 2

The Laplace equation

Having listed some classical results regarding existence of solutions to the Dirichlet problem, we move on to the global relation in regards to the Laplace equation. The work of [Ash13] reformulates this relation as an operator equation $T\boldsymbol{x} = \boldsymbol{y}$ between Banach spaces. A careful choice of these spaces yields boundedness and coercivity for the operator T; permitting a new Galerkin-type numerical method. We shall begin by setting up notation to describe the polygon, and the boundary data we will use. Then we will introduce a space of functions called the Paley–Wiener spaces which, in view of the existence Theorem of the previous Chapter, are ideal spaces to use when solving this operator equation. Using results in [Ash13], we give an implementation of a numerical method for solving the Laplace equation. Of special interest is the proof of spectral convergence given in Section 2.7 for sufficiently regular boundary data.

2.1 Initial set up

In this section, we follow the proof in [Ash13], which begins with reformulating the solution operator in terms of a linear operator equation. This builds on more general work in [Fok01, FK03] and [Ash12], where it is shown that, whenever a solution exists, the boundary data obeys a given relation, called the global relation.

We consider the following Dirichlet problem:

$$\begin{aligned} \Delta q &= 0 \quad \text{in } \Omega \\ q &= f_j \in H^1(\Gamma_j) \text{ for } j = 1, \dots, n, \end{aligned} \tag{2.1.1}$$

where Ω is a convex polygonal domain with edges $(\Gamma_j)_{j=1}^n$, and $H^1(\Gamma_j)$ is the Sobolev space of weakly differentiable functions on the line segment. We require that the Dirichlet data is continuous at each vertex $z_{j+1} \in \Gamma_j \cap \Gamma_{j+1}$, so that $f_j(z_{j+1}) = f_{j+1}(z_j)$.

Remark 2.1.1. *The approach in [Ash13] supposes the boundary data to be in $H_0^1(\Gamma_j)$ on*

each edge, which is the subspace of functions in $H^1(\Gamma_j)$ with vanishing trace. Equivalently, this is the closure of C_c^∞ functions in H^1 with the norm $\|f\|_{H_0^1} := \int |\nabla f|^2$. However we note that given any non-zero vertex values $f(z_j)$ at each vertex $\{z_j\}_{j=1}^n$, there exists a complex polynomial $p(x,y)$ attaining these values. The new function $u - \Re p(x,y)$ is also harmonic and solves the BVP with data $(f-p) \in H_0^1(\Gamma_j)$. Thus this additional condition is not a restriction.

We have seen above that this regularity is sufficient to ensure existence of a solution, and of the Dirichlet–Neumann (D2N) map. Rigorous results for existence and regularity of solutions are given in [BN08, Gri85, McL00, HW08, Dau88]. This new approach also yields an alternate proof of existence.

2.1.1 Pullback of boundary data

Ω may be defined by its vertices $\{z_j\}_{j=1}^n$ labelled anticlockwise around the origin, where each edge $\{\Gamma_j\}$ is from z_j to z_{j+1}. We also use the midpoint $m_j := (z_{j+1}+z_j)/2$ of the edge and the angle $\alpha_j := \arg(z_{j+1}-z_j)$ to denote the angle between Γ_j and the positive real axis. It is convenient to denote the difference, $(\alpha_k - \alpha_j)$, between two angles by Δ_{kj}. Each edge Γ_j of length $|\Gamma_j| = 2\sigma_j$ has a natural parameterisation

$$\gamma_j(t) = m_j + te^{\mathrm{i}\alpha_j}, \quad t \in [-\sigma_j \sigma_j]\,.$$

It will be necessary to pullback functions $f : \Gamma_j \to \mathbb{R}$ with this parameterisation, so that $\gamma_j^* f : [-\sigma_j\sigma_j] \to \mathbb{R}$, so we present this here for convenience.

Let Γ be a line segment, which we think of as an edge of the polygonal domain $\Omega \subset \mathbb{R}^2$, and let γ be its parameterisation. Then given $f : \Gamma \to \mathbb{R}$, we shall use the pullback $\psi^* f : [-\sigma, \sigma] \to \mathbb{R}$, of f by γ, which is defined as

$$(\gamma^* f)(\tau) := f(\gamma(\tau)).$$

For existence and regularity, we shall impose that the Dirichlet data $f_j \in H^1(\Gamma_j)$ for each $j = 1, \ldots, n$, and continuous at the vertices. However it is worth noting here one significant advantage of working in spectral space[1]:

Proposition 2.1.2 ([Rud91] p.199)**.** *If f is a distribution of compact support on $\mathbb{C}^n$, then define $\hat{f} : \mathbb{C}^n \to \mathbb{C}^n$ to be the formal Fourier transform of f:*

$$\hat{f}(y) := \langle f, e^{-\mathrm{i}x\cdot y}\rangle,$$

where the distribution acts on the x variable. Then $\hat{f} : \mathbb{C}^n \to \mathbb{C}^n$ is analytic. Furthermore

[1] This result is one of the *Paley–Wiener* Theorems, and we shall see special properties of these functions later on. A survey of Paley–Wiener spaces is given in Appendix B.

there exist constants N and r (relating to the distribution and its support) such that

$$|\hat{f}(z)| \lesssim (1+|z|)^N e^{r|\Im z|}, \quad z \in \mathbb{C}.$$

Remark 2.1.3. *We are only considering more regular boundary data $f_j \in H^1(\Gamma_j)$, and not simply distributional data. However, the Fokas method involves a relation between the Fourier transform of known and unknown functions. In view of Proposition 2.1.2, even for distributional boundary data, this global relation will be an equality of analytic functions. We have chosen to include the details about distributional boundary data here to highlight the power of the Fokas method in forming a smooth operator equation. To emphasise, we do not solve the Laplace problem for distributional boundary data but, using similar methods, one can* in principle *aim to solve the Laplace equation with point charges (Dirac data). However as we will see, rigorous proofs of convergence and stability are given only for more regular Dirichlet data.*

The pullback map introduced above has a natural extension to the space of distributions f on Γ (with the topology as given in [AF15a]) using the change of variables formula

$$\begin{aligned}\langle \gamma^* f, \Phi \rangle &= \int_{[-\sigma,\sigma]} f(\gamma(\tau))\Phi(\tau)\,\mathrm{d}\tau \\ &= \int_{\Gamma} f(y)((\gamma^{-1})^*\Phi)(y)|D\gamma^{-1}|(y)dy \\ &= \langle f, (\gamma^{-1})^*\Phi \cdot |D\gamma^{-1}| \rangle.\end{aligned}$$

As an example, suppose our boundary data were a delta function $\delta(x)$ at some point $x \in \partial\Omega$. An analysis for Laplace's equation with distributional boundary data is given in [BN08]; these kinds of boundary data are called *concentrated loads*, and are of interest in engineering settings. This data would correspond to a point charge at the boundary, and the potential may be found explicitly.

For example, suppose $f = \delta(m_j)$ is a Dirac mass at the midpoint of Γ_j. Since γ_j is the arclength parameterisation, then $|D\gamma_j^{-1}| = 1$ and $\gamma_j^* f = \delta_0$. We can check this by considering $\delta(m_j)$ as the limit of centered Gaussians, and calculating their pullbacks by γ_j.

2.1.2 Geometric identities

It will occasionally be useful to think of a given function in a number of coordinate frames. For example, given a function $q_C(z,\bar{z}) : \mathbb{C}^2 \to \mathbb{C}$, we may wish to find its normal derivative along some line $\Gamma \subset \mathbb{C}$ (i.e. the Neumann data). In this section we state some identities relating derivatives and the geometry of the problem, which will be used when inputting the Dirichlet data in the final sections. We note that our solution q can be represented in

a number of coordinate frames; in real (R) coordinates, in complex (C) coordinates, and in polygonal (P) coordinates:

$$q_R(x,y) = q_C(z,\bar{z}) = q_P(\tau, N).$$

The former are standard notation for complex variables and the final equality involves the tangent (τ) and normal (N) coordinates for a chosen edge Γ_k. Then the following identities hold:

$$\partial_z = \frac{1}{2}(\partial_x - \mathrm{i}\partial_y) = \frac{1}{2}e^{-\mathrm{i}\alpha_k}(\partial_\tau + \mathrm{i}\partial_N) \qquad \partial_x = \partial_z + \partial_{\bar{z}} \qquad \partial_\tau = e^{\mathrm{i}\alpha_k}\partial_z + e^{-\mathrm{i}\alpha_k}\partial_{\bar{z}} \tag{2.1.2a}$$

$$\partial_{\bar{z}} = \frac{1}{2}(\partial_x + \mathrm{i}\partial_y) = \frac{1}{2}e^{\mathrm{i}\alpha_k}(\partial_\tau - \mathrm{i}\partial_N) \qquad \partial_y = \mathrm{i}(\partial_z - \partial_{\bar{z}}) \qquad \partial_N = -\mathrm{i}(e^{\mathrm{i}\alpha_k}\partial_z - e^{-\mathrm{i}\alpha_k}\partial_{\bar{z}}) \tag{2.1.2b}$$

Example 2.1.4. *Consider the square with vertices at the four roots of unity, so that each edge has length $2\sigma_j = \sqrt{2}$. Consider the harmonic function $q_R(x,y) = xy$ which vanishes at the vertices. We wish to determine the parameterisation of the function $\vartheta_j := \gamma_j^*(\partial_\tau q)$: considering the first edge $\gamma_1(\tau) = \frac{1+\mathrm{i}}{2} + \tau e^{3\mathrm{i}\pi/4}$, observation tells us that since $y = 1 - x$ on the edge, we expect a reparameterisation in τ of the quadratic $x - x^2$. Thus the derivative is linear and decreasing as τ varies from $-\sqrt{2}/2$ to $\sqrt{2}/2$.*

This is realised by rewriting q_R as

$$q_C(z,\bar{z}) = \frac{1}{4\mathrm{i}}\left(z^2 - \bar{z}^2\right),$$

and using (2.1.2), we find

$$\partial_\tau q_P|_{\Gamma_1} = \left(e^{3\mathrm{i}\pi/4}\frac{z}{2\mathrm{i}} - e^{-3\mathrm{i}\pi/4}\frac{\bar{z}}{2\mathrm{i}}\right)\Big|_{z=\gamma_1(\tau)},$$

and so

$$\vartheta_1(\tau) = \tau\Im(e^{6\mathrm{i}\pi/4}) = -\tau,$$

as expected.

This example illustrates how we may computationally find the Dirichlet derivative data ϑ_j^t and by the same method, using identities (2.1.2), we may find the Neumann data from an already known harmonic function q. We shall use this fact in the later test cases to analyse our method.

2.2 The global relation

To form the global relation, suppose that q is a solution to the Laplace BVP (2.1.1). Then in coordinates $(z, \bar{z})$, and because of the identities (2.1.2), q satisfies the equation

$$q_{z\bar{z}}(z, \bar{z}) = 0. \tag{2.2.1}$$

Here and following, the subscripts in $q_{z\bar{z}}$, means partial derivatives of q with respect to these variables. Taking the 1-form $W(z, \bar{z}, k) = e^{-\mathrm{i}\lambda z} q_z \, \mathrm{d}z$, it follows that $dW = e^{-\mathrm{i}\lambda z} q_{z\bar{z}} \, \mathrm{d}\bar{z} \wedge \mathrm{d}z = 0$, so by Stokes' Theorem

$$\int_{\partial\Omega} e^{-\mathrm{i}\lambda z} q_z \, \mathrm{d}z = \int_{\Omega} \mathrm{d}W = 0.$$

This is the global relation from [Fok01, FK03]. Splitting these in to integrals along each edge Γ_j of the boundary, we introduce the *spectral functions*

$$\rho_j(\lambda) := \int_{z_j}^{z_{j+1}} e^{-\mathrm{i}\lambda z} q_z \, \mathrm{d}z,$$

and the global relation can be written more concisely as[2]

$$\sum_{j=1}^{n} \rho_j(\lambda) = 0, \quad \lambda \in \mathbb{C}. \tag{GR1}$$

Recall that, on the assumption of existence, it has been shown in [Fok01] that the solution to (2.1.1) can be written

$$q_z = \frac{1}{2\pi} \sum_{j=1}^{n} \int_{l_j} e^{\mathrm{i}\lambda z} \rho_k(\lambda) \, \mathrm{d}\lambda, \tag{2.2.2}$$

where l_j is the ray in $\mathbb{C}$ on which $\arg(\lambda) = -\alpha_j$. Using a similar representation for $q_{\bar{z}}$, the function q may be constructed as in [Fok08]:

$$q = 2\Re \int_{z_0}^{z} q_z \, \mathrm{d}z + \text{const},$$

however for the Laplace equation, the derivative of q is the more frequently used. From the tangential and normal coordinate frame on each edge Γ_j, and identities (2.1.2), the spectral functions may be written as

$$\rho_j(\lambda) = \frac{1}{2} e^{-\mathrm{i}\alpha_j} \int_{z_j}^{z_{j+1}} e^{-\mathrm{i}\lambda z} (q_\tau + \mathrm{i} q_N) \, \mathrm{d}z,$$

[2] This can be compared with (1.2.2) for the Helmholtz problem on a triangle.

where q_τ and q_N represent the tangential and normal derivatives respectively. Parameterising the edge by $\gamma_j(t) = m_j + te^{\mathrm{i}\alpha_j}$ we let ϑ and φ be the pullback of q_τ, q_N by γ_j respectively, i.e. $\vartheta_j(t) = q_\tau(\gamma_j(t))$. Then every spectral function involves the Dirichlet derivatives and the Neumann data:

$$\rho_j(\lambda) = \frac{e^{-\mathrm{i}\lambda m_j}}{2}\int_{-\sigma_j}^{\sigma_j} e^{-\mathrm{i}\lambda t e^{\mathrm{i}\alpha_j}}\,(\vartheta_j + \mathrm{i}\varphi_j)\,\mathrm{d}t = \frac{e^{-\mathrm{i}\lambda m_j}}{2}\left(\hat{\vartheta}_j(e^{\mathrm{i}\alpha_j}\lambda) + \mathrm{i}\hat{\varphi}_j(e^{\mathrm{i}\alpha_j}\lambda)\right), \quad j = 1,\dots,n, \tag{2.2.3}$$

where $\hat{\varphi}$ denotes the Fourier transform of the a function φ.

Define the vector valued data function $\mathbf{\Phi}^{\mathrm{Di}}(\lambda)$, defined component-wise as the Fourier transform of the derivative of the Dirichlet data:

$$\left(\Phi_1^{\mathrm{Di}}(\lambda),\dots,\Phi_n^{\mathrm{Di}}(\lambda)\right) = \left(\hat{\vartheta}_1(\lambda),\dots,\hat{\vartheta}_n(\lambda)\right).$$

Similarly we let $\mathbf{\Phi}^{\mathrm{Ne}}(\lambda)$ contain the Fourier transform of the (unknown) Neumann data

$$\left(\Phi_1^{\mathrm{Ne}}(\lambda),\dots,\Phi_n^{\mathrm{Ne}}(\lambda)\right) = \left(\hat{\varphi}_1(\lambda),\dots,\hat{\varphi}_n(\lambda)\right).$$

For each $k = 1,\dots,n$, multiply (2.2.3) by $e^{\mathrm{i}\lambda m_k}$ and replace λ by $\lambda e^{-\mathrm{i}\alpha_k}$. Then substituting these into the global relation (GR1), we obtain

$$0 = \sum_{j=1}^{n} e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k - m_j)\lambda}\left(\Phi_j^{\mathrm{Di}}(\lambda e^{-\mathrm{i}\Delta_{kj}}) + \mathrm{i}\Phi_j^{\mathrm{Ne}}(\lambda e^{-\mathrm{i}\Delta_{kj}})\right).$$

Given a vector function $\mathbf{\Phi}(\lambda)$, define the operator

$$(T\mathbf{\Phi})_k(\lambda) := \sum_{j=1}^{n} e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k - m_j)\lambda}\Phi_j(\lambda e^{-\mathrm{i}\Delta_{kj}}). \tag{2.2.4}$$

then we obtain a system of equations equivalent to the global relation:

$$T(\mathbf{\Phi}^{\mathrm{Di}} + \mathrm{i}\mathbf{\Phi}^{\mathrm{Ne}})(\lambda) = \mathbf{0}, \quad \lambda \in \mathbb{C}. \tag{GR2}$$

In view of (2.2.4), the global relation depends on the geometric properties, $(m_j)_{j=1}^n$ and $(\alpha_j)_{j=1}^n$, of our domain Ω. Because of this the results that will follow for boundedness of the operator T, use that our polygon Ω is *convex*. Indeed, we require precisely that whenever the polygon is rotated so that one of its sides Γ_j lies along the axis $\{\Im z = 0\}$, all other points on the perimeter, $\partial\Omega \setminus \overline{\Gamma_j}$, lie strictly above (or below) the axis. We shall remark on this in Section 2.4, where this property is used.

Remark 2.2.1. *It might appear that there is another equation in the background that we could use, namely the* Schwarz conjugate *of* (GR2). *Given an analytic function f, the*

function

$$\tilde{f}(z) := \overline{f(\bar{z})},$$

is also analytic. Thus we may consider the Schwarz conjugate of the global relation:

$$\overline{T(\mathbf{\Phi}^{\mathrm{Di}} + \mathrm{i}\mathbf{\Phi}^{\mathrm{Ne}})(\bar{\mu})} = \mathbf{0}, \quad \mu \in \mathbb{C}, \tag{2.2.5}$$

which is also an analytic function on $\mathbb{C}$*. However, since* (GR2) *holds for any* $\lambda \in \mathbb{C}$*, then* (2.2.5) *must also be satisfied, since for any fixed* $\mu \in \mathbb{C}$*, we can set* $\lambda = \bar{\mu}$ *in* (GR2) *and find that*

$$T(\mathbf{\Phi}^{\mathrm{Di}} + \mathrm{i}\mathbf{\Phi}^{\mathrm{Ne}})(\bar{\mu}) = \mathbf{0}.$$

We now proceed to analyse the properties of this operator T, as presented in [Ash13]. To accomplish this, we will use crucially that our boundary data functions $\Phi_j^{\mathrm{Di}}(\lambda) = \hat{\vartheta}_j(\lambda)$ are the Fourier transform of square-integrable functions on the boundary. Such functions belong to a class of spaces called Paley–Wiener spaces, so we consider these spaces here. The properties of these Paley–Wiener functions will be particularly important in our rigorous analysis of the operator T.

2.3 Paley–Wiener spaces

Let us first begin with a definition of the Paley–Wiener spaces, and then proceed to give some useful properties of these functions. In particular, such functions are analytic; satisfy certain exponential growth bounds, and the particular subspaces we are interested in also enjoy a symmetry property.

Definition 2.3.1. *For* $\sigma > 0$*, the Paley–Wiener space* PW^σ *is defined to be the space containing the Fourier transform of all complex valued square-integrable functions defined on* $[-\sigma, \sigma]$*:*

$$PW^\sigma := \mathcal{F}L^2\,[-\sigma,\sigma] \subset L^2(\mathbb{R}).$$

We also have the subspaces $PW^\sigma_{\mathrm{sym}} := \mathcal{F}L^2_{\mathbb{R}}\,[-\sigma,\sigma]$ *to be the Fourier transform of real-valued square integrable functions, and* $PW^\sigma_{\mathrm{asym}}$ *to be defined similarly for imaginary-valued functions.*

The classical Paley–Wiener Theorem (e.g. [Rud91]) states that this space is equal to

$$\{f : \mathbb{C} \to \mathbb{C} \text{ entire } : \|f\|_{L^2(\mathbb{R})} < \infty, |f(\lambda)| \lesssim_\epsilon e^{\sigma(|\lambda|+\epsilon)} \forall \epsilon > 0\}.$$

We say that functions satisfying such a pointwise bound are of *exponential type* σ. See also section B for more properties of these functions. However since our data is real-valued, we shall restrict our attention to the subspace $PW^\sigma_{\mathrm{sym}} \subset PW^\sigma$. Recall that there is a one-to-one correspondence between an L^2 function and its Fourier transform, and thus between

the Dirichlet data and the vector $\mathbf{\Phi}^{\mathrm{Di}}$. In addition, the subspaces $PW^{\sigma}_{\mathrm{sym}}$ and $PW^{\sigma}_{\mathrm{asym}}$ satisfy the following symmetry conditions.

Lemma 2.3.2 ([Ash13]). *$PW^{\sigma}_{\mathrm{sym}}$ and PW^{σ}_{asym} are closed subspaces of PW^{σ}, and*

$$f(\lambda) = \overline{f(-\bar{\lambda})}, \quad \forall f \in PW^{\sigma}_{\mathrm{sym}}$$
$$g(\lambda) = -\overline{g(-\bar{\lambda})}, \quad \forall g \in PW^{\sigma}_{asym}$$

Furthermore, from the definition of these spaces we have the decomposition

$$PW^{\sigma} = PW^{\sigma}_{\mathrm{sym}} \oplus PW^{\sigma}_{asym}.$$

This discussion means that these three Paley–Wiener spaces are Hilbert spaces when equipped with the standard L^2 inner product

$$(f_1, f_2) = \int_{\mathbb{R}} f_1(x)\overline{f_2(x)}\,\mathrm{d}x.$$

Finally, it is important to note the pseudo-compactness Lemma of [Ash13], which allows weaker-than-norm convergence for bounded subsequences[3]

Lemma 2.3.3 ([Ash13]). *Any norm-bounded sequence in PW^{σ} (or $PW^{\sigma}_{\mathrm{sym}}$, PW^{σ}_{asym}) contains a subsequence that converges pointwise and locally uniformly to an element of PW^{σ} (or $PW^{\sigma}_{\mathrm{sym}}$, PW^{σ}_{asym}) that obeys the same norm bound.*

Furthermore, we recall that the operator T is a composition of Paley–Wiener functions. Therefore whenever these functions converge in norm, the operator T also converges:

Lemma 2.3.4. *Given a sequence $\{\mathbf{\Phi}^{(l)}\}_{l\geq 1} \subset X_{\mathrm{sym}}$, such that $\mathbf{\Phi}^{(l)} \to 0$ locally uniformly. Then $T\mathbf{\Phi}^{(l)} \to \mathbf{0}$ locally uniformly in $\mathbb{C}^n$.*

Proof. For any compact set $K \subset \mathbb{C}$, and for any $j = 1, \ldots, n$ we have that

$$\lim_{l\to\infty} \sup_{\lambda\in K} \Phi_j^{(l)}(\lambda) = 0.$$

Recall that for any compact set K, and any continuous function $g : \mathbb{C} \to \mathbb{C}$, the set $g(K)$ is compact. Therefore by composition the functions $\Phi_j^{(l)}(g(\lambda)) \to 0$ locally uniformly as $l \to \infty$, since

$$\lim_{l\to\infty} \sup_{\lambda\in K} \Phi_j^{(l)}(g(\lambda)) = \lim_{l\to\infty} \sup_{\lambda\in g(K)} \Phi_j^{(l)}(\lambda) = 0.$$

[3]Indeed as [Ash13] notes, we cannot have a general bounded sequence admitting a norm-convergent subsequence, as this would mean the unit ball is sequentially compact. This is true for a Banach space if and only if it is finite-dimensional.

Defining for each $k, j = 1, \dots, n$, the continuous functions $f_{k,j}(\lambda) := e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k - m_j)\lambda}$ and $g_{k,j}(\lambda) := \lambda e^{-\mathrm{i}\Delta_{kj}}$, the components of $(T\mathbf{\Phi}^{(l)})_k(\lambda)$ are given by

$$\sum_{j=1}^{n} f_{k,j}(\lambda)\Phi_j^{(l)}(g_{k,j}(\lambda)).$$

Thus, on any compact set K,

$$\lim_{l\to\infty}\sup_{\lambda\in K}\left|f_{k,j}(\lambda)\Phi_j^{(l)}(g_{k,j}(\lambda))\right| \leq C_{k,j}\lim_{l\to\infty}\sup_{\lambda\in K}\left|\Phi_j^{(l)}(g_{k,j}(\lambda))\right| \to 0$$

locally uniformly. Therefore $(T\mathbf{\Phi}^{(l)})_k(\lambda) \to 0$ locally uniformly for each $k = 1, \dots, n$. □

In view of the pseudo-compactness Lemma 2.3.3, if $\{\mathbf{\Phi}^{(n)}\}_{n\geq 1}$ is a norm-bounded sequence, then there is a subsequence for which this result holds. This is particularly useful, as our Dirichlet and Neumann data lie in these Paley–Wiener spaces:

$$\begin{aligned}\mathbf{\Phi}^{\mathrm{Di}}(\lambda) &\in PW^{\sigma_1}_{\mathrm{sym}} \times \cdots \times PW^{\sigma_n}_{\mathrm{sym}}\\ \mathrm{i}\mathbf{\Phi}^{\mathrm{Ne}}(\lambda) &\in PW^{\sigma_1}_{\mathrm{asym}} \times \cdots \times PW^{\sigma_n}_{\mathrm{asym}}.\end{aligned}$$

Having suitably defined the spaces on which our functions $\mathbf{\Phi}$ are defined, in the next Section we identify suitable domain and range spaces for our operator T, on which it is bounded above and below. Specifically we shall see that the formal D2N map, $\mathbf{\Phi}^{\mathrm{Di}} \mapsto \mathbf{\Phi}^{\mathrm{Ne}}$ is a map between Paley–Wiener spaces.

2.4 Analysis of the operator equation

Let us denote the following spaces

$$\begin{aligned}X &:= PW^{\sigma_1} \times \cdots \times PW^{\sigma_n},\\ X_{\mathrm{sym}} &:= PW^{\sigma_1}_{\mathrm{sym}} \times \cdots \times PW^{\sigma_n}_{\mathrm{sym}},\\ Y &:= L^2(\mathbb{R}_{<0})^{\times n}.\end{aligned} \tag{2.4.1}$$

The global relation (GR2) may now be stated as an operator problem: Given $\mathbf{\Phi}^{\mathrm{Di}} \in X_{\mathrm{sym}}$, find $\mathbf{\Phi}^{\mathrm{Ne}} \in X_{\mathrm{sym}}$ such that

$$T\mathbf{\Phi}^{\mathrm{Ne}} = \mathrm{i}T\mathbf{\Phi}^{\mathrm{Di}}.$$

This amounts to determining that the following set is non-empty and contains only one function:

$$DN(\mathbf{\Phi}^{\mathrm{Di}}) := \left\{\mathbf{\Phi} \in X_{\mathrm{sym}} : T\mathbf{\Phi} = \mathrm{i}T\mathbf{\Phi}^{\mathrm{Di}}\right\}. \tag{2.4.2}$$

This problem is in two parts; first to identify the range of the operator T, and second to show that this range includes the set $\mathrm{i}T(X_{\mathrm{sym}})$. Recalling that $X_{\mathrm{sym}} \subset X$, the following

Theorem gives that the operator T is bounded above and below.

Theorem 2.4.1 ([Ash13]). *The operator $T : X \to Y$ is bounded. Furthermore T is injective and, as a restricted map $T : X_{\mathrm{sym}} \to Y$ has closed range. Thus it is bounded below, i.e. $\|T\boldsymbol{\Phi}\|_Y \gtrsim \|\boldsymbol{\Phi}\|_{X_{\mathrm{sym}}}$ for all $\boldsymbol{\Phi} \in X_{\mathrm{sym}}$.*

Since T is injective and bounded below, we know that its inverse is well defined and continuous on the range of T. Indeed, if we consider $T : X_{\mathrm{sym}} \to \mathrm{Ran}(T) \subset Y$, then $T^{-1} : \mathrm{Ran}(T) \to X_{\mathrm{sym}}$ satisfies

$$\|T^{-1}\boldsymbol{\Psi}\|_{X_{\mathrm{sym}}} \lesssim \|\boldsymbol{\Psi}\|_Y$$

by applying Theorem 2.4.1 with $\boldsymbol{\Psi} := T\boldsymbol{\Phi} \in \mathrm{Ran}(T)$. Eventually we will use this operator T to introduce a Galerkin scheme which reconstructs the Neumann data from the Dirichlet data. We are guaranteed a stable Galerkin scheme provided certain properties are satisfied and one of these is for a specific bilinear form $a : X_{\mathrm{sym}} \times X_{\mathrm{sym}} \to Y$ to be bounded and coercive. This follows by the Lax–Milgram Theorem 2.6.2, that we shall see later. Also coercivity of the bilinear form a will follow because T is bounded below, and boundedness holds also because T is continuous.

Corollary 2.4.2. *Since T is linear and injective, it follows that given Dirichlet data $\boldsymbol{\Phi}^{\mathrm{Di}} \in X_{\mathrm{sym}}$ the set $DN(\boldsymbol{\Phi}^{\mathrm{Di}})$ has at most one element, i.e. there is* at most *one function $\boldsymbol{\Phi}^{\mathrm{Ne}} \in X_{\mathrm{sym}}$ satisfying the global relation* (GR2).

We sketch one part of the proof of Theorem 2.4.1 from [Ash13], that T is a bounded operator, since similar ideas will be used for the Helmholtz problems in Chapter 3. Furthermore, these results hold precisely because the polygon is convex. This is because when one edge Γ_k of the polygon is rotated so that it lies along the axis $\{\Im z = 0\}$, all other edges lie in the half-plane $\{\Im z \geq 0\}$. So the vector

$$m_j + \tau e^{\mathrm{i}(\alpha_j - \alpha_k)} - m_k e^{\mathrm{i}\alpha_k},$$

between $m_k e^{\mathrm{i}\alpha_k}$ on the rotated edge Γ_k and any point $m_j + \tau e^{\mathrm{i}(\alpha_j - \alpha_k)}$ on the rotated edge Γ_j, must lie in the half-plane $\{\Im z \geq 0\}$. Thus this proof highlights the necessity of convexity in the analysis of T.

To prove that the operator T from (2.2.4) is bounded, uses the Fourier inversion Theorem on $L^2(\mathbb{R})$: since a generic term can be represented as the integral of the (compactly supported) boundary data we have

$$e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k - m_j)\lambda}\Phi_j(e^{-\mathrm{i}\Delta_{kj}}\lambda) = \frac{1}{2\pi}\int_{-\sigma_j}^{\sigma_j} e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k - m_j - \tau e^{\mathrm{i}\alpha_j})\lambda}\hat{\Phi}_j(-\tau)\,\mathrm{d}\tau$$

$$= \frac{1}{2\pi} e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}\left(m_k-(m_j-\sigma_j e^{\mathrm{i}\alpha_j})\right)} \int_0^{2\sigma_j} e^{-\mathrm{i}e^{-\mathrm{i}\alpha_k}\tau e^{\mathrm{i}\alpha_j}\lambda} \hat{\Phi}_j(-\tau+\sigma_j)\,\mathrm{d}\tau \tag{2.4.3}$$

$$= \frac{1}{2\pi} e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k-z_j)} \int_0^{2\sigma_j} e^{-\mathrm{i}e^{-\mathrm{i}\Delta_{kj}}\tau\lambda} \hat{\Phi}_j(-\tau+\sigma_j)\,\mathrm{d}\tau.$$

Edges which are *not* adjacent give an explicit exponential decay, because the vector $m_k - m_j - \tau e^{\mathrm{i}\alpha_j}$ between a point on Γ_k and a point on Γ_j lies strictly inside the edge Γ_k: for $j \neq k, k\pm 1$

$$-\pi/2 + \epsilon < \arg(\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k - m_j - \tau e^{\mathrm{i}\alpha_j})) < \pi/2 - \epsilon$$

so the exponential term

$$\left|e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}\left(m_k-m_j-\tau e^{\mathrm{i}\alpha_j}\right)\lambda}\right| \lesssim e^{-\epsilon|\lambda|}, \quad \text{for } \lambda \in \mathbb{R}_{<0}. \tag{2.4.4}$$

Then applying Cauchy–Schwarz to the first line of (2.4.3) gives, for $\lambda \in \mathbb{R}_{<0}$,

$$\begin{aligned}\left|e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k-m_j)\lambda}\Phi_j(e^{-\mathrm{i}\Delta_{kj}}\lambda)\right| &\lesssim \|\hat{\Phi}\|_{L^2(-\sigma_j,\sigma_j)} \left|\int_{-\sigma_j}^{\sigma_j} e^{-2\epsilon|\lambda|}\,\mathrm{d}t\right|^{1/2} \\ &\lesssim e^{-\epsilon|\lambda|}\|\Phi\|_{L^2(-\sigma_j,\sigma_j)},\end{aligned}$$

by Parseval's Theorem. Therefore $e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k-m_j)\lambda}\Phi_j(e^{-\mathrm{i}\Delta_{kj}}\lambda) \in L^2(\mathbb{R}_{<0})$ for non-adjacent edges $j \neq k, k\pm 1$.

Let us finally consider the case of two adjacent edges: suppose that $j = k+1$, so $m_k + \sigma_k e^{\mathrm{i}\alpha_k} = z_j = m_j - \sigma_j e^{\mathrm{i}\alpha_j}$ (the proof for $j = k-1$ is similar). Since these edges share a vertex, at this point the exponential term is imaginary and no longer contributes to decay. This means that there does not exist a strictly positive ϵ to use in our above estimate (2.4.4). To deal with this term, we shall look at the third line of (2.4.3). Since $e^{-\mathrm{i}\alpha_k(m_k-z_j)} = e^{-\mathrm{i}\sigma_k}$, this is an oscillatory term multiplied by a Laplace transform, and is still square-integrable as the following Lemma shows.

Lemma 2.4.3. *Let $f \in L^2(0,\infty)$ and consider the Laplace transform $\tilde{f}(z) := \int_0^\infty e^{-zt} f(t)\,\mathrm{d}t$. Then $\tilde{f} \in L^2(0,\infty)$.*

Furthermore, let $g(z) := e^{i\theta}z + b$ with $\theta \in (-\pi/2, \pi/2)$ such that for any $z \in \mathbb{R}_{>0}$, the function $p(z) := \Re g(z) \geq 0$. Then

$$\breve{f}(z) := \int_0^\infty e^{-g(z)t} f(t)\,\mathrm{d}t$$

is also in $L^2(0,\infty)$.

Proof.

$$\begin{aligned}|\tilde{f}(p)|^2 &\leq \left|\int_0^\infty e^{-pt/2}t^{1/4}t^{-1/4}e^{-pt/2}f(t)\,\mathrm{d}t\right| \\ &\leq \left(\int_0^\infty e^{-pt}t^{-1/2}\,\mathrm{d}t\right)\left(\int_0^\infty e^{-pt}t^{1/2}|f(t)|^2\,\mathrm{d}t\right) \\ &\leq \sqrt{\frac{\pi}{p}}\left(\int_0^\infty e^{-pt}t^{1/2}|f(t)|^2\,\mathrm{d}t\right)\end{aligned}$$

It follows then that

$$\begin{aligned}\int_0^\infty |\tilde{f}(p)|^2\,\mathrm{d}p &\leq \sqrt{\pi}\int_0^\infty \left(\int_0^\infty e^{-pt}p^{-1/2}\,\mathrm{d}p\right) t^{1/2}|f(t)|^2\,\mathrm{d}t \\ &\leq \sqrt{\pi}\int_0^\infty \sqrt{\frac{\pi}{t}}t^{1/2}|f(t)|^2\,\mathrm{d}t \\ &= \pi\|f\|_2\end{aligned}$$

The second part of the proof is similar: Noting that $|e^{-w}| = e^{-\Re w}$, we similarly obtain

$$\begin{aligned}|\breve{f}(z)|^2 &\leq \left|\int_0^\infty e^{-\Re(g(z))t}|f(t)|\,\mathrm{d}t\right|^2 \\ &\leq \left|\int_0^\infty e^{(-\Re b + z\cos\theta)t}|f(t)|\,\mathrm{d}t\right|^2 \\ &\leq \sqrt{\frac{\pi}{p(z)}}\int_0^\infty e^{-p(z)t}t^{1/2}|f(t)|^2\,\mathrm{d}t.\end{aligned}$$

Again then, we find the L^2 norm of this term. Partway through we use the substitution $u = p(z)$ and $\mathrm{d}u = \cos\theta\,\mathrm{d}z$:

$$\begin{aligned}\int_0^\infty |\breve{f}(z)|^2\,\mathrm{d}z &\leq \sqrt{\pi}\int_0^\infty \left(\int_0^\infty \frac{e^{-p(z)t}}{\sqrt{p(z)}}\,\mathrm{d}z\right) t^{1/2}|f(t)|^2\,\mathrm{d}t \\ &= \sqrt{\pi}\int_0^\infty \left(\int_{\Re(b)}^\infty \frac{e^{-ut}}{\sqrt{u}}\frac{\mathrm{d}u}{\cos\theta}\right) t^{1/2}|f(t)|^2\,\mathrm{d}t \\ &\leq \sqrt{\pi}\int_0^\infty \left(\int_0^\infty \frac{e^{-ut}}{\sqrt{u}}\frac{\mathrm{d}u}{\cos\theta}\right) t^{1/2}|f(t)|^2\,\mathrm{d}t \\ &\leq \frac{\pi}{\cos\theta}\int_0^\infty |f(t)|^2 = \frac{\pi\|f\|_2}{\cos\theta} \qquad (2.4.5)\end{aligned}$$

□

Remark 2.4.4. *We note that the bound in (2.4.5) becomes infinite as $\theta \to \pm\pi/2$. For*

$g(z)$ purely imaginary, the function looks like the Fourier transform

$$\breve{f}(z) = \int_0^\infty e^{-izt} f(t)\,\mathrm{d}t,$$

and our estimate replacing $p(z) \equiv 0$ in the integration range is too weak to deal with this case. (Note that even in the Fourier inversion Theorem, without prior knowledge of f, the Fourier transform exists only in a formal sense).

Using this result for the adjacent edge $j = k+1$, we know that $(-\Delta_{kj}) \in (\epsilon, \pi - \epsilon)$. Then by (2.4.3),

$$e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k - m_j)\lambda}\Phi_j(e^{-\mathrm{i}\Delta_{kj}}\lambda) = e^{-\mathrm{i}\sigma_k\lambda}\tilde{H}(-\lambda), \tag{2.4.6}$$

where $\tilde{H}(z) := \int_0^{2\sigma_j} e^{-g(z)\tau}\hat{\Phi}_j(-\tau + \sigma_j)\,\mathrm{d}\tau$ and $g(z) = -\mathrm{i}e^{-\mathrm{i}\Delta_{kj}}z$ has strictly positive real part for $z > 0$. Thus, by the preceding Lemma, $\tilde{H}(z) \in L^2(\mathbb{R}_{>0})$, and thus (2.4.6) is in $L^2(\mathbb{R}_{<0})$.

2.5 The set DN is non-empty

We have already seen that the set $DN(\mathbf{\Phi}^{\mathrm{Di}})$ has at most one element for each choice of $\mathbf{\Phi}^{\mathrm{Di}} \in X_{\mathrm{sym}}$. To conclude, we must show that for any $\mathbf{\Phi}^{\mathrm{Di}} \in X_{\mathrm{sym}}$ *there exists* a $\mathbf{\Phi}^{\mathrm{Ne}} \in X_{\mathrm{sym}}$ such that $T(\mathbf{\Phi}^{\mathrm{Di}} + \mathrm{i}\mathbf{\Phi}^{\mathrm{Ne}}) = 0$. This is equivalent to proving that there exists a function $\mathbf{\Phi}^{\mathrm{Ne}}$ such that

$$T\mathbf{\Phi}^{\mathrm{Ne}} = \mathrm{i}T\mathbf{\Phi}^{\mathrm{Di}}.$$

It is sufficient to prove that the range of T is equal to the range of $(\mathrm{i}T)$. However we should be careful, as X_{sym} is a real vector space, so the map $(\mathrm{i}T)$ is actually

$$\mathrm{i}T : \mathbf{\Phi}^{\mathrm{Di}} \mapsto \mathrm{i}\mathbf{\Phi}^{\mathrm{Di}} \mapsto T(\mathrm{i}\mathbf{\Phi}^{\mathrm{Di}}),$$

where the components, $\mathrm{i}\mathbf{\Phi}_j^{\mathrm{Di}}$, are elements of the corresponding $PW_{\mathrm{asym}}^{\sigma_j}$ spaces. However T^* is precisely the map that satisfies, for every $\mathbf{\Psi} \in Y$

$$\langle T\mathbf{\Phi}, \mathbf{\Psi}\rangle_Y = \sum_k \int_{-\infty}^{\infty} (T\mathbf{\Phi})_k(\lambda)\overline{\Psi_k(\lambda)}\,\mathrm{d}\lambda = \sum_k \int_{-\infty}^{0} \Phi_k(\lambda)\overline{(T^*\mathbf{\Psi})_k(\lambda)}\,\mathrm{d}\lambda = \langle \mathbf{\Phi}, T^*\mathbf{\Psi}\rangle_{X_{\mathrm{sym}}}.$$

By the definition of our operator $\mathrm{i}T$ above, it follows similarly that for every $\mathbf{\Psi} \in Y$

$$\begin{aligned}\langle (\mathrm{i}T)\mathbf{\Phi}, \mathbf{\Psi}\rangle_Y &= \sum_k \int_{-\infty}^{\infty} \mathrm{i}(T\mathbf{\Phi})_k(\lambda)\overline{\Psi_k(\lambda)}\,\mathrm{d}\lambda \\ &= \sum_k \int_{-\infty}^{0} \Phi_k(\lambda)\overline{-\mathrm{i}(T^*\mathbf{\Psi})_k(\lambda)}\,\mathrm{d}\lambda = \langle \mathbf{\Phi}, (-\mathrm{i}T^*)\mathbf{\Psi}\rangle_{X_{\mathrm{sym}}}\end{aligned}$$

and therefore we may write that $(\mathrm{i}T)^* : Y \to X_{\mathrm{sym}}$ is equal to $-\mathrm{i}(T^*) : Y \to X_{\mathrm{sym}}$.

Recall that $T : X_{\text{sym}} \to Y$ is a bounded linear map between Hilbert spaces (since X_{sym} is a closed subspace of X). It's important to note that X_{sym} is over the real numbers, whereas Y is over the complex numbers. As a result of these facts, the formal dual $T^* : Y^* \to X^*$ is defined and (by the Riesz representation Theorem) can be canonically represented as the unique map $T^* : Y \to X$ satisfying

$$\langle T\mathbf{\Phi}, \mathbf{\Psi} \rangle_Y = \langle \mathbf{\Phi}, T^*\mathbf{\Psi} \rangle_{X_{\text{sym}}} \quad \forall \mathbf{\Phi} \in X_{\text{sym}}, \mathbf{\Psi} \in Y.$$

(Furthermore we have the inner product identity $\langle \mathbf{\Phi}, \mathbf{\Psi} \rangle_{X_{\text{sym}}} \equiv \langle \mathbf{\Phi}, \mathbf{\Psi} \rangle_Y$ since the restriction of any element in X is also an element of Y). Because the range of T is closed, Banach's closed range Theorem states that

$$\text{Ran}(T) = (\text{Ker}(T^*))^{\perp}. \tag{2.5.1}$$

We have shown above that given the map $(\mathrm{i}T) : X_{\text{sym}} \to Y$, its adjoint is $(\mathrm{i}T)^* = -\mathrm{i}T^*$, so the kernels are equal: $\text{Ker}(T^*) = \text{Ker}((\mathrm{i}T)^*)$. Applying (2.5.1), we obtain

$$\text{Ran}(\mathrm{i}T) = \text{Ker}(T^*)^{\perp} = \text{Ran}(T).$$

More specifically, for any $\mathbf{\Psi} := \mathrm{i}T\mathbf{\Phi}^{\text{Di}} \in \text{Ran(iT)}$, there exists a $\mathbf{\Phi}^{\text{Ne}} \in X_{\text{sym}}$ such that $T\mathbf{\Phi}^{\text{Ne}} = \mathbf{\Psi}$. Equivalently, the set $DN(\mathbf{\Phi}^{\text{Di}}) \neq \emptyset$ for every $\mathbf{\Phi}^{\text{Di}} \in X_{\text{sym}}$, and thus the global relation has a solution.

2.6 Introducing a numerical method

We recall from the previous section, that the operator T is given explicitly as

$$(T\mathbf{\Phi})_k(\lambda) = \sum_{j=1}^{n} e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k - m_j)\lambda} \Phi_j(e^{-\mathrm{i}\Delta_{kj}}\lambda), \tag{2.6.1}$$

and we wish to solve $T(\mathbf{\Phi}^{\text{Ne}})_k(\lambda) = \mathrm{i}T(\mathbf{\Phi}^{\text{Di}})_k(\lambda)$ for all $\lambda \in \mathbb{C}$ and $k = 1, \ldots, n$. We have shown that functions in the range of T are contained in Y, and so are square integrable. In view of this, let us consider the following variational problem:

$$\arg_{\mathbf{\Phi} \in X_{\text{sym}}} \min E\left[\mathbf{\Phi}\right] : \quad E\left[\mathbf{\Phi}\right] := \sum_{k=1}^{n} \int_{\gamma} |T(\mathbf{\Phi}^{\text{Di}} + \mathrm{i}\mathbf{\Phi})_k(\lambda)|^2 \, \mathrm{d}s(\lambda), \tag{2.6.2}$$

where $\gamma : [0, \infty) \to \mathbb{C}$ is any curve, which eventually coincides with the negative real axis, i.e. there exists a $t_0 > 0$ such that $\gamma(t) \in \mathbb{R}_{<0}$ and $\gamma'(t) \neq 0$ for all $t > t_0$. Since the functions $\Phi_j(\lambda)$ are analytic, so also are $(T\mathbf{\Phi})_k(\lambda)$ for each $k = 1, \ldots, n$. Therefore, by the

identity Theorem, if

$$(T\boldsymbol{\Phi})_k(\lambda) = 0, \quad \forall \lambda \in \mathcal{A}$$

for any set $\mathcal{A}$ with an accumulation point, then $(T\boldsymbol{\Phi})_k(\lambda) \equiv 0$ in $\mathbb{C}$. We could also choose a domain $\mathcal{A} \subset \mathbb{C}$ in place of (2.6.2), which would involve a two-dimensional integration. Alternatively, if $\mathcal{A}$ is chosen as a countable set with a limit point, then an equivalent weak formulation could be constructed, where

$$\arg_{\boldsymbol{\Phi} \in X_{\text{sym}}} \min \mathcal{E}\left[\boldsymbol{\Phi}\right] : \quad \mathcal{E}\left[\boldsymbol{\Phi}\right] := \sum_{k=1}^{n} \sum_{\lambda \in \mathcal{A}} |T(\boldsymbol{\Phi}^{\text{Di}} + \mathrm{i}\boldsymbol{\Phi})_k(\lambda)|^2.$$

However, by choosing a semi-infinite curve γ as in (2.6.2), we will be able to prove coercivity for the related weak problem, and so to use the Lax–Milgram lemma. Furthermore, $E\left[\boldsymbol{\Phi}\right] < \infty$ for any $\boldsymbol{\Phi}^{\text{Di}}, \boldsymbol{\Phi} \in X_{\text{sym}}$, since $(T\boldsymbol{\Phi})_k \in L^2(\mathbb{R}_{<0})$ for $k = 1, \ldots, n$ by Theorem 2.4.1. For definiteness, we will use $\{\gamma\} = (-\infty, 0] \subset \mathbb{C}$ for the following; however let us make the following observation.

Remark 2.6.1. *Since the function $(T\boldsymbol{\Phi})_k(\lambda)$ is analytic, we know by Cauchy's Theorem that the integral along any closed curve is zero. Suppose $\{\gamma\} = (-\infty, 0]$, then in any wedge $(\pi, \pi \pm \delta) \subset \mathbb{C}$ where Jordan's Lemma applies (that is, where the integrand is an oscillatory term multiplied by a term which decays linearly), the integral along γ is equal to one along the rotated path $e^{\pm \mathrm{i}\delta}\gamma$. However we may choose this path to give optimum (exponential) decay of the integrand, and these rotations would improve numerical efficiency. As a proof-of-concept, and for verification of such a method we will pursue here only $\{\gamma\} = (-\infty, 0] \subset \mathbb{C}$, but highlight this improvement for future implementations.*

From this variational problem (2.6.2)

- If a solution to the Laplace equation exists, we may take $\boldsymbol{\Phi}^{\text{Ne}} = \boldsymbol{\Phi}$ to be the corresponding Neumann data, and $E\left[\boldsymbol{\Phi}^{\text{Ne}}\right] = 0$ is therefore a minimiser.
- In [Ash12] we see that solutions to the global relation correspond to solutions to the Laplace equation, so such a minimiser must be unique.

Since then a minimum $\boldsymbol{\Phi}$ does exist, for any perturbation $\boldsymbol{\eta} \in X_{\text{sym}}$, we have

$$0 = \frac{\mathrm{d}}{\mathrm{d}t} E\left[\boldsymbol{\Phi} + t\boldsymbol{\eta}\right]\Big|_{t=0} = \sum_{k=1}^{n} \frac{\mathrm{d}}{\mathrm{d}t} \int_{\gamma} \left|T\left(\boldsymbol{\Phi}^{\text{Di}} + \mathrm{i}\boldsymbol{\Phi}\right)_k(\lambda) + \mathrm{i}tT(\boldsymbol{\eta})_k(\lambda)\right|^2 \mathrm{d}s(\lambda)\Big|_{t=0},$$

and performing this differentiation we find that

$$\begin{aligned}0 &= \sum_{k=1}^{n} \int_\gamma (T\boldsymbol{\Phi}^{\mathrm{Di}})_k(\lambda)\overline{(\mathrm{i}T\boldsymbol{\eta})_k(\lambda)} + (\mathrm{i}T\boldsymbol{\Phi})_k(\lambda)\overline{(\mathrm{i}T\boldsymbol{\eta})_k(\lambda)} \\ &\qquad + \overline{(T\boldsymbol{\Phi}^{\mathrm{Di}})_k(\lambda)}(\mathrm{i}T\boldsymbol{\eta})_k(\lambda) + \overline{(T\boldsymbol{\Phi})_k(\lambda)}(\mathrm{i}T\boldsymbol{\eta})_k(\lambda)\,\mathrm{d}s(\lambda) \\ &= \sum_{k=1}^{n} \int_\gamma 2\Im\left((T\boldsymbol{\Phi}^{\mathrm{Di}})_k(\lambda)\overline{(\mathrm{i}T\boldsymbol{\eta})_k(\lambda)}\right) + 2\Re\left((\mathrm{i}T\boldsymbol{\Phi})_k(\lambda)\overline{(\mathrm{i}T\boldsymbol{\eta})_k(\lambda)}\right)\mathrm{d}s(\lambda).\end{aligned}$$

If we make the definitions of a bilinear operator $a : X_{\mathrm{sym}} \times X_{\mathrm{sym}} \to \mathbb{R}$ and a linear operator $\ell : X_{\mathrm{sym}} \to \mathbb{R}$ as

$$\begin{aligned}a(\boldsymbol{\Phi}, \boldsymbol{\eta}) &= \Re \sum_k \int_{-\infty}^{0} (T\boldsymbol{\Phi})_k(\lambda)\overline{(T\boldsymbol{\eta})_k(\lambda)}\,\mathrm{d}\lambda \\ \ell(\boldsymbol{\eta}) &= -\Im \sum_k \int_{-\infty}^{0} (T\boldsymbol{\Phi}^{\mathrm{Di}})_k(\lambda)\overline{(T\boldsymbol{\eta})_k(\lambda)}\,\mathrm{d}\lambda,\end{aligned} \tag{2.6.3}$$

we obtain the variational approach of [Ash13]:

$$a(\boldsymbol{\Phi}, \boldsymbol{\Phi}') = \ell(\boldsymbol{\Phi}'), \quad \forall \boldsymbol{\Phi}' \in X_{\mathrm{sym}}.$$

The Lax–Milgram result assures us of a unique minimiser to this variational problem, provided boundedness and coercivity properties can be proven for a, ℓ:

Theorem 2.6.2 (Lax–Milgram)**.** *Let X be a Hilbert space and $a : X \times X \to \mathbb{R}$ a bounded and coercive bilinear form. Let $\ell : X \to \mathbb{R}$ be a bounded linear functional on X, i.e. there exist constants c, C, M such that for every $\boldsymbol{\Phi}, \boldsymbol{\Phi}' \in X$ the following are satisfied:*

- $a(\boldsymbol{\Phi}, \boldsymbol{\Phi}') \leq C\|\boldsymbol{\Phi}\|_X \|\boldsymbol{\Phi}'\|_X$
- $a(\boldsymbol{\Phi}, \boldsymbol{\Phi}) \geq c\|\boldsymbol{\Phi}\|_X^2$
- $\ell(\boldsymbol{\Phi}') \leq M\|\boldsymbol{\Phi}'\|_X$.

Then there exists a unique $\boldsymbol{\Phi} \in X$ such that $a(\boldsymbol{\Phi}, \boldsymbol{\Phi}') = \ell(\boldsymbol{\Phi}')$ for every $\boldsymbol{\Phi}' \in X$.

Whenever the assumptions of Theorem 2.6.2 are satisfied, a further result gives explicit convergence rates of the approximate problems. From Céa's Lemma we will be able to deduce not only stability and convergence for our method, but also *spectral* convergence rates.

Lemma 2.6.3 (Céa's Lemma)**.** *Let X, a, l satisfy the assumptions of Theorem 2.6.2, and let $X_N \subseteq X$ be a subspace of X. Then denote $\boldsymbol{\Phi}_N \in X_N$ to be the unique solution in the subspace X_N to*

$$a(\boldsymbol{\Phi}_N, \boldsymbol{\Phi}') = \ell(\boldsymbol{\Phi}'), \quad \forall \boldsymbol{\Phi}' \in X_N.$$

Then the error between $\mathbf{\Phi}_N$ and the actual solution $\mathbf{\Phi}$ is bounded by a constant multiple of the best approximation $\mathbf{\Psi}$ to $\mathbf{\Phi}$ in the subspace X_N. That is,

$$\|\mathbf{\Phi} - \mathbf{\Phi}_N\|_X \leq \frac{C}{c} \inf_{\mathbf{\Psi} \in X_n} \|\mathbf{\Phi} - \mathbf{\Psi}\|_X. \tag{2.6.4}$$

These theorems require coercivity of the bilinear form a, for which we require that T is bounded below. Indeed, it is shown in [Ash13] that the assumptions of Theorem 2.6.2 are satisfied:

Lemma 2.6.4 ([Ash13, Lemma 5.2])**.** *The bilinear form $a : X_{\text{sym}} \to X_{\text{sym}}$ is bounded and coercive, and $\ell \in X^*_{\text{sym}}$.*

As a result, our weak formulation has a unique solution, and the Galerkin problem is stable and convergent. Indeed stronger results hold, and we proceed by showing that our method exhibits spectral convergence rates.

2.7 A spectral convergence Galerkin method

The main result of this section is a rigorous proof that for a certain class of boundary data, the convergence (2.6.4) is *exponentially* fast. This new result, given also in [AC15], is an important theoretical contribution of this thesis. This will be realised by using a Legendre polynomial basis on each edge, for which the rate of convergence is known whenever the data lies in a Sobolev space, H^m.

Remark 2.7.1. *In general problems, one may not expect such regularity for the Neumann data. Indeed, with less regular data we will not observe such fast convergence of the basis functions, and therefore we would expect slower-than-exponential rates of our Galerkin problem. However this Theorem proves that our method is rigorously justified, convergent, and with a controlled rate (depending on the regularity of the data). The previous implementations of the Galerkin method, for example in [FF11], have obtained good convergence rates, but no such proofs of convergence have been given. We therefore give this rigorous justification of our method here. In [FF11], the convergence rates compare well against finite element methods. The numerical results presented in this thesis also compare well, and are further justified by this Theorem.*

Theorem 2.7.2 (Spectral convergence rates)**.** *Let the Dirichlet data $\vartheta_j \in H^1[-\sigma_j, \sigma_j]$ for $1 \leq j \leq n$. Suppose that the unique solution to the global relation is such that for each $1 \leq j \leq n$, the Neumann data $\varphi_j \in H^m[-\sigma_j, \sigma_j]$ for all $m \geq 1$, i.e. that $\varphi_j \in C^\infty([-\sigma_j, \sigma_j])$. Then the approximate problems converge to the true solution:*

$$\|\varphi_j - \varphi_{N,j}\|^2_{L^2[-\sigma_j, \sigma_j]} \to 0,$$

with exponential rate.

To form this basis for the Galerkin problem, let us consider the finite-dimensional subspace of each $L^2_{\mathbb{R}}[-\sigma_j, \sigma_j]$, which is spanned by the normalised Legendre polynomials P_J, i.e.

$$f_{j,J}(t) = \frac{1}{2\pi}\sqrt{\frac{2J+1}{2\sigma_j}} P_J\left(\frac{t}{\sigma_j}\right), \quad j = 1, \dots, n; \quad J = 0, \dots, N-1. \tag{2.7.1}$$

By Parseval's Theorem, a basis for $PW^{\sigma_j}_{\text{sym}}$ is given by the Fourier transform of these Legendre functions $f_{j,J}$, which may be written explicitly in terms of Bessel functions [FF11]. Thus, working in spectral space we have a natural basis $e_{j,J}(\lambda) := \hat{f}_{j,J}(\lambda)$ for X. Let X_N be the subspace of X which is spanned by the first nN vectors $e_{j,J}$ for $j = 1, \dots, n$ and $J = 0, \dots, N-1$. For clarity, we shall denote these basis vectors as $\{\mathbf{e}_j\}_{j=1}^{nN}$. Our unknown vector $\mathbf{\Phi}^{\text{Ne}} = (\Phi_1^{\text{Ne}}, \dots, \Phi_n^{\text{Ne}})$ may be approximated in this subspace by

$$\mathbf{\Phi}^{\text{Ne}} \approx \mathbf{\Phi}_N^{\text{Ne}} = \sum_{j=1}^{nN} b_j \mathbf{e}_j(\lambda),$$

or in component form as

$$\Phi_j^{\text{Ne}} \approx \Phi_{N,j}^{\text{Ne}} = \sum_{J=0}^{N} b_{j,J} e_{j,J}(\lambda),$$

where the real coefficients $\{b_j\}_{j=1}^{nN}$ are to be determined.

Recalling that $\{\Phi_j^{\text{Ne}}\}_{j=1}^n$ contains the Fourier transform of the pullback of the Neumann data, we similarly write $\mathbf{\Phi}_N^{\text{Ne}} = \{\hat{\varphi}_{N,1}, \dots, \hat{\varphi}_{N,n}\}$. Then by Parseval's Theorem

$$\|\mathbf{\Phi}^{\text{Ne}} - \mathbf{\Phi}_N^{\text{Ne}}\|_X^2 = 2\pi \sum_{j=1}^{n} \|\varphi_j - \varphi_{N,j}\|^2_{L^2[-\sigma_j,\sigma_j]}.$$

By taking the infimum on both sides, we obtain an equality for the best approximation in X_N as

$$\inf_{\mathbf{\Psi}\in X_N} \|\mathbf{\Phi}^{\text{Ne}} - \mathbf{\Psi}\|_X^2 = 2\pi \sum_{j=1}^{n} \inf_{\psi \in V_{N,j}} \|\varphi_j - \psi_j\|^2_{L^2[-\sigma_j,\sigma_j]},$$

where $V_{N,j}$ is the span of $\{f_{j,J}\}_{J=0}^{N-1}$. Now if φ_j has sufficient regularity, say $\varphi_j \in H^m[-\sigma_j, \sigma_j]$, then we have the following well-known (see [CHQZ88, Section 9.1.2, p. 277]) estimate for the error in the Legendre polynomial approximation:

$$\inf_{\psi \in V_{N,j}} \|\varphi_j - \psi_j\|_{L^2[-\sigma_j,\sigma_j]} \lesssim N^{-m} \|\varphi_j\|_{H^m[-\sigma_j,\sigma_j]}.$$

Finally, by applying Céa's Lemma, we obtain the estimate

$$\sum_{j=1}^{n} \|\varphi_j - \varphi_{N,j}\|^2_{L^2[-\sigma_j,\sigma_j]} \lesssim N^{-2m} \sum_{j=1}^{n} \|\varphi_j\|^2_{H^m[-\sigma_j,\sigma_j]} = \mathcal{O}\left(\frac{1}{N^{2m}}\right). \tag{2.7.2}$$

So if the Dirichlet data is sufficiently regular so that $\varphi_j \in H^m[-\sigma_j, \sigma_j]$ for each $1 \leq j \leq n$, then the error between the pullback of the reconstructed Neumann data $(\varphi_{N,1}, \ldots, \varphi_{N,n})$ and the pullback of the exact solution $(\varphi_1, \ldots, \varphi_n)$ converges with rate N^{2m}.

Finally, we can deduce from (2.7.2), that if the Neumann data lies in every Sobolev space, the convergence is faster than any polynomial. A numerical scheme with such convergence rates has the *spectral convergence* property. We shall see that this spectral convergence is observed in our numerical experiments.

For our numerical tests, we will project the Dirichlet data $\mathbf{\Phi}^{\mathrm{Di}} = (\Phi_1^{\mathrm{Di}}, \ldots, \Phi_n^{\mathrm{Di}})$ used in (2.6.3) to a function $\mathbf{\Phi}_N^{\mathrm{Di}} \in X_N$:

$$\Phi_i^{\mathrm{Di}}(\lambda) \approx \Phi_{N,i}^{\mathrm{Di}}(\lambda) = \sum_{I=0}^{N-1} c_{i,I} e_{i,I}(\lambda),$$

and we want to find the coefficients of the minimiser $\mathbf{\Phi}^{\mathrm{Ne}}$ in our basis. Specifically we are searching for the coefficients $b_{i,I}$ such that $\Phi_i^{\mathrm{Ne}} \approx \Phi_{N,i}^{\mathrm{Ne}} = \sum_{I=0}^{N-1} b_{i,I} e_{i,I}(\lambda)$ solves the subspace problem

$$a(\mathbf{\Phi}_N^{\mathrm{Ne}}, \boldsymbol{e}_{j,J}) = \ell(\boldsymbol{e}_{j,J}), \quad \forall j = 1, \ldots, n \text{ and } J = 0, \ldots, N-1,$$

where we let $\boldsymbol{e}_{j,J}(\lambda) := (0, \ldots, 0, e_{j,J}(\lambda), 0, \ldots, 0)$ denote the vector function in the j-th position. Equivalently

$$\sum_{i=1}^{n} \sum_{I=0}^{N-1} b_{i,I} a(\boldsymbol{e}_{i,I}, \boldsymbol{e}_{j,J}) = \ell(\boldsymbol{e}_{j,J}), \quad \forall j = 1, \ldots, n \text{ and } J = 0, \ldots, N-1. \tag{2.7.3}$$

Defining the values

$$\begin{aligned} M_{i,I,j,J} :&= \sum_{k=1}^{n} \int_1^{\infty} (T\boldsymbol{e}_{i,I})_k(-t) \overline{(T\boldsymbol{e}_{j,J})_k(-t)} \, \mathrm{d}t \\ &= \sum_{k=1}^{n} \int_1^{\infty} e^{-\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k - m_i)t} e_{i,I}(-te^{-\mathrm{i}\Delta_{k,i}}) e^{\mathrm{i}e^{\mathrm{i}\alpha_k}\overline{(m_k - m_j)}t} e_{j,J}(-te^{-\mathrm{i}\Delta_{k,j}}) \, \mathrm{d}t, \end{aligned} \tag{2.7.4}$$

(2.7.3) takes the form of a matrix equation $\underline{\boldsymbol{A}} \cdot \boldsymbol{B} = \boldsymbol{L}$ where then

$$\begin{aligned} A_{(i,I),(j,J)} &:= \Re M_{i,I,j,J} \\ L_{(j,J)} &= -\Im \sum_{k=1}^{n} \int_1^\infty \left(\sum_i e^{-\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k - m_i)t} \Phi_{N,i}^{\mathrm{Di}}(-te^{-\mathrm{i}\Delta_{ki}}) \right) \overline{(T\boldsymbol{e}_{j,J})_k(-t)}\, \mathrm{d}t \\ &= -\Im \sum_{k,i=1}^{n} \sum_{I=0}^{N-1} c_{i,I} \int_1^\infty \left(\sum_i e^{-\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k - m_i)t} e_{i,I}(-te^{-\mathrm{i}\Delta_{ki}}) \right) \overline{(T\boldsymbol{e}_{j,J})_k(-t)}\, \mathrm{d}t \\ &= -\Im \sum_{i=1}^{n} \sum_{I=0}^{N-1} c_{i,I} M_{i,I,j,J}. \end{aligned} \tag{2.7.5}$$

Because of the double-indices, our notation $L_{(j,J)}$ means form a row vector out of the components $(j,J)_{j=1,J=0}^{n,N}$, and similarly for $a_{(i,I),(j,J)}$.

Remark 2.7.3. *As a computational note, we observe that a general matrix equation* (2.7.3) *would require* $(nN)^2 + nN$ *computations of terms in* (2.6.3). *This corresponds to* $n^2N(nN+1)$ *integrals. Here, in view of the elements* $M_{i,I,j,J}$ *we only require these terms, i.e.* $n(nN)^2$ *numerical integrations. This is further improved by the observation that*

$$M_{i,I,j,J} = \overline{M_{j,J,i,I}},$$

so indeed only the upper triangular entries of M *are required, amounting to* $\frac{1}{2}n^2N(nN+1)$ *integral computations; precisely half the number we may expect from* (2.7.3).

For the remainder of this chapter, we shall rewrite the operator T as an integral equation, and we shall give a new proof that the known data in the global relation (GR2) lies in the space Y. This proof may be extended to the Helmholtz problem, and from which boundedness of the linear form ℓ is obtained.

2.8 T as an integral operator

In the previous section, we have worked with the operator T as an injective, bounded operator between Banach spaces. In this section, we show that T can be thought of also as an integral operator, with a kernel. By representing T in this way, further results from Hilbert–Schmidt theory may be used. Furthermore, we use this representation to provide an alternative proof that the global relation has a unique solution (given valid Dirichlet data).

We say that T is written in the form of an integral operator, if there exists a vector function $\boldsymbol{K}(\lambda, y)$ such that for each pair of indices (k,j), the component function

$K_{k,j}(\lambda, y) \in L^2((-\infty, 0) \times \mathbb{R})$, and

$$(T\boldsymbol{\Phi})(\lambda) = \int \boldsymbol{K}(\lambda, y)\boldsymbol{\Phi}(y)\,\mathrm{d}y, \tag{2.8.1}$$

or in component form,

$$(T\boldsymbol{\Phi})_k(\lambda) = \sum_j \int_{\mathbb{R}} K_{k,j}(\lambda, y)\Phi_j(y)\,\mathrm{d}y.$$

From the definition (2.8.1) for K, the following equality must hold:

$$e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k - m_j)\lambda}\Phi_j(\lambda e^{-\mathrm{i}\Delta_{kj}}) = \int_{\mathbb{R}} K_{k,j}(\lambda, y)\Phi_j(y)\,\mathrm{d}y. \tag{2.8.2}$$

To obtain such an integral representation for $\Phi_j(\lambda)$, we need to understand the decay properties of functions in X_{sym}. In particular, recall that Paley–Wiener functions have specific exponential growth in the upper and lower half planes. Using this fact, along with Jordan's Lemma and Cauchy's integral Theorem we will be able to find the functions $K_{k,j}(\lambda)$ in (2.8.2).

2.8.1 Bounds in the complex plane

Consider one of the edge functions $\Phi_j(\lambda) \in PW^{\sigma_j}_{\mathrm{sym}}$. Recall also that such functions are analytic; in $L^2(\mathbb{R})$ and of exponential type σ_j:

$$|\Phi_j(\lambda)| \lesssim \|\Phi_j\|_{L^2(\mathbb{R})} e^{\sigma_j |\Im(\lambda)|}.$$

This tells us that along rays in the complex plane, the function cannot grow *more than* an exponential rate $\sigma_j|\Im(\lambda)|$. Since Φ_j is continuous and in $L^2(\mathbb{R})$, it must therefore be bounded on the real line (which also follows from this inequality). There are a class of results called Phragmén–Lindelöf Theorems (see Theorems B.0.3–B.0.5), which state that if a Paley–Wiener function is bounded on ∂D, for certain domains $D \subset \mathbb{C}$ (such as on two rays from the origin in the complex plane), the function also obeys this bound inside D. However we cannot apply these Phragmén–Lindelöf Theorems in this case, as the opening between the rays $\mathbb{R}_{>0}$ and $\mathbb{R}_{<0}$ is not strictly less than π. In fact the following argument demonstrates that we cannot expect boundedness along any ray (except the real axes) for

generic data: Choose $(\mathcal{F}^{-1}\Phi_j)(\tau) \equiv 1 \in L^2([-\sigma_j, \sigma_j])$, then

$$\begin{aligned}\Phi_j(\lambda) &= \frac{1}{2\pi}\int_{-\sigma_j}^{\sigma_j} e^{\mathrm{i}\lambda\tau}\,\mathrm{d}\tau \\ &= \frac{1}{2\pi\mathrm{i}\lambda}(e^{\mathrm{i}\lambda\sigma_j} - e^{-\mathrm{i}\lambda\sigma)_j}) \\ &= \frac{1}{\pi\lambda}\sin(\lambda\sigma_j),\end{aligned}$$

which grows exponentially along rays $\lambda = te^{\mathrm{i}\theta}$ for $\theta \notin \{0, \pi\}$.

This observation allows us to conclude that any decay we wish to have on functions (2.8.2) involving $\Phi_j(\lambda)$ away from the real line *must* also take into account the exponential function appearing there.

Consider once again the representation for $\Phi_j(\lambda)$, using the Fourier inversion Theorem:

$$\Phi_j(\lambda) = \frac{1}{2\pi}e^{-\mathrm{i}\sigma_j\lambda}\int_{-\sigma_j}^{\sigma_j} e^{\mathrm{i}\lambda(\tau+\sigma_j)}\hat{\Phi}_j(\tau)\,\mathrm{d}\tau,. \tag{2.8.3}$$

The integral is bounded as a function of λ for $\Im\lambda \geq 0$, and therefore

$$e^{\mathrm{i}\lambda\sigma_j}\Phi_j(\lambda)$$

is bounded for λ in the upper half-plane, $\mathbb{H}^+ := \{\lambda \in \mathbb{C} : \Im\lambda \geq 0\}$. Similarly we can write

$$\Phi_j(\lambda) = \frac{1}{2\pi}e^{\mathrm{i}\sigma_j\lambda}\int_{-\sigma_j}^{\sigma_j} e^{-\mathrm{i}\lambda(\tau+\sigma_j)}\hat{\Phi}_j(-\tau)\,\mathrm{d}\tau$$

so that $e^{-\mathrm{i}\lambda\sigma_j}\Phi_j(\lambda)$ is bounded on the lower half-plane $\mathbb{H}^- := \{\lambda \in \mathbb{C} : \Im\lambda \leq 0\}$.

Recall that we wish to find an integral kernel representation (i.e. an integral along the real line) for

$$e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k-m_j)\lambda}\Phi_j(\lambda e^{-\mathrm{i}\Delta_{kj}}),$$

and we are now able to determine for which values $\lambda \in \mathbb{C}$ these functions are bounded. Let us recall Jordan's Lemma for path integrations, as it applies for these functions. With this result, we will be able to use Cauchy's Theorem to deform contours to the real axis.

Lemma 2.8.1 (Jordan's Lemma)**.** *Let $\Phi(z)$ be analytic, and such that $e^{\mathrm{i}\sigma z}\Phi(z)$ is bounded in the upper half plane. Let the curved semi-circle of radius R be given by $\Gamma_R(t) := Re^{\mathrm{i}t}$ for $t \in [0, \pi]$. Then*

$$\int_{\Gamma_R}\frac{e^{\mathrm{i}\sigma z}\Phi(z)}{z}\,\mathrm{d}z \to 0, \quad \text{as } R \to \infty$$

Proof. Fix $\delta > 0$, and partition Γ_R into three parts: $\gamma_{1,R}(t)$ is for $t \in [0, \delta]$, $\gamma_{2,R}(t)$ is for $t \in [\delta, \pi - \delta]$ and $\gamma_{3,R}(t)$ is for $t \in [\pi - \delta, \pi]$.

Since $e^{\mathrm{i}\sigma z}\Phi(z)$ is bounded, the integral over $\gamma_{1,R}$ (similarly $\gamma_{3,R}$) can be bounded as

$$\left|\int_{\gamma_{1,R}} \frac{e^{\mathrm{i}\sigma z}\Phi(z)}{z}\,\mathrm{d}z\right| \lesssim \left|\int_{\gamma_{1,R}} \frac{1}{z}\,\mathrm{d}z\right| \leq C\delta.$$

For $\gamma_{2,R}$, first we observe from the representation (2.8.3) that

$$\begin{aligned}
\left|e^{\mathrm{i}\sigma z}\Phi(z)\right| &= \left|\frac{1}{2\pi}\int_0^{2\sigma} e^{\mathrm{i}z\tau}\hat{\Phi}(t-\sigma)\,\mathrm{d}\tau\right| \\
&\leq \frac{\|\Phi\|_2}{2\pi}\left(\int_0^{2\sigma} e^{-2|z|\tau\sin\delta}\right)^{1/2} \\
&\leq \frac{\|\Phi\|_2}{2\pi}\left(\frac{1-e^{-4\sigma|z|\sin\delta}}{2|z|\sin\delta}\right)^{1/2} \\
&\leq \frac{\|\Phi\|_2}{2\pi(2z\sin\delta)^{1/2}}.
\end{aligned}$$

Using this bound on the contour $\gamma_{2,R}$, this additional decay of $z^{1/2}$ gives decay $R^{1/2}$ of the resulting integral:

$$\begin{aligned}
\left|\int_{\gamma_{2,R}} \frac{e^{\mathrm{i}\sigma z}\Phi(z)}{z}\,\mathrm{d}z\right| &\leq \pi R(1-2\delta)\sup_{\gamma_{2,R}}\left|\frac{e^{\mathrm{i}\sigma z}\Phi(z)}{z}\right| \\
&= \pi(1-2\delta)\frac{\|\Phi\|_2}{2\pi(2\sin\delta)^{1/2}R^{1/2}}. \qquad (2.8.4)
\end{aligned}$$

Therefore, given $\epsilon > 0$, choose $0 < \delta < \frac{\epsilon}{3C}$ and R such that (2.8.4) is less than $\epsilon/3$. Then the integral

$$\left|\int_{\Gamma_R} \frac{e^{\mathrm{i}\sigma z}\Phi(z)}{z}\,\mathrm{d}z\right| < \epsilon.$$

□

Continuing with our search for a kernel representation for the operator T, in order to use Cauchy's Theorem we need a function that decays in the relevant half-plane. Let us fix two edges j, k and let $\theta := \Delta_{jk}$. First suppose that $\theta \in (0, \pi)$, so $\lambda e^{\mathrm{i}\theta}$ is in the *lower*

half-plane $\mathbb{H}^-$ for $\lambda \in \mathbb{R}_{<0}$. Then our expression can be manipulated:

$$\begin{aligned} e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k-m_j)\lambda}\Phi_j(\lambda e^{-\mathrm{i}\Delta_{kj}}) &= e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k-m_j)\lambda}e^{\mathrm{i}\lambda e^{\mathrm{i}\theta}\sigma_j}\left(e^{-\mathrm{i}\lambda e^{\mathrm{i}\theta}\sigma_j}\Phi_j(\lambda e^{\mathrm{i}\theta})\right) \\ &= e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k-m_j)\lambda}e^{\mathrm{i}\lambda e^{\mathrm{i}\theta}\sigma_j}\left(\frac{1}{2\pi\mathrm{i}}\int_{B_\epsilon(\lambda e^{\mathrm{i}\theta})}\frac{e^{-\mathrm{i}z\sigma_j}\Phi_j(z)}{z-\lambda e^{\mathrm{i}\theta}}\,\mathrm{d}z\right) \\ &= e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k-m_j)\lambda}e^{\mathrm{i}\lambda e^{\mathrm{i}\theta}\sigma_j}\left(\frac{-1}{2\pi\mathrm{i}}\int_{-\infty}^{\infty}\frac{e^{-\mathrm{i}z\sigma_j}\Phi_j(z)}{z-\lambda e^{\mathrm{i}\theta}}\,\mathrm{d}z\right) \\ &= e^{\mathrm{i}\lambda e^{-\mathrm{i}\alpha_k}\left(m_k-(m_j-\sigma_j e^{\mathrm{i}\alpha_j})\right)}\left(\frac{-1}{2\pi\mathrm{i}}\int_{-\infty}^{\infty}\frac{e^{-\mathrm{i}z\sigma_j}\Phi_j(z)}{z-\lambda e^{\mathrm{i}\theta}}\,\mathrm{d}z\right), \end{aligned} \tag{2.8.5}$$

for any $\lambda \in \mathbb{R}_{<0}$ and $\theta \in (0,\pi)$. We have used that the integral is taken *anti-clockwise* in the lower half-plane, and that the integrand decays exponentially away from the real axis, so Jordan's Lemma allows us to take the contour to an infinite semi-circle, with contribution vanishing on the curved path.

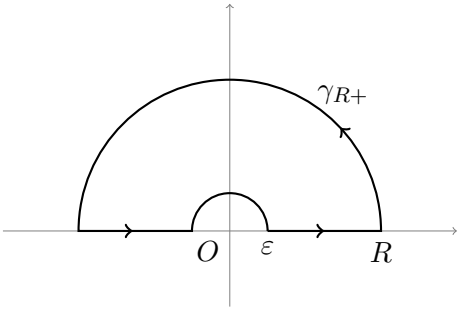
If instead $\theta \in (\pi, 2\pi)$, then a similar calculation allows us to write

$$\begin{aligned} e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k-m_j)\lambda}\Phi_j(\lambda e^{-\mathrm{i}\Delta_{kj}}) &= e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k-m_j)\lambda}e^{-\mathrm{i}\lambda e^{\mathrm{i}\theta}\sigma_j}\left(e^{\mathrm{i}\lambda e^{\mathrm{i}\theta}\sigma_j}\Phi_j(\lambda e^{\mathrm{i}\theta})\right) \\ &= e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k-m_j)\lambda}e^{-\mathrm{i}\lambda e^{\mathrm{i}\theta}\sigma_j}\left(\frac{1}{2\pi\mathrm{i}}\int_{B_\epsilon(\lambda e^{\mathrm{i}\theta})}\frac{e^{\mathrm{i}z\sigma_j}\Phi_j(z)}{z-\lambda e^{\mathrm{i}\theta}}\,\mathrm{d}z\right) \\ &= e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k-m_j)\lambda}e^{-\mathrm{i}\lambda e^{\mathrm{i}\theta}\sigma_j}\left(\frac{1}{2\pi\mathrm{i}}\int_{-\infty}^{\infty}\frac{e^{\mathrm{i}z\sigma_j}\Phi_j(z)}{z-\lambda e^{\mathrm{i}\theta}}\,\mathrm{d}z\right) \\ &= e^{\mathrm{i}\lambda e^{-\mathrm{i}\alpha_k}\left(m_k-(m_j+\sigma_j e^{\mathrm{i}\alpha_j})\right)}\left(\frac{1}{2\pi\mathrm{i}}\int_{-\infty}^{\infty}\frac{e^{\mathrm{i}z\sigma_j}\Phi_j(z)}{z-\lambda e^{\mathrm{i}\theta}}\,\mathrm{d}z\right), \end{aligned} \tag{2.8.6}$$

Finally we ask, what happens for $\theta = \pi$, since any deformation of a contour about $\lambda e^{\mathrm{i}\theta} \in \mathbb{R}_{>0}$ for $\lambda \in \mathbb{R}_{<0}$ must lie in both half planes. We guess a solution as being a linear combination of the above two results, i.e. equations (2.8.5) and (2.8.6), and this is stated in the following Lemma.

Lemma 2.8.2. *Let $f(z)$ be analytic in $\mathbb{C}$. Suppose also that for some $\sigma > 0$, $e^{\mathrm{i}\sigma(z-a)}f(z)$ is bounded in $\mathbb{H}^+$ and $e^{-\mathrm{i}\sigma(z-a)}f(z)$ is bounded in $\mathbb{H}^-$. Then for any $a \in \mathbb{R}$, $f(a)$ has an integral representation given by*

$$\int_{\mathbb{R}} \operatorname{sinc}(\sigma(z-a))f(z)\,\mathrm{d}z = \frac{\pi f(a)}{\sigma}. \tag{2.8.7}$$



Proof. Fix $\epsilon > 0$ and let Γ_R be a perturbation of the line segment $[-R, R]$, containing the points $[-R, a-\epsilon] \cup \{a + \epsilon e^{\mathrm{i}\phi} : \phi \in [-\pi, 0]\} \cup [a+\epsilon, R]$. Define also the semi-circular contours $\gamma_{R+} = \{Re^{\mathrm{i}t} : t \in [0, \pi]\}$ and $\gamma_{R-} = \{Re^{-\mathrm{i}t} : t \in [0, \pi]\}$. Noting that $\operatorname{sinc}(\sigma(z-a)) = \frac{e^{\mathrm{i}\sigma(z-a)} - e^{-\mathrm{i}\sigma(z-a)}}{2\mathrm{i}\sigma(z-a)}$, we can apply Cauchy's residue Theorem to conclude that

$$\int_{\Gamma_R \cup \gamma_{R+}} \frac{e^{\mathrm{i}\sigma(z-a)}}{2\mathrm{i}\sigma(z-a)} f(z)\,\mathrm{d}z = \frac{\pi f(a)}{\sigma} \tag{2.8.8}$$

$$\int_{\Gamma_R \cup \gamma_{R-}} \frac{e^{-\mathrm{i}\sigma(z-a)}}{2\mathrm{i}\sigma(z-a)} f(z)\,\mathrm{d}z = 0. \tag{2.8.9}$$

Using Jordan's Lemma 2.8.1, we see that as $R \to \infty$, the contribution over the outer curved contours $\gamma_{R_\pm}$ tends to zero. Denote the inner curve by $\gamma_\epsilon(t) = \epsilon e^{\mathrm{i}t}$ for $t \in [-\pi, 0]$, then since $\operatorname{sinc}(\sigma(z-a))$ has a removable singularity, it is bounded in a region around a so that

$$\left| \int_{\gamma_\epsilon} \operatorname{sinc}(\sigma(z-a)) f(z)\,\mathrm{d}z \right| \leq C\epsilon \to 0 \quad \text{as } \epsilon \to 0.$$

Therefore, by subtracting (2.8.9) from (2.8.8) and taking the limits $R \to \infty$ and $\epsilon \to 0$, we are left with an integral only along the real line:

$$\begin{aligned} \frac{\pi f(a)}{\sigma} &= \int_{\mathbb{R}} \frac{e^{\mathrm{i}\sigma(z+\lambda)} - e^{-\mathrm{i}\sigma(z+\lambda)}}{2\mathrm{i}\sigma(z+\lambda)} f(z) dz \\ &= \int_{\mathbb{R}} \operatorname{sinc}(\sigma(z+\lambda)) f(z)\,\mathrm{d}z. \end{aligned}$$

□

Remark 2.8.3. *We emphasise that this result holds only for those analytic functions f that satisfy the boundedness conditions: $\left|e^{\pm\mathrm{i}\sigma(z-a)} f(z)\right| \leq C$ in $\mathbb{H}^\pm$ respectively. Using the Paley–Wiener Theorem, this condition precisely coincides with f being the Fourier transform of a function in $L^2[-\sigma, \sigma]$; and so Lemma 2.8.2 holds for all $f \in PW^\sigma$ (noting that $\sigma > 0$ is fixed but arbitrary).*

Corollary 2.8.4. *The results above may be extended for the other two cases, where $\lambda e^{\mathrm{i}\theta} \in$*

$\mathbb{H}^+$ *or* $\mathbb{H}^-$. *Beginning with the right-hand side of* (2.8.6)

$$e^{\mathrm{i}\lambda e^{-\mathrm{i}\alpha_k}(m_k-m_j)}\left(\frac{1}{2\pi\mathrm{i}}\int_{-\infty}^{\infty}\frac{e^{\mathrm{i}\sigma_j(z-\lambda e^{\mathrm{i}\theta})}\Phi_j(z)}{z-\lambda e^{\mathrm{i}\theta}}\,\mathrm{d}z\right).$$

Letting $\Gamma=[-R,R]\cup\gamma_{R-}$ *be the semi-circular contour in* $\mathbb{H}^-$, *we see again that*

$$\frac{1}{2\pi\mathrm{i}}\int_{\Gamma}\frac{e^{-\mathrm{i}\sigma_j(z-\lambda e^{\mathrm{i}\theta})}\Phi_j(z)}{z-\lambda e^{\mathrm{i}\theta}}\,\mathrm{d}z=0. \tag{2.8.10}$$

Subtracting these two expressions, we obtain a sinc *integral*

$$\begin{aligned}e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k-m_j)\lambda}\Phi_j(\lambda e^{\mathrm{i}\theta}) &= e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k-m_j)\lambda}\left(\frac{1}{2\pi\mathrm{i}}\int_{\mathbb{R}}\frac{\sigma_j\left(e^{\mathrm{i}\sigma_j(z-\lambda e^{\mathrm{i}\theta})}-e^{-\mathrm{i}\sigma_j(z-\lambda e^{\mathrm{i}\theta})}\right)}{\sigma_j(z-\lambda e^{\mathrm{i}\theta})}\,\mathrm{d}z\right)\\ &= e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k-m_j)\lambda}\left(\frac{\sigma_j}{\pi}\int_{\mathbb{R}}\operatorname{sinc}(\sigma_j(z-\lambda e^{\mathrm{i}\theta}))\Phi_j(z)\,\mathrm{d}z\right).\end{aligned} \tag{2.8.11}$$

Therefore the representation (2.8.11) *is valid for all values of* $\theta\in[0,2\pi)$.

In conclusion, the operator T has the integral representation

$$(T\boldsymbol{\Phi})_k(\lambda)=\sum_j\int_{\mathbb{R}}K_{k,j}(\lambda,y)\Phi_j(y)\,\mathrm{d}y,$$

for

$$K_{k,j}(\lambda,y)=\frac{\sigma_j e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k-m_j)\lambda}}{\pi}\operatorname{sinc}(\sigma_j(y-\lambda e^{-\mathrm{i}\Delta_{kj}})). \tag{2.8.12}$$

Considering the inner product $\langle T\boldsymbol{\Phi},\boldsymbol{\Psi}\rangle$[4]:

$$\begin{aligned}\langle T\boldsymbol{\Phi},\boldsymbol{\Psi}\rangle &= \sum_{k,j}\int_{-\infty}^{0}\int_{\mathbb{R}}K_{k,j}(\lambda,y)\Phi_j(y)\overline{\Psi_k(\lambda)}\,\mathrm{d}y\,\mathrm{d}\lambda\\ &= \sum_j\int_{\mathbb{R}}\Phi_j(y)\overline{\left(\sum_k\int_{-\infty}^{0}\overline{K_{k,j}(\lambda,y)}\Psi_k(\lambda)\,\mathrm{d}\lambda\right)},\end{aligned}$$

we use the formal identity $\langle T\boldsymbol{\Phi},\boldsymbol{\Psi}\rangle=\langle\boldsymbol{\Phi},T^*\boldsymbol{\Psi}\rangle$, to obtain a representation for adjoint operator T^*:

$$(T^*\boldsymbol{\Psi})_j(\mu)=\sum_k\int_{-\infty}^{0}L_{j,k}(\mu,z)\Psi_a(z)\,\mathrm{d}z,\quad\text{where}$$

$$L_{j,k}(\mu,z)=\overline{K_{k,j}(z,\mu)}=\frac{\sigma_j e^{-\mathrm{i}e^{\mathrm{i}\alpha_k}\overline{(m_k-m_j)}z}}{\pi}\operatorname{sinc}(\sigma_j(\bar{\mu}-ze^{\mathrm{i}\Delta_{kj}})).$$

[4]recall that the domain of T^* is $Y=L^2(-\infty,0)$.

In components, T^* has the integral representation

$$(T^*\boldsymbol{\Psi})_j(\mu) = \sum_k \int_{-\infty}^{0} \frac{\sigma_j e^{-\mathrm{i}e^{\mathrm{i}\alpha_k}\overline{(m_k - m_j)}z}}{\pi} \operatorname{sinc}(\sigma_j(\bar{\mu} - ze^{\mathrm{i}\Delta_{kj}}))\Psi_k(z)\,\mathrm{d}z. \tag{2.8.13}$$

Using (2.8.13), we are able to give a second proof that the set $DN(\boldsymbol{\Phi}^{\mathrm{Di}})$ is non-empty for all $\boldsymbol{\Phi}^{\mathrm{Di}} \in X_{\mathrm{sym}}$, i.e. that the Dirichlet–Neumann map has a solution. Because of our earlier discussion, we know that $DN(\boldsymbol{\Phi}^{\mathrm{Di}})$ has at most one element, so it follows again that a unique solution to the global relation exists.

2.9 A new proof that DN is non-empty

In Section 2.5 we gave a proof that $DN(\boldsymbol{\Phi}^{\mathrm{Di}})$ is non-empty. This proof relied on the fact that the *same* operator T acts on both the known Dirichlet data $\boldsymbol{\Phi}^{\mathrm{Di}}$ and the unknown Neumann data $\boldsymbol{\Phi}^{\mathrm{Ne}}$ in the global relation, i.e. that the global relation is given by

$$T\boldsymbol{\Phi}^{\mathrm{Ne}} = \mathrm{i}T\boldsymbol{\Phi}^{\mathrm{Di}}. \tag{2.9.1}$$

That is, our earlier proof used strongly the specific knowledge that we are solving the Laplace BVP with Dirichlet data. The proof given in Section 2.5 considers the range of the operator $(\mathrm{i}T)$, to show that the range is the same as the range of T. This cannot be directed extended to the Helmholtz case, as the operators are substantially different. Indeed, for the Helmholtz equation, the right-hand side will now become a new function $\boldsymbol{\Psi}$ that depends on the Dirichlet data, but cannot be reduced to the function $\mathrm{i}T\boldsymbol{\Phi}^{\mathrm{Di}}$.

As one step to overcoming this obstruction in the proof, we would like to use our new integral representations (2.8.12) and (2.8.13) to give an alternative (and more generic) proof that $DN(\boldsymbol{\Phi}^{\mathrm{Di}})$ is non-empty. This proof is more generic in the sense that we form an integral relation which, by Banach's closed range Theorem, is shown to be zero. The exact nature of the integral relation relies on the equation we are solving, but such an integral equation can be formulated for the Helmholtz problems. We have been unable to extend this proof to the Helmholtz cases in this thesis, but by presenting the approach here, we hope that this result may be proven in the future by this method. The key identity is in the proof of Theorem 2.9.3 where, using the integral relations for T and T^*, the term $T^*\eta$ is obtained. Since $\eta \in \operatorname{Ker}(T^*)$, the integral is shown to be zero. A proof for the Helmholtz equations may attempt to similarly identify these vanishing terms in the integral.

Beginning with the proof, recall that the pullback of our Dirichlet data f_j is given as $\vartheta_j = \psi_j^*(f_j)$, so that $\boldsymbol{\Phi}^{\mathrm{Di}} = (\Phi_1^{\mathrm{Di}}, \ldots, \Phi_n^{\mathrm{Di}})$ is defined component-wise by the Fourier transform of the derivative of ϑ_j, i.e.

$$\Phi_j^{\mathrm{Di}}(\lambda) = \big(\vartheta_j'\big)\hat{}\,(\lambda).$$

We will also need a vector consisting only of the Fourier transform of this data, ϑ_j, which we will denote $\mathbf{\Theta}^{\mathrm{Di}} = (\Theta_1^{\mathrm{Di}}, \dots, \Theta_n^{\mathrm{Di}})$ with

$$\Theta_j^{\mathrm{Di}}(\lambda) := \hat{\vartheta_j}(\lambda).$$

By construction both $\mathbf{\Theta}^{\mathrm{Di}}, \mathbf{\Phi}^{\mathrm{Di}} \in X_{\mathrm{sym}}$.

In our derivation of the global relation for the Laplace problem, we used the complex form of Stokes' Theorem

$$\int_{\partial\Omega} e^{-\mathrm{i}\lambda z} q_z \, \mathrm{d}z = \int_{\Omega} \mathrm{d}W = 0,$$

which was possible because the Laplace equation can be written as $q_{z\bar{z}} = 0$, or equivalently that $W(z, \bar{z}) := q_z(z, \bar{z}) \, \mathrm{d}z$ is closed. This means in essence we could work with the tangential and normal derivatives of q along the boundaries; putting the outward derivative (Neumann) and the tangential (Dirichlet) derivative data on equal footing. Let us re-derive the global relation using Green's Theorem, as we will have to do for the Helmholtz case. We provide a sketch here; however the full derivation is found in the next section, by reducing to the case $\beta = 0$.

For $\lambda \in \mathbb{C}$, we set $\zeta(\lambda) = (\lambda, \mathrm{i}\lambda)$ as a parameterisation of one part of the algebraic variety, $Z_P = \{(\lambda_1, \lambda_2) \in \mathbb{C}^2 : \lambda_1^2 + \lambda_2^2 = 0\}$. If $v_\beta(\lambda, x, y) := e^{-\mathrm{i}\zeta(\lambda)\cdot(x,y)}$, then for any fixed $\lambda \in \mathbb{C}$ and any harmonic function u inside Ω,

$$v_\beta \Delta_{x,y} u - u \Delta_{x,y} v_\beta = 0, \quad \forall \, x, y \in \Omega.$$

So by Green's Theorem we obtain an equality, which is equivalent to the global relation:

$$0 = \iint_{\Omega} [v_\beta \Delta u - u \Delta v_\beta] \, \mathrm{d}x \, \mathrm{d}y = \sum_{j=1}^{n} \int_{\Gamma_j} [v_\beta \partial_\nu u + \mathrm{i}(\zeta \cdot \nu_k) v_\beta u] \, \mathrm{d}\Gamma_j(x, y).$$

Rearranging this in to an equation for the Neumann data; making the substitution $\lambda \mapsto \lambda e^{-\mathrm{i}\alpha_k}$, and multiplying by $e^{\mathrm{i}\lambda m_k}$, we obtain the global relation, this time involving the Dirichlet data f_k, and not the derivative:

$$(T\mathbf{\Phi})(\lambda) = \mathbf{\Psi}(\lambda), \tag{2.9.2}$$

where T is the same operator given above, and $\mathbf{\Psi}(\lambda)$ is given in components as

$$\Psi_k(\lambda) := \sum_{j=1}^{n} e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k - m_j)\lambda} \left(-\lambda e^{-\mathrm{i}\Delta_{kj}}\right) \Theta_j^{\mathrm{Di}}(\lambda e^{-\mathrm{i}\Delta_{kj}}). \tag{2.9.3}$$

It has been assumed in [Ash13, AC15] that $\Psi_k(\lambda)$ is square-integrable. The following result states that $\mathbf{\Psi} := \mathrm{i}T\mathbf{\Phi}^{\mathrm{Di}}$, so the relations (2.9.1) and (2.9.2) are indeed equivalent. The proof of this follows from the later Theorem 3.1.4, in the more general case for the

Helmholtz and modified-Helmholtz problems.

Proposition 2.9.1 (Boundedness of $\boldsymbol{\Psi}$ for Laplace)**.** *The function $\boldsymbol{\Psi}(\lambda)$ defined in (2.9.3) is equivalent to $\mathrm{i}(T\boldsymbol{\Phi}^{\mathrm{Di}})(\lambda)$ for all $\lambda \in \mathbb{C}$, and $\boldsymbol{\Phi}^{\mathrm{Di}} \in X_{\mathrm{sym}}$. Thus $\Psi_k(\lambda) \in L^2(\mathbb{R}_{<0})$ for each $k = 1, \dots, n$.*

Remark 2.9.2. *This equality is special for the Laplace problem: for Helmholtz, the functions $\Psi_k(\lambda)$ cannot be written purely in terms of the operator T, and it is not clear that $\Psi_k(\lambda) \in L^2(\mathbb{R}_{<0})$.*

Using for now the result of Proposition 2.9.1, we deduce that the linear operator ℓ in the weak formulation is valid, even with this representation $\boldsymbol{\Psi}(\lambda)$ using the functions $\boldsymbol{\Theta}(\lambda)$. Let us conclude by giving an alternative proof using the integral representation for T that the set $DN(\boldsymbol{\Phi}^{\mathrm{Di}})$ is non-empty for all $\boldsymbol{\Phi}^{\mathrm{Di}} \in X_{\mathrm{sym}}$. Recall that because T has closed range, Banach's closed range Theorem gives the equality

$$\mathrm{Ran}(T) = \mathrm{Ker}(T^*)^{\perp};$$

so to show that $\boldsymbol{\Psi} \in \mathrm{Ran}(T)$, it suffices to prove that $\langle \boldsymbol{\Psi}, \boldsymbol{\eta} \rangle = 0$ for every $\boldsymbol{\eta} \in \mathrm{Ker}(T^*)$.

Theorem 2.9.3 (Existence of a solution to the global relation)**.** *The function $\boldsymbol{\Psi} = \mathrm{i}(T\boldsymbol{\Phi}^{\mathrm{Di}}) \in \mathrm{Ran}(T)$.*

Proof. Suppose that $T^*\boldsymbol{\eta} = 0$ for some $\boldsymbol{\eta} \in Y$. Then using Lemma 2.8.2 and the integral expression (2.8.13) for T^*, we calculate

$$\begin{aligned}
\langle \boldsymbol{\Psi}, \boldsymbol{\eta} \rangle &= \sum_{k,j} \int_{-\infty}^{0} \mathrm{i} e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k - m_j)\lambda} \Phi_j^{\mathrm{Di}}(\lambda e^{-\mathrm{i}\Delta_{kj}}) \overline{\eta_k(\lambda)} \, \mathrm{d}\lambda \\
&= \sum_{k,j} \frac{\mathrm{i}\sigma_j}{\pi} \int_{-\infty}^{0} \left(\int_{\mathbb{R}} e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k - m_j)\lambda} \operatorname{sinc}(\sigma_j(z - \lambda e^{-\mathrm{i}\Delta_{kj}})) \Phi_j^{\mathrm{Di}}(z) \overline{\eta_k(\lambda)} \, \mathrm{d}z \right) \mathrm{d}\lambda \\
&= \sum_{k,j} \frac{\mathrm{i}\sigma_j}{\pi} \int_{\mathbb{R}} \Phi_j^{\mathrm{Di}}(z) \overline{\left(\int_{-\infty}^{0} e^{-\mathrm{i}e^{\mathrm{i}\alpha_k}\overline{(m_k - m_j)}\lambda} \operatorname{sinc}(\sigma_j(z - \lambda e^{\mathrm{i}\Delta_{kj}})) \eta_k(\lambda) \, \mathrm{d}\lambda \right)} \, \mathrm{d}z \\
&= \sum_{j} \int_{\mathbb{R}} \mathrm{i} \Phi_j^{\mathrm{Di}}(z) \overline{(T^*\boldsymbol{\eta})_j(z)} \, \mathrm{d}z \\
&= 0.
\end{aligned}$$

□

CHAPTER 3

The Helmholtz equation

Many of the results we discussed above for the Laplace equation can be extended to the Helmholtz and modified-Helmholtz equation. Consider, for a fixed parameter β^2, the Dirichlet problem

$$\begin{aligned} -\Delta u + 4\beta^2 u &= 0 \quad \text{in } \Omega \\ u &= f_k \quad \text{on } \Gamma_k. \end{aligned} \tag{3.0.1}$$

This corresponds to Helmholtz ($\beta^2 < 0$) and modified-Helmholtz ($\beta^2 > 0$) problems respectively. As a special case, $\beta^2 = 0$ is the Dirichlet Laplace problem. This motivates the consideration that these Helmholtz problems are perturbations of the Laplace problem, and in considering the global relation as an operator equation, indeed the new operator T_β is a perturbation of T. We will see that this perturbation is *compact*, and that T_β lies in a class of *upper semi-Fredholm operators*. An upper semi-Fredholm operator, $T : X \to Y$, is a bounded operator between Banach spaces X and Y, such that the range, $\mathrm{Ran}(T) \subset Y$, is closed and the kernel, $\mathrm{Ker}(T)$, is finite dimensional. We have shown that $T : X_{\mathrm{sym}} \to Y$ has a trivial kernel, but there are a discrete set of values β^2, for which the operator equation $T_\beta \boldsymbol{x} = \boldsymbol{y}$ is not invertible. These are the Dirichlet eigenvalues of the Laplacian. For now fix $4\beta^2 \in \mathbb{R}$ which is *not* an eigenvalue of the Laplacian.

Ignoring boundary values, the function $v_\beta(z, \bar{z}, \lambda) = e^{-\mathrm{i}\lambda z + \mathrm{i}\beta^2 \bar{z}/\lambda}$ is a solution to the Helmholtz equation inside Ω, and we may alternatively write $v_\beta = e^{-\mathrm{i}\zeta\cdot(x,y)}$ in standard coordinates for

$$\zeta(\lambda) = \left(\lambda - \beta^2/\lambda, \mathrm{i}(\lambda + \beta^2/\lambda)\right).$$

Let us again denote the pullback of the Dirichlet data to Γ_j by $\vartheta_j := \psi_j^*(f_j)$. We form the vector functions $\boldsymbol{\Theta}^{\mathrm{Di}} = (\hat{\vartheta}_1, \ldots, \hat{\vartheta}_n)$, and similarly $\boldsymbol{\Phi}^{\mathrm{Ne}}$ for the pullback of the unknown Neumann data, g_j, on each edge. Noting that the outward normal, ν_j, to Γ_j is

$$\nu_j = (\sin(\alpha_j), -\cos(\alpha_j)),$$

we apply Stokes' Theorem over Ω to obtain an equation over the boundary:

$$0 = \iint_\Omega (v_\beta \Delta u - u \Delta v_\beta)\,\mathrm{d}x\,\mathrm{d}y = \sum_{j=1}^{n} \int_{\Gamma_j} (v_\beta g_j + \mathrm{i}(\zeta \cdot \nu_j) v_\beta f_j)\,\mathrm{d}\Gamma_j(x,y). \tag{3.0.2}$$

Let us denote the term involving our Dirichlet data f_j by

$$F(\lambda) = -\mathrm{i} \sum_{j=1}^{n} \int_{\Gamma_j} (\zeta(\lambda) \cdot \nu_j) v_\beta(\lambda) f_j\,\mathrm{d}\Gamma_j(x,y).$$

This will be the *known* boundary data term appearing in the global relation, and recall that for each edge Γ_j, there is the parameterisation $\gamma_j(t) = m_j + te^{\mathrm{i}\alpha_j}$. The dot product appearing in (3.0.2) is

$$\zeta(\lambda) \cdot \nu_j = -\mathrm{i}\lambda e^{\mathrm{i}\alpha_j} - \frac{\mathrm{i}\beta^2 e^{-\mathrm{i}\alpha_j}}{\lambda}.$$

Using these substitutions, we can rewrite $F(\lambda)$ as a Fourier transform of the Dirichlet data:

$$F(\lambda) = -\sum_{j=1}^{n} \left(\lambda e^{\mathrm{i}\alpha_j} + \frac{\beta^2 e^{-\mathrm{i}\alpha_j}}{\lambda} \right) \int_{-\sigma_j}^{\sigma_j} e^{-\mathrm{i}\lambda m_j + \mathrm{i}\beta^2 \overline{m_j}/\lambda} e^{-\mathrm{i}\lambda e^{\mathrm{i}\alpha_j} + \mathrm{i}\beta^2 e^{-\mathrm{i}\alpha_j}/\lambda} \vartheta_j(t)\,\mathrm{d}t. \tag{3.0.3}$$

Multiplying by $e^{\mathrm{i}\lambda m_k - \mathrm{i}\beta^2 \overline{m_k}/\lambda}$ and making the substitution $\lambda \mapsto \lambda e^{-\mathrm{i}\alpha_k}$, we may define

$$-(S_\beta \boldsymbol{\Theta}^{\mathrm{Di}})_k(\lambda) := e^{\mathrm{i}\lambda m_k e^{-\mathrm{i}\alpha_k} - \mathrm{i}\beta^2 \overline{m_k} e^{\mathrm{i}\alpha_k}/\lambda} F(\lambda e^{-\mathrm{i}\alpha_k}),$$

The same substitution for the Neumann data gives an operator T_β defined as

$$(T_\beta \boldsymbol{\Phi})_k(\lambda) := \sum_{j=1}^{n} e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k - m_j)\lambda - \mathrm{i}\beta^2 e^{\mathrm{i}\alpha_k} \overline{(m_k - m_j)}/\lambda} \Phi_j \left(\lambda e^{-\mathrm{i}\Delta_{kj}} - \frac{\beta^2 e^{\mathrm{i}\Delta_{kj}}}{\lambda} \right). \tag{3.0.4}$$

The operator S_β is similar to (3.0.4) for T_β, but with an additional multiplicative term:

$$\begin{aligned}(S_\beta \boldsymbol{\Theta})_k(\lambda) = \sum_{j=1}^{n} & e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k - m_j)\lambda - \mathrm{i}e^{\mathrm{i}\alpha_k}\beta^2 (\overline{m_k - m_j})/\lambda} \\ & \times \left(\lambda e^{-\mathrm{i}\Delta_{kj}} + \frac{\beta^2 e^{\mathrm{i}\Delta_{kj}}}{\lambda} \right) \Theta_j \left(\lambda e^{-\mathrm{i}\Delta_{kj}} - \frac{\beta^2 e^{\mathrm{i}\Delta_{kj}}}{\lambda} \right).\end{aligned} \tag{3.0.5}$$

Equating these parameterisations of (3.0.2), we obtain the global relation for the Helmholtz and modified-Helmholtz problems:

$$(T_\beta \boldsymbol{\Phi}^{\mathrm{Ne}})_k(\lambda) = -(S_\beta \boldsymbol{\Theta}^{\mathrm{Di}})_k(\lambda), \quad \forall \lambda \in \mathbb{C} \setminus \{0\},\ k = 1, \ldots, n. \tag{3.0.6}$$

In the case $\beta = 0$, this reduces to the global relation for the Laplace problem, obtained

previously. Let $\boldsymbol{\Psi}(\lambda) = (\Psi_1(\lambda), \dots, \Psi_n(\lambda))$ be defined component-wise from the known Dirichlet data, so that

$$\Psi_k(\lambda) := -(S_\beta \boldsymbol{\Theta}^{\mathrm{Di}})_k(\lambda), \qquad \text{for each } k = 1, \dots, n.$$

In this way, the D2N map can be restated as the following problem: Given $\boldsymbol{\Theta}^{\mathrm{Di}} \in X_{\mathrm{sym}}$, find $\boldsymbol{\Phi}^{\mathrm{Ne}} \in X_{\mathrm{sym}}$ such that

$$(T_\beta \boldsymbol{\Phi}^{\mathrm{Ne}})(\lambda) = \boldsymbol{\Psi}(\lambda), \quad \forall \lambda \in \mathbb{C} \setminus \{0\}. \tag{3.0.7}$$

Remark 3.0.1. *Notice that the global relation holds for all functions $v_\beta(\lambda, x, y)$ defined by $\zeta(\lambda) = \big(\lambda - \beta^2/\lambda, \mathrm{i}(\lambda + \beta^2/\lambda)\big)$ above. However a new function $e^{-\mathrm{i}\mu\cdot(x,y)}$ could also be used in Stokes' Theorem, for*

$$\mu(\lambda) = \big(\lambda - \beta^2/\lambda, -\mathrm{i}(\lambda + \beta^2/\lambda)\big)\,.$$

In this case, using the symmetry $f(\lambda) = \overline{f(-\bar{\lambda})}$ for all $f \in PW^{\sigma}_{\mathrm{sym}}$, we find that the global relation following from this representation is

$$\overline{(T\boldsymbol{\Phi}^{\mathrm{Ne}})(-\bar{\lambda})} = \overline{\boldsymbol{\Psi}(-\bar{\lambda})}, \quad \forall\, \lambda \in \mathbb{C} \setminus \{0\}.$$

which is equivalent to the system of equations (3.0.7).

3.1 A Galerkin method for Helmholtz and modified-Helmholtz equations

To solve the global relation (3.0.6), we appeal similarly to the variational problem

$$\arg_{\boldsymbol{\Phi} \in X_{\mathrm{sym}}} \min E_\beta[\boldsymbol{\Phi}]: \quad E_\beta[\boldsymbol{\Phi}] := \sum_{k=1}^{n} \int_{\gamma_k} |T_\beta(\boldsymbol{\Phi}^{\mathrm{Ne}})_k(\lambda) - \boldsymbol{\Psi}_k(\lambda)|^2 \, \mathrm{d}s(\lambda), \tag{3.1.1}$$

which may be compared with (2.6.2) for the Laplace problem. Again, if the global relation can be solved on any set $\mathcal{A}$ with a limit point, then by analyticity of the functions, the relation holds on the entire domain $\mathbb{C} \setminus \{0\}$. As a result, we may choose γ_k to be the line segment from -1 to ∞ coinciding with the negative real axis. This is to ensure we stay away from the $1/\lambda$ singularity at zero. Recall that for the Laplace problem, we could choose γ_k to be the entire real axis, which leads us to define Y in (2.4.1) to be the space

of square-integrable functions on $(-\infty, 0]$. Let us now re-define[1]

$$Y := L^2((-\infty, -1])^{\times n}.$$

We will show that both $T_\beta \mathbf{\Phi}^{\mathrm{Di}}$ and $\mathbf{\Psi}$ lie in this space Y. If a solution $\mathbf{\Phi} = \mathbf{\Phi}^{\mathrm{Ne}}$ to the global relation exists, then $E_\beta\left[\mathbf{\Phi}^{\mathrm{Ne}}\right] = 0$ is a minimiser. Differentiating, we obtain the relation

$$0 = \left.\frac{\mathrm{d}E_\beta(\mathbf{\Phi}^{\mathrm{Ne}} + t\boldsymbol{\eta})}{\mathrm{d}t}\right|_{t=0} = \sum_k \int_{-\infty}^{-1} 2\Re((T\mathbf{\Phi})_k(\overline{T\boldsymbol{\eta}_k})) - 2\Im(\Psi_k\overline{(T\boldsymbol{\eta})_k})\,\mathrm{d}\lambda.$$

For functions $\mathbf{\Phi}, \boldsymbol{\eta} \in X_{\mathrm{sym}}$, let us define the bilinear and linear forms

$$a(\mathbf{\Phi}, \boldsymbol{\eta}) := \Re \sum_k \int_{-\infty}^{-1} (T\mathbf{\Phi})_k(\lambda)\overline{((T\boldsymbol{\eta})_k(\lambda))}\,\mathrm{d}\lambda \tag{3.1.2}$$

$$\ell(\boldsymbol{\eta}) := -\Im \sum_k \int_{-\infty}^{-1} \Psi_k(\lambda)\overline{(T\boldsymbol{\eta})_k(\lambda)}\,\mathrm{d}\lambda. \tag{3.1.3}$$

Then the variational problem becomes: Given $\mathbf{\Theta}^{\mathrm{Di}} \in X_{\mathrm{sym}}$, find $\mathbf{\Phi}^{\mathrm{Ne}} \in X_{\mathrm{sym}}$ such that

$$a(\mathbf{\Phi}^{\mathrm{Ne}}, \mathbf{\Phi}') = \ell(\mathbf{\Phi}'), \quad \forall \mathbf{\Phi}' \in X_{\mathrm{sym}}. \tag{3.1.4}$$

To solve the global relation, it suffices to prove that this variational problem has a unique solution. In view of the Lax–Milgram Theorem 2.6.2, the four properties to show are: for any $\mathbf{\Phi}, \mathbf{\Phi}' \in X_{\mathrm{sym}}$,

1. $|a(\mathbf{\Phi}, \mathbf{\Phi}')| \lesssim \|\mathbf{\Phi}\|_2 \|\mathbf{\Phi}'\|_2$, which follows from T_β being bounded.
2. $|a(\mathbf{\Phi}, \mathbf{\Phi})| \gtrsim \|\mathbf{\Phi}\|_2^2$, which follows from T_β being bounded below.
3. $\ell(\mathbf{\Phi}') \lesssim \|\mathbf{\Phi}'\|_2$, which follows from showing that $\|\mathbf{\Phi}'\|_2 < \infty$.
4. For all valid Dirichlet data, f, the function $\mathbf{\Psi} = -(S_\beta \mathbf{\Theta}^{\mathrm{Di}}) \in \mathrm{Ran}(T_\beta)$.

By valid Dirichlet data, we mean that $f_j \in H^1(\Gamma_j)$ for $j = 1, \ldots, n$ and are compatible (continuous) at the vertices. For convenience, we shall write

$$T_\beta = T_0 + K_\beta,$$

where it was shown by the other author in [AC15] that T_β is a perturbation of T_0 by the compact operator K_β, and is therefore upper semi-Fredholm. Using this fact, when $4\beta^2$ is not a Dirichlet eigenvalue, the operator T_β is injective with closed range. The following

[1] The arguments we shall present for well-posedness on this new space Y still hold for the Laplace problem. This highlights the freedom we have in our choice of curves γ_k.

Theorem deduces therefore that T_β is bounded above and below. It then follows that the bilinear form a is bounded and coercive, and the weak problem has a unique solution:

Theorem 3.1.1 ([AC15]). *For $4\beta^2$ not a Dirichlet eigenvalue, the weak problem (3.1.4) admits a unique solution $\mathbf{\Phi}^{\mathrm{Ne}} \in X_{\mathrm{sym}}$.*

In the following sections we reproduce the proof by the other author, that T_β is bounded above and below, and that S_β has finite norm, which is sufficient to deduce properties 1-3 above. With regard to property 4, let us comment briefly on the question of existence for the Helmholtz problem:

Remark 3.1.2. *For the Laplace equation we showed that $DN(\mathbf{\Phi})$ is non-empty for all valid Dirichlet data, by finding a representation for T^* and showed that $\mathbf{\Psi}$ lies in $Ran(T) = Ker(T^*)^\perp$. For the Helmholtz equation, similar representations to (2.8.13) and (2.8.12) hold for T_β and T_β^*: Setting $q_{kj}(\lambda) := \lambda e^{-\mathrm{i}\Delta_{kj}} - \beta^2 e^{\mathrm{i}\Delta_{kj}}/\lambda$, we have*

$$\Phi_j(q_{kj}(\lambda)) = \frac{\sigma_j}{\pi}\int_{\mathbb{R}} \operatorname{sinc}\left(\sigma_j(z - q_{kj}(\lambda))\right)\Phi_j(z)\,\mathrm{d}z, \quad \forall\, \lambda \in \mathbb{C}. \tag{3.1.5}$$

Similarly then for Helmholtz we have

$$(T_\beta \mathbf{\Phi})_k(\lambda) = \sum_{j=1}^{n}\int_{\mathbb{R}} \frac{\sigma_j}{\pi} e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k-m_j)\lambda - \mathrm{i}\beta^2 e^{\mathrm{i}\alpha_k}\overline{(m_k-m_j)}/\lambda} \operatorname{sinc}(\sigma_j(y - q_{kj}(\lambda)))\Phi_j(y)\,\mathrm{d}y$$

$$(T^* \mathbf{\Psi})_j(\mu) = \sum_{k=1}^{n}\int_{-\infty}^{0} \frac{\sigma_j}{\pi} e^{-\mathrm{i}e^{\mathrm{i}\alpha_k}\overline{(m_k-m_j)}z + \mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k-m_j)\overline{\beta^2}/z} \operatorname{sinc}(\sigma_j(\bar{\mu} - \overline{q_{kj}(z)}))\Psi_k(z)\,\mathrm{d}z.$$

We know from classical results that for valid Dirichlet data a solution exists, and this is proven separately in [AF15b]. It's hoped that in the future, the proof in Section 2.9 for existence of the Laplace BVP (using integral representations for T and T^*), may also be extended to give an additional proof of existence for the Helmholtz problem.

3.1.1 T_β is bounded

Using the Fourier transform representation of $\Phi_j(z)$, as in the Laplace case, we intend to rewrite each term in T_β as a Laplace transform. From this we shall deduce boundedness in Y. Recall that $(T_\beta \Phi)_k(\lambda)$ is a sum of terms

$$e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k-m_j)\lambda - \mathrm{i}\beta^2 e^{\mathrm{i}\alpha_k}\overline{(m_k-m_j)}/\lambda}\Phi_j\left(\lambda e^{-\mathrm{i}\Delta_{kj}} - \frac{\beta^2 e^{\mathrm{i}\Delta_{kj}}}{\lambda}\right).$$

Using the Fourier inversion Theorem, we have the identity

$$\Phi_j(\lambda e^{-\mathrm{i}\Delta_{kj}} - \beta^2 e^{\mathrm{i}\Delta_{kj}}/\lambda) = \frac{1}{2\pi}\int_{-\sigma_j}^{\sigma_j} e^{-\mathrm{i}\tau\left(\lambda e^{-\mathrm{i}\Delta_{kj}} - \beta^2 e^{\mathrm{i}\Delta_{kj}}/\lambda\right)}\hat{\Phi}_j(-\tau)\,\mathrm{d}\tau,$$

for every $j, k = 1, \ldots, n$. Making the substitution $\tau \to \tau + \sigma_j$, this integral has a positive range $[0, 2\tau]$ and we can apply the earlier Lemma 2.4.3 to bound the Laplace transform. Specifically we calculate that the integral is equal to

$$\begin{aligned} &e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k - m_j)\lambda - \mathrm{i}\beta^2 e^{\mathrm{i}\alpha_k}\overline{(m_k - m_j)}/\lambda} \frac{1}{2\pi} \int_0^{2\sigma_j} e^{-\mathrm{i}(\tau-\sigma_j)\left(\lambda e^{-\mathrm{i}\Delta_{kj}} - \beta^2 e^{\mathrm{i}\Delta_{kj}}/\lambda\right)} \hat{\Phi}_j(-\tau)\,\mathrm{d}\tau \\ &= e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k - (m_j - \sigma_j e^{\mathrm{i}\alpha_j}))\lambda} e^{-\mathrm{i}\beta^2 \overline{e^{-\mathrm{i}\alpha_k}(m_k - (m_j - \sigma_j e^{\mathrm{i}\alpha_j}))}/\lambda} \frac{1}{2\pi} \int_0^{2\sigma_j} e^{-g(\lambda)\tau} \hat{\Phi}_j(-\tau)\,\mathrm{d}\tau \end{aligned} \tag{3.1.6}$$

where $g(\lambda) = \mathrm{i}e^{-\mathrm{i}\Delta_{kj}}\lambda - \mathrm{i}\beta^2 e^{\mathrm{i}\Delta_{kj}}/\lambda$. As in the proof of the Laplace case, for $j \neq k, k \pm 1$, this expression is observed to decay exponentially for $\lambda \in \mathbb{R}_{<0}$ (and in particular is in $L^2(-\infty, -1)$).

The case for $j = k + 1$ gives $\theta := -\Delta_{kj} \in (\epsilon, \pi - \epsilon)$. Since a bounded function is in L^2 if and only if it is in L^2 for λ sufficiently large, we shall examine the large λ behaviour of (3.1.6).

$$\tilde{g}(\lambda) := \mathrm{i}e^{\mathrm{i}\epsilon/2}\lambda,$$

then eventually $\Re g(\lambda) \geq \Re \tilde{g}(\lambda) > 0$ for $\lambda \in \mathbb{R}_{<0}$. In the case $j = k + 1$, the integral (3.1.6) becomes

$$e^{-\mathrm{i}\sigma_j\lambda} e^{\mathrm{i}\beta^2\sigma_j/\lambda} \frac{1}{2\pi} \int_0^{2\sigma_j} e^{-g(\lambda)\tau} \hat{\Phi}_j(-\tau)\,\mathrm{d}\tau,$$

and for λ sufficiently large, it is estimated from above by

$$\int_0^{2\sigma_j} e^{-\tilde{g}(\lambda)\tau} |\Phi_j(-\tau)|\,\mathrm{d}\tau;$$

and this function is in $L^2(-\infty, -1)$ by Lemma (2.4.3).

The similar case of $j = k - 1$ is proven by making the substitution $\tau \to \sigma_j - \tau$ in the integral; the case $j = k$ by observing it is proportional to the norm $\|\Phi_j\|_2$, and the other cases since the leading exponential gives decay which may be uniformly bounded. In every case, the L^2 bound depends only on the fixed geometry and $\|\Phi_j\|_2$ for $j = 1, \ldots, n$, thus the operator T_β satisfies

$$\|T_\beta \Phi\|_2 \leq C(\Omega)\|\Phi\|_2.$$

3.1.2 T_β is bounded below

We know that an operator $T : X \to Y$ between Banach spaces is bounded below if and only if it is injective and has closed range, and it was shown in [Ash13] that T_0 is bounded below. Since T_0 is injective it has nullity $\{0\}$, and thus is upper semi-Fredholm. We observe that when considered as an operator

$$T_0 : X \to \mathrm{Ran}(T_0),$$

T_0 has index 0, where the index of a Fredholm operator is the dimension of the kernel minus the dimension of the co-kernel. Since K_β is compact, it is shown in [Kat95] that T_β is also upper semi-Fredholm. If $(-4\beta^2)$ is not an eigenvalue of the Laplace problem, then there is at most one solution to the Helmholtz boundary value problem. Thus the linear problem $T_\beta \boldsymbol{\Phi} = \boldsymbol{\Psi}$ is uniquely solvable for all $\boldsymbol{\Psi} \in \mathrm{Ran}(T_\beta)$. Since T_β is injective, it follows that T_β is bounded below, provided it has closed range; which we now prove.

Proposition 3.1.3. *The operator $T_\beta : X_{\mathrm{sym}} \to Y$ has closed range.*

Proof. Suppose $\boldsymbol{\Psi}_n = T_\beta \boldsymbol{\Phi}_n$ and that $\boldsymbol{\Psi}_n \to \boldsymbol{\Psi}$, for some $\boldsymbol{\Psi} \in X_{\mathrm{sym}}$. We claim that $\boldsymbol{\Psi} \in \mathrm{Ran}(T_\beta)$. By normalising the sequences to $\boldsymbol{\varphi}_n$ and $\boldsymbol{\psi}_n$ respectively, it suffices to prove the result for these sequences.

- $\boldsymbol{\varphi}_n$ is a bounded sequence in X_{sym} and thus by the pseudo-compactness Lemma 2.3.3, $\boldsymbol{\varphi}_n \to \boldsymbol{\varphi}$ locally uniformly for a subsequence. Also since K_β is compact, $K_\beta \boldsymbol{\varphi}_n \to \boldsymbol{\psi}^{(K)} \in Y$ for a subsequence. It follows that $K_\beta \boldsymbol{\varphi} = \boldsymbol{\psi}^{(K)}$:

$$\|K_\beta \boldsymbol{\varphi} - \boldsymbol{\psi}^{(K)}\|_2 \leq \|K_\beta \boldsymbol{\varphi} - K_\beta \boldsymbol{\varphi}_n\|_2 + \|K_\beta \boldsymbol{\varphi}_n - \boldsymbol{\psi}^{(K)}\|_2,$$

  where the first term on the right-hand side tends to zero since $(\boldsymbol{\varphi}_n - \boldsymbol{\varphi}) \to \mathbf{0}$; and the second term tends to zero by assumption.

- It follows that $T_0 \boldsymbol{\varphi}_n = \boldsymbol{\psi}_n - K_\beta \boldsymbol{\varphi}_n \to \boldsymbol{\psi} - \boldsymbol{\psi}^{(K)}$. Since T_0 has closed range, the right-hand side must be equal to $T_0 \boldsymbol{\varphi}^{(T)}$ for some $\boldsymbol{\varphi}^{(T)} \in X_{\mathrm{sym}}$. We claim that $\boldsymbol{\varphi}^{(T)} = \boldsymbol{\varphi}$:

  Since T_0 is bounded below and $T_0(\boldsymbol{\varphi}_n - \boldsymbol{\varphi}^{(T)}) \to \mathbf{0}$, it must be the case that $\boldsymbol{\varphi}_n - \boldsymbol{\varphi}^{(T)} \to \mathbf{0}$ a.e. and locally uniformly. As $\boldsymbol{\varphi}_n \to \boldsymbol{\varphi}$, $\boldsymbol{\varphi} = \boldsymbol{\varphi}^{(T)}$.

- Therefore $T_0 \boldsymbol{\varphi} = \boldsymbol{\psi} - \boldsymbol{\psi}^{(K)}$ and so $T_0 \boldsymbol{\varphi} + K_\beta \boldsymbol{\varphi} = \boldsymbol{\psi}$ as required.

□

3.1.3 $S_\beta \boldsymbol{\Theta}^{\mathrm{Di}}$ has finite norm

In this section, we will show that the right-hand side of the global relation, $\Psi_k(\lambda) := -(S_\beta \boldsymbol{\Theta}^{\mathrm{Di}})_k(\lambda) \in L^2(-\infty, -1)$ for each $k = 1, \ldots, n$. It will be convenient to make the substitution $q_{k,j}(\lambda) := \lambda e^{-\mathrm{i}\Delta_{kj}} - \beta^2 e^{\mathrm{i}\Delta_{kj}}/\lambda$. We recall that $\boldsymbol{\Psi}(\lambda)$ is given by

$$\begin{aligned}\Psi_k(\lambda) = \mathrm{i} \sum_{j=1}^{n} & e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k - m_j)\lambda - \mathrm{i}e^{\mathrm{i}\alpha_k}\beta^2(\overline{m_k - m_j})/\lambda} \\ & \times \left(\mathrm{i} q_{k,j}(\lambda) + \frac{2\mathrm{i}\beta^2 e^{\mathrm{i}\Delta_{kj}}}{\lambda} \right) \Theta_j^{\mathrm{Di}}\left(q_{k,j}(\lambda)\right).\end{aligned} \tag{3.1.7}$$

Since (3.1.7) involves a multiplication by λ, this motivates us to consider the Fourier transform of the *derivative* of ϑ_j. This proof is an extension of the one from Section 2.9 where it was shown that $\boldsymbol{\Psi} = \mathrm{i}T\boldsymbol{\Phi}^{\mathrm{Di}}$. Recall again that the Dirichlet data $f_j \in H^1(\Gamma_j)$, satisfies $f_j(z_j) = f_{j+1}(z_j)$. Thus the pullback functions $\vartheta_j \in H^1$ and are continuous across the vertices:

$$\vartheta_j(\sigma_j) = \vartheta_{j+1}(-\sigma_j), \quad j = 1, \dots, n,$$

where we make the identification that $\vartheta_{n+1} = \vartheta_1$. Integrating by parts we have, for each[2] $j = 1, \dots, n$

$$\mathrm{i}\lambda\hat{\vartheta}_j(\lambda) = e^{\mathrm{i}\lambda\sigma_j}\vartheta_j(-\sigma_j) - e^{-\mathrm{i}\lambda\sigma_j}\vartheta_j(\sigma_j) + \int_{-\sigma_j}^{\sigma_j} e^{-\mathrm{i}\lambda\tau}\vartheta_j'(\tau)\,\mathrm{d}\tau.$$

Making this substitution in to (3.1.7) for λ replaced by $q_{k,j}(\lambda)$, we have

$$\begin{aligned}\Psi_k(\lambda) = \mathrm{i}\sum_{j=1}^{n} e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k-m_j)\lambda - \mathrm{i}e^{\mathrm{i}\alpha_k}(\overline{m_k-m_j})/\lambda}\left(e^{\mathrm{i}q_{k,j}(\lambda)\sigma_j}\vartheta_j(-\sigma_j) - e^{-\mathrm{i}q_{k,j}(\lambda)\sigma_j}\vartheta_j(\sigma_j)\right)\\ + \mathrm{i}\sum_{j=1}^{n} e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k-m_j)\lambda - \mathrm{i}e^{\mathrm{i}\alpha_k}\beta^2(\overline{m_k-m_j})/\lambda}\Phi_j^{\mathrm{Di}}(q_{k,j}(\lambda))\\ - \sum_{j=1}^{n} e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k-m_j)\lambda - \mathrm{i}e^{\mathrm{i}\alpha_k}\beta^2(\overline{m_k-m_j})/\lambda}\frac{2\beta^2 e^{\mathrm{i}\Delta_{kj}}}{\lambda}\Theta_j^{\mathrm{Di}}\left(q_{k,j}(\lambda)\right).\end{aligned} \tag{3.1.8}$$

The centre operator is precisely $(\mathrm{i}T_\beta\boldsymbol{\Phi}^{\mathrm{Di}})(\lambda)$, and let us denote the final one as a remainder

$$-(\tilde{S}_\beta\boldsymbol{\Theta})_k(\lambda) := -\sum_{j=1}^{n} e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k-m_j)\lambda - \mathrm{i}e^{\mathrm{i}\alpha_k}\beta^2(\overline{m_k-m_j})/\lambda}\frac{2\beta^2 e^{\mathrm{i}\Delta_{kj}}}{\lambda}\Theta_j^{\mathrm{Di}}\left(q_{k,j}(\lambda)\right). \tag{3.1.9}$$

Since $\left|\frac{2\beta^2 e^{\mathrm{i}\Delta_{kj}}}{\lambda}\right| \lesssim 1$ for $\lambda \in (-\infty, -1)$ and any values $k, j = 1, \dots, n$, both of these terms $(\mathrm{i}T_\beta\boldsymbol{\Phi}^{\mathrm{Di}})_k, (\tilde{S}_\beta\boldsymbol{\Theta})_k \in L^2(-\infty, -1)$. Thus, it remains for us to consider the first line of (3.1.8). We will deduce that

$$\sum_j e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k-m_j)\lambda - \mathrm{i}e^{\mathrm{i}\alpha_k}(\overline{m_k-m_j})/\lambda}\left(e^{\mathrm{i}q_{k,j}(\lambda)\sigma_j}\vartheta_j(-\sigma_j) - e^{-\mathrm{i}q_{k,j}(\lambda)\sigma_j}\vartheta_j(\sigma_j)\right) \tag{3.1.10}$$

is in $L^2(-\infty, -1)$, by showing that this term is identically zero, as the following result states.

Theorem 3.1.4 (Boundedness of $\boldsymbol{\Psi}$)**.** *Let $\boldsymbol{\Theta}^{\mathrm{Di}}$ be the function corresponding to any valid Dirichlet data $\{f_j\}_{j=1}^n$, which are continuous across the vertices and lie in $H^1(\Gamma_j)$ for each*

[2] weakly differentiable functions are continuous on $\mathbb{R}$, so this is well-defined. However all these arguments follow through assuming $\vartheta_j \in C^\infty([-\sigma_j, \sigma_j])$ with continuity across the vertices. Then our conclusion follows from the density of these functions in H^1.

$j = 1, \dots, n$. *For any* $\beta^2 \in \mathbb{R}$, *the operator* $-S_\beta \boldsymbol{\Theta}^{\mathrm{Di}}$ *is given by*

$$-(S_\beta \boldsymbol{\Theta}^{\mathrm{Di}})(\lambda) = \mathrm{i}(T_\beta \boldsymbol{\Phi}^{\mathrm{Di}})(\lambda) - (\tilde{S}_\beta \boldsymbol{\Theta})(\lambda),$$

and as such $-(S_\beta \boldsymbol{\Theta}^{\mathrm{Di}}) \in Y$. *Furthermore, for* $\beta^2 = 0$, *we have the equality* $-(S_0 \boldsymbol{\Theta}^{\mathrm{Di}})(\lambda) = \mathrm{i}(T \boldsymbol{\Phi}^{\mathrm{Di}})(\lambda)$, *as stated in Section 2.9.*

Proof. It suffices to prove that (3.1.10) is zero, which follows precisely from the continuity of our boundary across the vertices. Consider two adjacent edges i and $j = i + 1$. Noting the equality $m_i + \sigma_i e^{\mathrm{i}\alpha_i} = m_j - \sigma_j e^{\mathrm{i}\alpha_j}$, we consider the terms of (3.1.10) involving $\vartheta_i(\sigma_i)$ and $\vartheta_j(-\sigma_j)$ at the vertex z_j. The i-th term is

$$\begin{aligned}
+ (i\text{-th term}) &= -e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k - m_i)\lambda - \mathrm{i}e^{\mathrm{i}\alpha_k}\beta^2(\overline{m_k - m_i})/\lambda} e^{-\mathrm{i}\sigma_j\left(\lambda e^{-\mathrm{i}\Delta_{ki}} - \beta^2 e^{\mathrm{i}\Delta_{ki}}/\lambda\right)} \vartheta_i(\sigma_i) \\
&= -e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}\left(m_k - \left[m_i + \sigma_i e^{\mathrm{i}\alpha_i}\right]\right)\lambda - \mathrm{i}\beta^2 \overline{e^{-\mathrm{i}\alpha_k}\left(m_k - \left[m_i + \sigma_i e^{\mathrm{i}\alpha_i}\right]\right)}/\lambda} \vartheta_i(\sigma_i) \\
&= -e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}\left(m_k - \left[m_j - \sigma_j e^{\mathrm{i}\alpha_j}\right]\right)\lambda - \mathrm{i}\beta^2 \overline{e^{-\mathrm{i}\alpha_k}\left(m_k - \left[m_j - \sigma_i e^{\mathrm{i}\alpha_j}\right]\right)}/\lambda} \vartheta_j(-\sigma_j) \\
&= -e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k - m_j)\lambda - \mathrm{i}\beta^2 e^{\mathrm{i}\alpha_k}\overline{(m_k - m_j)}\lambda} e^{\mathrm{i}\sigma_j\left(\lambda e^{-\mathrm{i}\Delta_{kj}} - \beta^2 e^{\mathrm{i}\Delta_{kj}}/\lambda\right)} \vartheta_j(-\sigma_j) \\
&= -\left(j\text{-th term}\right).
\end{aligned}$$

Therefore all terms in the sum (3.1.10) cancel, and we can write our operator simply as

$$\Psi_k(\lambda) = \mathrm{i}(T_\beta \boldsymbol{\Phi}^{\mathrm{Di}})_k(\lambda) - (\tilde{S}_\beta \boldsymbol{\Theta})_k(\lambda), \tag{3.1.11}$$

which reduces to the Laplace case $\Psi_k(\lambda) = \mathrm{i}(T \boldsymbol{\Phi}^{\mathrm{Di}})_k(\lambda)$ for $\beta = 0$. In particular, $\Psi_k(\lambda) \in L^2(-\infty, -1)$. □

CHAPTER 4

Numerical results for 2D polygons

In this final chapter for two-dimensional problems, we will present numerical results of the Galerkin method we have introduced. We will be particularly interested in the spectral convergence rates which are demonstrated, and that compare well to recent results [FFX04, SSF10, FF11, HFS15]. We also introduce a related method for identifying eigenvalues of the Dirichlet Laplacian; which are values $-4\beta^2 \in \mathbb{R}$, such that there does *not* exist a unique solution to the global relation. Equivalently, these are values for which the homogeneous problem

$$\begin{aligned} -\Delta u &= -4\beta^2 u \quad \text{in } \Omega \\ u &= 0 \qquad\quad \text{on } \Gamma_k \end{aligned}$$

has a non-zero solution $u_\beta(x, y)$. This function u_β is the eigenfunction corresponding to $-4\beta^2$. It is known that all eigenvalues of the Dirichlet Laplacian are strictly positive ($4\beta^2 < 0$) and bounded away from zero. The smallest modulus eigenvalue has special properties, and is called the *principal eigenvalue*[1] [McL00, Eva10, pp. 249 & 357 resp.].

4.1 An implementation

In the previous chapter we introduced the new Galerkin method for the Helmholtz and modified-Helmholtz equation with Dirichlet boundary conditions (3.0.1). This is valid for the Laplace equation with $\beta^2 = 0$ as a special case. Recall the definition of an approximating subspace, $X_N \subset X_{\text{sym}}$ from Section 2.7, such that for each edge $\{\Gamma_j\}_{j=1}^n$ we have a basis for a subspace of $L^2_{\mathbb{R}}[-\sigma_j, \sigma_j]$ consisting of the normalised Legendre polynomials

$$f_{j,J}(t), \quad j = 1, \ldots, n; \quad J = 0, \ldots, N-1.$$

[1] We are talking here about Dirichlet eigenvalues, which are those where zero Dirichlet data has been prescribed over the entire boundary. Comparison between these and Neumann eigenvalues (as well as mixed boundary data) has been an area of some interest. One such example is studying the smallest-modulus eigenvalues of each, and some results are given in [Fri91].

The Fourier transform $e_{j,J}(\lambda) := \hat{f}_{j,J}(\lambda)$ of these vectors forms a natural basis for X_{sym}, and a specific function of the basis is

$$\boldsymbol{e}_{j,J}(\lambda) := (0, \dots, e_{j,J}(\lambda), 0, \dots, 0),$$

meaning the J-th basis element on face j is described as a vector-valued function. Then the unknown Neumann vector $\boldsymbol{\Phi}^{\text{Ne}}$ is approximated component-wise in this subspace by

$$\Phi_j^{\text{Ne}} \approx \Phi_{N,j}^{\text{Ne}} = \sum_{J=0}^{N-1} c_{j,J} \mathbf{e}_{j,J},$$

for the real coefficients $\{c_{j,J}\}_{j,J}$ to be determined. In view of Lax–Milgram and Céa's Lemma, in Section 2.7 we proved that when the true Neumann data, $\varphi_j = \mathcal{F}^{-1}(\Phi_j^{\text{Ne}})$, are in $C^\infty([-\sigma_j, \sigma_j])$ for each $j = 1, \dots, n$, the convergence on each edge will be exponentially fast:

$$\|\varphi_j - \varphi_{N,J}\|^2_{L^2[-\sigma_j,\sigma_j]} \to 0.$$

$\boldsymbol{\Phi}^{\text{Di}}$ may also be approximated by $\boldsymbol{\Phi}_N^{\text{Di}} \in X_N$:

$$\Phi_j^{\text{Di}}(\lambda) \approx \Phi_{N,i}^{\text{Di}}(\lambda) = \sum_{I=0}^{N-1} c_{i,I} e_{i,I}(\lambda), \qquad \text{for each } \; i = 1, \dots, n$$

and in vector form the approximation is given by

$$\boldsymbol{\Phi}^{\text{Di}}(\lambda) \approx \boldsymbol{\Phi}_N^{\text{Di}}(\lambda) = \sum_{i=1}^{nN} c_{i,I} \boldsymbol{e}_{i,I}(\lambda),$$

where the projection coefficients $c_{i,I} \in \mathbb{R}$ for $i = 1, \dots, n$ and $I = 0, \dots, N-1$. Then also, if we project the function $\boldsymbol{\Psi}(\lambda) = -(S_\beta \boldsymbol{\Phi}^{\text{Di}})$ to X_N, we find a representation in terms of the functions $e_{i,I}(\lambda)$ too:

$$\begin{aligned}
\Psi_{N,k}(\lambda) &= (S_\beta \boldsymbol{\Phi}_N^{\text{Di}})_k(\lambda) \\
&= \sum_{i=1}^{n} \sum_{I=0}^{N-1} c_{i,I} (S_\beta \boldsymbol{e}_{i,I})_k(\lambda) \\
&= \sum_{i=1}^{n} \sum_{I=0}^{N-1} c_{i,I} e^{\mathrm{i}e^{-\mathrm{i}\alpha_k}(m_k - m_i)\lambda - \mathrm{i}e^{\mathrm{i}\alpha_k}\beta^2(\overline{m_k - m_i})/\lambda} \\
&\qquad\qquad \times \left(\lambda e^{-\mathrm{i}\Delta_{ki}} + \frac{\beta^2 e^{\mathrm{i}\Delta_{ki}}}{\lambda}\right) e_{i,I} \left(\lambda e^{-\mathrm{i}\Delta_{ki}} - \frac{\beta^2 e^{\mathrm{i}\Delta_{ki}}}{\lambda}\right)
\end{aligned}$$

As we did in (2.7.3) for the Laplace problem, we can form a matrix problem $\underline{\boldsymbol{A}} \cdot \boldsymbol{B} = \boldsymbol{L}$, where we again denote the matrix and vector components by $A_{(i,I),(j,J)}$ and $L_{(j,J)}$. The

relevant integral terms appearing in the weak formulation are

$$M_{i,I,j,J} := \sum_{k=1}^{n} \int_1^\infty (T_\beta \boldsymbol{e}_{i,I})_k(-t)\overline{(T_\beta \boldsymbol{e}_{j,J})_k(-t)}\,\mathrm{d}t \tag{4.1.1}$$

Then $A_{i,I,j,J} = \Re M_{i,I,j,J}$ and in view of (3.1.11),

$$L_{j,J} = -\Im \sum_{i=1}^{n}\sum_{I=0}^{N-1} c_{i,I} M_{i,I,j,J} + \Im \sum_{k=1}^{n} \int_1^\infty (\tilde{S}_\beta \boldsymbol{\Theta})_k(-t)\overline{(T_\beta \boldsymbol{e}_{j,J})_k(-t)}\,\mathrm{d}t. \tag{4.1.2}$$

However, using the above expression, we still require an approximation of $\Theta_i(\lambda)$. So we may use the full expression for $\boldsymbol{\Psi}(\lambda)$ with the coefficients

$$\Theta_i^d(\lambda) \approx \Sigma_{N,i}^d(\lambda) = \sum_{I=0}^{N-1} \mathfrak{c}_{i,I} e_{i,I}(\lambda),$$

for projection coefficients $\mathfrak{c}_{\mathfrak{i},\mathfrak{J}}$ with $i = 1, \ldots, n$ and $I = 0, \ldots, N-1$. Therefore

$$L_{j,J} = \Im \sum_{k,i=1}^{n}\sum_{I=0}^{N-1} \mathfrak{c}_{i,I} \int_1^\infty (S_\beta \boldsymbol{e}_{i,I})_k(\lambda)\overline{(T_\beta \boldsymbol{e}_{j,J})_k(-t)}\,\mathrm{d}t, \tag{4.1.3}$$

and we shall use this representation for our numerical examples.

Remark 4.1.1. *In general (and we shall see this is a problem for the three-dimensional case), our basis functions do not satisfy the compatibility conditions of continuity across the vertices of the polygon, described in Section 0.2.5. In this case, the integral (4.1.3) may not be finite. However for the examples we choose, this problem does not seem to occur. The term (4.1.2) takes in to account consistency of data at the vertices, and so the operator $\tilde{S}_\beta$ no longer has a growth factor $\lambda e^{-\mathrm{i}\Delta_{ki}}$, but only a decay factor in λ. Thus an implementation along these lines, using the values $M_{i,I,j,J}$ previously calculated for the bilinear form a, may indeed increase accuracy and numerical efficiency.*

In either case, the Galerkin method to recover the approximate solution $\boldsymbol{\Phi}_N^{\mathrm{Ne}} \in X_N$, is given by the linear problem: Find coefficients $\{b_{i,I}\}_{i,I}$ such that

$$\sum_{i=1}^{n}\sum_{I=0}^{N-1} b_{i,I} a_\beta(\boldsymbol{e}_{i,I}, \boldsymbol{e}_{j,J}) = \ell_\beta(\boldsymbol{e}_{j,J}), \quad \forall j = 1, \ldots, n \text{ and } J = 0, \ldots, N-1.$$

The right-hand side vector ℓ is formed as a row vector out of the components $L_{i,I}$, and similarly for the matrix a along each row and column.

Remark 4.1.2. *As we showed for the Laplace equation in Remark 2.7.3, the symmetries*

in $M_{i,I,j,J}$ are still true for the Helmholtz BVP:

$$M_{i,I,j,J} = \overline{M_{j,J,i,I}}.$$

This symmetry reduces the number of computations required to find all the values $M_{i,I,j,J}$. Recall that for the Laplace problem, the total number of integrations required to form the linear problem is

$$\frac{1}{2}n^2N(nN+1) = \mathcal{O}(n^3N^2)$$

For the Helmholtz problem though, the matrix elements, $L_{j,J}$, can no longer be reduced entirely to terms involving the projection coefficients, $c_{i,I}$, and $M_{i,I,j,J}$. Thus the number of computations required is greater for the Helmholtz BVPs, than for Laplace. However, it should be noted that the additional $1/t$ decay in the integrand of the second term in (4.1.2), does ensure that this integral converges faster: indeed, we see from (3.1.9) that the operator $\tilde{S}$ acting on a basis vector $\boldsymbol{e}_{i,I}(\lambda)$, is given by

$$(\tilde{S}\boldsymbol{e}_{i,I})_k(\lambda) = \frac{2\beta^2 e^{\mathrm{i}\Delta_{kj}}}{\lambda}(T\boldsymbol{e}_{i,I})_k(\lambda).$$

The total number of integral terms needed is $\frac{1}{2}n^2N(nN+1)$ for $M_{i,I,j,J}$, and an additional $n(nN)$ terms for $L_{j,J}$. The total number of integrations is therefore

$$\frac{1}{2}n^2N(nN+3),$$

which is still $\mathcal{O}(n^3N^2)$, with the same constant for sufficiently large values n, N.

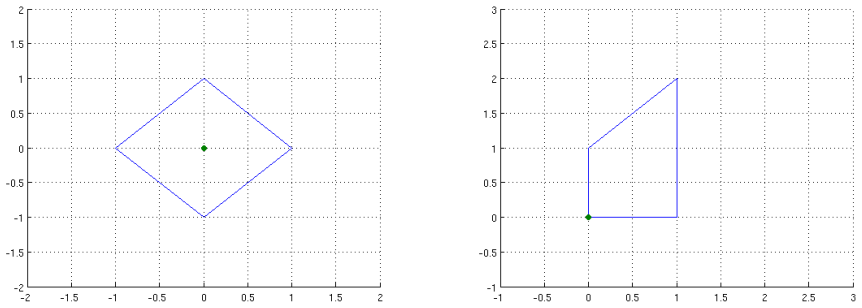
4.2 Numerical results

We present here a few test cases for the method presented in Chapter 3. We shall do this in the two domains shown in Figure 4.1. Consider the following general solution to the Helmholtz equation, $-\Delta u + 4\beta^2 = 0$ with $\beta^2 < 0$:

$$u(x,y) = (A_1\cos(\mu_1 x) + A_2\sin(\mu_1 x))\,(B_1\cos(\mu_2 y) + B_2\sin(\mu_2 y))\,, \tag{4.2.1}$$

for A_i and B_j arbitrary, and $\mu_1^2 + \mu_2^2 = |4\beta^2|$. For our purposes we shall identify the test cases with the domain (A or B) and a number corresponding to $\mu_1 = \sqrt{3|\beta^2|}, \mu_2 = \sqrt{|\beta^2|}$ and

1. $4\beta^2 = -1$; 6 basis vectors; variables $(A_1, A_2, B_1, B_2) = (1, 0, 1, 0)$,
2. $4\beta^2 = -1$; 6 basis vectors; variables $(1, 2, 3/2, 5/2)$,
3. $4\beta^2 = -16$; 8 basis vectors; variables $(1, 0, 1, 0)$,



(a) Domain A, vertices at $\{1, \mathrm{i}, -1, -\mathrm{i}\}$ (b) Domain B, vertices at $\{0, 1, 1+2\mathrm{i}, \mathrm{i}\}$

Figure 4.1: Two test domains, A and B.

4. $4\beta^2 = -16$; 8 basis vectors; variables $(1, 2, 3/2, 5/2)$.

Each of the Figures 4.2-4.9 shows the exact Neumann data along each edge compared with the approximate Neumann data for a given test case. In each Figure, the top four plots show the exact data and the reconstructed data over each of the edges, and the bottom four plots are the absolute pointwise error between these two.

Figure 4.10 demonstrates spectral accuracy as the number of basis vectors, N, is increased for test case 2 above. In particular we observe extraordinarily low condition numbers for both these domains. These results are comparable to [SSF10, FIS15, HFS15], which solve the global relation via a pointwise collocation method. In [SSF10], numerical results are given with a Fourier basis, and with a polynomial (Chebyshev) basis. The former case has comparably low condition numbers to the results presented here, but slower, polynomial, convergence rates. The latter case has fast (exponential) convergence with higher condition numbers. The results presented here have a big advantage: by using a polynomial (Legendre) basis, we have proven exponential convergence for smooth boundary data, and we still have low condition numbers.

In these figures, the maximum error is the largest calculated L^∞-norm error between the two functions, across the whole perimeter. This is a particularly good numerical result, since the spectral convergence Theorem 2.7.2 and rate (2.7.2) are for the weaker L^2 norm convergence.

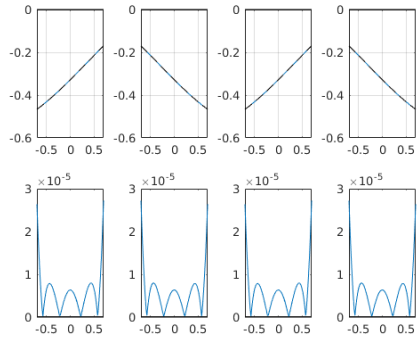


Figure 4.2: Test case 1, domain A

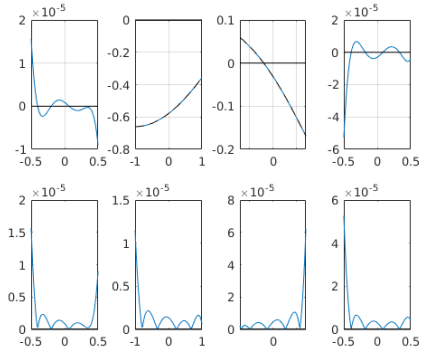


Figure 4.3: Test case 1, domain B

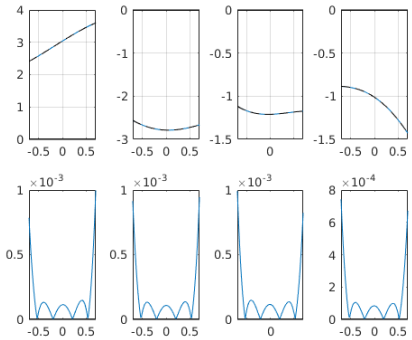


Figure 4.4: Test case 2, domain A

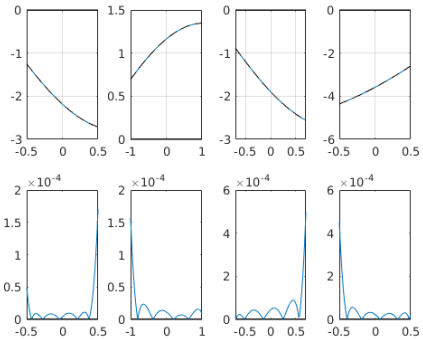


Figure 4.5: Test case 2, domain B

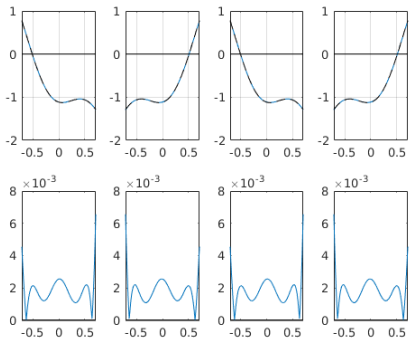


Figure 4.6: Test case 3, domain A

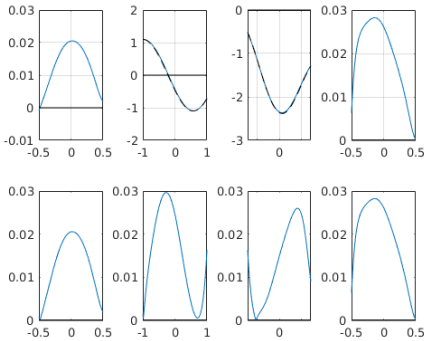


Figure 4.7: Test case 3, domain B

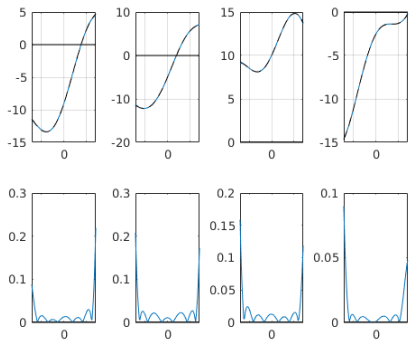


Figure 4.8: Test case 4, domain A

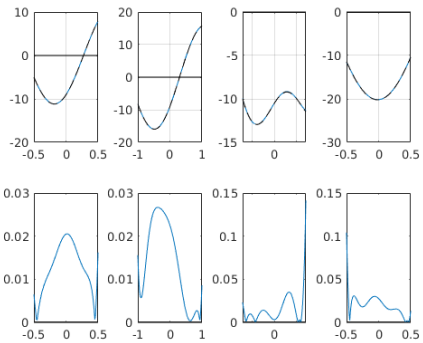
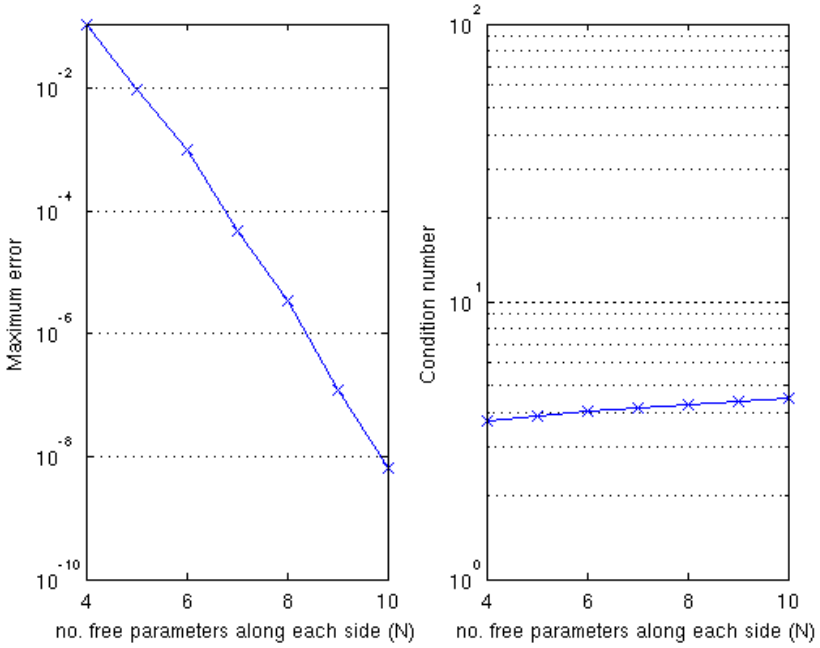
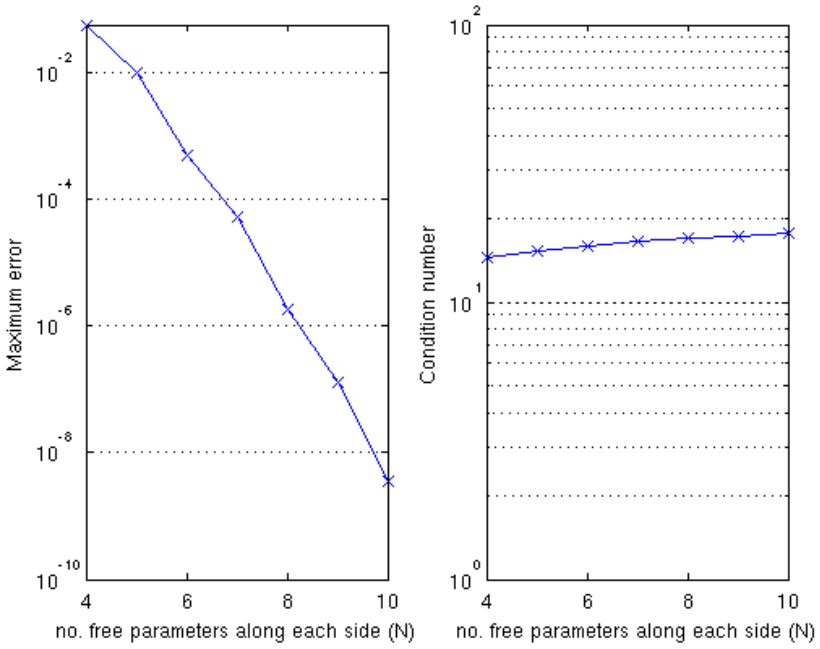


Figure 4.9: Test case 4, domain B



(a) Square domain



(b) Wedge domain

Figure 4.10: Helmholtz equation: Maximum absolute errors and condition numbers for the resulting Galerkin matrices compared against the number of basis vectors, N, on each edge.

4.3 Additional results

By changing the value of β^2, we can equally solve the global relation for the modified-Helmholtz equations. An example of a generic solution is given similarly to (4.2.1):

$$u(x,y) = \left(A_1\cosh(\mu_1 x) + A_2\sinh(\mu_1 x)\right)\left(B_1\cosh(\mu_2 y) + B_2\sinh(\mu_2 y)\right), \tag{4.3.1}$$

where again $\mu_1^2 + \mu_2^2 = 4\beta^2 > 0$. Using the same parameters $(A_1, A_2, B_1, B_2) = (1, 2, 3/2, 5/2)$, we observe spectral convergence towards the true solution as shown in Figure 4.11.

It is also possible to modify these linear forms to permit *mixed* boundary data. For simplicity, let us briefly describe this extension for the Laplace problem, for which the global relation is

$$T\mathbf{\Phi}^{\mathrm{Ne}} = \mathrm{i}T\mathbf{\Phi}^{\mathrm{Di}}.$$

In this equation, our unknown data has previously been $\mathbf{\Phi}^{\mathrm{Di}}$, which is a vector comprising of the Fourier transform of derivatives of the Dirichlet data; whereas $\mathbf{\Phi}^{\mathrm{Ne}}$ is the Fourier transform of the Neumann data. Suppose instead for some subset $\mathcal{D} \subset \{1, \ldots, n\}$, we are given the Dirichlet data on edge Γ_j, for $j \in \mathcal{D}$, and else we are given the Neumann data. Let us construct the known Dirichlet data vector as $\mathbf{\Phi}^{d,K} = (\Phi_1^{d,K}, \ldots, \Phi_n^{d,K})$ with zeros where data has not been prescribed:

$$\Phi_j^{d,K} = \begin{cases} \Phi_j^{\mathrm{Di}}, & j \in \mathcal{D} \\ 0, & \text{else.} \end{cases}$$

This can be rephrased as a projection operator $P : X_{\mathrm{sym}} \to X_{\mathrm{sym}}$ by $P : \mathbf{\Phi}^{\mathrm{Di}} \mapsto \mathbf{\Phi}^{d,K}$. A similar construction for the unknown Neumann data gives the known boundary data function

$$\mathbf{\Phi}^K(\lambda) := \mathbf{\Phi}^{d,K}(\lambda) + \mathbf{\Phi}^{n,K}(\lambda),$$

or equivalently $\mathbf{\Phi}^K = P\mathbf{\Phi}^{\mathrm{Di}} + (I - P)\mathbf{\Phi}^{\mathrm{Ne}}$. Constructing similarly the *unknown* data function $\mathbf{\Phi}^U = (I - P)\mathbf{\Phi}^{\mathrm{Di}} + P\mathbf{\Phi}^{\mathrm{Ne}}$ and noting that $P^2 = P$, the global relation may be rewritten as

$$TP\mathbf{\Phi}^U - \mathrm{i}T(I - P)\mathbf{\Phi}^U = \mathrm{i}\left[TP\mathbf{\Phi}^K + \mathrm{i}T(I - P)\mathbf{\Phi}^K\right]. \tag{4.3.2}$$

Since for mixed boundary data, assurance of existence is not guaranteed (e.g. for entirely Neumann data, we further require the zero-average condition over the boundary), we will not pursue the formal analysis of (4.3.2) here. Instead, we present in Figure 4.12 a numerical test of the same problem that was studied in [FF11]; where a solution is known to exist. This includes the same domain B as was used there, while the domain A is for

comparison with our previous tests. The solution inside the domains is

$$u(x, y) = e^{1+x} \cos(2 + y),$$

and Neumann data is given between the third and fourth vertices in our domains 4.1; while Dirichlet data is prescribed on the other three edges.

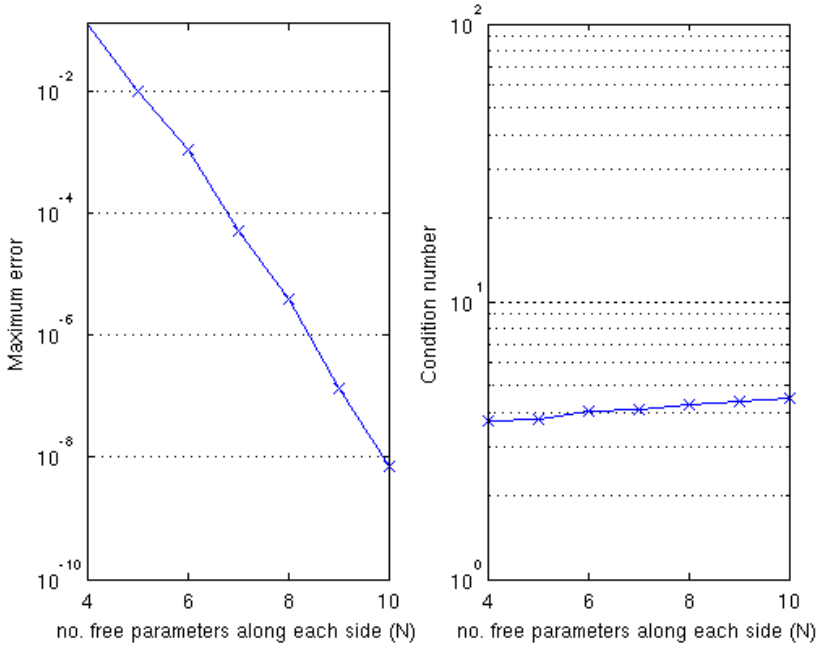
Remark 4.3.1. *These modified equations are similar in style to the operator T, and so some properties of T can be used, such as boundedness and closed range. An alternative approach would be to use the same operator T, but instead to modify the domains of the functions. E.g. in a triangular domain with Neumann data given on the final edge we could consider*

$$\begin{aligned} \tilde{\mathbf{\Phi}}^K &= (\Phi_1^{\mathrm{Di}}, \Phi_2^{\mathrm{Di}}, \mathrm{i}\Phi_3^{\mathrm{Ne}}) \\ \tilde{\mathbf{\Phi}}^U &= (\Phi_1^{\mathrm{Ne}}, \Phi_2^{\mathrm{Ne}}, -\mathrm{i}\Phi_3^{\mathrm{Di}}) \end{aligned} \tag{4.3.3}$$

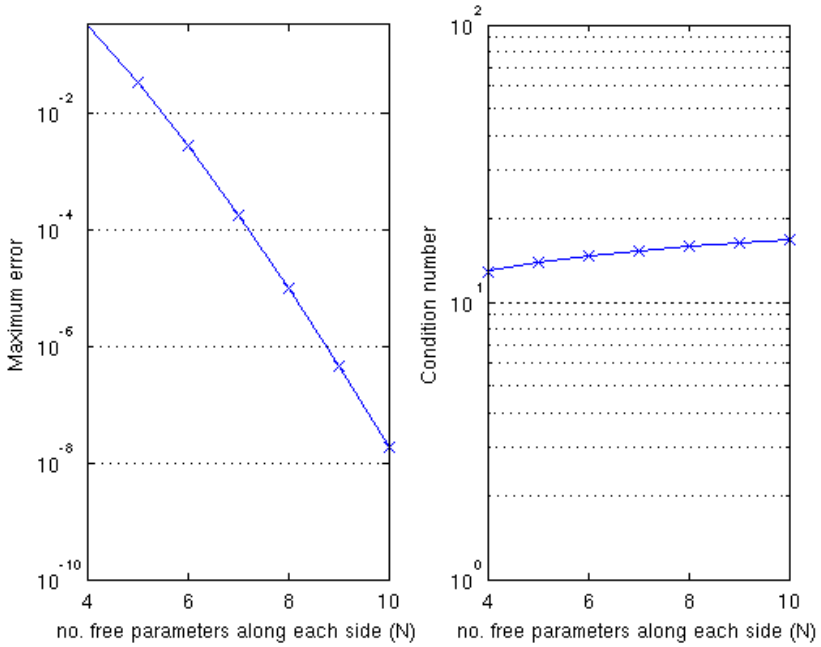
Then the global relation remains $T\tilde{\mathbf{\Phi}}^U = \mathrm{i}T\tilde{\mathbf{\Phi}}^K$. However due to a multiplication by i*, the domain of T involves components in X_{asym} as well as X_{sym}. Indeed, if we set*

$$X_{\mathcal{D}} := PW_{\mathrm{sym}}^{\sigma_1} \times PW_{\mathrm{sym}}^{\sigma_2} \times \left(\mathrm{i}PW_{\mathrm{sym}}^{\sigma_3}\right) = PW_{\mathrm{sym}}^{\sigma_1} \times PW_{\mathrm{sym}}^{\sigma_2} \times PW_{\mathrm{asym}}^{\sigma_3},$$

then T must be considered as an operator $T : X_P \to Y$.

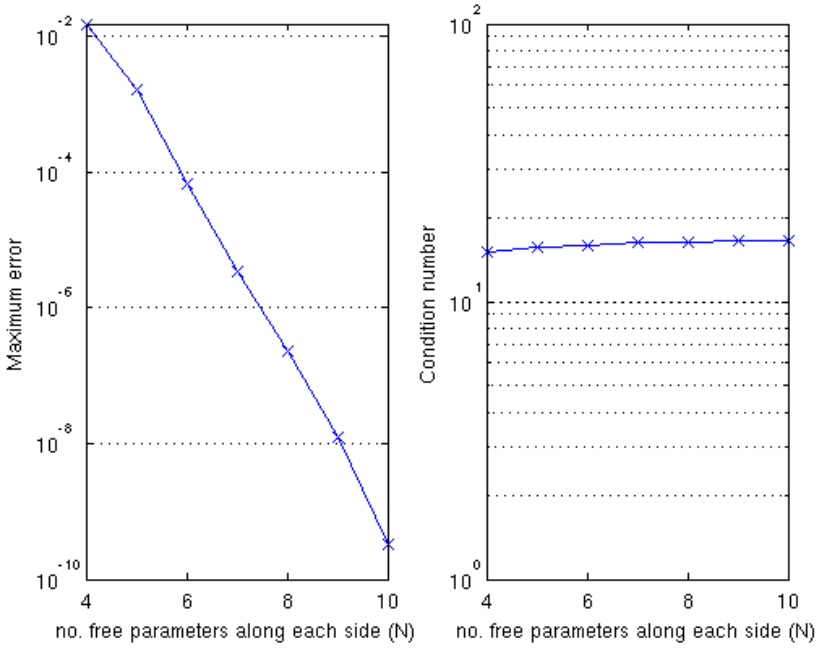


(a) Square domain

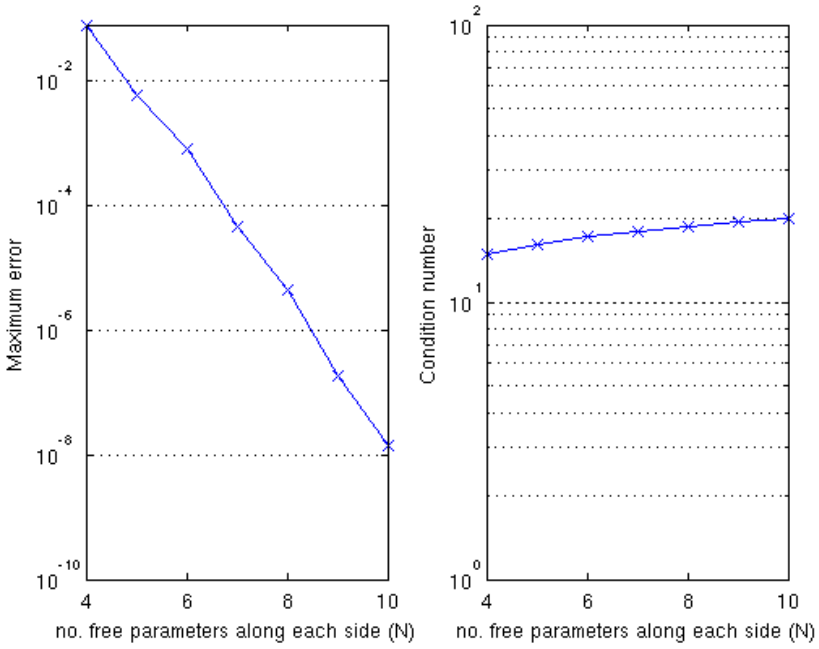


(b) Wedge domain

Figure 4.11: modified-Helmholtz equation: Maximum absolute errors and condition numbers for the resulting Galerkin matrices compared against the number of basis vectors, N, on each edge.



(a) Square domain



(b) Wedge domain

Figure 4.12: Laplace equation with mixed boundary data: Maximum absolute errors and condition numbers for the resulting Galerkin matrices compared against the number of basis vectors, N, on each edge.

4.3.1 Less regular data

In the previous sections, we have used a known smooth solution to the BVPs, and compared the actual Neumann data to the reconstructed data, with good results also comparable to those found in [FF11]. Our numerical experiments also agree with the spectral convergence Theorem 2.7.2, where the Neumann data is known to be smooth on each edge. However, for real-valued problems, the Neumann data will not be as smooth, and as such we would not expect such rapid convergence.

In this section, we consider some numerical experiments using only the Dirichlet data. We will approximate the error by calculating the numerical solution for a larger number of basis vectors ($N = 20$ on each edge), and comparing our results to these. We will do this for the two domains as above: Domain A is a square, and Domain B is the wedge domain from [FF11]. The four BVPs we will test are:

1. Using constant Dirichlet data, $f \equiv 3$, over the whole boundary, solving the Helmholtz problem $-\Delta u + 4\beta^2 u = 0$, for $4\beta^2 = -1$.

2. Using constant Dirichlet data, $f \equiv 3$, over the whole boundary, solving the Helmholtz problem $-\Delta u + 4\beta^2 u = 0$, for $4\beta^2 = -16$.

3. Using zero Dirichlet data over edges 1,2 and 4, and a 'hat' function (described below) over the third edge. We will solve the Helmholtz problem $-\Delta u + 4\beta^2 u = 0$, for $4\beta^2 = -1$.

4. Using zero Dirichlet data over edges 1,2 and 4, and a 'hat' function (described below) over the third edge. We will solve the Helmholtz problem $-\Delta u + 4\beta^2 u = 0$, for $4\beta^2 = -16$.

In domain B, this 'hat' function corresponds to being on the top (sloped) edge of the domain, where one of the interior angles is greater than $\pi/2$, and one angle is less than $\pi/2$. Over an edge parameterised by $\gamma_3 : [-\sigma_3, \sigma_3] \to \mathbb{R}$, the Dirichlet data 'hat' function is

$$\vartheta_3(t) = \begin{cases} 1 + \frac{t}{\sigma_3}, & -\sigma_3 < t < 0 \\ 1 - \frac{t}{\sigma_3}, & 0 < t < \sigma_3. \end{cases}$$

Figures 4.13-4.16 show the error plots between the constructed solution with 8 basis vectors on each edge (solid line) compared with the more precise solution (dashed line). The errors in this section are greater, partly because using this method, even small Dirichlet data gives large values and gradients of the Neumann data, especially in Figure 4.16. Figures 4.17-4.18 plot the maximum absolute error between the given solution and the $N = 20$ control solution, as the number of basis vectors on each edge is increased.

Of particular interest for the first two Test Cases in domain A, is that by symmetry, the reconstructed Neumann data is expected to be the same on every side, as shown in

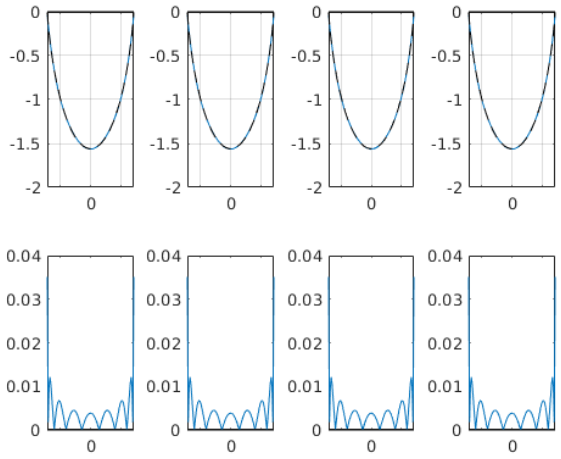


Figure 4.13: Test case 1, domain A

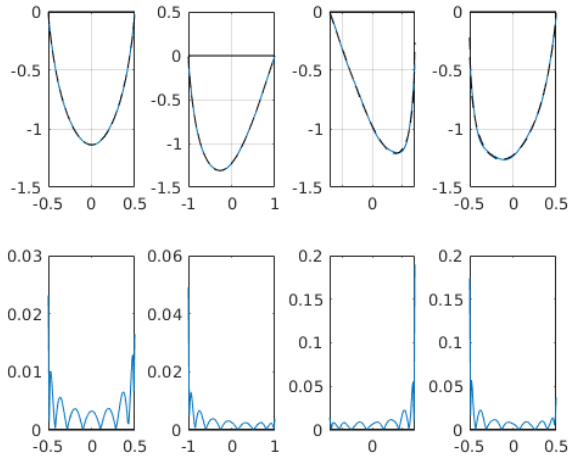


Figure 4.14: Test case 1, domain B

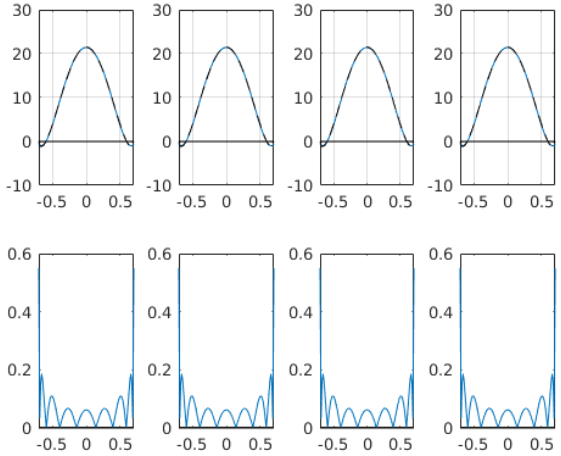


Figure 4.15: Test case 2, domain A

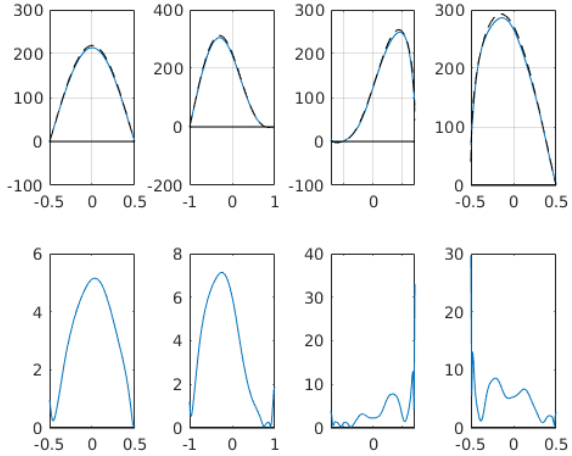
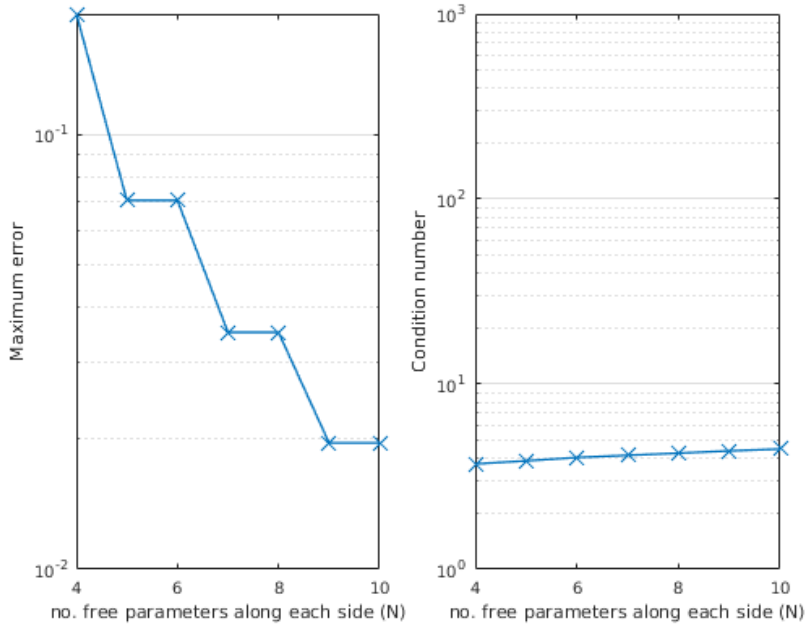


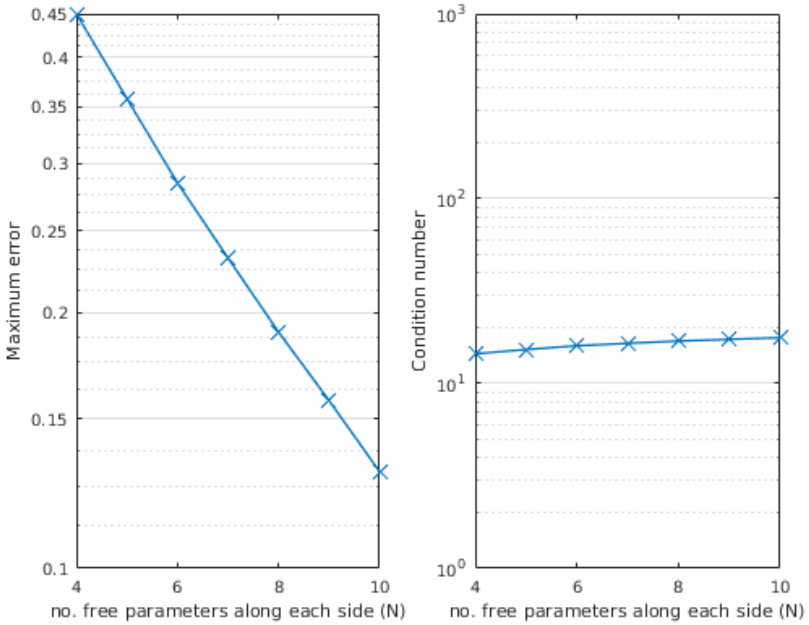
Figure 4.16: Test case 2, domain B

Figures 4.13 and 4.15. But also, we observe a 'staircasing' in the error plots 4.17(a) and 4.18(a). This is likewise to be expected:

Since the problem is symmetric, the Neumann data must be an even function over each edge. Recall that for the Legendre basis, the terms $P_0, P_2, \ldots$ are even functions. Therefore we will only obtain an increase in accuracy of approximation when using an odd number of basis vectors. Except for small numerical errors, using only P_0 and P_1 would not give a better approximation than using only P_0, since the coefficient of P_1 in the best-approximation is 0.

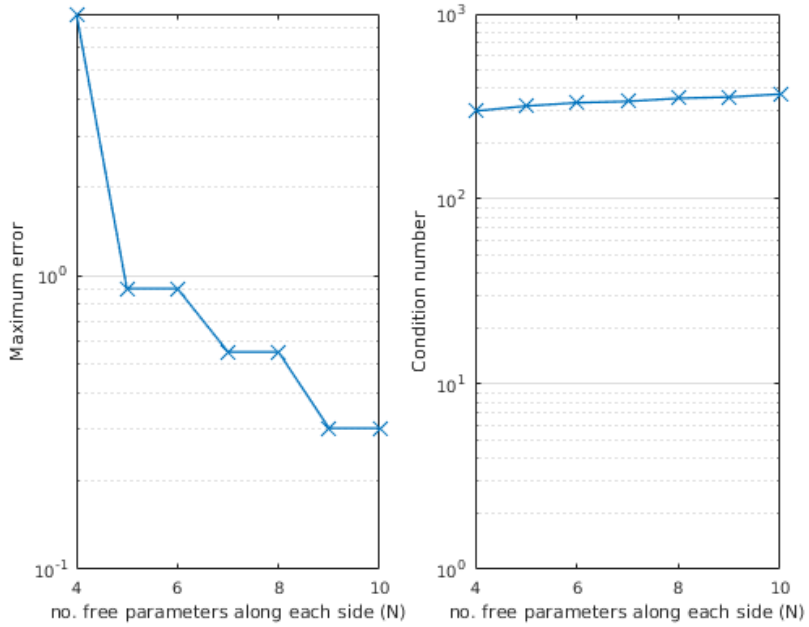


(a) Square domain

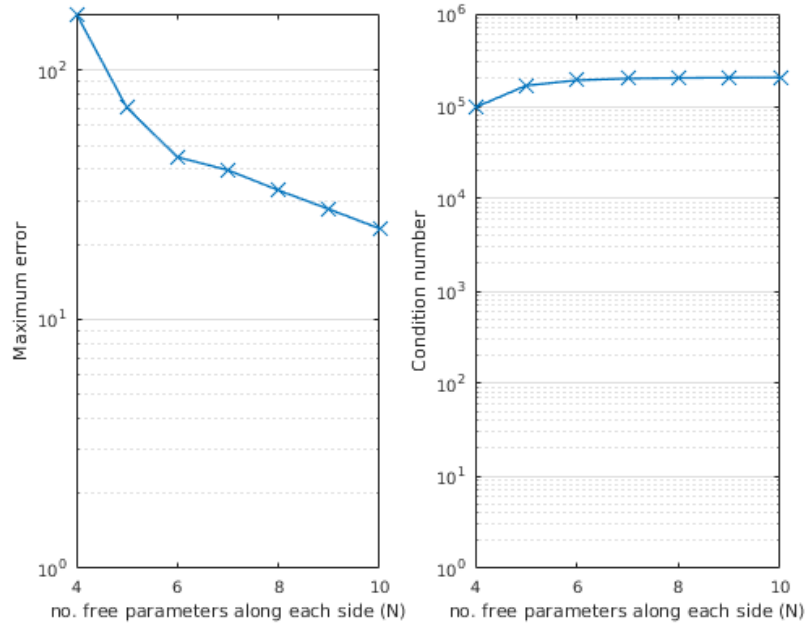


(b) Wedge domain

Figure 4.17: Helmholtz equation with $4\beta^2 = -1$ for Test Case 1: Maximum absolute errors and condition numbers for the resulting Galerkin matrices compared against the number of basis vectors, N, on each edge.



(a) Square domain



(b) Wedge domain

Figure 4.18: Helmholtz equation with $4\beta^2 = -16$ for Test Case 2: Maximum absolute errors and condition numbers for the resulting Galerkin matrices compared against the number of basis vectors, N, on each edge.

Figures 4.19-4.22 show the errors for Test cases 3 and 4, where the hat function is prescribed on each edge. In particular, the data on the third edge appears to be much less regular, and the difference between the two functions is more noticeable at points where the true solution appears to be less smooth. Indeed, for the square domain, an alternative approach to compare our method would be to use separation of variables to construct the solution as a Fourier series. Then, a numerical computation of the Fourier series could also be used to test the accuracy of our solution.

Because of the apparent lower regularity of the constructed Neumann data, for Test cases 3 and 4, we will instead plot the maximum L^2-error over the entire boundary (that is, the maximum of the L^2-errors over each individual face). Figures 4.23-4.24 show how the maximum L^2-error changes as the number of basis vectors is increased.

It is possible using these L^2-error plots to estimate the convergence rate for a given problem. Let us choose Domain A for Test Case 3, as shown in Figure 4.23(a). On the *assumption* that a straight line can be fitted to the data in this log plot, a relation between the error, e, and the number of basis vectors, N, must be of the form

$$e = Ae^{-cN},$$

where $A, c \in \mathbb{R}_{>0}$ are to be determined. Given a point (N, e) on this line,

$$\log e = -cN + \log A.$$

Looking at the plot in Figure 4.23(a), in this case it is reasonable for us to choose the extremal data points to lie on our line[2]. Let us consider the points $(N_1, e_1) = (4, 0.9853)$ and $(N_2, e_2) = (10, 0.4292)$. By solving these equations,

$$c = \frac{1}{N_2 - N_1} \log\left(\frac{e_1}{e_2}\right) \approx 0.1385,$$

which gives that $A = e_1 e^{4c} \approx 1.715$. Therefore, for this BVP we have estimated that

$$\|\varphi_j - \varphi_{N,j}\|^2_{L^2[-\sigma_j,\sigma_j]} \leq Ae^{-cN}, \quad \text{where} \quad A = 1.715, c = 0.1385.$$

Figure 4.25 shows the comparison between this line of exponential convergence, and L^2-error plot from Figure 4.23(a). In general, by plotting on a semi-logarithmic scale, any convergence which appears linear is convergence of an exponential rate, with some factor which can be calculated. Although these are slower than the rates we observed numerically for smooth data in Section 4.2, we can still observe exponential convergence rates for these numerical examples.

[2]Moving the line parallel to itself changes the value of A, but not the convergence rate c, which is of primary interest.

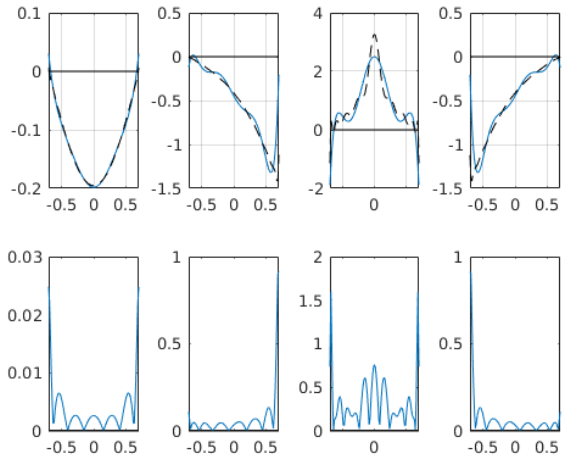


Figure 4.19: Test case 1, domain A

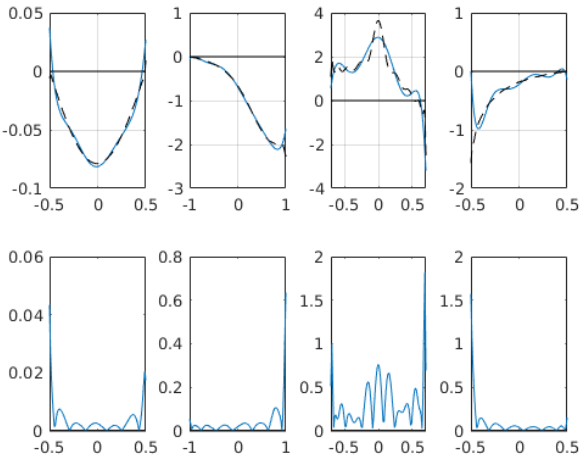


Figure 4.20: Test case 1, domain B

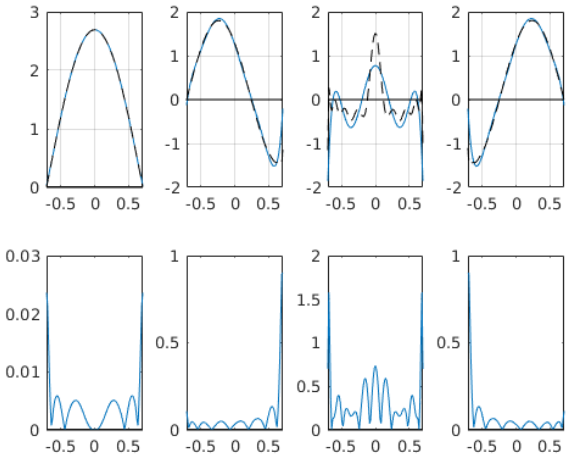


Figure 4.21: Test case 2, domain A

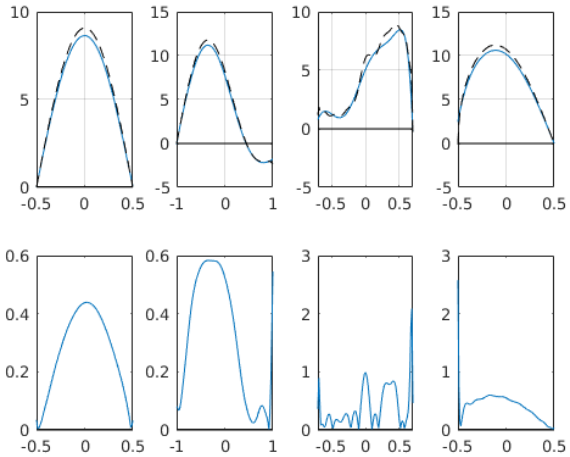
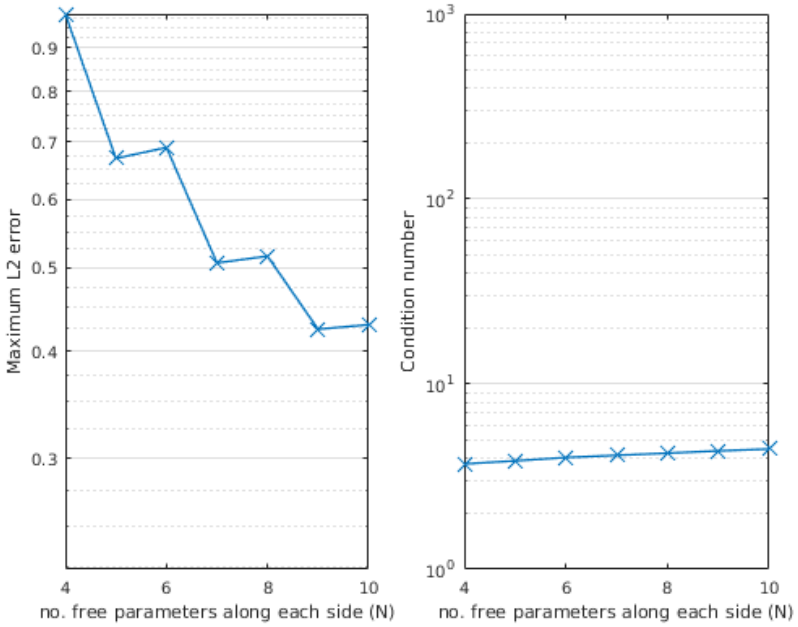
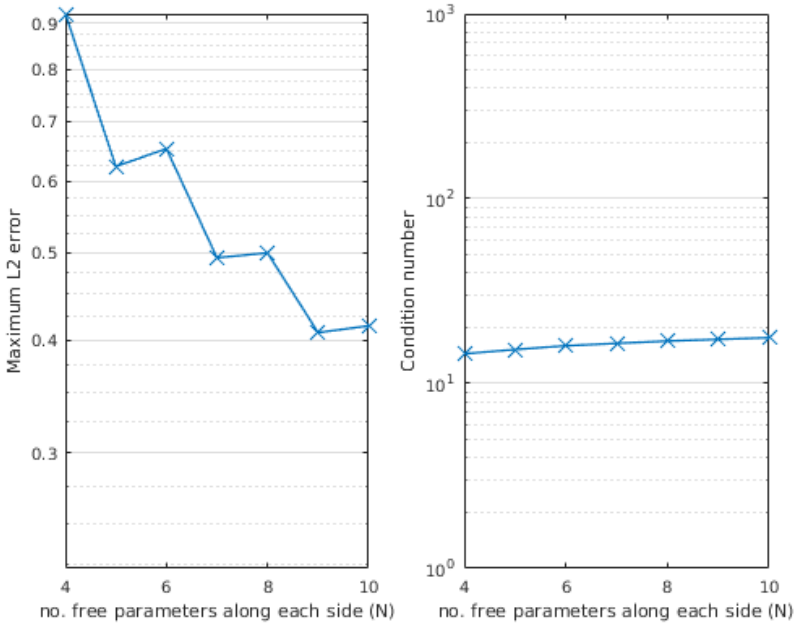


Figure 4.22: Test case 2, domain B

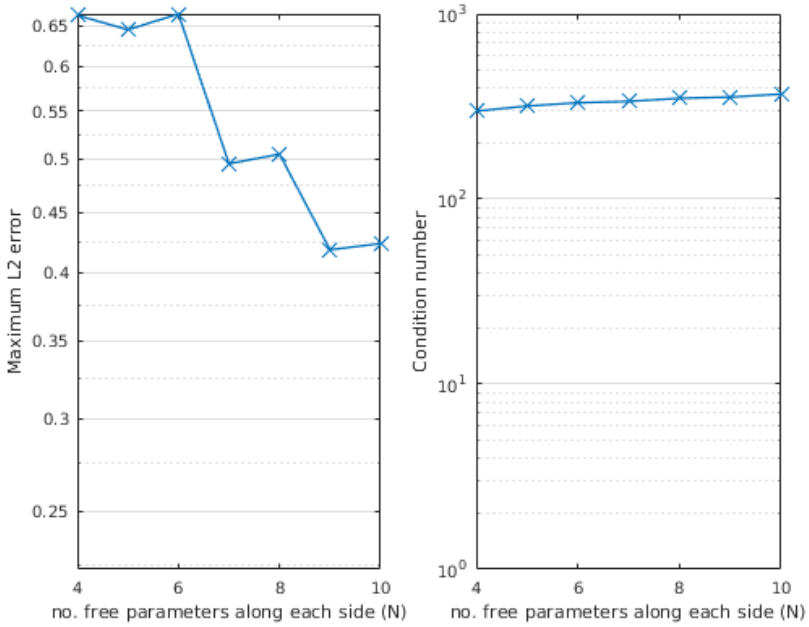


(a) Square domain

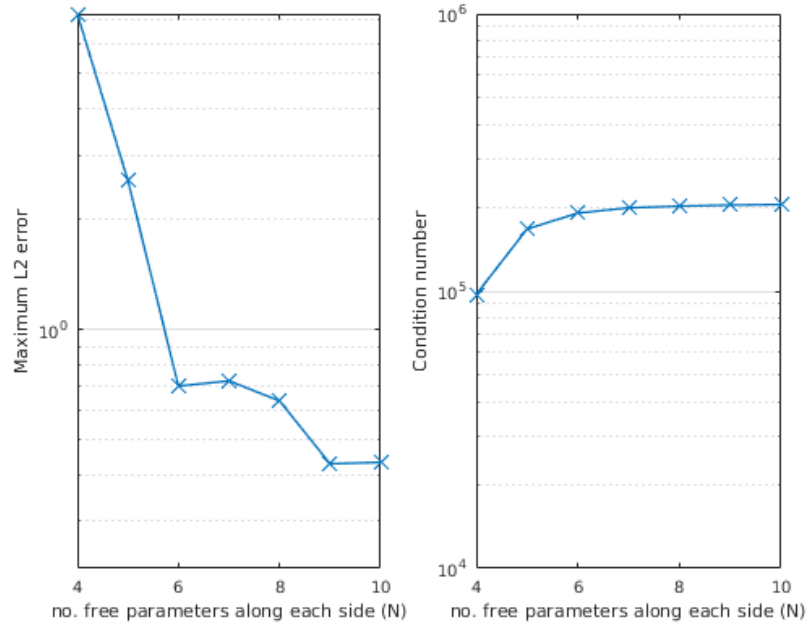


(b) Wedge domain

Figure 4.23: Helmholtz equation with $4\beta^2 = -1$ for Test Case 3: Maximum L^2 errors and condition numbers for the resulting Galerkin matrices compared against the number of basis vectors, N, on each edge.



(a) Square domain



(b) Wedge domain

Figure 4.24: Helmholtz equation with $4\beta^2 = -16$ for Test Case 4: Maximum L^2 errors and condition numbers for the resulting Galerkin matrices compared against the number of basis vectors, N, on each edge.

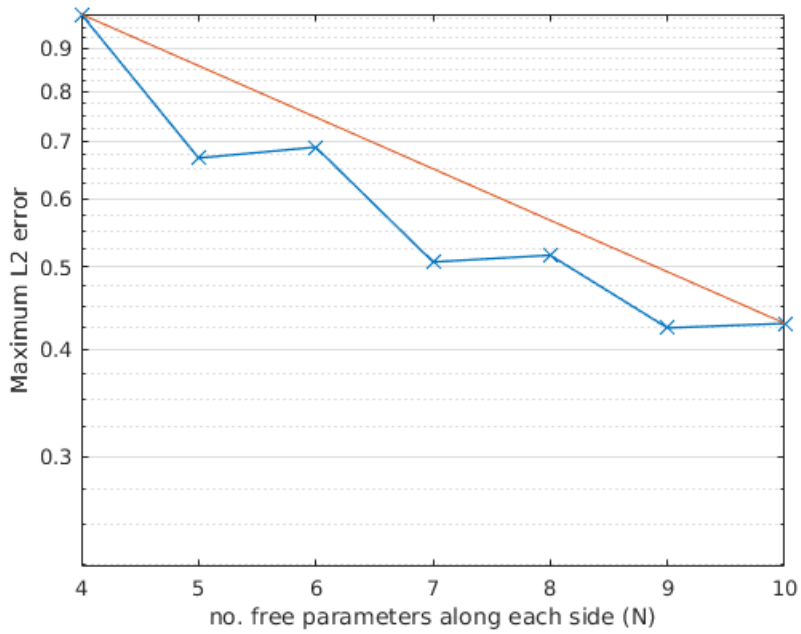


Figure 4.25: L^2-error plot from Figure 4.23(a), showing the error for Test Case 3 on the square domain A. The figure includes the calculated line with exponential convergence rate factor $c = -0.1385$.

4.4 The Dirichlet eigenvalue problem

The Dirichlet eigenvalue problem is a non-unique solution to the Helmholtz equation. More specifically, we seek pairs $(u, 4\beta^2)$ such that[3]

$$\begin{aligned} -\Delta u - 4\beta^2 u &= 0 \ \text{ in } \Omega \\ u &= 0 \ \text{ on } \Gamma_j, \ \ j = 1, \ldots, n. \end{aligned} \tag{4.4.1}$$

Recall that the linear operator T_β for recovering the unknown Neumann data is Fredholm. T_β is injective (that is, it has nullity zero) precisely when the Laplace equation has a unique solution. Since the $-\Delta$ is a symmetric elliptic operator, standard results (e.g. [Eva10, p.355]) yield that every eigenvalue of $-\Delta$ is real and positive. Consequently the following observation holds

Remark 4.4.1. *The operator $T_\beta : X \to Y$, which is upper semi-Fredholm, is injective if and only if $4\beta^2 \in \mathbb{R} \setminus 0$ and not equal to one of the strictly positive Dirichlet–eigenvalues of the Laplacian.*

This result is a restatement of the Theorem for elliptic operators. The consequence of

[3]We have used a different sign for this equation in the current section only. This is to emphasise that the eigenvalues are positive values of $4\beta^2$, corresponding to the Helmholtz equation.

this fact is that by fixing a domain Ω we may *identify* eigenvalues, by studying the condition number of the linear Galerkin system. This is the content of the following Theorem from [AC15]. Because we are dealing with limits for $\beta \in \mathbb{C}$, the bilinear form a is slightly modified

$$\tilde{a}_\beta(\mathbf{\Phi}, \mathbf{\Phi}') := \Re\langle T_\beta \mathbf{\Phi}, T_{\overline{\beta}} \mathbf{\Phi}' \rangle_Y \tag{4.4.2}$$

Theorem 4.4.2. *(i) Suppose* $\{(\mathbf{\Phi}_m, \beta_m)\}_{m\geq 1}$ *satisfies the Galerkin problem* (4.4.2) *and*

$$\lim_{m\to\infty} \beta_m = \beta \in (0, \infty).$$

Then $4\beta^2$ *is an eigenvalue of the Laplacian.*

(ii) For each $\beta \in (0, \infty)$ *such that* $4\beta^2$ *is an eigenvalue of the Laplacian, there exists a sequence of pairs* $\{(\mathbf{\Phi}_m, \beta_m)\}_{m\geq 1}$ *that satisfy the Galerkin problem* (4.4.2) *with* $\|\mathbf{\Phi}_m\|_X = 1$ *such that*

$$\lim_{m\to\infty} |\beta - \beta_m| = 0, \quad \lim_{m\to\infty} \inf_{\ker T(\beta)} \|\mathbf{\Phi} - \mathbf{\Phi}_m\|_X = 0.$$

Let us define the matrix

$$\mathsf{T}^{(m)}_{ij}(\beta) = a_\beta(\mathbf{e}_i, \mathbf{e}_j), \quad 1 \leq i, j \leq m.$$

If a sequence $\{\beta_m\}_{m\geq 1}$ in $\mathbb{R}$ defined by $\det \mathsf{T}^{(m)}(\beta_m) = 0$ converges, then

$$\beta = \lim_{m\to\infty} \beta_m$$

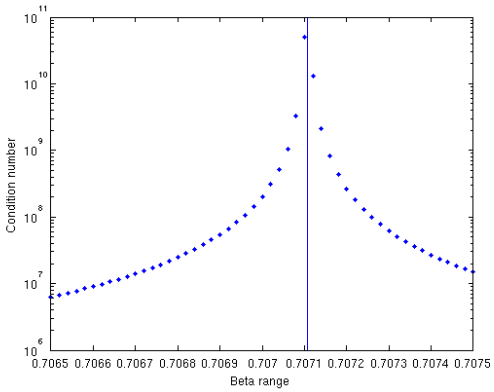
will be a true Dirichlet eigenvalue.

To demonstrate this approach, let us consider a square domain with four vertices at 0, π, $\pi(1+\mathrm{i})$ and $\pi\mathrm{i}$ respectively, where explicit eigenfunctions are given as

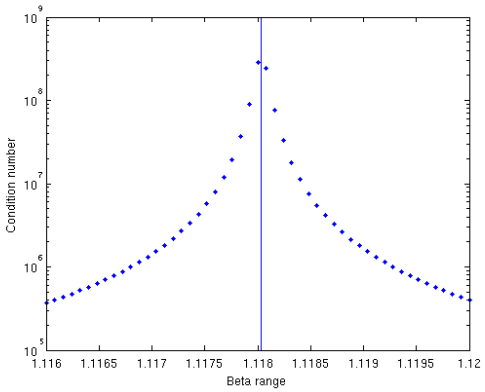
$$u(x, y) = \sin(kx)\sin(ly), \quad \text{for } k, l \in \mathbb{Z}$$

and $4\beta^2 = k^2 + l^2$. Using $\{\mathbf{e}_j\}_{j=1}^{nN}$ as a basis for an approximating subspace in X from Section 4.1, let us form the Galerkin matrix $\mathsf{T}^{(nN)}(\beta)$. Figure 4.26 plots the condition numbers of $\mathsf{T}^{(nN)}(\beta)$ around the first three eigenvalues. In each case, spikes in the condition numbers correctly reveal the eigenvalue's location. We observe that each spike is a number of orders of magnitude greater than nearby values. Figure 4.27 highlights the true eigenvalues, even over a wider range where the condition numbers vary by multiple orders of magnitude.

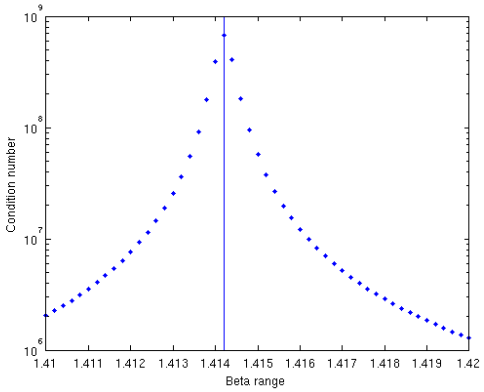
We note that there is a double approximation involved in the application of Theorem 4.4.2. First there is the approximation that, for β an eigenvalue of the Helmholtz problem, a given Galerkin problem defined by the matrix $T^{(n)}$ may have an eigenvalue $\beta_n \neq \beta$. For this value β_n, $\det T^{(n)}(\beta_n) = 0$, and the Theorem states that these values will converge, so



(a) $\beta = \sqrt{2}/2$



(b) $\beta = \sqrt{5}/2$



(c) $\beta = \sqrt{8}/2$

Figure 4.26: The condition numbers of $\mathsf{T}^{(nN)}(\beta)$ around the first three eigenvalues for a square domain ($n = 4$) using 9 basis vectors on each edge ($N = 9$). In each case, the exact eigenvalue is marked by a vertical line.

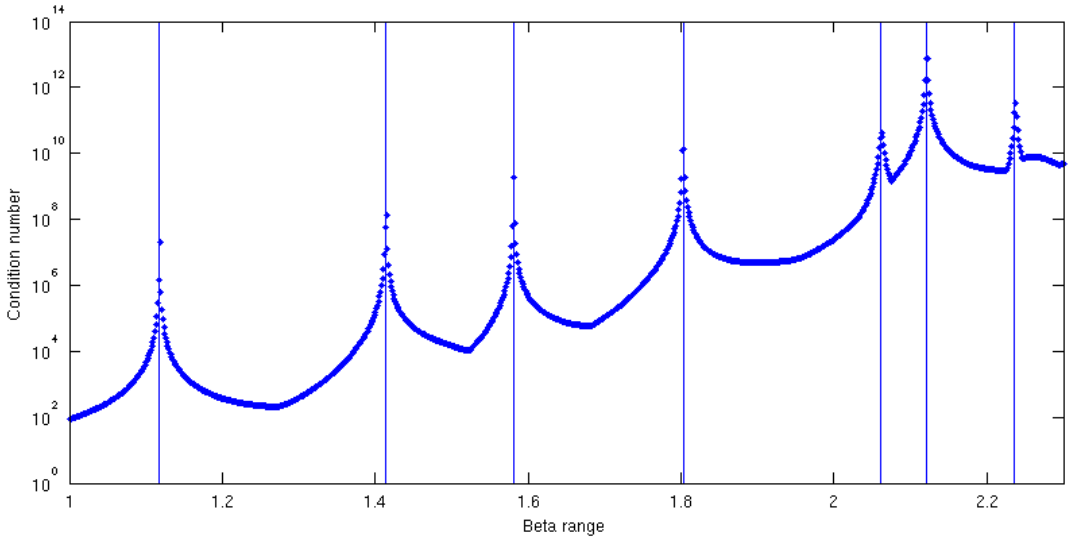


Figure 4.27: The condition numbers of $\mathsf{T}^{(nN)}(\beta)$ for a wider range of β values with $n = 4$ and $N = 9$. Exact eigenvalues are marked by vertical lines.

$\beta = \lim_{n\to\infty} \beta_n$. Because of this, it is certainly possible, for a given problem, that these approximate eigenvalues lie in $\mathbb{C} \setminus \mathbb{R}$, even though $\beta \in (0, \infty)$.

Second, there is the approximation in our numerical implementation that we will observe a 'spike' in the condition number of a well-defined problem, $T^{nN}(\beta_{nN,j})$ (for a fixed value nN) as $(\beta_{nN,j})_{j>1}$ approaches an approximate eigenvalue β_{nN}. One should take in to account these factors when using this method to find eigenvalues, and let us remark on this.

Remark 4.4.3. *Sometimes, a peak may not be observed, even at a known eigenvalue β. This could occur for a number of reasons, for example:*

- *The range over which we are searching for an eigenvalue is too broad, so the spike will not be observed unless the resolution at which we calculate the condition numbers of $T^{nN}(\beta_{nN,j})$ is enough for the narrow spike to be revealed.*
- *By the first approximation, since the true eigenvalue β is the limit of the values $(\beta_m)_{m\geq 1}$ for which $\det T^{(m)}(\beta_m) = 0$; if the range we are searching is too small around β, then β_m may lie outside of this range. In this case, the spike may not be observed.*

4.5 Summary of two-dimensional Helmholtz

We have shown how Fokas' unified method provides a continuous map between the unknown Neumann data and the known Dirichlet data for the Helmholtz problem in a polygonal domain Ω. This map, which depends on $\beta \in \mathbb{C}$, is realised by solving an operator

equation $T_\beta \mathbf{\Phi} = \mathbf{\Psi}$, where T_β is a compact perturbation of a similar operator studied for Laplace problem (where $\beta = 0$). By rewriting the global relation as a linear operator equation for the unknown function $\mathbf{\Phi}^{\text{Ne}}$ and utilising the Paley–Wiener spaces, we have proved that this operator is upper semi-Fredholm. Using results for such operators and the strong properties following from analyticity, we have obtained existence and uniqueness of solutions away from an isolated set of eigenvalues β.

For such values, we have proposed a Galerkin method for reconstructing the unknown data $\mathbf{\Phi}^{\text{Ne}}$. The validity of such a method follows from the functional analytic properties T_β which we have established in Section 3.1. Numerical tests for this method in two domains are shown in figure 4.10 and demonstrate spectral convergence rates comparable to those in [FF11], and remarkably low matrix condition numbers. We have also tested our implementation with more general boundary data, where the exact solution is not known, and have obtained slower convergence rates. These convergence rates still appear to be exponential, and we have shown how this rate can be approximated numerically. Our approach to solving these BVPs requires a numerical integration for each matrix entry, but we emphasise that the integrand is *analytic* away from zero. This property allows for efficient numerical integration, with the use of contour deformation to ensure exponential convergence of the integrands.

Previous numerical studies have followed a pointwise evaluation of the global relation at special collocation points [FFX04, Dav08, SFFS08, FF11]; for example [SSF10] establishes quadratic convergence rates using a Fourier basis. The convergence properties and condition numbers are due to a good choice of collocation points, either along rays in $\mathbb{C}$, or specially distributed points, called *Halton nodes*, described in [FF11, Appendix A]. More recent work in [FIS15, HFS15, FP15] has resulted in similarly low condition numbers, and which are independent of β. Some convergence results have been provided in [FP15, Ch. 6], and a survey of these pointwise collocation approaches is given, including the type of basis functions (polynomial or Fourier) and the choice of the collocation points that were used. These approaches use the Dirichlet data, and solve numerically for the Neumann data, $\partial_n q$, around the boundary. In contrast, the approach presented here from [Ash13, AC15] considers the Fourier transform, $\mathbf{\Phi}^{\text{Ne}}$, of this Neumann data, which lies in a Paley–Wiener space of analytic functions, with known bounds. Importantly, our results introduce a rigorous justification of a second (Galerkin) numerical approach which has not featured in these earlier studies. Furthermore, the calculations involve integration of analytic functions, and so these numerical results hold without calculating the global relation at well-chosen points in the complex plane. In this way, the method we have presented can be easily extended to any Laplace or Helmholtz BVP on a convex polygon, and the convergence results of Theorem 2.7.2 remain true.

With regard to the Dirichlet eigenvalues of the Laplacian, we have shown that for any sequence $\{\beta_m\}_{m\geq 1}$ tending towards a true eigenvalue $\beta \in (0, \infty)$, the condition numbers

of the corresponding matrices $\{\mathsf{T}^{(m)}(\beta_m)\}_{m\geq 1}$ increase without bound. By considering the known eigenvalues for a square, we have shown the effectiveness of this method for determining eigenvalues. Indeed, for a fixed matrix size, figure 4.27 highlights noticeable spikes in the values $\mathsf{T}^{(nN)}(\beta)$. From numerical experiments, these spikes are typically several orders of magnitude.

The work here has been confined to regions of convex polygons, however these can in principle be extended to more general planar domains. One such extension for future study would be as curvilinear domains, for example convex polygons where each edge is permitted to be a smooth curve that keeps the shape convex.

CHAPTER 5

The Laplace problem on three-dimensional polyhedra

Two recent papers [Ash14b, Ash14a] have extended the earlier two-dimensional work in convex polygonal domains, to their three-dimensional analogue: convex polyhedra. This extension uses many of the ideas from our two-dimensional problems, and as we shall see, the global relation may again be written as an operator equation $T\boldsymbol{x} = \boldsymbol{y}$ between Banach spaces, where T is a continuous and injective linear operator. For a polyhedral domain, our boundary data will be supported on the faces, and the related Fourier transforms will lie in similarly defined Paley–Wiener spaces. For two-dimensional BVPs, we defined the Paley–Wiener spaces PW_j^σ to be $\mathcal{F}L^2\left[-\sigma_j, \sigma_j\right]$; whereas the Paley–Wiener spaces relevant to three-dimensional problems will consist of the Fourier transform of functions in $L^2(Q_j)$, for polygonal domains Q_j. We begin in a similar fashion, noting the comparisons between this and the polygonal cases. We will then proceed to propose a numerical implementation in detail, taking care to explain specific numerical difficulties for a few reasons:

1. Because the numerics will require two-dimensional integration (which is proportionally *more* difficult numerically), we wish to highlight areas where efficiency can be improved.

2. This is the first time a three-dimensional implementation of the Fokas method has been attempted, and it is hoped that by providing additional details, we will aid future work in this area.

3. Some difficulties arise that were present in the two-dimensional case, but that were easier to manage than for the three-dimensional case. We refer specifically to the integration-by-parts required to ensure that the numerical integrals in our weak formulation are finite, when calculated on basis functions. This arises because our basis functions *do not* lie in a subspace required for boundedness of the integrals, even though their sum does. We take care in presenting this subtle point in Section 5.5.

With regard to point 3, we provide a coordinate-independent integration-by-parts that alleviates the issue of boundedness. In doing so we introduce a *fundamentally new* representation for the global relation, which will lead to a new weak formulation for the Laplace and Helmholtz problems in polyhedral domains. This new weak formulation is explored in Sections 5.5-5.6. As a result, we provide the first numerical tests of the Fokas method in three-dimensions and, as we have shown for 2D domains, this method is stable and convergent. Let us begin with the relevant notation for the Laplace problem on three-dimensional polyhedra.

Suppose Ω is a convex polyhedron, which is defined by its polygonal faces $\{\Sigma_i\}_{i=1}^n$. Throughout this section, we let bold symbols $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, \lambda_2)$ and $\boldsymbol{x} = (x_1, x_2, x_3)$ denote vectors in $\mathbb{C}^3$ and $\mathbb{R}^3$ respectively; while their respective un-bolded coordinates λ, x denote the projection onto the first two components: $\boldsymbol{\lambda} = (\lambda, \lambda_3)$ and $\boldsymbol{x} = (x, x_3)$. Then the three-dimensional Laplace problem is

$$\Delta q = 0, \quad \text{in } \Omega \tag{5.0.1}$$

$$q = f_j, \quad \text{on } \Sigma_j,\ j = 1, \dots, n. \tag{5.0.2}$$

To ensure existence of a solution, it is sufficient that $f_j \in H^1(\Omega)$ and $f_i = f_j$ on $\overline{\Sigma_i} \cap \overline{\Sigma_j}$ [Dau88]. This means compatibility at the edges, and is analogous to vertex continuity in the 2D polygonal case. Let

$$\delta(\lambda) = \mathrm{i}\sqrt{\lambda_1^2 + \lambda_2^2},$$

where the positive real part in the square root is taken. Then the algebraic variety $Z_P := \{\boldsymbol{\lambda} \in \mathbb{C}^3 : \lambda_1^2 + \lambda_2^2 + \lambda_3^2 = 0\}$ is equal to the union of the set $Z_P^+ = \{\boldsymbol{\lambda} : \lambda \in \mathbb{C}^2, \lambda_3 = \delta(\lambda)\}$ with the corresponding set, Z_P^-, where the negative square root is taken for $\delta(\lambda)$.

For any $\boldsymbol{\lambda} \in Z_P$, the function $v_{\boldsymbol{\lambda}}(\boldsymbol{x}) := e^{-\mathrm{i}\boldsymbol{\lambda}\cdot\boldsymbol{x}}$ solves $\Delta v_{\boldsymbol{\lambda}} = 0$, and so applying Green's identity

$$\int_\Omega \left[q\Delta v_{\boldsymbol{\lambda}} - v_{\boldsymbol{\lambda}}\Delta q\right] \mathrm{d}\boldsymbol{x} = \sum_{j=1}^n \int_{\Sigma_j} \left[q\partial_{\boldsymbol{n}_j} v_{\boldsymbol{\lambda}} - v_{\boldsymbol{\lambda}}\partial_{\boldsymbol{n}_j} q\right] \mathrm{d}\sigma_j(\boldsymbol{x}), \tag{5.0.3}$$

where $\mathrm{d}\sigma_j(\boldsymbol{x})$ denotes the corresponding surface measure over Σ_j. The left-hand side vanishes for any solution q of the Laplace equation, so the boundary terms yield the global relation

$$\begin{aligned} &\sum_{j=1}^n \rho_j(\boldsymbol{\lambda}) = 0, \quad \forall\, \boldsymbol{\lambda} \in Z \\ &\rho_j(\boldsymbol{\lambda}) := \int_{\Sigma_j} e^{-\mathrm{i}\boldsymbol{\lambda}\cdot\boldsymbol{x}} \left[\partial_{\boldsymbol{n}_j} q(\boldsymbol{x}) + \mathrm{i}(\boldsymbol{\lambda}\cdot\boldsymbol{n}_j) f_j(\boldsymbol{x})\right] \mathrm{d}\sigma_j(\boldsymbol{x}) \end{aligned} \tag{5.0.4}$$

The faces can be conveniently parameterised by a map $\psi_j : \mathbb{R}^2 \to \mathbb{R}^3$, using an orthogonal matrix R_j which rotates the outward normal $\boldsymbol{n}_i$ to $\boldsymbol{e}_z = (0,0,1)^t$: For $X = (X_1, X_2)^t$

$$\psi_j : X \mapsto \boldsymbol{m}_j + R_j^t \begin{pmatrix} X \\ 0 \end{pmatrix}.$$

With this parameterisation, if we let $\vartheta_j := \psi_j^* f_j$ be the pullback of f_j to a polygon Q_j in the plane, and similarly $\varphi_j := \psi_j^*(\partial_{\boldsymbol{n}} q)$, we write

$$\rho_j(\boldsymbol{\lambda}) = e^{-\mathrm{i}\boldsymbol{\lambda}\cdot\boldsymbol{m}_j} \int_{Q_j} e^{-\mathrm{i}(R_j\boldsymbol{\lambda})_1 X_1 - \mathrm{i}(R_j\boldsymbol{\lambda})_2 X_2} \left[\varphi_j + \mathrm{i}(R_j\boldsymbol{\lambda})_3 \vartheta_j\right] \mathrm{d}X.$$

In a similar way to the two-dimensional case, we may multiply the global relation by $e^{\mathrm{i}\boldsymbol{\lambda}\cdot\boldsymbol{m}_k}$ and make the substitution $\boldsymbol{\lambda} \mapsto R_k^t\boldsymbol{\lambda}$. If we do this, and denote new vectors for the Fourier transform of our data

$$\boldsymbol{\Theta}^{\mathrm{Di}} = (\hat{\vartheta}_1(\lambda), \ldots, \hat{\vartheta}_n(\lambda))^t, \quad \boldsymbol{\Phi}^{\mathrm{Ne}} = (\hat{\varphi}_1(\lambda), \ldots, \hat{\varphi}_n(\lambda))^t, \tag{5.0.5}$$

then the global relation may be written in the equivalent form

$$(T\boldsymbol{\Phi}^{\mathrm{Ne}})_k(\lambda) + (S\boldsymbol{\Theta}^{\mathrm{Di}})_k(\lambda) = 0, \quad \forall \lambda \in \mathbb{C}^2, \tag{5.0.6}$$

where if we use the rotation $\Delta_{kj}\boldsymbol{\lambda} := R_j R_k^t \boldsymbol{\lambda}$, the operators T and S are defined componentwise as

$$\begin{aligned} (T\boldsymbol{\Phi}^{\mathrm{Ne}})_k(\lambda) &:= \sum_{j=1}^{n} e^{-\mathrm{i}(\boldsymbol{m}_j - \boldsymbol{m}_k)\cdot R_k^t\boldsymbol{\lambda}} \Phi_j^{\mathrm{Ne}}((\Delta_{kj}\boldsymbol{\lambda})_1, (\Delta_{kj}\boldsymbol{\lambda})_2) \\ (S\boldsymbol{\Theta}^{\mathrm{Di}})_k(\lambda) &:= \sum_{j=1}^{n} \mathrm{i} e^{-\mathrm{i}(\boldsymbol{m}_j - \boldsymbol{m}_k)\cdot R_k^t\boldsymbol{\lambda}} (\Delta_{kj}\boldsymbol{\lambda})_3 \Theta_j^{\mathrm{Di}}((\Delta_{kj}\boldsymbol{\lambda})_1, (\Delta_{kj}\boldsymbol{\lambda})_2). \end{aligned} \tag{5.0.7}$$

Remark 5.0.1. *Although the global relation here is for $\boldsymbol{\lambda} = (\lambda, \delta(\lambda)) \in Z_P^+$, as remarked in [Ash14b], by taking complex conjugates and relabeling λ_1 and λ_2, the global relation must also hold for $\boldsymbol{\lambda} \in Z_P^-$, and therefore on the whole of Z_P.*

The Paley–Wiener space for a polygon Q is defined as the Fourier transform of the space $L^2(Q)$. By the Paley–Wiener Theorem this is equal to

$$PW_{Q,\mathrm{sym}} := \{f : \mathbb{C}^2 \to \mathbb{C} : f|_{\mathbb{R}^2} \in L^2(\mathbb{R}^2), |f(z)| \lesssim \|f\|_2 e^{\sup_{y\in Q}(\Im z\cdot y)}\}$$

and functions $f \in PW_{Q,\mathrm{sym}}$ satisfy the symmetry relation

$$f(\lambda) = \overline{f(-\bar{\lambda})}, \quad \forall\, \lambda \in \mathbb{C}^2.$$

We define the spaces $Y = L^2(\mathbb{R}^2)^{\times n}$ and

$$X_{\text{sym}} = PW^2_{Q_1,\text{sym}} \times \cdots \times PW^2_{Q_n,\text{sym}} \simeq L^2(\partial\Omega). \tag{5.0.8}$$

By construction, the Neumann data must satisfy that the integral over $\partial\Omega$ is zero, and we have also assumed that the Dirichlet data is continuous across the vertices. The Neumann data then, lies in the subspace $\{\mathbf{\Phi} \in X_{\text{sym}} : \sum_i \Phi_i(0) = 0\}$.

Since we know that solving the global relation is equivalent to solving the PDE (5.0.1), the problem may be restated as follows: For valid Dirichlet data $\mathbf{\Theta}^{\text{Di}} \in X_{\text{sym}}$, define $\Psi_k(\lambda) := -(S\mathbf{\Theta}^{\text{Di}})_k(\lambda)$, and find $\mathbf{\Phi}^{\text{Ne}} \in X_{\text{sym}}$ such that

$$(T\mathbf{\Phi}^{\text{Ne}})_k(\lambda) = \Psi_k(\lambda) \quad \text{for every} \quad k = 1, \ldots, n.$$

This requires studying the operator equation involving T, and uses similar machinery as for the two-dimensional case: indeed the pseudo-compactness lemma 2.3.3 for the Paley–Wiener space still holds.

Lemma 5.0.2 ([Ash14b, Lemma 1]). *Every bounded sequence in X_{sym} contains a subsequence that converges locally uniformly in $\mathbb{C}^2$ to an element of X_{sym} which obeys the same norm bound.*

Using the form of T, indeed existence and uniqueness of solutions to the global relation are possible:

Theorem 5.0.3 ([Ash14b, Theorem 2]). *The map $T : X_{\text{sym}} \to Y$ is bounded above and below:*

$$\|\mathbf{\Phi}\|_Y \lesssim \|T\mathbf{\Phi}\|_{X_{\text{sym}}} \lesssim \|\mathbf{\Phi}\|_Y, \quad \forall\, \mathbf{\Phi} \in X_{\text{sym}}.$$

As such it is an injective linear map with closed range. Furthermore for any admissible boundary data $\{f_j\}_{j=1}^n$, the function $\mathbf{\Psi} := -S\mathbf{\Theta}^{\text{Di}}$ lies in $Ker(T^*)^\perp$; perpendicular to the kernel of the formal adjoint operator, T^*, to T. So by Banach's closed range Theorem

$$Ran(T) = Ker(T^*)^\perp,$$

and there exists a solution $\mathbf{\Phi}^{\text{Ne}}$ to the global relation. By injectivity, this solution is unique.

5.1 The weak problem

Since the operator T has been shown to define a linear map from X_{sym} to Y, and yields a unique solution to the global relation, we may proceed to define the associated weak problem. Details are given in [Ash14b, Ash14a], and such a numerical approach is possible because the operator T is bounded below. We will introduce three weak problems with different properties:

- The first weak problem was introduced in [Ash14b] and the forms will be denoted by the forms $a(\mathbf{\Phi}, \mathbf{\Phi}')$ and $\ell(\mathbf{\Phi}')$. This problem comes from a quadratic minimisation, and is analogous to the weak problem introduced in (2.6.3) for the Laplace problem, by integrating over a curve on the negative real line.

- The second weak problem is proposed here for the first time. This is analogous to the weak problem for the two-dimensional Helmholtz equation, where the integral is taken from $-\infty$ to -1 only. In this case we may choose to exclude any compact set K from the domain of integration, and will be denoted by the forms $a_K(\mathbf{\Phi}, \mathbf{\Phi}')$ and $\ell_K(\mathbf{\Phi}')$. This has the significant advantage that the numerical integration will not need to be performed near $\mathbf{0}$, and as such is the one we shall pursue for our numerical tests in the following chapters.

- The third weak problem is also given in [Ash14b], and will be denoted by $\tilde{a}(\mathbf{\Phi}, \mathbf{\Phi}')$ and $\tilde{\ell}(\mathbf{\Phi}')$. This is especially interesting, since the proof given for coercivity in Theorem 4.1 of this paper, may be used to give an *explicit* coercivity bound for the bilinear form a. We give this proof in Section sec:coercivity. This coercivity bound, combined with Céa's Lemma and the boundedness constant for a (attainable from the bound for T) would give a specific control on the convergence of the Galerkin problems. As such this is a recommended area for a future implementation to compare with the new implementation of the second weak problem.

Because of the boundedness properties of T, the Lax–Milgram and Céa Lemmas apply to all three weak formulations, giving numerical stability and convergence for the resulting finite-dimensional problems. Having demonstrated this approach in the two-dimensional case, we proceed quickly, but highlight the notable changes:

First, the weak formulation is defined on a sub-domain $\{\lambda \in \mathbb{R}^2\} \subset \mathbb{C}^2$ instead of a curve, but again real values for λ are used.

Second, by the pseudo-compactness lemma, we do not need to consider values near zero to avoid numerical difficulties. Indeed, we may exclude any compact set K, and consider the integrals over $\mathbb{R}^2 \setminus K$, which is analogous to the curve from $(-\infty, -1) \subset \mathbb{R}_{<0}$ in the two-dimensional case. This is the content of Theorem 5.1.4 and yields an entirely new weak formulation for 3D elliptic problems.

Thirdly, an alternative weak approach is given, which yields explicit coercivity bounds for the weak problem. By Céa's Lemma, these bounds give estimates for the rate of convergence. In the numerical tests, very similar linear forms are considered, after an integration by parts.

Finally, since the boundary of a polygon consists of line segments, we had a wide choice of good bases for a line segment, and for which we have an explicit Fourier transform representation (the Legendre and Bessel functions). For generic two-dimensional polygonal domains, a good choice of basis vectors is not as clear. We have chosen here to minimise

arbitrariness and choose a standard polynomial basis for each face Q_j:

$$f_{j,\alpha}(x,y) = x^{\alpha_1}y^{\alpha_2}, \quad \text{for multi-indices } \alpha = (\alpha_1,\alpha_2);\ |\alpha| \leq N.$$

This consists of the first $M := \frac{1}{2}(N+1)(N+2)$ polynomials on a given face. Over the n faces of the polyhedron, this corresponds to $\frac{n}{2}(N+1)(N+2)$ basis vectors $\{\boldsymbol{f}_j\}_{j=1}^{nM}$. The Fourier transform will be given explicitly in terms of a finite sum over the boundary and geometric quantities from the domain. However it is admitted that this choice could be improved upon for specific domains, or a better general choice of basis vectors.

With these considerations the weak formulation of the global relation may be obtained:

Theorem 5.1.1 ([Ash14b])**.** *For fixed $\boldsymbol{\Psi} = -S\boldsymbol{\Phi}^{\mathrm{Di}} \in Y$, we have the following linear and bilinear forms on X and $X \times X$ respectively*

$$\ell : \boldsymbol{\Phi}' \mapsto \langle \boldsymbol{\Psi}, T\boldsymbol{\Phi}' \rangle_Y, \quad a : (\boldsymbol{\Phi}, \boldsymbol{\Phi}') \mapsto \langle T\boldsymbol{\Phi}, T\boldsymbol{\Phi}' \rangle_Y.$$

Then the weak problem is: given $\boldsymbol{\Psi} \in Y$, find $\boldsymbol{\Phi} \in X_{\mathrm{sym}}$ such that

$$a(\boldsymbol{\Phi}, \boldsymbol{\Phi}') = \ell(\boldsymbol{\Phi}'), \quad \textit{for all } \boldsymbol{\Phi}' \in X_{\mathrm{sym}}.$$

This problem is well-posed, and furthermore for $\boldsymbol{\Psi} = -S\boldsymbol{\Theta}^{\mathrm{Di}}$ in the range of T, this unique weak solution solves the classical problem $T\boldsymbol{\Phi}^{\mathrm{Ne}} = \boldsymbol{\Psi}$.

We observed for the 2D global relation that the operator T is a finite sum of exponential terms multiplied by the component functions Φ_j evaluated along rays, and as such $(T\boldsymbol{\Phi}_l)$ converges to zero whenever a sequence $\{\boldsymbol{\Phi}_l\}_{l\geq 1}$ does. We shall use this Lemma again to derive a new weak formulation on a sub-domain $\mathbb{R}^2 \setminus K$. This flexibility will permit us to avoid removable singularities at the origin, as well as using symmetry to yield a more efficient numerical scheme. The proof of this result is identical to Lemma 2.3.4.

Lemma 5.1.2. *For any sequence $\{\boldsymbol{\Phi}_l\}_{l\geq 1} \subset X_{\mathrm{sym}}$ tending locally uniformly to zero, $(T\boldsymbol{\Phi}_l)_k(\lambda) \to 0$ locally uniformly as a function of λ, and for each $k = 1,\ldots,n$.*

The second result we shall need is that convergence of the bilinear form implies convergence of $\boldsymbol{\Phi}_l$, and thus of the sequence $T\boldsymbol{\Phi}_l$.

Proposition 5.1.3. *If $\boldsymbol{\Phi}_l$ is a sequence, such that $a(\boldsymbol{\Phi}_l, \boldsymbol{\Phi}_l) \to a(\boldsymbol{\Phi}, \boldsymbol{\Phi}) = 0$ for some $\boldsymbol{\Phi} \in X_{\mathrm{sym}}$, then $T\boldsymbol{\Phi} = \mathbf{0}$ and $\boldsymbol{\Phi} = \mathbf{0}$.*

Proof. In [Ash14b] it is shown that T is coercive, so that for any $\boldsymbol{\Phi} \in X_{\mathrm{sym}}$,

$$a(\boldsymbol{\Phi}, \boldsymbol{\Phi}) = \|T\boldsymbol{\Phi}\|_Y^2 \gtrsim \|\boldsymbol{\Phi}\|_{X_{\mathrm{sym}}}^2. \tag{5.1.1}$$

As such the sequence $\{\boldsymbol{\Phi}_l\}$ is uniformly bounded, so by 2.3.3 [Ash13, Lemma 4.6] a subsequence (call this $\boldsymbol{\Phi}_l$) converges pointwise and locally uniformly to some $\boldsymbol{\Phi} \in X_{\mathrm{sym}}$. Since

T is continuous and $T\mathbf{\Phi}_l \to \mathbf{0}$ it follows that $T\mathbf{\Phi} = \mathbf{0}$ almost everywhere. However, since $T\mathbf{\Phi}$ is an analytic function in $\mathbb{C}^2$, $T\mathbf{\Phi} \equiv \mathbf{0}$. By coercivity, we find that $\mathbf{\Phi} = \mathbf{0}$. □

Theorem 5.1.4 (New weak formulation)**.** *Let $K \subset \mathbb{R}^2$ be any compact set. Then the above Theorem holds for Y replaced by $Y_K := L^2(\mathbb{R}^2 \setminus K)^{\times n}$. That is to say for*

$$a_K(\mathbf{\Phi}, \mathbf{\Phi}') = \sum_{k=1}^{n} \int_{\mathbb{R}^2 \setminus K} (T\mathbf{\Phi})_k(\lambda) \overline{(T\mathbf{\Phi}')_k(\lambda)} \, \mathrm{d}\lambda \tag{5.1.2}$$

$$\ell_K(\mathbf{\Phi}') = \sum_{k=1}^{n} \int_{\mathbb{R}^2 \setminus K} -(S\mathbf{\Theta}^{\mathrm{Di}})_k(\lambda) \overline{(T\mathbf{\Phi}')_k(\lambda)} \, \mathrm{d}\lambda. \tag{5.1.3}$$

Proof. We now appeal to the Lax–Milgram result for existence and uniqueness of the weak problem: it suffices to prove that the linear form ℓ_K is bounded, and the bilinear form a_K is bounded and coercive. Since

$$|\ell_K(\mathbf{\Phi}')| \leq \langle \mathbf{\Psi}, T\mathbf{\Phi}' \rangle_{Y_K} \leq \langle \mathbf{\Psi}, T\mathbf{\Phi}' \rangle_Y \leq C,$$

where the final inequality was proven for ℓ in [Ash14a]. Similarly $|a_K(\mathbf{\Phi}, \mathbf{\Phi}')| \leq C\|\mathbf{\Phi}\|_{X_{\mathrm{sym}}}\|\mathbf{\Phi}'\|_{X_{\mathrm{sym}}}$, and it remains then to prove that a_K is coercive:

Suppose this is not the case. Then there is a sequence $\mathbf{\Phi}_l \in X_{\mathrm{sym}}$ with $\|\mathbf{\Phi}_l\|_{X_{\mathrm{sym}}} = 1$ such that $a_K(\mathbf{\Phi}_l, \mathbf{\Phi}_l) \to 0$. Since $\mathbf{\Phi}_l$ is a bounded sequence, Proposition 5.1.3 gives that $\mathbf{\Phi}_l \to \mathbf{\Phi} = \mathbf{0}$ pointwise and locally uniformly for a subsequence. Lemma 5.1.2 ensures local uniform convergence of $T\mathbf{\Phi}_l \to 0$, so that the integral over a compact set converges:

$$\lim_{l\to\infty} \sum_{k=1}^{n} \int_K |(T\mathbf{\Phi}_l)_k(\lambda)|^2 \, \mathrm{d}\lambda = \sum_{k=1}^{n} \int_K \lim_{l\to\infty} |(T\mathbf{\Phi}_l)_k(\lambda)|^2 \, \mathrm{d}\lambda = 0.$$

Finally by the coercivity estimate (5.1.1) for a over the entire domain Y, we deduce coercivity over Y_K, because

$$\begin{aligned} \|\mathbf{\Phi}_l\|^2_{X_{\mathrm{sym}}} \lesssim \|T\mathbf{\Phi}_l\|^2_Y &= \sum_{k=1}^{n} \left(\int_{\mathbb{R}^2 \setminus K} |(T\mathbf{\Phi}_l)_k(\lambda)|^2 \, \mathrm{d}\lambda + \int_K |(T\mathbf{\Phi}_l)_k(\lambda)|^2 \, \mathrm{d}\lambda \right) \\ &\leq a_K(\mathbf{\Phi}_l, \mathbf{\Phi}_l) + \sum_{k=1}^{n} \int_K |(T\mathbf{\Phi}_l)_k(\lambda)|^2 \, \mathrm{d}\lambda \to 0, \end{aligned}$$

and thus $\|\mathbf{\Phi}_l\|_{X_{\mathrm{sym}}} \to 0$, which contradicts our assumption. □

5.1.1 Explicit coercivity bounds

In (5.1.2) we considered a new weak formulation for the global relation, and proved that the forms satisfy the assumption of Lax–Milgram. Importantly, Céa's Lemma applies, which gives a convergence rate of the Galerkin problem, using only the coercivity and

boundedness constants. Another weak approach motivated by [Ash14b, Eq. 4.2] is to consider the modified weak problem $\tilde{a}(\boldsymbol{\Phi}, \boldsymbol{\Phi}') = \tilde{\ell}(\boldsymbol{\Phi}')$ for all $\boldsymbol{\Phi}' \in X_{\mathrm{sym}}$, where

$$\begin{aligned}\tilde{a}(\boldsymbol{\Phi}, \boldsymbol{\Phi}') &:= \Re \int_{\mathbb{R}^2} \Big(T\boldsymbol{\Phi}(\lambda) \cdot L\boldsymbol{\Phi}'(-\lambda) - LT\boldsymbol{\Phi}(\lambda) \cdot \boldsymbol{\Phi}'(-\lambda) - 2MT\boldsymbol{\Phi}(\lambda) \cdot \boldsymbol{\Phi}'(-\lambda) \Big) \frac{\mathrm{d}\lambda}{|\lambda|} \\ -\tilde{\ell}(\boldsymbol{\Phi}') &:= \Re \int_{\mathbb{R}^2} \Big(S\boldsymbol{\Theta}^{\mathrm{Di}}(\lambda) \cdot L\boldsymbol{\Phi}'(-\lambda) - LS\boldsymbol{\Theta}^{\mathrm{Di}}(\lambda) \cdot \boldsymbol{\Phi}'(-\lambda) - 2MS\boldsymbol{\Theta}^{\mathrm{Di}}(\lambda) \cdot \boldsymbol{\Phi}'(-\lambda) \Big) \frac{\mathrm{d}\lambda}{|\lambda|},\end{aligned}$$

and the operators M and L are defined on X_{sym} as

$$(M\boldsymbol{\Phi})_k(\lambda) = \mathrm{i}(\boldsymbol{m}_k \cdot R_k^t \boldsymbol{\lambda})\Phi_k(\lambda), \qquad (L\boldsymbol{\Phi})_k(\lambda) = \lambda_1 \frac{\partial \Phi_k}{\partial \lambda_2} + \lambda_2 \frac{\partial \Phi_k}{\partial \lambda_1}. \tag{5.1.4}$$

This weak problem is motivated by an identity that is used to prove that the operator T is bounded below, and this weak approach follows by substituting occurrences of $T\boldsymbol{\Phi}^{\mathrm{Ne}}$ in the definition of $\tilde{a}$ by $-S\boldsymbol{\Theta}^{\mathrm{Di}}$. Therefore any function $\boldsymbol{\Phi}^{\mathrm{Ne}} \in X_{\mathrm{sym}}$ solving the global relation also solves the weak problem. If we can show that $\tilde{a}, \tilde{\ell}$ are bounded and that $\tilde{a}$ is coercive, then the Lax–Milgram Theorem 2.6.2 guarantees that this is the unique solution to the global relation $T\boldsymbol{\Phi}^{\mathrm{Ne}} = -S\boldsymbol{\Theta}^{\mathrm{Di}}$, for given valid Dirichlet data $\boldsymbol{\Theta}^{\mathrm{Di}}$. And indeed in [Ash14b], boundedness is shown and using properties of this weak formulation, $T : X_{\mathrm{sym}} \to Y$ is shown to be injective.

This result may be extended to give an *explicit* coercivity bound for a, which is explicit from the geometry. This remarkable fact, combined with Céa Lemma gives optimal lower bounds on the convergence rate for the Galerkin method associated to $\tilde{a}$ and $\tilde{\ell}$. Let us recall that the matrices are constructed so that $R_k^t \mathbf{e}_z = \mathbf{n}_k$, where $\boldsymbol{n}_k$ is the outward normal of the k-th face, and $\boldsymbol{m}_k$ is the midpoint vector for the k-th face. Optimal convergence is assured when coordinates are chosen such that $m := \inf_k \mathbf{m}_k \cdot \mathbf{n}_k$ is maximised, so that we suppose the point $(0, 0, 0)$ lies inside the polyhedron.

Recall that for $\lambda \in \mathbb{R}^2$ and $\Phi_j \in PW_{Q_j,\mathrm{sym}}$, $\Phi_j(\lambda) = \overline{\Phi_j(-\lambda)}$. A similar proof using only the definition of the Fourier transform gives the identity

$$-\frac{\partial \Phi_j}{\partial \lambda_i}(-\lambda) = \overline{\frac{\partial \Phi_j}{\partial \lambda_i}(\lambda)}, \quad i = 1, 2.$$

Making these substitutions, we calculate

$$\begin{aligned}\Phi_k(\lambda)(L\boldsymbol{\Phi})_k(-\lambda) &= \Phi_k(\lambda) \left[-\lambda_1 \frac{\partial \Phi_k}{\partial \lambda_1}(-\lambda) - \lambda_2 \frac{\partial \Phi_k}{\partial \lambda_2}(-\lambda) \right] \\ &= \overline{\Phi_k(-\lambda)} \overline{\left[\lambda_1 \frac{\partial \Phi_k}{\partial \lambda_1}(\lambda) + \lambda_2 \frac{\partial \Phi_k}{\partial \lambda_2}(\lambda) \right]} \\ &= \overline{(L\boldsymbol{\Phi})_k(\lambda)\Phi_k(-\lambda)},\end{aligned} \tag{5.1.5}$$

so that $\Im(\Phi_k(\lambda)(L\boldsymbol{\Phi})_k(-\lambda) + (L\boldsymbol{\Phi})_k(\lambda)\Phi_k(-\lambda)) = 0$. The following Theorem uses this fact

to give explicit coercivity bounds for the weak problem. These arguments are taken from [Ash14b, Lemma 4.7], where (5.1.7) is derived to prove that T is injective. Our proof here directly shows that this identity yields a coercivity bound which, by Céa's Lemma, may be used to estimate convergence rates for this method.

Theorem 5.1.5 (Explicit coercivity bounds)**.** *Given the polyhedron Ω defined as above, suppose (by a translation of our coordinates) that the origin is contained inside Ω, so that all the midpoint vectors $\mathbf{m}_i$ point outwards, i.e. $\mathbf{m}_k \cdot \mathbf{n}_k > 0$. Let $m := \inf_k \mathbf{m}_k \cdot \mathbf{n}_k$ be the least such value over all the faces Σ_k. Then*

$$a(\boldsymbol{\Phi}, \boldsymbol{\Phi}) \geq 2m\|\boldsymbol{\Phi}\|_X^2, \qquad \text{for every } \boldsymbol{\Phi} \in X_{\mathrm{sym}}.$$

In particular, by Céa's Lemma, our solution $\boldsymbol{\Phi}_N$ in a subspace $X_N \subsetneq X_{\mathrm{sym}}$ differs from the exact solution $\boldsymbol{\Phi} \in X_{\mathrm{sym}}$ by at most a constant multiple of the subspace error, $\inf_{\boldsymbol{\Phi}' \in X_N} \|\boldsymbol{\Phi} - \boldsymbol{\Phi}'\|_{X_{\mathrm{sym}}}$:

$$\|\boldsymbol{\Phi} - \boldsymbol{\Phi}_N\|_{X_{\mathrm{sym}}} \leq \frac{C}{2m} \inf_{\boldsymbol{\Phi}' \in X_N} \|\boldsymbol{\Phi} - \boldsymbol{\Phi}'\|_{X_{\mathrm{sym}}},$$

where C is the boundedness constant for a.

Proof. We first use the identity [Ash14a, Eq.. 4.2]

$$\begin{aligned}\int_{\mathbb{R}^2} \Big(T\boldsymbol{\Phi}(\lambda) \cdot L\boldsymbol{\Phi}(\lambda) - LT\boldsymbol{\Phi}(\lambda) \cdot \boldsymbol{\Phi}(-\lambda) - 2MT\boldsymbol{\Phi}(\lambda) \cdot \boldsymbol{\Phi}(-\lambda) \Big) \frac{\mathrm{d}\lambda}{|\lambda|} \\ = \int_{\mathbb{R}^2} \Big(\boldsymbol{\Phi}(\lambda) \cdot L\boldsymbol{\Phi}(-\lambda) - L\boldsymbol{\Phi}(\lambda) \cdot \boldsymbol{\Phi}(-\lambda) - 2M\boldsymbol{\Phi}(\lambda) \cdot \boldsymbol{\Phi}(-\lambda) \Big) \frac{\mathrm{d}\lambda}{|\lambda|}.\end{aligned}$$

Let us consider the first two terms $H(\lambda) := \boldsymbol{\Phi}(\lambda) \cdot L\boldsymbol{\Phi}(-\lambda) - L\boldsymbol{\Phi}(\lambda) \cdot \boldsymbol{\Phi}(-\lambda)$ on the right-hand side. For $\lambda \in \mathbb{R}^2$, it is quickly seen that $\overline{H(\lambda)} = -H(\lambda)$, so the function is purely imaginary. Therefore we can simplify

$$\begin{aligned} a(\boldsymbol{\Phi}, \boldsymbol{\Phi}) &= \Re \int_{\mathbb{R}^2} -2M\boldsymbol{\Phi}(\lambda) \cdot \boldsymbol{\Phi}(-\lambda) \frac{\mathrm{d}\lambda}{|\lambda|} \\ &= \Re \sum_{k=1}^{n} \int_{\mathbb{R}^2} -2\mathrm{i}(\mathbf{m}_k \cdot R_k^t \boldsymbol{\lambda}) |\Phi_k(\lambda)|^2 \frac{\mathrm{d}\lambda}{|\lambda|}, \end{aligned} \tag{5.1.6}$$

from the definition of the multiplication operator M and $\boldsymbol{\Phi}(-\lambda) = \overline{\boldsymbol{\Phi}(\lambda)}$. Recall that the matrix R_i^t and vector $\mathbf{m}_i$ components are real, and that the vector $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, \mathrm{i}|\lambda|)^t$. Consequently only the third component of $\boldsymbol{\lambda}$ contributes to the real part of the integral,

and

$$\begin{aligned} a(\mathbf{\Phi}, \mathbf{\Phi}) &= \sum_{k=1}^{n} \int_{\mathbb{R}^2} 2\mathbf{m}_k \cdot R_k^t(0,0,|\lambda|)^t |\Phi_k(\lambda)|^2 \frac{\mathrm{d}\lambda}{|\lambda|} \\ &= \sum_{k=1}^{n} 2\mathbf{m}_k \cdot \mathbf{n}_k \int_{\mathbb{R}^2} |\Phi_k(\lambda)|^2 \,\mathrm{d}\lambda \\ &\geq 2m \|\mathbf{\Phi}\|^2_{X_{\mathrm{sym}}}. \end{aligned} \tag{5.1.7}$$

□

We remark that the operator L in (5.1.4) uses derivatives of the Paley–Wiener functions $\Phi_k(\lambda)$, which is valid since all functions are analytic. In Section 5.5, we will see a new weak formulation, derived via a coordinate-independent integration-by-parts. In this approach too, we will see a similar representation of a directional derivative $(a,b)\cdot\nabla\Phi_k(\lambda)$, which can be compared with the operator L. To see the necessity of a new method, we now set up the Galerkin method for our initial modified weak problem (5.1.2).

5.2 Constructing a basis

Recall that a good choice of basis for polygonal domains is less clear than for 2D problems, but that we have decided to use the polynomials

$$f_{j,\alpha}(X) = X^\alpha, \quad j = 1,\dots,n;\ |\alpha| \leq N$$

as a basis for $L^2(Q_j)$ and $X = (X_1, X_2)$, as proposed in [Ash14a]. Thus a function $\phi_j \in L^2(Q_j)$ may be approximated by a linear combination of polynomials $f_{j,\alpha}(X) := X_1^{\alpha_1} X_2^{\alpha_2}$ as

$$\phi_j(X) \approx \phi_{N,j}(X) = \sum_{|\alpha|\leq N} c_{j,\alpha} X^\alpha.$$

This has the significant advantage that the Fourier transforms are given precisely: for a given polygon Q in the plane,

$$\int_Q X^\alpha e^{-\mathrm{i}\lambda\cdot X}\,\mathrm{d}X = (-D)^\alpha \int_Q e^{-\mathrm{i}\lambda\cdot X}\,\mathrm{d}X.$$

It is sufficient then to find this integral, where we shall write the vector $\lambda = (\lambda_1, \lambda_2)$ throughout. We have

$$\int_Q e^{-\mathrm{i}\lambda\cdot X} = \int_Q \frac{\partial}{\partial X_1}\left(\frac{e^{-\mathrm{i}\lambda\cdot X}}{-\mathrm{i}\lambda_1}\right)\mathrm{d}X \equiv \int_Q \frac{\partial}{\partial X_2}\left(\frac{e^{-\mathrm{i}\lambda\cdot X}}{-\mathrm{i}\lambda_2}\right)\mathrm{d}X. \tag{5.2.1}$$

Concentrating on the first of these equalities, Green's Theorem gives us an integral over the boundary:

$$\int_{\partial Q} \frac{e^{-\mathrm{i}\lambda\cdot X}}{-\mathrm{i}\lambda_1}\,\mathrm{d}X_2.$$

As the boundary is now a polygon, this is a sum over line segments: let us fix $(Y,Z) := (X_i, X_{i+1})$ for some $i \in \{1,\dots,n\}$. Using the vector parameterisation $X = Y + t(Z-Y)$, we find

$$\frac{-1}{\mathrm{i}\lambda_1}\int_0^1 e^{-\mathrm{i}\lambda\cdot(Y+t(Z-Y))}(Z_2-Y_2)\,\mathrm{d}t = \frac{-1}{\mathrm{i}\lambda_1}(Z_2-Y_2)\frac{e^{-\mathrm{i}\lambda\cdot Z}-e^{-\mathrm{i}\lambda\cdot Y}}{-\mathrm{i}\lambda\cdot(Z-Y)}.$$

The contribution over all edges of ∂Q is given precisely as

$$F_Q^{(1)}(\lambda) = \frac{-1}{\lambda_1}\sum_{j=1}^{m}\frac{(X_{j+1}-X_j)_2}{\lambda\cdot(X_{j+1}-X_j)}\left(e^{-\mathrm{i}\lambda\cdot X_{j+1}}-e^{-\mathrm{i}\lambda\cdot X_j}\right),$$

noting that $(X_{j+1}-X_j)_2$ involves only the *second component* of $X_{j+1}-X_j$. By a similar calculation to (5.2.1), we find that an equivalent representation $F_Q^{(1)}(\lambda)$ is given by

$$F_Q^{(2)}(\lambda) = \frac{1}{\lambda_2}\sum_{j=1}^{m}\frac{(X_{j+1}-X_j)_1}{\lambda\cdot(X_{j+1}-X_j)}\left(e^{-\mathrm{i}\lambda\cdot X_{j+1}}-e^{-\mathrm{i}\lambda\cdot X_j}\right)$$

and also

$$F_Q(\lambda) = \frac{1}{2\lambda_1\lambda_2}\sum_{j=1}^{m}\frac{(\lambda_1,-\lambda_2)\cdot(X_{j+1}-X_j)}{\lambda\cdot(X_{j+1}-X_j)}\left(e^{-\mathrm{i}\lambda\cdot X_{j+1}}-e^{-\mathrm{i}\lambda\cdot X_j}\right).$$

Remark 5.2.1. *An important note here is that all of these functions are the Fourier transform of $\int_Q e^{-\mathrm{i}\lambda\cdot X}dX$, and hence are holomorphic*[1] *as functions in $\mathbb{C}^2$. In particular,*

$$F_Q^{(1)}(\lambda) = F_Q^{(2)}(\lambda) = F_Q(\lambda), \quad \forall\,\lambda\in\mathbb{C},$$

however we have identified these uniquely by their a-priori singularity. I.e. given the functions, it is immediately clear e.g. for $F_Q^{(1)}$ that there is no λ_2 singularity, whereas it is not immediately clear (but nevertheless true) that the λ_1 singularity is removable. In fact all singularities (except at ∞) are removable.

This remark has computational effects, as we would like to avoid computing removable singularities, and so for the sequel, near the axis $\lambda_2 = 0$ we will always use $F_Q^{(1)}$, and vice versa. Away from both axes, F_Q has clear quadratic decay, however we have found it best in MATLAB to limit the number of distinct (but equal) functions used. This seems to aid numerical precision, so we divide $\mathbb{C}^2$ into distinct regions where $F_Q^{(1)}(\lambda)$ and $F_Q^{(2)}(\lambda)$ are

[1] A function $f:\mathbb{C}^n\to\mathbb{C}^n$ is holomorphic if it is holomorphic in each coordinate separately.

used.

Because $F_Q^{(i)}$ still involve an explicit $1/\lambda_i$ term; when λ_i is near zero, we shall avoid using this representation for $F_Q(\lambda)$. Since all three are functionally equivalent, we shall settle on the following representation:

$$F_Q(\lambda) := \begin{cases} F_Q^{(1)}(\lambda), & |\lambda_1| \geq |\lambda_2| \\ F_Q^{(2)}(\lambda), & |\lambda_2| > |\lambda_1|. \end{cases}$$

With this representation, $F_Q(\lambda)$ (being the Fourier transform of a compactly supported function) is still analytic; in $L^2(\mathbb{R})$ and a Schwartz ('rapid decay') function.

It therefore follows that an approximation $\mathbf{\Phi}_N \approx \mathbf{\Phi} \in X_{\text{sym}}$ may be given in terms of these functions:

$$\Phi_{N,j}(\lambda) = \sum_{|\alpha| \leq N} c_{j,\alpha} (-1)^\alpha D^\alpha F_{Q_j}(\lambda).$$

So it will be useful to have an analytical form for these derivatives $D^\alpha F_Q(\lambda)$. Recall that the Leibniz formula for multi-index derivatives is

$$D^\alpha (FG)(\lambda) = \sum_{\beta \leq \alpha} \binom{\alpha}{\beta} D^{\alpha-\beta} F(\lambda) D^\beta G(\lambda).$$

To derive the derivatives of F_Q we will use the following identities:

$$\begin{aligned} D^\alpha \left(\frac{1}{\lambda_1} \right) &= \frac{(-\mathrm{i})^\alpha (-1)^\alpha \alpha!}{\lambda_1^{\alpha_1+1}} \mathbf{1}_{\alpha_2=0} \\ D^\alpha (e^{-\mathrm{i}\lambda \cdot X_{j+1}} - e^{-\mathrm{i}\lambda \cdot X_j}) &= (-\mathrm{i})^\alpha (-\mathrm{i})^\alpha \left(X_{j+1}^\alpha e^{-\mathrm{i}\lambda \cdot X_{j+1}} - X_j^\alpha e^{-\mathrm{i}\lambda \cdot X_j} \right), \end{aligned} \tag{5.2.2}$$

with the convention that a multi-index α acts either like $\alpha = (\alpha_1, \alpha_2)$ or like $\alpha_1 + \alpha_2$.

As we observed above, the functions $F_Q(\lambda)$ have removable singularities. To assist the numerics, we shall rewrite these as sinc functions, to more clearly identify these removable singularities. Let us first work with $F_Q^{(1)}(\lambda)$: recalling that

$$F_Q^{(1)}(\lambda) = \frac{-1}{\lambda_1} \sum_{j=1}^m \frac{(X_{j+1} - X_j)_2}{\lambda \cdot (X_{j+1} - X_j)} \left(e^{-\mathrm{i}\lambda \cdot X_{j+1}} - e^{-\mathrm{i}\lambda \cdot X_j} \right),$$

we see the exponential part is equivalent to

$$\begin{aligned} F_Q^{(1)}(\lambda) &= \frac{-1}{\lambda_1} \sum_{j=1}^m \frac{(X_{j+1} - X_j)_2}{\lambda \cdot (X_{j+1} - X_j)} e^{-\frac{\mathrm{i}}{2}\lambda \cdot (X_{j+1} + X_j)} \left(e^{-\frac{\mathrm{i}}{2}\lambda \cdot (X_{j+1} - X_j)} - e^{-\frac{\mathrm{i}}{2}\lambda \cdot (X_{j+1} - X_j)} \right) \\ &= \frac{\mathrm{i}}{\lambda_1} \sum_{j=1}^m (X_{j+1} - X_j)_2 e^{-\frac{\mathrm{i}}{2}\lambda \cdot (X_{j+1} + X_j)} \operatorname{sinc}\left(\frac{\lambda}{2} \cdot (X_{j+1} - X_j) \right). \end{aligned} \tag{5.2.3}$$

In a similar way we may calculate the derivatives, $D^\alpha F_Q^{(1)}(\lambda_1, \lambda_2)$. Letting $\operatorname{sinc}^{(k)}(z)$ denote the k-th derivative of sinc,

$$\begin{aligned}
D^\alpha F_Q^{(1)}(\lambda) &= \sum_{j=1}^{m} \sum_{\substack{\beta \le \alpha \\ \gamma \le \beta}} \binom{\alpha}{\beta}\binom{\beta}{\gamma} D^{\alpha-\beta}\left(\frac{\mathrm{i}(X_{j+1}-X_j)_2}{\lambda_1}\right) D^{\beta-\gamma}\left(e^{-\frac{\mathrm{i}}{2}\lambda\cdot(X_{j+1}+X_j)}\right) \\
&\qquad \times D^\gamma\left(\operatorname{sinc}\left(\frac{\lambda}{2}\cdot(X_{j+1}-X_j)\right)\right) \\
&= \sum_{j=1}^{m} \sum_{\substack{\beta \le \alpha, \beta_2 = \alpha_2 \\ \gamma \le \beta}} (-\mathrm{i})^\alpha \binom{\alpha}{\beta}\binom{\beta}{\gamma} \left(\frac{\mathrm{i}(X_{j+1}-X_j)_2(\alpha-\beta)_1!(-1)^{\alpha-\beta}}{\lambda_1^{\alpha_1-\beta_1+1}}\right) \\
&\qquad \times \left(\frac{(-\mathrm{i})^{\beta-\gamma}(X_{j+1}+X_j)^{\beta-\gamma}}{2^{\beta-\gamma}} e^{-\frac{\mathrm{i}}{2}\lambda\cdot(X_{j+1}+X_j)}\right) \\
&\qquad\qquad \times \frac{(X_{j+1}-X_j)^\gamma}{2^\gamma} \operatorname{sinc}^{(|\gamma|)}\left(\frac{\lambda}{2}\cdot(X_{j+1}-X_j)\right) \\
&= \sum_{j=1}^{m} \sum_{\substack{\beta \le \alpha, \beta_2 = \alpha_2 \\ \gamma \le \beta}} \frac{\mathrm{i}(-1)^\beta(-\mathrm{i})^{\alpha+\beta-\gamma}(X_{j+1}-X_j)_2\alpha!}{\gamma!(\beta-\gamma)!\lambda_1^{\alpha_1-\beta_1+1}} e^{-\frac{\mathrm{i}}{2}\lambda\cdot(X_{j+1}+X_j)} \\
&\qquad \times \frac{(X_{j+1}+X_j)^{\beta-\gamma}(X_{j+1}-X_j)^\gamma}{2^\beta} \operatorname{sinc}^{(|\gamma|)}\left(\frac{\lambda}{2}\cdot(X_{j+1}-X_j)\right).
\end{aligned}$$

Similarly for $D^\alpha F_Q^{(2)}(\lambda)$,

$$\begin{aligned}
D^\alpha F_Q^{(2)}(\lambda) &= \sum_{j=1}^{m} \sum_{\substack{\beta \le \alpha, \beta_1 = \alpha_1 \\ \gamma \le \beta}} \frac{\mathrm{i}(-1)^\beta(-\mathrm{i})^{\alpha+\beta-\gamma}(X_{j+1}-X_j)_1\alpha!}{\gamma!(\beta-\gamma)!\lambda_2^{\alpha_2-\beta_2+1}} e^{-\frac{\mathrm{i}}{2}\lambda\cdot(X_{j+1}+X_j)} \\
&\qquad \times \frac{(X_{j+1}+X_j)^{\beta-\gamma}(X_{j+1}-X_j)^\gamma}{2^\beta} \operatorname{sinc}^{(|\gamma|)}\left(\frac{\lambda}{2}\cdot(X_{j+1}-X_j)\right).
\end{aligned}$$

Remark 5.2.2. *Since* $\operatorname{sinc} : \mathbb{C} \to \mathbb{C}$ *is entire,* (5.2.3) *is analytic in the sub-region specified. Therefore so are all of its derivatives. However it may be that* $\lambda \cdot (X_{j+1} - X_j) = 0$ *for some* j *and* $\lambda \in \mathbb{R}^2$. *Since there is not an explicit implementation of* sinc *as an entire function in MATLAB (i.e. an implementation such that an evaluation of its derivatives near zero is stable), we choose to use the Taylor expansion*

$$\operatorname{sinc}(z) = \sum_{k \ge 0} a_k z^k$$

for points z *near zero. This is convenient, since the derivative is also given as*

$$\frac{\mathrm{d}}{\mathrm{d}z}\operatorname{sinc}(z) = \sum_{k \ge 1} k a_k z^{k-1},$$

and so in our implementation we shall use the first few Taylor terms to approximate $\mathrm{sinc}(z)$ *for small-modulus values of* z*. This will remove potential inaccuracies due to MATLAB's computation of derivatives of* sinc *near zero.*

5.3 A stable orthogonalisation

Our basis of polynomials is no longer orthogonal, so for our Galerkin problem, we would like to create a new basis from our initial basis. This is particularly useful, since we are work with the Fourier transform of these functions. Recall that by Parseval's identity, if we orthogonalise these vectors, their Fourier transforms are also orthogonalised. Furthermore, by using orthogonal vectors in our basis, it becomes easier to numerically project the known Dirichlet data to our basis, and only work with integrals involving these known basis vectors. For example, we shall see in Section 6.2, that the number of numerical integrations to calculate the Galerkin matrices may be reduced, because we are only considering terms on individual basis vectors.

$$f_{j,\alpha}(X) = X_1^{\alpha_1} X_2^{\alpha_2}, \qquad \text{for each face } Q_j, \text{ and } |\alpha| \leq N.$$

The Stone–Weierstrass Theorem states that any continuous function, $f \in C^0(Q_j)$, can be uniformly approximated by the set of polynomials $\{X_1^{\alpha_1} X_2^{\alpha_2} : \alpha_1, \alpha_2 \in \mathbb{N}\}$. Since continuous functions are dense in $L^2(Q_j)$, these functions form an *approximating basis*[2] for $L^2(Q_j)$. Fixing a face Q_i for now, we shall label the vectors spanning a subspace of $L^2(Q_j)$ as $\{f_j\}_{j=1}^M$, for $M = \frac{1}{2}(N+1)(N+2)$. Since each face is compact, we can easily calculate integrals over the faces, so we shall orthogonalise these vectors by the Gram–Schmidt algorithm:

$$\begin{aligned} u_1 &:= f_1 \\ u_2 &:= f_2 - \frac{\langle f_2, u_1 \rangle}{\langle u_1, u_1 \rangle} u_1 \\ &\vdots \\ u_M &:= f_M - \sum_{j=1}^{M-1} \frac{\langle f_n, u_j \rangle}{\langle u_j, u_j \rangle} u_j. \end{aligned} \tag{5.3.1}$$

[2] This means that for any $g \in L^2(Q_j)$ and $\epsilon > 0$ there exists a constant N_ϵ and a linear combination $g_\epsilon = \sum_{|\alpha| \leq N_\epsilon} c_\alpha f_{j,\alpha}$ such that $\|g - g_\epsilon\|_{L^2(Q_j)} < \epsilon$.

Defining a matrix $\Lambda = (\Lambda_{n,j})_{n,j=1}^{M}$ as

$$\Lambda_{n,j} := \begin{cases} \frac{\langle f_n, u_j \rangle}{\langle u_j, u_j \rangle}, & n > j \\ 1, & n = j \\ 0, & \text{else} \end{cases},$$

we write $\mathbf{f} = \Lambda \mathbf{u}$ or equivalently $f_n = \sum_{j=1}^{n} \Lambda_{n,j} u_j$. Thus if a function F is a linear combination of u_j,

$$\begin{aligned} F = \sum_{j=1}^{M} \alpha_j u_j &= \sum_{j=1}^{M} \alpha_j \left(\sum_{n=1}^{M} \Lambda_{j,n}^{-1} f_n \right) \\ &= \boldsymbol{\alpha} \cdot \Lambda^{-1} \mathbf{f} \\ &= \sum_{n=1}^{M} \left(\sum_{j=1}^{M} \Lambda_{j,n}^{-1} \alpha_j \right) f_n \end{aligned} \tag{5.3.2}$$

So $F = \sum_{n=1}^{M} \beta_n f_n$ for $\beta_n = \sum_{j=1}^{M} \Lambda_{j,n}^{-1} \alpha_j$.

Suppose then that we have a known function F and wish to project it to a subspace spanned by $(f_n)_{n=1}^{M}$. We write

$$F \approx \sum_{j=1}^{M} \alpha_j u_j,$$

where by orthogonality, it's quickly checked that the coefficients α_j are given as

$$\alpha_j = \frac{\langle F, u_j \rangle}{\langle u_j, u_j \rangle} = \sum_{m=1}^{M} \frac{\Lambda_{j,m}^{-1} \langle F,\ f_m \rangle}{\langle u_j, u_j \rangle}.$$

Since we can write β_n in terms of α_j,

$$F \approx F_M = \sum_{n=1}^{M} \beta_n f_n, \quad \text{for } \beta_n = \sum_{j,m=1}^{M} \Lambda_{j,n}^{-1} \Lambda_{j,m}^{-1} \frac{\langle F,\ f_m \rangle}{\langle u_j, u_j \rangle}. \tag{5.3.3}$$

Because of Parseval's Theorem, $\hat{F}$ can also be approximated by $\hat{f}_n$ using the same coefficients $(\beta_n)_{n=1}^{M}$ (up to a scaling factor). Thus we have a basis for $X_N \subset X$ by $e_{i,\alpha}(\lambda) := \hat{f}_{i,\alpha}(\lambda)$ for $1 \leq i \leq n$ and $|\alpha| \leq N$, let us denote this basis by $\{\boldsymbol{e}_j\}_{j=1}^{nM}$. Then we have

$$\boldsymbol{\Phi}^{\mathrm{Di}} \approx \boldsymbol{\Phi}_N^{\mathrm{Di}} = \sum_{l=1}^{nM} c_l \boldsymbol{e}_l,$$

where the coefficients $c_l = c_{i,\alpha}$ for $|\alpha| \leq N$, are precisely the coefficients $\{\beta_j\}_{j=1}^{\frac{1}{2}(N+1)(N+2)}$

on the i-th face. And so the linear form $\ell_K(\boldsymbol{e}_j)$ in the subspace X_N is

$$\ell_K(\boldsymbol{e}_j) = \sum_{k=1}^{n}\sum_{l=1}^{nM} c_l \int_{\mathbb{R}^2\setminus K} -(S\boldsymbol{e}_l)_k\overline{(T\boldsymbol{e}_j)_k}\,\mathrm{d}x\,\mathrm{d}y \equiv \sum_{l=1}^{nM} c_l \left\langle -S\boldsymbol{e}_l, T\boldsymbol{e}_j\right\rangle .$$

5.3.1 A stable orthogonalisation

An issue with the Gram–Schmidt approach to orthogonalisation, is that numerical round-off error occurs in each step where $\langle f_n, u_j\rangle$ is calculated. This propagates through the orthogonalisation because of the terms $(u_j)_{j=1}^{n-1}$ occurring in the expression for u_n. As a result, such a procedure is numerically unstable. However this is *not* the case for our method: by providing an analytical expression for these inner products, we may eliminate such numerical errors from propagating in (5.3.1). Indeed, these inner products can be reduced to an analytic expression depending only on the geometry of the polygonal face Q.

Indeed, suppose the vertices of Q are given by $(X^{(1)}, X^{(2)}, \ldots, X^{(n)}, X^{(n+1)} = X^{(1)})$, where each $X^{(j)} = (X_1^{(j)}, X_2^{(j)}) \in \mathbb{R}^2$ represents the coordinates of a vertex. We wish to integrate a generic basis vector $x^p y^q$ over the domain enclosed by Q. Crucially such functions are separable in x and y so an application of Stokes' Theorem reduces this integral to one over the boundary:

$$\begin{aligned}\int_Q x^p y^q\,\mathrm{d}x\,\mathrm{d}y &= \int_Q \mathrm{d}\left(\frac{x^{p+1}y^q}{p+1}\,\mathrm{d}y\right)\\ &= \int_{\partial Q}\frac{x^{p+1}y^q}{p+1}\,\mathrm{d}y\\ &= \sum_{j=1}^{n}\int_{\Gamma_j}\frac{x^{p+1}y^q}{p+1}\,\mathrm{d}y\end{aligned}$$

We can parameterise $\Gamma_j(t) = X^{(j)} + t(X^{(j+1)} - X^{(j)}) =: Y + t(Z - Y)$ so we have $\mathrm{d}y = (Z-Y)_2\,\mathrm{d}t$ and the integral over Γ_j becomes

$$\frac{1}{p+1}\int_0^1 (Y_1 + t(Z-Y)_1)^{p+1}(Y_2 + t(Z-Y)_2)^q (Z-Y)_2\,\mathrm{d}t.$$

This can be expanded using the binomial Theorem:

$$(a + t(b-a))^n = \sum_{k=0}^{n}\binom{n}{k}a^k(b-a)^{n-k}t^{n-k},$$

giving an integral only in powers of t

$$\sum_{k=0}^{n+1}\sum_{\tilde{k}=0}^{n}\frac{1}{p+1}\binom{p+1}{k}\binom{q}{\tilde{k}}Y_1^k Y_2^{\tilde{k}}(Z-Y)_1^{p+1-k}(Z-Y)_2^{q-\tilde{k}}\int_0^1 t^{p+q+1-k-\tilde{k}}\,\mathrm{d}t$$

The integral gives $(p+q+2-k-\tilde{k})^{-1}$, so summing over all such faces Γ_j yields an analytic expression for our integral

$$\begin{aligned} I_{p,q,Q} &:= \int_Q x^p y^q \,\mathrm{d}x\,\mathrm{d}y \\ &= \sum_{j=1}^{n}\sum_{k=0}^{p+1}\sum_{\tilde{k}=0}^{q}\frac{1}{(p+1)(p+q+2-k-\tilde{k})}\binom{p+1}{k}\binom{q}{\tilde{k}}\dots \\ &\qquad \dots (X^{(j)})_1^k (X^{(j)})_2^{\tilde{k}} (X^{(j+1)}-X^{(j)})_1{}^{p+1-k}(X^{(j+1)}-X^{(j)})_2{}^{q-\tilde{k}} \end{aligned} \tag{5.3.4}$$

In particular then, the coefficients $\Lambda_{n,j}$ are given precisely in terms of the geometry. Thus the Gram–Schmidt procedure will be correct to machine precision. To highlight this, let us use a 1-1 correspondence between $n \in \mathbb{Z} \leftrightarrow (\alpha_1(n), \alpha_2(n)) \in \mathbb{Z}^2$ which, where unambiguous, we shall implicitly use (α_1, α_2). Suppose $u_1, \dots, u_{n-1}$ have been calculated and coefficients $a_{k,\alpha}$, such that $u_k = \sum_{j\le k} a_{k,\alpha(k)} f_{\alpha(k)} = \sum_\alpha a_{k,\alpha} x^{\alpha_1} y^{\alpha_2}$.

$$\langle f_n, u_j\rangle = \sum_{k\le j}\langle e_n, a_{j,\alpha(k)}\rangle = \sum_{k\le j} I_{p(k),q(k),Q}, \qquad \text{for } p(k)=\alpha_1(n)+\alpha_1(k),\ q(k)=\alpha_2(n)+\alpha_2(k)$$

Similarly the norm of u_j is given by a double sum

$$\langle u_j, u_j\rangle = \sum_{k,\tilde{k}\le j} I_{p(k,\tilde{k}),q(k,\tilde{k}),Q}, \qquad \text{for } p(k,\tilde{k})=\alpha_1(k)+\alpha_1(\tilde{k}),\ q(k,\tilde{k})=\alpha_2(k)+\alpha_2(\tilde{k}).$$

In summary, this approach does not store the functions u_j, but rather a matrix $(a_{k,\alpha})_{k,\alpha}$ where the k-th row is the coefficients for u_k in terms of e_α. This matrix can be built up row-by-row using the exact expressions for $I_{p,q,Q}$ given here. Once all the values $a_{k,\alpha}$ are known, the coefficients β_j only require a numerical integration for $\langle F, f_m\rangle$ in (5.3.3).

5.3.2 Applying to our linear problem

Recall that our Dirichlet data on the i-th face Σ_i is f_i. Using the pullback map ψ_i, this face is a flat polygon Q_i in the plane. The Dirichlet data, $\vartheta_i^{\mathrm{Di}} = \psi_i^* f_i$, can therefore be approximated

$$\vartheta_i^{\mathrm{Di}}(X) \approx \sum_{|\gamma|\le N} b_{i,\gamma} X^\gamma, \quad X \in Q_i.$$

The known data for the linear problem is given as a vector

$$\mathbf{\Phi}^{\mathrm{Di}}(\lambda) := \begin{pmatrix} \widehat{\vartheta_1^{\mathrm{Di}}} \\ \vdots \\ \widehat{\vartheta_n^{\mathrm{Di}}} \end{pmatrix}(\lambda), \quad \lambda \in \mathbb{C}^2,$$

which can be approximated by

$$\mathbf{\Phi}_N^{\mathrm{Di}}(\lambda) := \begin{pmatrix} \sum_{|\gamma|\leq N} b_{1,\gamma} X^\gamma \mathbf{I}_{Q_1} \\ \vdots \\ \sum_{|\gamma|\leq N} b_{n,\gamma} X^\gamma \mathbf{I}_{Q_n} \end{pmatrix}\widehat{\ }(\lambda) = \begin{pmatrix} \sum_{|\gamma|\leq N} b_{1,\gamma} (-D)^\gamma F_{Q_1}(\lambda) \\ \vdots \\ \sum_{|\gamma|\leq N} b_{n,\gamma} (-D)^\gamma F_{Q_n}(\lambda) \end{pmatrix}, \quad \lambda \in \mathbb{C}^2$$

where we have simplified using the calculations of Section 5.2. For the purpose of generality, we may use here any approximating basis, and so we assume that the Fourier transform of such functions (in this case $(-D)^\gamma F_{Q_i}(\lambda_1, \lambda_2)$) is given as a vector

$$\mathbf{e}_{j,\gamma} := (0, \ldots, \underbrace{e_{j,\gamma}}_{j\text{-th place}}, \ldots, 0),$$

where $e_{j,\gamma}$ represents one of the basis vectors which reconstruct the Dirichlet data on the j-th polygon Q_j. In our case

$$e_{j,\gamma}(\lambda) = (-D)^\gamma F_{Q_j}(\lambda) = \mathrm{i}^{\gamma_1+\gamma_2}\, \partial_{\lambda_2}^{\gamma_2}\, \partial_{\lambda_1}^{\gamma_1}\, F_{Q_j}(\lambda).$$

Our full basis therefore are the vectors

$$\{\mathbf{e}_{j,\gamma} : j = 1, \ldots, n, |\gamma| \leq N\}.$$

Applying the operator $(-S)$ to this known data, we have

$$\begin{aligned} (-S\Phi_N^d)_k(\lambda) &= \sum_{l=1}^{n} -\mathrm{i} e^{-\mathrm{i}(\boldsymbol{m}_l - \boldsymbol{m}_k)\cdot R_k^t \boldsymbol{\lambda}} (\Delta_{kl}\boldsymbol{\lambda})_3 \left(\sum_{|\gamma|\leq N} b_{l,\gamma} (-D)^\gamma F_{Q_l}(\boldsymbol{\lambda}) \right) \\ &= \sum_{\gamma,l} \beta_{l,\gamma} (-S\mathbf{e}_{l,\gamma})_k(\lambda). \end{aligned} \tag{5.3.5}$$

Returning to our full linear problem, we must solve for the unknown coefficients $c_{i,\alpha}$ such that

$$\sum_{i=1}^{n} \sum_{|\alpha|\leq N} c_{i,\alpha} a_K(\mathbf{e}_{i,\alpha}, \mathbf{e}_{j,\beta}) = \ell(\mathbf{e}_{l,\beta}), \quad \forall\, l = 1, \ldots, n, |\beta| \leq N,$$

which, written in full using our calculations above, is

$$\begin{aligned}\sum_{i=1}^{n}\sum_{|\alpha|\leq N} c_{i,\alpha}\sum_{k=1}^{n}\int_{\mathbb{R}^2\setminus K}(T\mathbf{e}_{i,\alpha})_k(\lambda)\overline{(T\mathbf{e}_{j,\beta})_k(\lambda)}\,\mathrm{d}\lambda \\ =\sum_{l=1}^{n}\sum_{|\gamma|\leq N}\beta_{l,\gamma}\sum_{k=1}^{n}\int_{\mathbb{R}^2\setminus K}-S(\mathbf{e}_{l,\gamma})_k(\lambda)\overline{(T\mathbf{e}_{j,\beta})_k(\lambda)}\,\mathrm{d}\lambda,\end{aligned} \tag{5.3.6}$$

for all $j=1,\ldots,n$ and $|\beta|\leq N$.

5.4 Observations using the cube as a special case

We have obtained the weak formulation (5.1.2), and constructed basis functions $\{\boldsymbol{e}_l\}_{l=1}^{nM}\in X_{\mathrm{sym}}$ such that, for any valid Dirichlet data $\boldsymbol{\Theta}^{\mathrm{Di}}\in X_{\mathrm{sym}}$, we can approximate by

$$\boldsymbol{\Theta}^{\mathrm{Di}}\approx\boldsymbol{\Theta}^{\mathrm{Di}}_N=\sum_{l=1}^{nM}b_l\boldsymbol{e}_l.$$

However there is a hidden issue here, because these basis functions do not necessarily satisfy the continuity requirements across the polyhedral edges, that the functions Θ_j satisfy. Recall that for two-dimensions in Remark 4.1.1, the additional decay term in the integrand meant that we could use the Legendre polynomials as a basis, even though an individual basis function on an edge did not vanish at the vertices. In the same way the given Dirichlet data $\boldsymbol{\Theta}^{\mathrm{Di}}$ must lie in a strict subset of X_{sym}, of those functions which are continuous across the edges of the polyhedron. It is this property that permits the function $(S\boldsymbol{\Theta}^{\mathrm{Di}})_k(\lambda)$ to lie in $\in L^2(\mathbb{R}^2)$ for every $k=1,\ldots,n$. To illustrate that this is *not* true for our basis functions, let us give a brief example of this effect, and then prove that this issue *does* arise, at least for the BVP on a cube. Then we will show that this problem can be overcome by similarly introducing an additional decay term in the function $(S\boldsymbol{\Theta}^{\mathrm{Di}})_k(\lambda)$, and we shall do this in Section 5.5.

Example 5.4.1. *Consider the trivial zero function $f(x)=0$. Then it is possible to write $f(x)=g(x)-2h(x)$, where $g(x):=2$ and $h(x):=-1$, and so it is true that*

$$\int_{\mathbb{R}}f(x)\,\mathrm{d}x=\int_{\mathbb{R}}g(x)-2h(x),$$

but it does not follow that this integral can be rewritten as a sum of integrals $\int g-2\int h$, as each individual term is infinite. Although $f\in L^2(\mathbb{R})$, this is not true for the functions g,h (even though their linear combination may do).

This example shows that we have to be careful exchanging the integral of a linear combination of functions to give a sum of the integrals over each function, *unless* we know

that these individual functions are also integrable. Now let us show the danger here by proving that the cube, $S(\boldsymbol{e}_\alpha)$ does not lie in the space $L^2(\mathbb{R}^2 \setminus K)$. We will fix this issue in the following sections by using the continuity of $\boldsymbol{\Theta}$ at the vertices to form an entirely new expression for S for which $S(\boldsymbol{e}_\alpha) \in L^2(\mathbb{R}^2 \setminus K)$, and which is equivalent to S for valid Dirichlet data $\boldsymbol{\Theta}$.

Consider then the cube where each parameterised face Q_j has vertices at $(\pm 1/2, \pm 1/2)$ in each quadrant. Then we can calculate $F_Q(\lambda)$ exactly:

$$\iint_Q e^{-\mathrm{i}\lambda\cdot X}\,\mathrm{d}X = \frac{(e^{-\mathrm{i}\lambda_1/2} - e^{\mathrm{i}\lambda_1/2})(e^{-\mathrm{i}\lambda_2/2} - e^{\mathrm{i}\lambda_2/2})}{-\lambda_1\lambda_2} \tag{5.4.1}$$

$$= \frac{4\sin(\lambda_1/2)\sin(\lambda_2/2)}{\lambda_1\lambda_2} \tag{5.4.2}$$

$$= \operatorname{sinc}(\lambda_1/2)\operatorname{sinc}(\lambda_2/2), \tag{5.4.3}$$

from which it follows that if we set $\boldsymbol{\Phi}(\lambda) = (F_{Q_1}(\lambda), 0, \ldots, 0)$, we have

$$(T\boldsymbol{\Phi})_k(\lambda) = e^{-\mathrm{i}(m_1 - m_k)\cdot R_k^t\lambda} \operatorname{sinc}\left(\frac{(\Delta_{k,1}\lambda)_1}{2}\right) \operatorname{sinc}\left(\frac{(\Delta_{k,1}\lambda)_2}{2}\right).$$

The parameterisation of the first face is

$$\psi_1 : \begin{pmatrix} x \\ y \end{pmatrix} \mapsto \underbrace{\begin{pmatrix} 1 \\ 1/2 \\ 1/2 \end{pmatrix}}_{m_1} + \underbrace{\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}}_{R_1^t} \begin{pmatrix} x \\ y \\ 0 \end{pmatrix}$$

However, there is a problem here if we attempt to consider the right-hand side term $\ell(\boldsymbol{e}_{j,\beta})$: suppose we wish to calculate $\langle -S\boldsymbol{\Theta}^{\mathrm{Di}}, T\boldsymbol{e}_{j,\beta}\rangle$. As before, we approximate $\boldsymbol{\Theta}^{\mathrm{Di}} = (\Theta_1^{\mathrm{Di}}, \ldots, \Theta_n^{\mathrm{Di}})$ in our subspace as

$$\Theta_l^{\mathrm{Di}}(\lambda) \approx \sum_{|\gamma|\leq N} b_{l,\gamma} e_{l,\gamma}(\lambda), \quad l = 1, \ldots, n.$$

Then one may expect (though we shall see this is incorrect) that $\ell(\boldsymbol{e}_{j,\beta})$ is given as a term-wise sum by

$$\sum_{k,l=1}^{n} \sum_{|\gamma|\leq N} b_{l,\gamma} \iint_{\mathbb{R}^2\setminus K} -\mathrm{i}e^{-\mathrm{i}(m_l - m_k)\cdot R_k^t\lambda} (\Delta_{kl}\lambda)_3 e_{l,\gamma}(\lambda)\overline{(T\boldsymbol{e}_{j,\beta})_k(\lambda)}\,\mathrm{d}\lambda. \tag{5.4.4}$$

To show that (5.4.4) is invalid, let us consider this term for $k = l = j = 1$ and $\beta = \gamma = (0, 0)$ on the cube. Since we know $e_{l,\gamma}(\lambda) = F_{Q_1}(\lambda)$ exactly from (5.4.3), the integrand would be

$$-\mathrm{i}|\lambda| \operatorname{sinc}\left(\frac{\lambda_1}{2}\right)^2 \operatorname{sinc}\left(\frac{\lambda_2}{2}\right)^2, \tag{5.4.5}$$

as $\overline{\operatorname{sinc}(z)} = \operatorname{sinc}(\bar{z})$. However this term is *not* integrable, so there must be a mistake in the step where $\mathbf{\Phi}^{\mathrm{Di}}$ is approximated and the integral and sum are exchanged!

Notice that for our given Dirichlet boundary data (in H^1 and continuous across the faces), a solution to the Laplace equation *must* exist. Therefore the linear forms a, ℓ are bounded, provided we stay in this space. The function $\mathbf{\Theta}^{\mathrm{Di}}$ lies in our space, by construction. However, when we project to the basis vectors $\boldsymbol{e}_{j,\beta}$, these *no longer* satisfy the consistency requirement along the edges individually - only when summed.

As an analogy, think of a function which vanishes at the endpoints of a line segment. If we write this function in a generic polynomial basis, it may well be the case that individual functions take non-zero values at the boundary. The same effect is here, that the integral of the projected function may satisfy consistency requirements, but the individual basis vectors in the sum do not.

To overcome this difficulty, we must find a new representation, for $(-S\mathbf{\Theta}^{\mathrm{Di}})_k(\lambda)$ which agrees with this operator for all valid Dirichlet data $\mathbf{\Theta}^{\mathrm{Di}}$, but which is square-integrable on our basis vectors $\boldsymbol{e}_{j,\beta}$. From (5.4.5) we see that a growth of $|\lambda|$ is our issue, so we hope this may be solved by an integration-by-parts. The equality follows by showing the boundary integral is identically zero precisely because of our consistency requirement.

This may be compared with the two-dimensional problem, where in Section 3.1.3 we took an integral $\int \lambda \hat{q}_j(\lambda)\,\mathrm{d}\lambda$ and rewrote with $\int \hat{q}_j'(\lambda)\,\mathrm{d}\lambda$. Since we worked always with the *derivative* of the Dirichlet data, the integrals were bounded. For two-dimensions this was derived in [Fok01] for the Laplace problem directly, beginning by writing Laplace's equation in complex coordinates. In three-dimensions, it may be that a different application of Green's theorem in (5.0.3) would give the analogous form similarly for the Laplace problem. We have found it easier to work directly from the current representation, and this also has the advantage that we can do a similar integration-by-parts for the Helmholtz equation in the following Chapter.

5.5 Constructing a new weak formulation

In this section we shall derive an integral identity which gives additional decay. We obtain an identity involving our operator S, but such that the integral of individual basis terms is finite. For clarity, we'll do this in a coordinate-independent form, so that the resulting integrals are over the polyhedron Ω itself and the faces Σ_j. One advantage of this approach is that we may work with the boundaries of Σ_j directly, as being a member of two faces, whereas considering the corresponding planar faces Q_j would make such identifications more difficult to observe. In particular, we shall obtain integrals of the form $\int_\Gamma \mathbf{F} \cdot \hat{\mathbf{t}}\,\mathrm{d}s$

along an edge $\Gamma \in \Sigma_i \cap \Sigma_j$, from which we can deduce that the contributions from Σ_i and Σ_j cancel out. The purpose of this integration-by-parts is to establish a completely new representation for S - which is equal for valid Dirichlet functions $\boldsymbol{\Theta}^{\mathrm{Di}}$ that satisfy the compatibility requirements, but that has an extension as an operator to the whole space X_{sym}. Importantly this space includes our basis functions $\boldsymbol{e}_{j,\beta}(\lambda)$, giving numerical stability. In doing so, we will obtain a completely new weak formulation for the global relation.

Theorem 5.5.1. *The operator S can be re-written as a new operator given in (5.5.6), which we call S_X. This new operator has the property that*

$$S\boldsymbol{\Theta}^{\mathrm{Di}} = S_X\boldsymbol{\Theta}^{\mathrm{Di}},$$

for all valid Dirichlet data given in the space X_{sym}, and satisfying compatibility across the edges. Furthermore $S_X\boldsymbol{\Phi} \in Y_K := L^2(\mathbb{R}^2 \setminus K)^{\times n}$, for any $\boldsymbol{\Phi} \in X_{\mathrm{sym}}$, and in particular

$$-(S_X\boldsymbol{e}_{j,\beta})_k(\lambda) \in L^2(\mathbb{R} \setminus K), \tag{5.5.1}$$

for any $j,k = 1,\dots,n$, any multi-index β, and any compact set $K \subset \mathbb{R}^2$.

Remark 5.5.2. *The boundedness statement (5.5.1) gives a completely new representation for the global relation, and one which may be tested on basis functions which individually do not lie in X. Thus the problem observed earlier is solved: Given $\boldsymbol{\Phi}_N = \sum_{l=1}^{nM}\sum_\gamma c_l\boldsymbol{e}_l(\lambda)$,*

$$S\left(\sum_{l=1}^{nM} c_l\boldsymbol{e}_l\right) = S_X\left(\sum_{l=1}^{nM} c_l\boldsymbol{e}_l\right) = \sum_{l=1}^{nM} c_l S_X\boldsymbol{e}_l,$$

and the individual terms, $(S_X\boldsymbol{e}_l)(\lambda) \in Y$, may be integrated alongside $(T\boldsymbol{e}_j)(\lambda)$.

To prove this important result, let us consider the vector identity for vector fields $\mathbf{A} = \mathbf{A}(\mathbf{x})$ and $\mathbf{B} = \mathbf{B}(\mathbf{x})$:

$$\nabla \times (\mathbf{A} \times \mathbf{B}) = \mathbf{A}(\nabla \cdot \mathbf{B}) - (\mathbf{A} \cdot \nabla)\mathbf{B} - \mathbf{B}(\nabla \cdot \mathbf{A}) + (\mathbf{B} \cdot \nabla)\mathbf{A}.$$

Consider a fixed face Σ with outward normal $\mathbf{n}$. Let $\mathbf{A} := \mathbf{n}_k$ for some fixed $k \in \{1,\dots,n\}$ and $\mathbf{B} := \left(f(\mathbf{x})e^{-\mathrm{i}\boldsymbol{\lambda}\cdot\mathbf{x}}\right)\boldsymbol{\lambda}$. Then we find that

$$\begin{aligned}\nabla \cdot \mathbf{B} &= \boldsymbol{\lambda} \cdot \nabla\left(f(\mathbf{x})e^{-\mathrm{i}\boldsymbol{\lambda}\cdot\mathbf{x}}\right) \\ &= \boldsymbol{\lambda} \cdot (\nabla f(\mathbf{x}))e^{-\mathrm{i}\boldsymbol{\lambda}\cdot\mathbf{x}} - \mathrm{i}(\boldsymbol{\lambda}\cdot\boldsymbol{\lambda})f(\mathbf{x})e^{-\mathrm{i}\boldsymbol{\lambda}\cdot\mathbf{x}}\end{aligned} \tag{5.5.2}$$

and

$$(\mathbf{n}_k \cdot \nabla)\mathbf{B} = \boldsymbol{\lambda}\left[\mathbf{n}_k \cdot (\nabla f(\mathbf{x}))\, e^{-\mathrm{i}\boldsymbol{\lambda}\cdot\mathbf{x}} - \mathrm{i}(\mathbf{n}_k \cdot \boldsymbol{\lambda})\left(f(\mathbf{x})e^{-\mathrm{i}\boldsymbol{\lambda}\cdot\mathbf{x}}\right)\right].$$

Then, noting that $\mathbf{n}_k$ is a constant vector; for any $\boldsymbol{\lambda}$ with $|\boldsymbol{\lambda}|^2 = 0$ we find the identity

$$\begin{aligned}\nabla\times\left[\mathbf{n}_k\times\left(\boldsymbol{\lambda}f(\mathbf{x})e^{-\mathrm{i}\boldsymbol{\lambda}\cdot\mathbf{x}}\right)\right]\cdot\mathbf{n} &= (\mathbf{n}_k\cdot\mathbf{n})\nabla\cdot\mathbf{B}-\mathbf{n}\cdot(\mathbf{n}_k\cdot\nabla)\mathbf{B}\\ &= (\mathbf{n}_k\cdot\mathbf{n})\boldsymbol{\lambda}\cdot(\nabla f(\mathbf{x}))e^{-\mathrm{i}\boldsymbol{\lambda}\cdot\mathbf{x}}-(\boldsymbol{\lambda}\cdot\mathbf{n})\,\mathbf{n}_k\cdot(\nabla f(\mathbf{x}))\,e^{-\mathrm{i}\boldsymbol{\lambda}\cdot\mathbf{x}}+\mathrm{i}\,(\boldsymbol{\lambda}\cdot\mathbf{n})\,(\boldsymbol{\lambda}\cdot\mathbf{n}_k)\,f(\mathbf{x})e^{-\mathrm{i}\boldsymbol{\lambda}\cdot\mathbf{x}}\\ &= \Big((\mathbf{n}_k\cdot\mathbf{n})\boldsymbol{\lambda}-(\boldsymbol{\lambda}\cdot\mathbf{n})\mathbf{n}_k\Big)\cdot\nabla f(\mathbf{x})e^{-\mathrm{i}\boldsymbol{\lambda}\cdot\mathbf{n}}+\mathrm{i}\,(\boldsymbol{\lambda}\cdot\mathbf{n})\,(\boldsymbol{\lambda}\cdot\mathbf{n}_k)\,f(\mathbf{x})e^{-\mathrm{i}\boldsymbol{\lambda}\cdot\mathbf{x}}.\end{aligned}$$

From this, we obtain the integral identity

$$\begin{aligned}\int_\Sigma \mathrm{i}\,(\boldsymbol{\lambda}\cdot\mathbf{n})\,f(\mathbf{x})e^{-\mathrm{i}\boldsymbol{\lambda}\cdot\mathbf{x}}\,\mathrm{d}\sigma(\mathbf{x}) &= \frac{1}{\boldsymbol{\lambda}\cdot\mathbf{n}_k}\int_{\partial\Sigma}\left[\mathbf{n}_k\times\left(\boldsymbol{\lambda}f(\mathbf{x})e^{-\mathrm{i}\boldsymbol{\lambda}\cdot\mathbf{x}}\right)\right]\cdot\hat{\mathbf{t}}\,\mathrm{d}s\\ &\quad-\frac{1}{\boldsymbol{\lambda}\cdot\mathbf{n}_k}\int_\Sigma\Big((\mathbf{n}_k\cdot\mathbf{n})\boldsymbol{\lambda}-(\boldsymbol{\lambda}\cdot\mathbf{n})\mathbf{n}_k\Big)\cdot\nabla f(\mathbf{x})e^{-\mathrm{i}\boldsymbol{\lambda}\cdot\mathbf{n}}\,\mathrm{d}\sigma(\mathbf{x}),\end{aligned}\tag{5.5.3}$$

Where we have used Stokes' Theorem that for a vector field $\mathbf{C}(\mathbf{x})$,

$$\int_\Sigma(\nabla\times\mathbf{C})\cdot\mathbf{n}\,\mathrm{d}\sigma(\mathbf{x}) = \int_{\partial Q}\mathbf{C}\cdot\hat{\mathbf{t}}\,\mathrm{d}s.$$

Initially it appears from (5.5.3) that we need to know the derivative, ∇f, of f at each point on the plane. This is not in general possible since f is prescribed *only* on Σ, so its normal derivative is unknown. However, on closer inspection, we see that the term

$$\Big((\mathbf{n}_k\cdot\mathbf{n})\boldsymbol{\lambda}-(\boldsymbol{\lambda}\cdot\mathbf{n})\mathbf{n}_k\Big)\cdot\nabla f(\mathbf{x})$$

is actually the directional derivative of f in the direction $\tilde{\boldsymbol{\lambda}} = (\mathbf{n}_k\cdot\mathbf{n})\boldsymbol{\lambda}-(\boldsymbol{\lambda}\cdot\mathbf{n})\mathbf{n}_k$. It is readily checked that $\tilde{\boldsymbol{\lambda}}$ lies parallel to Σ; indeed $\tilde{\boldsymbol{\lambda}}\cdot\mathbf{n} = (\mathbf{n}_k\cdot\mathbf{n})(\boldsymbol{\lambda}\cdot\mathbf{n})-(\boldsymbol{\lambda}\cdot\mathbf{n})(\mathbf{n}_k\cdot\mathbf{n}) = 0$. Thus, only the values $f|_\Sigma$ are required.

Considering the first boundary term in (5.5.3), let us sum over every face $(\Sigma_j)_{j=1}^n$:

$$\sum_{j=1}^n\int_{\partial\Sigma_j}f(\mathbf{x})e^{-\mathrm{i}\boldsymbol{\lambda}\cdot\mathbf{x}}\,[\mathbf{n}_k\times\boldsymbol{\lambda}]\cdot\hat{\mathbf{t}}\,\mathrm{d}s.\tag{5.5.4}$$

This term involves integrals of f over each edge of the polygon. Specifically, a fixed edge Γ is in the boundary of precisely two faces Σ_i and Σ_j. Assuming that f is continuous across the edges: for $\mathbf{x}_0\in\Sigma_i\cap\Sigma_j$,

$$\lim_{\substack{\mathbf{x}\to\mathbf{x}_0\\ \mathbf{x}\in\Sigma_i}}f(\mathbf{x}) = \lim_{\substack{\mathbf{x}\to\mathbf{x}_0\\ \mathbf{x}\in\Sigma_j}}f(\mathbf{x}).$$

Suppose that $\Gamma\in\Sigma_i\cap\Sigma_j$ is positively oriented with respect to Σ_i. Then it is necessarily negatively oriented with respect to Σ_j (since the faces lie on opposite sides of Γ), so the

contribution to (5.5.4) from the edge Γ is

$$\int_\Gamma f(\mathbf{x}) e^{-\mathrm{i}\boldsymbol{\lambda}\cdot\mathbf{x}} \left[\mathbf{n}_k \times \boldsymbol{\lambda}\right] \cdot \left(\hat{\mathbf{t}} - \hat{\mathbf{t}}\right) \mathrm{d}s = 0.$$

Considering first the left-hand side of (5.5.3), we apply the parameterisation

$$\psi_j : (X_1, X_2, 0)^t \mapsto \mathbf{m}_j + R_j^t (X_1, X_2, 0)^t.$$

Since the transformation R_j is orthogonal, the map ψ_j preserves area, and so this integral is equal to

$$e^{-\mathrm{i}\boldsymbol{\lambda}\cdot\mathbf{m}_j} \int_{Q_j} -\mathrm{i}(\boldsymbol{\lambda}\cdot\mathbf{n}_j) e^{-\mathrm{i}R_j\boldsymbol{\lambda}\cdot(X,0)^t} q_j^d(X)\,\mathrm{d}X.$$

By replacing $\boldsymbol{\lambda} \mapsto R_k^t\boldsymbol{\lambda}$, and noting that $\boldsymbol{\lambda}\cdot\mathbf{n}_j = \boldsymbol{\lambda}\cdot R_j^t(0,0,1)^t = (R_j\boldsymbol{\lambda})_3$, we obtain

$$e^{-\mathrm{i}R_k^t\boldsymbol{\lambda}\cdot\mathbf{m}_j} \int_{Q_j} -\mathrm{i}(\Delta_{kj}\boldsymbol{\lambda})_3 e^{-\mathrm{i}(\Delta_{kj}\boldsymbol{\lambda})\cdot(X,0)^t} q_j^d(X)\,\mathrm{d}X.$$

Multiplying this by $e^{\mathrm{i}R_k^t\mathbf{m}_k}$ gives

$$-\mathrm{i}(\Delta_{kj}\boldsymbol{\lambda})_3 e^{-\mathrm{i}(\mathbf{m}_j-\mathbf{m}_k)\cdot R_k^t\boldsymbol{\lambda}} \int_{Q_j} e^{-\mathrm{i}(\Delta_{kj}\boldsymbol{\lambda})\cdot(X,0)^t} q_j^d(X)\,\mathrm{d}X,$$

which is precisely the j-th term in the sum for $-(S\boldsymbol{\Theta}^{\mathrm{Di}})_k(\boldsymbol{\lambda})$.

It remains then to evaluate the right-hand side terms in (5.5.3). Taking the first term, we consider the pullback of

$$\Big((\mathbf{n}_k\cdot\mathbf{n})\boldsymbol{\lambda} - (\boldsymbol{\lambda}\cdot\mathbf{n})\mathbf{n}_k\Big)\cdot\nabla f(\mathbf{x})$$

Letting $\vartheta_j^d(X) = (\psi_j^* f)(X) = f(\psi_j(X))$, we see that the directional derivative $D_{\mathbf{z}} f(\mathbf{x})$ in a direction $\mathbf{z}$, is equal to $D_{\mathbf{w}} q_j(X)$ for $\mathbf{w} = R_j\mathbf{z}$ and $X = \psi_j^{-1}(\mathbf{x})$. So

$$\begin{aligned}
\boldsymbol{w} = (X_1, X_2, 0)^t &= R_j\Big((\mathbf{n}_k\cdot\mathbf{n}_j)\boldsymbol{\lambda} - (\boldsymbol{\lambda}\cdot\mathbf{n}_j)\mathbf{n}_k\Big) \\
&= R_j\Big((\mathbf{n}_k\cdot\mathbf{n}_j)\boldsymbol{\lambda} - (R_j\boldsymbol{\lambda}\cdot R_j\mathbf{n}_j)\mathbf{n}_k\Big) \\
&= (\mathbf{n}_k\cdot\mathbf{n}_j)R_j\boldsymbol{\lambda} - (R_j\boldsymbol{\lambda}\cdot R_j\mathbf{n}_j)R_j\mathbf{n}_k \\
&= (\mathbf{n}_k\cdot\mathbf{n}_j)R_j\boldsymbol{\lambda} - (R_j\boldsymbol{\lambda})_3 R_j\mathbf{n}_k.
\end{aligned} \tag{5.5.5}$$

Making the substitution again that $\boldsymbol{\lambda} \mapsto R_k^t\boldsymbol{\lambda}$, the derivative of q_j is taken in the direction

$$\boldsymbol{\mu}^{(j)}(\boldsymbol{\lambda}) := (\mathbf{n}_k\cdot\mathbf{n}_j)\,(\Delta_{kj}\boldsymbol{\lambda}) - (\Delta_{kj}\boldsymbol{\lambda})_3 R_j\mathbf{n}_k.$$

In the case that $j = k$, we may observe that $\boldsymbol{\mu}^{(j)}(\boldsymbol{\lambda}) = (\lambda_1, \lambda_2, 0)$. By our discussion above, the third component of $\boldsymbol{\mu}^{(j)}(\boldsymbol{\lambda})$ is always zero. The term involving derivatives of q_j is

$$\boldsymbol{\mu}_1^{(j)}(\boldsymbol{\lambda})\frac{\partial \vartheta_j^d}{\partial X_1}(X) + \boldsymbol{\mu}_2^{(j)}(\boldsymbol{\lambda})\frac{\partial \vartheta_j^d}{\partial X_2}(X).$$

Using the same parameterisation, our term may be represented as an integral over Q_j by

$$\frac{1}{R_k^t \boldsymbol{\lambda}\cdot\mathbf{n}_k} e^{-\mathrm{i}R_k\boldsymbol{\lambda}\cdot\mathbf{m}_j}\int_{Q_j} e^{-\mathrm{i}\Delta_{kj}\boldsymbol{\lambda}\cdot X}\left[\boldsymbol{\mu}_1^{(j)}(\boldsymbol{\lambda})\frac{\partial \vartheta_j^d}{\partial X_1}(X) + \boldsymbol{\mu}_2^{(j)}(\boldsymbol{\lambda})\frac{\partial \vartheta_j^d}{\partial X_2}(X)\right]\mathrm{d}X.$$

Thus, we have the following identity for the term $-(S\boldsymbol{\Theta}^{\mathrm{Di}})_k(\lambda)$ that appears in the global relation:

$$\begin{aligned}-(S\boldsymbol{\Theta}^{\mathrm{Di}})_k(\lambda) :&= \sum_{j=1}^{n} -\mathrm{i}(\Delta_{kj}\boldsymbol{\lambda})_3 e^{-\mathrm{i}(\mathbf{m}_j-\mathbf{m}_k)\cdot R_k^t\boldsymbol{\lambda}}\int_{Q_j} e^{-\mathrm{i}(\Delta_{kj}\boldsymbol{\lambda})\cdot X}\vartheta_j^d(X)\,\mathrm{d}X\\ &= \sum_{j=1}^{n}\frac{1}{\mathrm{i}|\lambda|}e^{-\mathrm{i}(\mathbf{m}_j-\mathbf{m}_k)\cdot R_k^t\boldsymbol{\lambda}}\int_{Q_j} e^{-\mathrm{i}\Delta_{kj}\boldsymbol{\lambda}\cdot X}\left[\boldsymbol{\mu}_1^{(j)}(\boldsymbol{\lambda})\frac{\partial \vartheta_j^d}{\partial X_1}(X) + \boldsymbol{\mu}_2^{(j)}(\boldsymbol{\lambda})\frac{\partial \vartheta_j^d}{\partial X_2}(X)\right]\mathrm{d}X.\end{aligned} \tag{5.5.6}$$

5.6 A new Galerkin method

In the previous section, we showed how the operator S may be rewritten in a new way with the property that these functions are defined and equivalent for valid Dirichlet data functions; however the latter is also defined for all functions in X_{sym}. In particular, the latter is defined on our basis functions. In view of (5.5.6), we may construct this new Galerkin method. Let us begin with setting notation to simplify our later expressions. Let $(\mathbf{e}_j)_{j=1}^n$ denote the standard basis for $\mathbb{R}^n$, and, for a multi-index $\alpha = (\alpha_1, \alpha_2) \in \mathbb{N}^2$, let

$$e_{i,\alpha}(\lambda) := \int_{Q_i} e^{-\mathrm{i}\lambda\cdot X} X^\alpha\,\mathrm{d}X,$$

be the Fourier transform of a polynomial over the polygon Q_i. Roman letters i, j, k, l will always be integers and when they appear in a summation, will be from 1 to n. Finally, we use Greek letters α, β, γ to be multi-indices and summed over a modulus at most N.

The Galerkin problem is to find $\boldsymbol{\Phi}^{\mathrm{Ne}} \in X_{\mathrm{sym}}$ such that

$$a_K(\boldsymbol{\Phi}^{\mathrm{Ne}}, \boldsymbol{\Phi}') = \ell(\boldsymbol{\Phi}'), \quad \forall \boldsymbol{\Phi}' \in X_{\mathrm{sym}}. \tag{5.6.1}$$

As we have seen above, this problem is well-posed and can be approximated by solving on

subspaces [Ash14b]. Define a subspace $X_N \subset X_{\text{sym}}$ to be the one spanned by the vectors

$$\boldsymbol{e}_{i,\alpha}(\lambda) := e_{i,\alpha}(\lambda)\boldsymbol{e}_i, \quad 1 \leq i \leq n, |\alpha| \leq N.$$

Then we wish to find $\boldsymbol{\Phi}_N^{\text{Ne}} \approx \boldsymbol{\Phi}^{\text{Ne}}$ which is given as a linear combination

$$\boldsymbol{\Phi}_N^{\text{Ne}}(\lambda) = \sum_{l,\gamma} c_{l,\gamma}\boldsymbol{e}_{l,\gamma}(\lambda).$$

We recall that

$$\begin{aligned} a_K(\boldsymbol{e}_{i,\alpha}, \boldsymbol{e}_{j,\beta}) &= \sum_k \int_{\mathbb{R}^2\setminus K} (T\boldsymbol{e}_{i,\alpha})_k(\lambda)\overline{(T\boldsymbol{e}_{j,\beta})_k(\lambda)}\,\mathrm{d}\lambda \\ &= \sum_k \int_{\mathbb{R}^2\setminus K} e^{-\mathrm{i}(\mathbf{m}_j-\mathbf{m}_k)\cdot R_k^t\boldsymbol{\lambda}} e_{i,\alpha}((\Delta_{ki}\lambda)_1, (\Delta_{ki}\lambda)_2) \\ &\qquad \times e^{\mathrm{i}(\mathbf{m}_i-\mathbf{m}_k)\cdot R_k^t\bar{\boldsymbol{\lambda}}}\overline{e_{j,\beta}((\Delta_{kj}\lambda)_1, (\Delta_{kj}\lambda)_2)}\,\mathrm{d}\lambda \end{aligned} \tag{5.6.2}$$

where we shall denote the integral term by $A^{(k)}_{i,\alpha,j,\beta}$. Similarly, if our Dirichlet data projected to the subspace X_N is given by the vector function

$$\boldsymbol{\Theta}_N^{\text{Di}} = (\Theta_{N,1}^{\text{Di}}, \ldots, \Theta_{N,n}^{\text{Di}}),$$

then since each $\vartheta_i^d(\lambda) \in H^1(Q_i)$, the derivatives can also be approximated in X_N: for $a \in \{1,2\}$, suppose the projection is

$$\frac{\partial \vartheta_l^d}{\partial X_a}(\lambda) \approx \sum_\gamma c_{X_a,l,\gamma}e_{l,\gamma}(\lambda),$$

where $c_{X_a,l,\gamma}$ are the projection coefficients for the basis functions $e_{l,\gamma}(\lambda)$. Using (5.5.6), we have

$$\begin{aligned} \ell(\boldsymbol{e}_{j,\beta}) &= \sum_k \int_{\mathbb{R}^2\setminus K} \left(-S\boldsymbol{\Phi}^{\text{Di}}\right)_k(\lambda)\overline{(T\boldsymbol{e}_{j,\beta})_k(\lambda)}\,\mathrm{d}\lambda \\ &= \sum_{k,l,\gamma} \int_{\mathbb{R}^2\setminus K} \frac{1}{\mathrm{i}|\lambda|} e^{-\mathrm{i}(\mathbf{m}_j-\mathbf{m}_k)\cdot R_k^t\boldsymbol{\lambda}} \left[c_{X_1,l,\gamma}\boldsymbol{\mu}_1^{(l)}(\lambda) + c_{X_2,l,\gamma}\boldsymbol{\mu}_2^{(l)}(\lambda)\right] e_{l,\gamma}((\Delta_{kl}\lambda)_1, (\Delta_{kl}\lambda)_2) \\ &\qquad \times e^{\mathrm{i}(\mathbf{m}_i-\mathbf{m}_k)\cdot R_k^t\bar{\boldsymbol{\lambda}}}\overline{e_{j,\beta}((\Delta_{kj}\lambda)_1, (\Delta_{kj}\lambda)_2)}\,\mathrm{d}\lambda, \end{aligned} \tag{5.6.3}$$

where we denote this integral term by $L^{(k)}_{l,\gamma,j,\beta}$. We highlight again that the final integrals (5.6.3) exist because the derivatives of ϑ_l^d are in $L^2(Q_l)$, and because $1/|\lambda|$ is uniformly bounded on $\mathbb{R}^2 \setminus K$. In summary, the finite-dimensional Galerkin problem is: find the

coefficients $(c_{i,\alpha})_{i,\alpha}$ such that

$$\sum_{i,\alpha} c_{i,\alpha} \left(\sum_{k} A^{(k)}_{i,\alpha,j,\beta} \right) = \sum_{k,l,\gamma} L^{(k)}_{l,\gamma,j,\beta}, \quad \forall\, 1 \leq j \leq n,\ |\beta| \leq N. \tag{5.6.4}$$

We emphasise here, that the projection coefficients $\{c_{l,\gamma}, c_{X_1,l,\gamma}, c_{X_2,l,\gamma}\}_{l,\gamma}$ are obtained via an orthogonalisation in Section 5.3.1 using Gram–Schmidt. In general this method is unstable due to a propagation of error at each stage. However in view of (5.3.4) and following, the required inner products can be given precisely at each stage, i.e. there is *no numerical integration* required in the Gram–Schmidt process itself. Thus the projection coefficients may be obtained to arbitrary precision. The integrals required for the coefficients in (5.6.4) do require integration, which are obtained numerically in MATLAB. We have noticed a significant increase in difficulty for MATLAB to compute these integrals, when compared with the 2D elliptic problems. Although MATLAB's `quad2d` and `integral2` routines have seemed optimal for our purposes, we provide in the following section a brief summary of a statistical integration technique which proves powerful, particularly as the number of dimensions increases. If these methods were to be extended to higher dimensions, a statistical integrator may be especially useful.

5.7 Monte–Carlo Integration

We have discussed above some of the numerical difficulties involved in finding the terms $a(\boldsymbol{e}_{i,\alpha}, \boldsymbol{e}_{j,\beta})$; and particularly $\ell(\boldsymbol{e}_{j,\beta})$ requiring an integration by parts. Even with these considerations, we have found numerical integration to be difficult in MATLAB. It is possible this is primarily due to the removable singularities of $F_Q(\lambda)$ in (3.0.4). These singularities occur along a line in $\mathbb{R}^2$ and so (unlike the two-dimensional Laplacian) must be integrated throughout the entire approximation to $\mathbb{R}^2 \setminus K$.

For a generic integration of dimension d, employing an integration using trapezoidal rule has an error bound $O(N^{-2/d})$ using N points. In general, convergence of integrations with such methods become slower as the dimension d is increased. However with Monte–Carlo integration, the average error scales as $O(1/\sqrt{N})$ [Pre92, p.295]. This is slower but, crucially, does not deteriorate as d is increased. Therefore such integration can be particularly useful in statistical physics. We provide a brief description of the Metropolis–Hastings Monte–Carlo integration here, and direct the reader to [Hal70] for a survey of Monte–Carlo integration.

Consider a $d-$dimensional domain Ω and functions $g(x) = f(x)p(x) : \Omega \to \mathbb{R}$. For the Metropolis–Hastings algorithm, p must be normalised so that it is a probability distribution, so we require that $V := \int_\Omega p(x)\,\mathrm{d}x < \infty$. To agree with this, we could consider $V = (\mathbb{R}^2 \setminus K) \cap B_R$ for a ball B_R, and calculate error bounds separately. We wish to

calculate numerically the integral

$$I := \int_\Omega g(x)\,\mathrm{d}x = \int_\Omega f(x)p(x)\,\mathrm{d}x.$$

The general Monte–Carlo integration states that we may choose $x_1, \ldots, x_N \in \Omega$ uniformly at random (this approach supposes the volume of Ω; $\mathrm{Vol}(\Omega) < \infty$). The approximation to I is the finite sum

$$I_N := \frac{\mathrm{Vol}(\Omega)}{N} \sum_{i=1}^{N} g(x_i).$$

The average error in I_N is defined to be the square route of the variance of I_N: letting the sample variance of g be $\sigma_N^2 := \frac{1}{N-1}\sum_{i=1}^{N}(g(x_I) - I_N)^2$, this gives

$$\sqrt{\mathrm{Var}(I_N)} = \sqrt{\frac{\mathrm{Vol}(\Omega)^2}{N}\mathrm{Var(g)}} = \frac{\mathrm{Vol}(\Omega)\sigma_N}{\sqrt{N}}$$

which tends to zero provided $(\sigma_N)_{N\geq 1}$ is a bounded sequence.

Although this method is valid as an integration estimator, a number of improvements are possible to such a naive choice of points $x_1, \ldots, x_N$. One of the more well-known modifications is the Metropolis–Hastings algorithm, which falls in to a class of 'importance sampling' methods. The idea is that instead of picking $(x_i)_{i=0}^N$ uniformly in Ω, we may sample using a distribution which reflects the function we are integrating. Intuitively, we are more likely to choose points which give a greater contribution to the integral. In doing so, we expect to converge to the true value more efficiently[3]. The algorithm is as follows:

1. Pick an arbitrary $x_1 \in \Omega$, and a probability density $Q(x|y)$ which is symmetric: $Q(x|y) = Q(y|x)$. For example, take the vector analogue of the normal distribution $\frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{|x-y|^2}{2\sigma^2}}$.
2. Given k and x_k, propose a new point $y = Q(x|x_k)$.
3. With probability $P = p(y)/p(x_k)$ we set $x_{k+1} = y$ (or if $P > 1$); else we set $x_{k+1} = x_k$.
4. Repeat steps 2 and 3 until $x_1, \ldots, x_N$ have been generated inductively.
5. The approximation to I is

$$I_N := \frac{1}{N}\sum_{i=1}^{N} \frac{g(x_i)}{p(x_i)/V} = \frac{V}{N}\sum_{i=1}^{N} f(x_i).$$

Let us now apply this algorithm to our integral $a(e_{i,\alpha}, e_{j,\beta})$. Fixing i, α and j, β, the

[3] imagine a table with many coins of various values. By preferentially counting the large coins first we expect, in a given time, to be closer to the true value.

k-th term in $\langle Te_{i,\alpha}, Te_{j,\beta}\rangle$ is

$$\iint_{\mathbb{R}^2\setminus K} e^{-\mathrm{i}(\mathbf{m}_i-\mathbf{m}_k)\cdot R_k^t\boldsymbol{\lambda}}\overline{e^{-\mathrm{i}(\mathbf{m}_j-\mathbf{m}_k)\cdot R_k^t\boldsymbol{\lambda}}}\left(\iint_{Q_i} e^{-\mathrm{i}\Delta_{ki}\boldsymbol{\lambda}\cdot X}X^\alpha\,\mathrm{d}X\right)\dots \\ \dots\overline{\left(\iint_{Q_j} e^{-\mathrm{i}\Delta_{kj}\boldsymbol{\lambda}\cdot Y}Y^\beta\,\mathrm{d}Y\right)}\,\mathrm{d}\lambda_1\,\mathrm{d}\lambda_2 \tag{5.7.1}$$

Since $\boldsymbol{\lambda} = (\lambda, \mathrm{i}|\lambda|)$, the real part of the exponents can be separated: for real-valued functions $r(X,Y), s(X,Y,\lambda_1,\lambda_2)$ we have

$$\int_{(\mathbb{R}^2\setminus K)\times Q_i\times Q_j} e^{-r(X,Y)|\lambda|}e^{-\mathrm{i}s(X,Y,\lambda)}X^\alpha Y^\beta\,\mathrm{d}\lambda\,\mathrm{d}X\,\mathrm{d}Y.$$

The imaginary part of $\Delta_{ki}\lambda$ is

$$\Delta_{ki}(0,0,|\lambda|)^t = R_iR_k^t(0,0,|\lambda|)^t = |\lambda|R_i\mathbf{n}_k,$$

so $\Im\left(\Delta_{ki}\lambda\cdot(X_1,X_2,0)^t\right) = |\lambda|R_j^t(X_1,X_2,0)^t\cdot\mathbf{n}_k$. Then $r:\mathbb{R}^4\to\mathbb{R}$ and $s:\mathbb{R}^6\to\mathbb{R}$ are given by

$$\begin{aligned} -r(X_1,X_2,Y_1,Y_2) &:= \left[(\mathbf{m}_i+\mathbf{m}_j-2\mathbf{m}_k)+R_i^t(X_1,X_2,0)^t+R_j^t(Y_1,Y_2,0)^t\right]\cdot\mathbf{n}_k \\ s(X_1,X_2,Y_1,Y_2,\lambda_1,\lambda_2) &:= \left[\mathbf{m}_i-\mathbf{m}_j+R_i^t(X_1,X_2,0)^t-R_j^t(Y_1,Y_2,0)\right]\cdot R_k^t(\lambda_1,\lambda_2,0)^t. \end{aligned}$$

Observing also that for any vector $\mathbf{x} = (a,b,0)\in\mathbb{R}^3$ the point $\mathbf{m}_i + R_i^t\mathbf{x}\in\Sigma_i$, means that we can view the terms in square brackets as the difference between various points in Σ_i and Σ_j.

Lemma 5.7.1. *The function $r(X,Y)\geq 0$ with equality only in the following cases*

1. *$i=k$ and*
   - *$j=k$, or*
   - *Σ_j shares an edge with Σ_k and $(Y,0)$ lies on the pullback of this edge: $\mathbf{m}_j+R_j^t(Y,0)^t\in\Sigma_j\cap\Sigma_k$.*
2. *$j=k$ and Σ_i shares an edge with Σ_k and $(X,0)$ lies on the pullback of this edge: $\mathbf{m}_i+R_i^t(X,0)^t\in\Sigma_i\cap\Sigma_k$.*

Proof. The point $\mathbf{m}_i+R_i^t(X,0)^t\in\Sigma_i$. It is clear that for $i=k$, this point is perpendicular to the normal, $\mathbf{n}_k$, of Σ_k. For $i\neq k$ and by convexity $\left(\mathbf{m}_i+R_i^t(X,0)^t\in\Sigma_i\right)\cdot\mathbf{n}_k\leq 0$ with equality if and only if $\mathbf{m}_i+R_i^t(X,0)^t\in\Sigma_i\cap\Sigma_k$. The same argument holds for j. □

With these exceptions then, we may set our probability distribution $p(X,Y,\lambda) :=$

$e^{-r(X,Y)|\lambda|}$ and our function $f(X,Y,\lambda) := e^{-\mathrm{i}s(X,Y,\lambda)}X^\alpha Y^\beta$, and

$$V = \int_{(\mathbb{R}^2\setminus K)\times Q_i\times Q_j} e^{-|\lambda|\left[2\mathbf{m}_k-\left(\mathbf{m}_i+R_i^t(X_1,X_2,0)^t\right)-\left(\mathbf{m}_j+R_j^t(Y_1,Y_2,0)^t\right)\right]\cdot\mathbf{n}_k}\,\mathrm{d}\lambda\,\mathrm{d}X\,\mathrm{d}Y.$$

CHAPTER 6

Extension to the Helmholtz problem

In this section, we extend the theory introduced in the previous section for the Laplace equation to the Helmholtz equation ($\epsilon < 0$):

$$-\Delta q + \epsilon q = 0, \quad \text{in } \Omega \tag{6.0.1}$$

$$q = f_i, \quad \text{on } \Sigma_i,\ i = 1, \dots, n. \tag{6.0.2}$$

For $\epsilon > 0$, this is the modified-Helmholtz equation. As shown in [Ash14a], any constant coefficient elliptic differential operator may be written as the Helmholtz or modified-Helmholtz equation after a change of coordinates. Specifically, the general form of such a PDE is

$$P(D) = \sum_{i,j=1}^{3} A_{ij} D_i D_j + \sum_{i=1}^{3} B_i D_i + C,$$

where $D = (-\mathrm{i}\partial_1, -\mathrm{i}\partial_2, -\mathrm{i}\partial_3)^t$ and A_{ij} is symmetric and positive definite. Suppose u solves the BVP

$$\begin{aligned} P(D)u &= 0, \quad \Omega \\ u &= f_i, \quad \text{on } \Sigma_i,\ i = 1, \dots, n \end{aligned} \tag{6.0.3}$$

in a polyhedron Ω with faces Σ_i. Suppose also that $f_i \in H^1(\Sigma_i)$ and continuous across the boundaries: $f_i = f_j$ on $\overline{\Sigma_i} \cap \overline{\Sigma_j}$. Then after a change of coordinates, solving this general PDE is equivalent to solving for

$$P(D) = -\Delta + \epsilon,$$

which is precisely the Helmholtz or modified-Helmholtz equation (6.0.1).

Let $\lambda \in \mathbb{C}^2$, and $\boldsymbol{\lambda} = (\lambda, \lambda_3) \in \mathbb{C}^3$ be such that

$$\boldsymbol{\lambda} \cdot \boldsymbol{\lambda} + \epsilon = 0, \tag{6.0.4}$$

then the function $v_{\boldsymbol{\lambda}}(\mathbf{x}) := e^{-\mathrm{i}\boldsymbol{\lambda}\cdot\boldsymbol{x}}$ solves (6.0.1). By the divergence Theorem

$$\begin{aligned} 0 &= \int_{\Omega} \left[uP(D)v_{\boldsymbol{\lambda}} - v_{\boldsymbol{\lambda}}P(D)u\right] \mathrm{d}\sigma(\boldsymbol{x}) \\ &= \sum_{i=1}^{n} \int_{\Sigma_i} e^{-\mathrm{i}\boldsymbol{\lambda}\cdot\boldsymbol{x}} \left[\frac{\partial u}{\partial \boldsymbol{n}_i} + \mathrm{i}\boldsymbol{\lambda}\cdot\boldsymbol{n}_i f_i\right] \mathrm{d}\sigma(\boldsymbol{x}). \end{aligned} \tag{6.0.5}$$

The global relation is then

$$\sum_{i=1}^{n} \int_{\Sigma_i} e^{-\mathrm{i}\boldsymbol{\lambda}\cdot\boldsymbol{x}} \frac{\partial u}{\partial \boldsymbol{n}_i} \mathrm{d}\sigma(\boldsymbol{x}) = -\mathrm{i}\sum_{i=1}^{n} \int_{\Sigma_i} e^{-\mathrm{i}\boldsymbol{\lambda}\cdot\boldsymbol{x}} (\boldsymbol{\lambda}\cdot\boldsymbol{n}_i) f_i \, \mathrm{d}\sigma(\boldsymbol{x}). \tag{6.0.6}$$

Making the same substitutions as for the Laplace equation, and found in [Ash14a], we may define the operators similarly to (5.0.7) as

$$\begin{aligned} (T_\epsilon \boldsymbol{\Phi})_k(\lambda) &= \sum_{j=1}^{n} e^{-\mathrm{i}(\boldsymbol{m}_j - \boldsymbol{m}_k)\cdot R_k^t \boldsymbol{\lambda}} \Phi_j((\Delta_{kj}\boldsymbol{\lambda})_1, (\Delta_{kj}\boldsymbol{\lambda})_2) \\ (S_\epsilon \boldsymbol{\Theta})_k(\lambda) &= \sum_{j=1}^{n} \mathrm{i} e^{-\mathrm{i}(\boldsymbol{m}_j - \boldsymbol{m}_k)\cdot R_k^t \boldsymbol{\lambda}} (\Delta_{kj}\boldsymbol{\lambda})_3 \Theta_j((\Delta_{kj}\boldsymbol{\lambda})_1, (\Delta_{kj}\boldsymbol{\lambda})_2), \end{aligned} \tag{6.0.7}$$

and the global relation is

$$(T_\epsilon \boldsymbol{\Phi}^{\mathrm{Ne}})_k(\lambda) = -(S_\epsilon \boldsymbol{\Theta}^{\mathrm{Di}})_k(\lambda), \quad k = 1, \ldots, n. \tag{6.0.8}$$

This is only valid for values $\boldsymbol{\lambda}\cdot\boldsymbol{\lambda} = -\epsilon$; one part of which can be parameterised by $\lambda_3 = \delta(\lambda)$ where

$$\delta(\lambda) = \mathrm{i}|\lambda| \left(1 + \frac{\epsilon}{|\lambda|^2}\right)^{1/2},$$

so that $\boldsymbol{\lambda} = (\lambda, \delta(\lambda))$, and $\lambda = (\lambda_1, \lambda_2)$. Indeed, if the global relation holds for the positive square root, it necessarily holds also for the negative, and thus we shall adopt the part where $\Im(\delta(\lambda)) > 0$. That is, setting $Z_P^+ := \{\boldsymbol{\lambda} : \lambda = (\lambda_1, \lambda_2) \in \mathbb{C}^2, \lambda_3 = \delta(\lambda)\}$, the global relation (6.0.8) is equivalent to the linear problem

$$(T_\epsilon \boldsymbol{\Phi}^{\mathrm{Ne}})_k(\lambda) = -(S_\epsilon \boldsymbol{\Theta}^{\mathrm{Di}})_k(\lambda), \quad 1 \le k \le n, \ (\lambda, \delta(\lambda)) \in Z_P^+. \tag{6.0.9}$$

Notice that the ϵ dependence is implicit in the set Z_P^+ on the right-hand side.

Returning to (6.0.6), we may follow the same principle as in Section 5.5: following an integration-by-parts we obtain a relation which is the analogue of (5.5.3). The only change will be that $\boldsymbol{\lambda}\cdot\boldsymbol{\lambda} = -\epsilon \neq 0$, so the extra term from (5.5.2) does not cancel. Following the

same derivation, we have

$$\begin{aligned}\int_\Sigma \mathrm{i}\,(\boldsymbol{\lambda}\cdot\mathbf{n})\,f(\mathbf{x})e^{-\mathrm{i}\boldsymbol{\lambda}\cdot\mathbf{x}}\,\mathrm{d}\sigma(\mathbf{x}) &= \frac{1}{\boldsymbol{\lambda}\cdot\mathbf{n}_k}\int_{\partial\Sigma}\left[\mathbf{n}_k\times\left(\boldsymbol{\lambda}f(\mathbf{x})e^{-\mathrm{i}\boldsymbol{\lambda}\cdot\mathbf{x}}\right)\right]\cdot\hat{\mathbf{t}}\,\mathrm{d}s\\ &\quad-\frac{1}{\boldsymbol{\lambda}\cdot\mathbf{n}_k}\int_\Sigma\Big((\mathbf{n}_k\cdot\mathbf{n})\boldsymbol{\lambda}-(\boldsymbol{\lambda}\cdot\mathbf{n})\mathbf{n}_k\Big)\cdot\nabla f(\mathbf{x})e^{-\mathrm{i}\boldsymbol{\lambda}\cdot\mathbf{n}}\,\mathrm{d}\sigma(\mathbf{x})\\ &\quad+\frac{\mathrm{i}\epsilon}{\boldsymbol{\lambda}\cdot\mathbf{n}_k}\int_\Sigma(\boldsymbol{n}_k\cdot\boldsymbol{n})fe^{-\mathrm{i}\boldsymbol{\lambda}\cdot\boldsymbol{x}}\,\mathrm{d}\sigma(\boldsymbol{x}).\end{aligned} \tag{6.0.10}$$

Again if we use the parameterisation $\Psi_l : (X_1, X_2, 0)^t \mapsto \mathbf{m}_l + R_l^t(X_1, X_2, 0)^t$ for Σ_l; multiply by $e^{\mathrm{i}\boldsymbol{\lambda}\cdot\boldsymbol{m}_l}$, and substitute $\boldsymbol{\lambda}\mapsto R_k^t\boldsymbol{\lambda}$, we obtain the following identity for S_ϵ:

$$\begin{aligned}-\left(S_\epsilon\boldsymbol{\Theta}^{\mathrm{Di}}\right)_k(\boldsymbol{\lambda}) &= \sum_{l=1}^n\frac{1}{\lambda_3}e^{-\mathrm{i}(\mathbf{m}_l-\mathbf{m}_k)\cdot R_k^t\boldsymbol{\lambda}}\int_{Q_l}e^{-\mathrm{i}\Delta_{kl}\boldsymbol{\lambda}\cdot X}\left[\boldsymbol{\mu}_1^{(l)}(\boldsymbol{\lambda})\frac{\partial\vartheta_l^d}{\partial X_1}(X)+\boldsymbol{\mu}_2^{(l)}(\boldsymbol{\lambda})\frac{\partial\vartheta_l^d}{\partial X_2}(X)\right]\mathrm{d}X\\ &\quad+\sum_{l=1}^n\frac{\mathrm{i}\epsilon(\boldsymbol{n}_k\cdot\boldsymbol{n}_l)}{\lambda_3}e^{-\mathrm{i}(\boldsymbol{m}_l-\boldsymbol{m}_k)\cdot R_k^t\boldsymbol{\lambda}}\int_{\Sigma_l}\vartheta_l^d(X)e^{-\mathrm{i}R_k^t\boldsymbol{\lambda}\cdot(X,0)^t}\,\mathrm{d}X.\end{aligned} \tag{6.0.11}$$

6.1 A new weak formulation for Helmholtz

Similarly to the weak problem defined by the linear forms a_K and ℓ_K in Theorem 5.1.4, and the analysis in Sections 5.5-5.6, we may propose a new weak problem for the Helmholtz BVPs. We will proceed in a similar fashion to the previous Chapter: first we will define the linear forms $a_{K,\epsilon}$ and $\ell_{K,\epsilon}$, and secondly we will use an integration-by-parts to achieve a new representation, with which we can use our polynomial basis.

Let us again consider Dirichlet data ϑ_j which are defined on each face Σ_j of the polyhedron, and which are continuous across the edges. The Fourier transform of this data, $\boldsymbol{\Theta}^{\mathrm{Di}}\in X_{\mathrm{sym}}$, is defined as in (5.0.5). Then given this valid Dirichlet data $\boldsymbol{\Theta}^{\mathrm{Di}}\in X_{\mathrm{sym}}$, the weak problem is to find $\boldsymbol{\Phi}^{\mathrm{Ne}}\in X_{\mathrm{sym}}$ such that

$$a_{K,\epsilon}(\boldsymbol{\Phi}^{\mathrm{Ne}},\boldsymbol{\Phi}') = \ell_{K,\epsilon}(\boldsymbol{\Phi}'),\quad\forall\,\boldsymbol{\Phi}'\in X_{\mathrm{sym}},$$

where

$$\begin{aligned}a_{K,\epsilon}(\boldsymbol{\Phi},\boldsymbol{\Phi}') &:= \sum_k\langle(T_\epsilon\boldsymbol{\Phi})_k,(T_\epsilon\boldsymbol{\Phi}')_k\rangle_{L^2(\mathbb{R}^2\setminus K)}\\ \ell_{K,\epsilon}(\boldsymbol{\Phi}') &:= \sum_k\langle(-S_\epsilon\boldsymbol{\Theta}^{\mathrm{Di}})_k,(T_\epsilon\boldsymbol{\Phi}')_k\rangle_{L^2(\mathbb{R}^2\setminus K)}.\end{aligned} \tag{6.1.1}$$

Using (6.0.10) and (6.0.11), we can rewrite this as an equivalent weak problem that is numerically tractable on our basis vectors $\boldsymbol{e}_{j,\alpha}(\lambda)$. Indeed, let us use the same notation as

in the previous chapter, and set

$$\begin{aligned}A^{(k)}_{i,\alpha,j,\beta} &:= \int_{\mathbb{R}^2\setminus K} e^{-\mathrm{i}(\mathbf{m}_i-\mathbf{m}_k)\cdot R_k^t\boldsymbol{\lambda}} e_{i,\alpha}\left((\Delta_{ki}\lambda)_1,(\Delta_{ki}\lambda)_2\right)\\ &\qquad e^{\mathrm{i}(\mathbf{m}_j-\mathbf{m}_k)\cdot R_k^t\bar{\boldsymbol{\lambda}}}\overline{e_{j,\beta}\left((\Delta_{kj}\lambda)_1,(\Delta_{kj}\lambda)_2\right)}\,\mathrm{d}\lambda\\ L^{(k)}_{l,\gamma,j,\beta} &:= \int_{\mathbb{R}^2\setminus K} \frac{1}{\delta(\lambda)} e^{-\mathrm{i}(\mathbf{m}_l-\mathbf{m}_k)\cdot R_k^t\boldsymbol{\lambda}}\left[c_{X_1,l,\gamma}\boldsymbol{\mu}_1^{(l)}(\lambda)+c_{X_2,l,\gamma}\boldsymbol{\mu}_2^{(l)}(\lambda)\right] e_{l,\gamma}\left((\Delta_{kl}\lambda)_1,(\Delta_{kl}\lambda)_2\right)\\ &\qquad e^{\mathrm{i}(\mathbf{m}_j-\mathbf{m}_k)\cdot R_k^t\bar{\boldsymbol{\lambda}}}\overline{e_{j,\beta}\left((\Delta_{kj}\lambda)_1,(\Delta_{kj}\lambda)_2\right)}\,\mathrm{d}\lambda,\end{aligned} \tag{6.1.2}$$

where again

$$\boldsymbol{\mu}^{(l)}(\lambda) := (\mathbf{n}_k\cdot\mathbf{n}_l)\,(\Delta_{kl}\boldsymbol{\lambda}) - (\Delta_{kl}\boldsymbol{\lambda})_3 R_j\mathbf{n}_k.$$

We recognise an additional term in (6.0.11) arising as a result of ϵ in the Helmholtz problem. We denote the terms arising from this perturbation by

$$\begin{aligned}\mathcal{L}^{(k)}_{l,\gamma,j,\beta} = \int_{\mathbb{R}^2\setminus K} &\frac{\mathrm{i}\epsilon(\boldsymbol{n}_k\cdot\boldsymbol{n}_j)}{\delta(\lambda)} e^{-\mathrm{i}(\mathbf{m}_l-\mathbf{m}_k)\cdot R_k^t\boldsymbol{\lambda}} c_{l,\gamma}e_{l,\gamma}\left((\Delta_{kl}\lambda)_1,(\Delta_{kl}\lambda)_2\right)\\ &e^{\mathrm{i}(\mathbf{m}_j-\mathbf{m}_k)\cdot R_k^t\bar{\boldsymbol{\lambda}}}\overline{e_{j,\beta}\left((\Delta_{kj}\lambda)_1,(\Delta_{kj}\lambda)_2\right)}\,\mathrm{d}\lambda.\end{aligned} \tag{6.1.3}$$

Thus this new Galerkin problem for Helmholtz is realised as a perturbation of that for Laplace:

$$\sum_{i,\alpha} c_{i,\alpha}\left(\sum_k A^{(k)}_{i,\alpha,j,\beta}\right) = \sum_{k,l,\gamma}\left(L^{(k)}_{l,\gamma,j,\beta}+\mathcal{L}^{(k)}_{l,\gamma,j,\beta}\right),\quad \forall\, 1\le j\le n,\ |\beta|\le N. \tag{6.1.4}$$

6.2 Remarks on implementation

We have seen that the global relation gives rise to an operator equation which, in view of the Lax–Milgram lemma, may be reduced to a weak problem. This in turn results in the finite-dimensional Galerkin problem (6.1.4) for the class of Helmholtz problems (any value of $\epsilon\in\mathbb{R}$ is permitted). This may be solved numerically, and for any approximating basis is stable and convergent as the number, $(N+1)(N+2)/2$, of basis vectors tends to infinity. Also of interest, however, is the speed of calculation, and we now discuss a technique for calculating the values $A^{(k)}_{i,\alpha,j,\beta}$, $L^{(k)}_{l,\gamma,j,\beta}$ and $\mathcal{L}^{(k)}_{l,\gamma,j,\beta}$: by using specific properties of the operator T we can show objectively how numerical work can be reduced.

Proposition 6.2.1. *Suppose our weak problem is such that the compact set K is symmetric about either axis through the origin. Let $\lambda=(\lambda_1,\lambda_2)\in\mathbb{R}$, $\boldsymbol{\lambda}=(\lambda,\delta(\lambda))$ and $\boldsymbol{\Phi},\boldsymbol{\Theta}\in X_{\mathrm{sym}}$, the Paley–Wiener space. Then the following identities hold:*

- $(T_\epsilon\boldsymbol{\Phi})_k(-\lambda) = \overline{(T_\epsilon\boldsymbol{\Phi})_k(\lambda)}$

- $(S_\epsilon \boldsymbol{\Theta})_k(-\lambda) = \overline{(S_\epsilon \boldsymbol{\Theta})_k(\lambda)}$
- $A^{(k)}_{i,\alpha,j,\beta}, L^{(k)}_{l,\gamma,j,\beta}, \mathcal{L}^{(k)}_{l,\gamma,j,\beta} \in \mathbb{R}$ *for all values* i, j, k *and* α, β, γ *in their respective ranges.*

Proof. Given $\lambda \in \mathbb{R}^2$, we notice that $\delta(-\lambda) = \delta(\lambda)$, so let us denote $\tilde{\boldsymbol{\lambda}} := (-\lambda_1, -\lambda_2, \delta(\lambda))$, to be the component in the expression for $(T_\epsilon \Phi)_k(-\lambda)$ in (6.0.7). Then for any k, if we set

$$R^t_k \boldsymbol{\lambda} = R^t_k(\lambda, 0)^t + \mathrm{i} R^t_k(0, 0, \delta(\lambda))^t = \boldsymbol{a} + \mathrm{i}\boldsymbol{b}, \quad \boldsymbol{a}, \boldsymbol{b} \in \mathbb{R}^3,$$

then $R^t_k \tilde{\boldsymbol{\lambda}} = -\boldsymbol{a} + \mathrm{i}\boldsymbol{b}$. In particular, $-\mathrm{i} R^t_k \tilde{\boldsymbol{\lambda}} = -\mathrm{i}\boldsymbol{a} + \boldsymbol{b} = \overline{-\mathrm{i} R^t_k \boldsymbol{\lambda}}$, so that

$$e^{-\mathrm{i}(\boldsymbol{m}_j - \boldsymbol{m}_k)\cdot R^t_k \tilde{\boldsymbol{\lambda}}} = \overline{e^{-\mathrm{i}(\boldsymbol{m}_j - \boldsymbol{m}_k)\cdot R^t_k \boldsymbol{\lambda}}}.$$

To conclude the proof for our operator T_ϵ, we note that since $\boldsymbol{\Phi} \in X_{\mathrm{sym}}$, the component functions Φ_j are in the Paley–Wiener space over the j-th polygon Q_j, so they satisfy the symmetry property $\Phi_j(-\bar{z}) = \overline{\Phi_j(z)}$ for any $z \in \mathbb{C}^2$. Denoting similarly the two-dimensional vector $((\Delta_{kj}\boldsymbol{\lambda})_1, (\Delta_{kj}\boldsymbol{\lambda})_2) =: a + \mathrm{i}b$ for $a, b \in \mathbb{R}^2$, we find that

$$\Phi_j((\Delta_{kj}\tilde{\boldsymbol{\lambda}})_1, (\Delta_{kj}\tilde{\boldsymbol{\lambda}})_2) = \Phi_j(-\overline{(a + \mathrm{i}b)}) = \overline{\Phi_j(a + \mathrm{i}b)} = \overline{\Phi_j(\Delta_{kj}\boldsymbol{\lambda})_1, (\Delta_{kj}\boldsymbol{\lambda})_2)},$$

proving our claim for T_ϵ. By comparison of S_ϵ with T_ϵ, it suffices to show that $\mathrm{i}(\Delta_{kj}\tilde{\boldsymbol{\lambda}})_3 = \overline{\mathrm{i}(\Delta_{kj}\boldsymbol{\lambda})_3}$, which follows similarly.

Finally, to prove the claims for components of A, L and $\mathcal{L}$ we fix values i, j, k and α, β, and denote a given integrand by $G(\lambda) := (T\boldsymbol{e}_{i,\alpha})_k(\lambda)\overline{(T\boldsymbol{e}_{j,\beta})_k(\lambda)}$. Without loss of generality, assume that K is symmetric along the λ_2 axis. Then we may rewrite $A^{(k)}_{i,\alpha,j,\beta}$ as an integral over the right half-plane only:

$$A^{(k)}_{i,\alpha,j,\beta} = \int_{(\mathbb{R}^2 \setminus K) \cap \{\lambda_1 > 0\}} G(\lambda) + \overline{G(\lambda)}\, \mathrm{d}\lambda = 2\Re \int_{(\mathbb{R}^2 \setminus K) \cap \{\lambda_1 > 0\}} G(\lambda)\, \mathrm{d}\lambda.$$

A similar proof holds for L, where the difference is that we also require

$$\frac{c_{X_1,l,\gamma}\boldsymbol{\mu}^{(l)}_1(-\lambda) + c_{X_2,l,\gamma}\boldsymbol{\mu}^{(l)}_2(-\lambda)}{\delta(\lambda)} = \overline{\left(\frac{c_{X_1,l,\gamma}\boldsymbol{\mu}^{(l)}_1(\lambda) + c_{X_2,l,\gamma}\boldsymbol{\mu}^{(l)}_2(\lambda)}{\delta(\lambda)}\right)},$$

which follows since $\delta(\lambda)$ is purely imaginary, and $\mathrm{i}\boldsymbol{\mu}(-\lambda) = \overline{\mathrm{i}\boldsymbol{\mu}(\lambda)}$. □

Corollary 6.2.2. *The integrals in the weak formulation* (6.1.4) *may be performed over a smaller domain* $\left(\mathbb{R}^2 \setminus K\right) \cap \{\lambda_1 > 0\}$. *Furthermore for every fixed* i, j, k *and* α, β *we have the identity*

$$A^{(k)}_{i,\alpha,j,\beta} = A^{(k)}_{j,\beta,i,\alpha},$$

which is to say that the resulting Galerkin matrix is symmetric.

As a consequence of these equalities, the apparent numerical difficulty has been reduced by at least a factor of two: firstly the integration range is smaller, and secondly that symmetry in the Galerkin matrix means the lower diagonal entries need not be computed, but instead are given directly from the upper diagonal ones. Furthermore, since we are confident that all integrals are real valued, we may enforce this in the definition of the integrand in MATLAB. A priori the integrand is complex-valued, however $\Re \int f = \int (\Re f)$. So integrating a function which is known to be real valued has a noticeable reduction in computation time (which is to be expected, since a complex-valued number is defined in memory by two real numbers).

In the final chapter we provide the first numerical examples of the Fokas method in three dimensions, using this fundamentally new weak formulation of the global relation.

CHAPTER 7

Numerical results for 3D polyhedra

In the previous chapters, we introduced a new numerical method for the three-dimensional Laplace, Helmholtz and modified-Helmholtz Dirichlet BVPs using a weak formulation involving the linear forms a_K, ℓ_K and $a_{K,\epsilon}, \ell_{K,\epsilon}$ for the Laplace and (modified-)Helmholtz problems respectively. Following an integration-by-parts of the related operators S and S_ϵ, we were able to propose a numerical method which is convergent, and such that the individual terms could be calculated on basis vectors (a motivation for seeking this alternate form was given in Section 5.4).

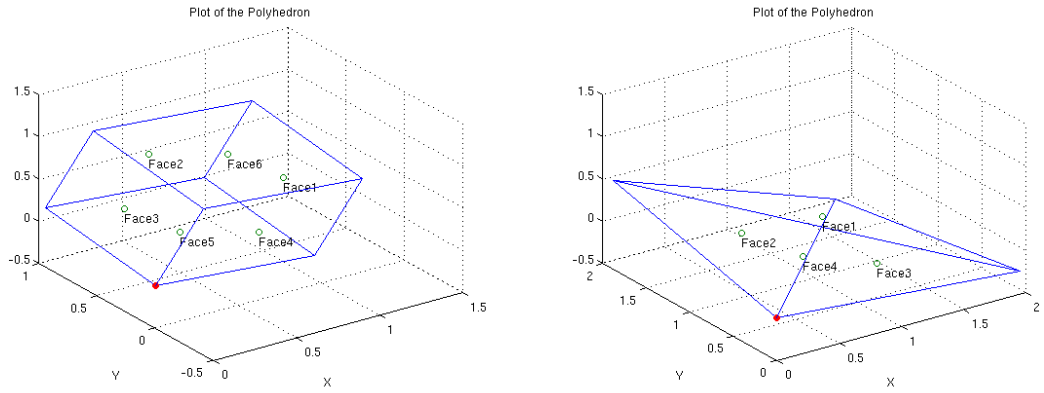
In this section, we have used MATLAB to present a numerical implementation of this Galerkin method, in two domains and for multiple test cases. In each case, we take a known solution to the PDE, and insert the trace of this function as the Dirichlet data. The numerical solution to the global relation (i.e. the projected Neumann data) can then be compared with the actual Neumann data, as well as the the projected Neumann data.

Remark 7.0.1. *For the two-dimensional Laplace problem, we also demonstrated solutions for mixed boundary data types (where each edge was prescribed with either Dirichlet or Neumann data). In view of the integration by parts in Section 5.5, we may similarly treat the Neumann boundary value problem, and the mixed boundary value problem. Care must be taken to ensure that a solution does indeed exist; indeed it follows from Green's Theorem that the Neumann data must integrate to zero over the boundary:*

$$\int_{\partial\Omega} \partial_\nu u \, \mathrm{d}A = 0.$$

We have discussed compatibility criteria for the two-dimensional Dirichlet-only problem in section 0.2.4, and similar conditions must hold at the boundaries for the three-dimensional problem also - see [Dau88]. However on the assumption *that a solution to the global relation exists, the BVP is solved [Ash12, Ash13, AF15b].*

Recall that we have chosen to use the standard polynomial functions as a basis of



(a) Cube domain A

(b) Pyramid domain B

Figure 7.1: Two test domains, A and B.

$L^2(Q_j)$. By Parseval's Theorem, our basis for $X_N \subset X$ is given as

$$\boldsymbol{e}_{i,\alpha}(\lambda) := e_{i,\alpha}(\lambda)\boldsymbol{e}_i, \quad 1 \leq i \leq n, |\alpha| \leq N.$$

where $e_{i,\alpha}(\lambda)$ is the Fourier transform of $f_\alpha(X) := X^\alpha$ over the i-th polygon Q_i. In the following examples, we set $N = 3$, which amounts to approximating the data on each face by polynomials up to degree 3. We expect this to give a good approximation of the exact boundary data for the problems we choose. For more oscillatory boundary data, this value N may be changed accordingly.

We have taken the standard unit cube with a vertex at zero and the pyramid with vertices at $(0,0,0), (2,0,0), (0,2,0)$ and $(1/2,1/2,1)$. To make these domains more generic, we have rotated them by angle $3\pi/10$ around the vector $(1,1,1)$, see Fig 7.1.

7.1 Numerical Examples

Let us consider three examples:

(Lap): For this example we take the function

$$u(x,y,z) = z + x^2 - y^2,$$

which solves the Laplace problem, and is approximated exactly in our subspace. The error over the first face is given in figure 7.2 for the pyramid and for the cube.

(Helm): Here we take the function

$$u(x,y,z) = 4\cos(x/2),$$

which solves $-\Delta u - \frac{1}{4}u = 0$, the Helmholtz problem for $\epsilon = -1/4$; see figure 7.3.

(m-Helm): We take the function

$$u(x, y, z) = yz\cosh(x),$$

which solves $-\Delta u + u = 0$, the modified-Helmholtz problem for $\epsilon = 1$; see figure 7.4.

In each case, the plot shows the absolute difference between the Neumann data obtained numerically via the global relation, and the exact Neumann data, which is known for each problem. The 'best possible error' is the absolute difference between this exact data, and the best possible approximation in this subspace. Also note that the convergence results ensure L^2-convergence only, not pointwise convergence, and so this low pointwise error is a good indicator of the accuracy of this approximation. In future experiments, it would be good to extend these tests to more realistic data, and to compare L^2-convergence rates, as shown for the two-dimensional cases in Section 4.3.1. Also our numerical experiments show that the coefficients of the exact projected data, $\mathbf{\Phi}_N^{\text{Ne}}$, and the reconstructed data $\tilde{\mathbf{\Phi}}_N^n$ differ by a magnitude of order 10^{-3}, and it is expected that more accurate numerical integration would also improve this accuracy.

The following plots in this Chapter highlight the error over one of the faces for our two domains and for the Laplace, Helmholtz and modified-Helmholtz BVPs. The plots over the other faces are similar, and have been included in Appendix A. These plots are the first three-dimensional numerical implementation of the Fokas method, and help to show that our proposed methods in the previous two Chapters (which are stable) are worthy of future study, to apply to Helmholtz problems with less-regular boundary data.

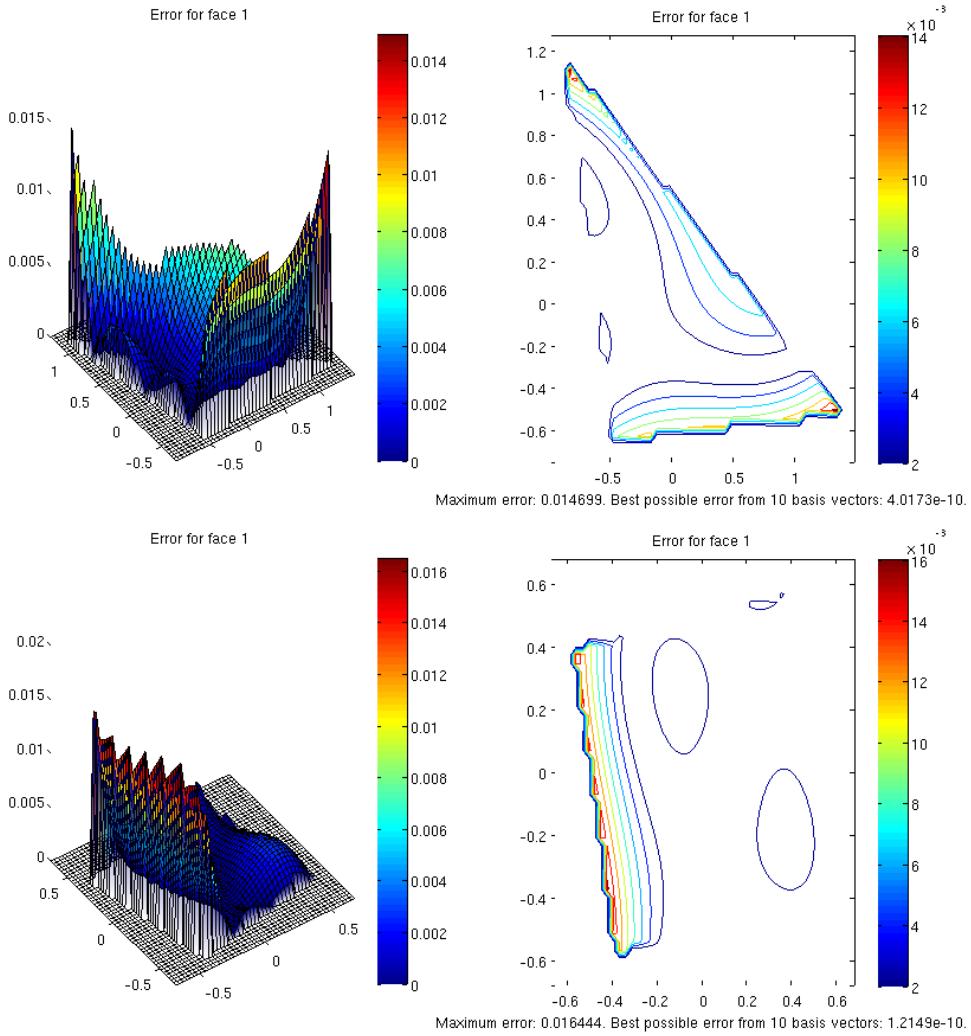


Figure 7.2: Error over face 1 for the Laplace problem. Top: Pyramid domain. Bottom: Cube domain.

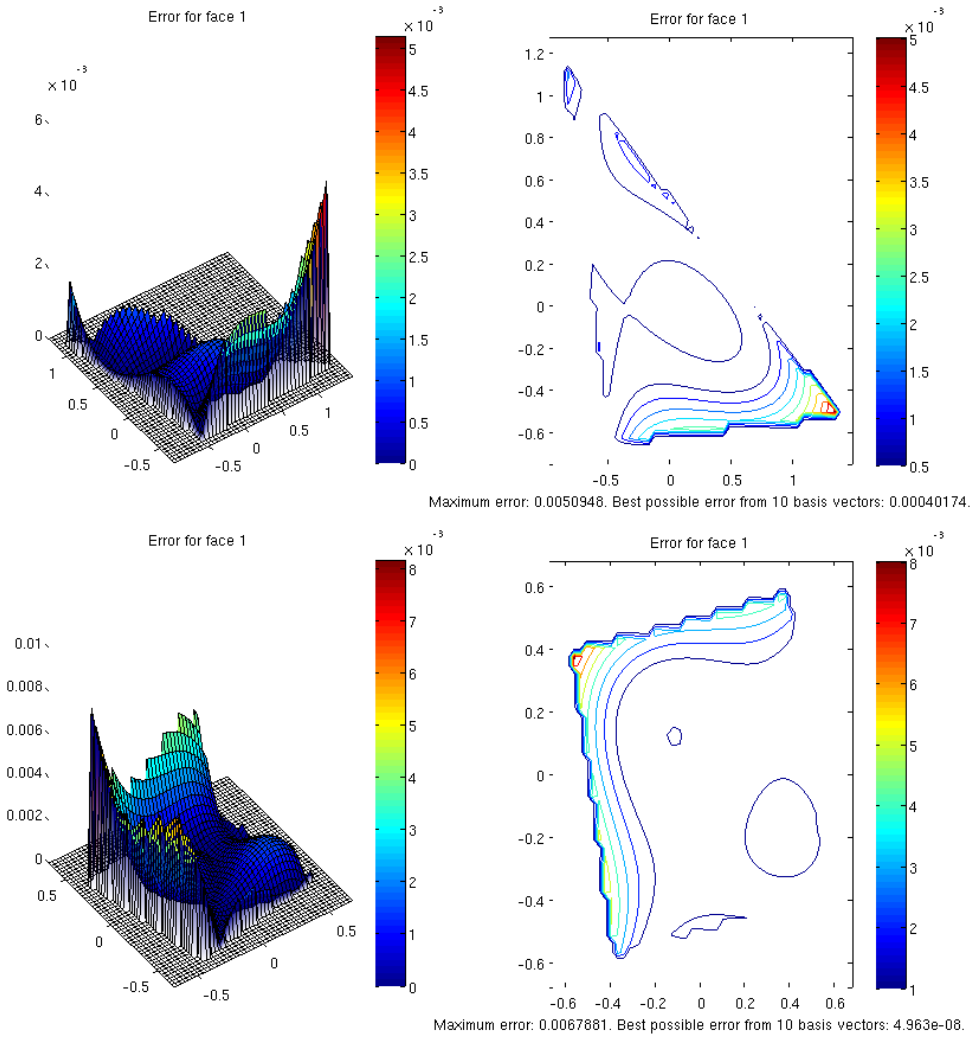


Figure 7.3: Error over face 1 for the Helmholtz problem. Top: Pyramid domain. Bottom: Cube domain.

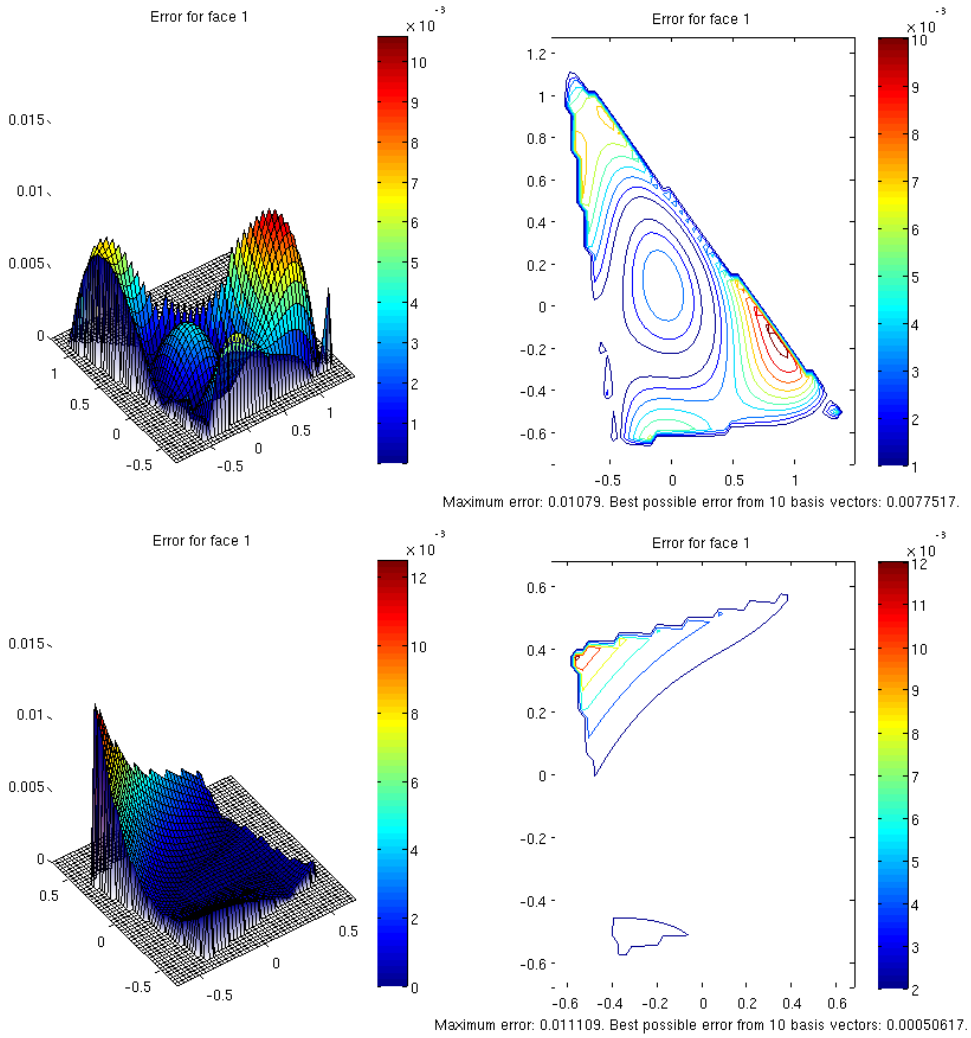


Figure 7.4: Error over face 1 for the modified-Helmholtz problem. Top: Pyramid domain. Bottom: Cube domain.

Conclusion

In this thesis we have presented an application of the Fokas method to linear PDEs in two and three dimensions. The global relation for these problems can be written as a continuous map, $T\mathbf{\Phi}^{\mathrm{Ne}} = -S\mathbf{\Theta}^{\mathrm{Di}}$, between the unknown Neumann data and the known Dirichlet data. For the Helmholtz and modified-Helmholtz problems, this operator equation has the form $T_\beta\mathbf{\Phi}^{\mathrm{Ne}} = -S_\beta\mathbf{\Theta}^{\mathrm{Di}}$, where T_β is a compact perturbation of T and the right-hand side is square-integrable. This operator T_β is upper semi-Fredholm and, using results from complex analysis and properties of the Paley–Wiener spaces, the global relation is well-posed away from Laplace Dirichlet eigenvalues, as shown in [Ash13, Ash14a, Ash14b, AC15]. For the two-dimensional problem, we have achieved the following:

- Using functional properties of T_β from [Ash14b], we have existence and uniqueness of solutions to the global relation. Utilising the Paley–Wiener spaces, we have derived a completely new class of variational problems, leading to a new weak formulation.
- In view of the Lax–Milgram Theorem, this weak problem has a unique solution and is numerically tractable.
- We have proposed a Galerkin implementation that is is stable and convergent, and gave a rigorous proof of *spectral convergence rates* for smooth boundary data.
- These exponential convergence rates were demonstrated numerically; compare well with recent results from [FF11], and have comparatively low condition numbers consistent with results from [FF11, FFX04, Dav08, SSF10].
- We have shown how our presentation for the Dirichlet BVP could be extended to accept mixed boundary data over the polygon; and provided a numerical test using an example from [FF11].
- Because the Helmholtz BVP *is not* uniquely solvable at eigenvalues of the Laplacian, we have shown that the condition numbers of the finite-dimensional problem must become unbounded in a neighbourhood of these eigenvalues.
- We have demonstrated that these Dirichlet eigenvalues can be identified numerically, by observing these 'spikes' in the condition numbers.

In the second half of this thesis, we have worked towards a numerical implementation of the Fokas method for three-dimensional polyhedral domains, using the global relation constructed in [Ash14b, Ash14a]. We have proposed a new class of variational problems, for which linear operators are defined on $\mathbb{R}^2 \setminus K$, for *any* compact set $K \subset \mathbb{R}^2$, and shown that this admits a unique solution. Stability and convergence of this method have been proven for the Laplace, Helmholtz and modified-Helmholtz BVPs. At this point, we must choose a basis for each face, Q_j, of the polygon: The Legendre basis is good for $L^2[-\sigma, \sigma]$; however this does not have an obvious extension to a basis for $L^2(Q_j)$. We have provided the following framework to overcome these difficulties:

- Using a standard polynomial basis, the Fourier transform of these functions on each face was calculated precisely in terms of the geometry of Q_j in 5.2.
- Via the Gram–Schmidt algorithm in 5.3 we obtained an L^2-orthogonalisation of these basis functions, with respect to Q_j. Crucially, this orthogonalisation is *exact* since the relevant inner products can be calculated precisely in terms of the geometry of Q_j.
- Using compatibility of the Dirichlet data across the edges of the polyhedron, we have constructed an entirely new weak formulation in 5.5 for the Laplace BVP and 6.1 for the (modified-)Helmholtz BVP. This gives a practical numerical implementation, and avoids divergence when computing the linear forms on our basis functions (as they *do not* individually satisfy these compatibility requirements).
- To further aid our numerical implementation, in Section 6.2 we have identified symmetries in the matrix coefficients for the Galerkin problem, thus reducing the number of computations needed and increasing efficiency.
- Finally in the previous Chapter we provided a proof-of-concept numerical implementation for some Laplace, Helmholtz and modified-Helmholtz examples, which demonstrates the validity of this approach.

Our approach has been as generic as possible and future work could optimise the choice of basis vectors; as well as the orthogonalisation and integration for specific problems.

In summary, the results we have obtained for two-dimensions exhibits spectral convergence rates for sufficiently smooth data, and a formal proof of this convergence was given.

For previous collocation approaches of the Fokas method, for example in [FF11, FIS15, HFS15], formal proofs of convergence were not provided even for regular boundary data, though recently some proofs in this area have been provided in [FP15, Ch. 6]. However these methods did demonstrate low condition numbers and good convergence rates in

practice. In 4.5 we have compared our approach with these implementations, and in particular with [FF11], which was itself shown to perform well alongside classical boundary integral methods for the three test cases they studied.

For this reason, I believe that the proof of spectral convergence given in Theorem 2.7.2 for smooth data, and the numerical results in Section 4.2, places this method alongside the current state of the art finite element methods for Dirichlet BVPs with smooth data. It is admitted that finite element methods perform extremely well in situations not considered in this thesis, and so further work should be done to test the Fokas method and our proposed numerical implementation in these further situations.

Furthermore we have remarked that the collocation approaches aim to recover the unknown Neumann data from the known Dirichlet data over the boundary. In contrast, the unknown data we have considered in this thesis has always been the *Fourier transform* of the Dirichlet and Neumann data. In solving for the Fourier transform of these functions, we have been able to use strong properties from Complex Analysis, since the Fourier transform of these functions, and related linear operators are all analytic functions. This has enabled the strong theoretical results in [Ash13, AC15, Ash14b, Ash14a], leading to the new numerical methods and implementations given in this thesis. This thesis thus provides a rigorously justified numerical implementation of the Fokas method for polygonal and polyhedral domains, and in particular it contains the first three-dimensional numerical implementation of the Fokas method.

APPENDIX A

3D Plots

In Section 7.1, we provided plots for the Laplace, Helmholtz and modified-Helmholtz BVPs for the rotated cube and rotated pyramid domains over the first face. We provide here the remaining error plots for these test cases over the remaining faces. We notice that the maximum errors seem to occur at the boundaries of the regions. Such errors could possibly be improved in future implementations by using a different choice of basis vectors, or by imposing the Neumann zero-average condition

$$\sum_{j=1}^{n} \int_{\Sigma_j} \partial_{\boldsymbol{n}_j} q(\boldsymbol{x}) \, \mathrm{d}\sigma(\boldsymbol{x}) = 0$$

on our finite-dimensional subspaces. Our Dirichlet data is chosen such that the exact solution does respect this condition, however we have not imposed this on our subspace. We also note however that the errors away from these boundaries are significantly lower over every face, and for each test case. Figures A.1 and A.2 plot the absolute errors for the Laplace problem for the two domains, and Figures A.3-A.6 demonstrate the numerical implementation for the Helmholtz and modified-Helmholtz examples.

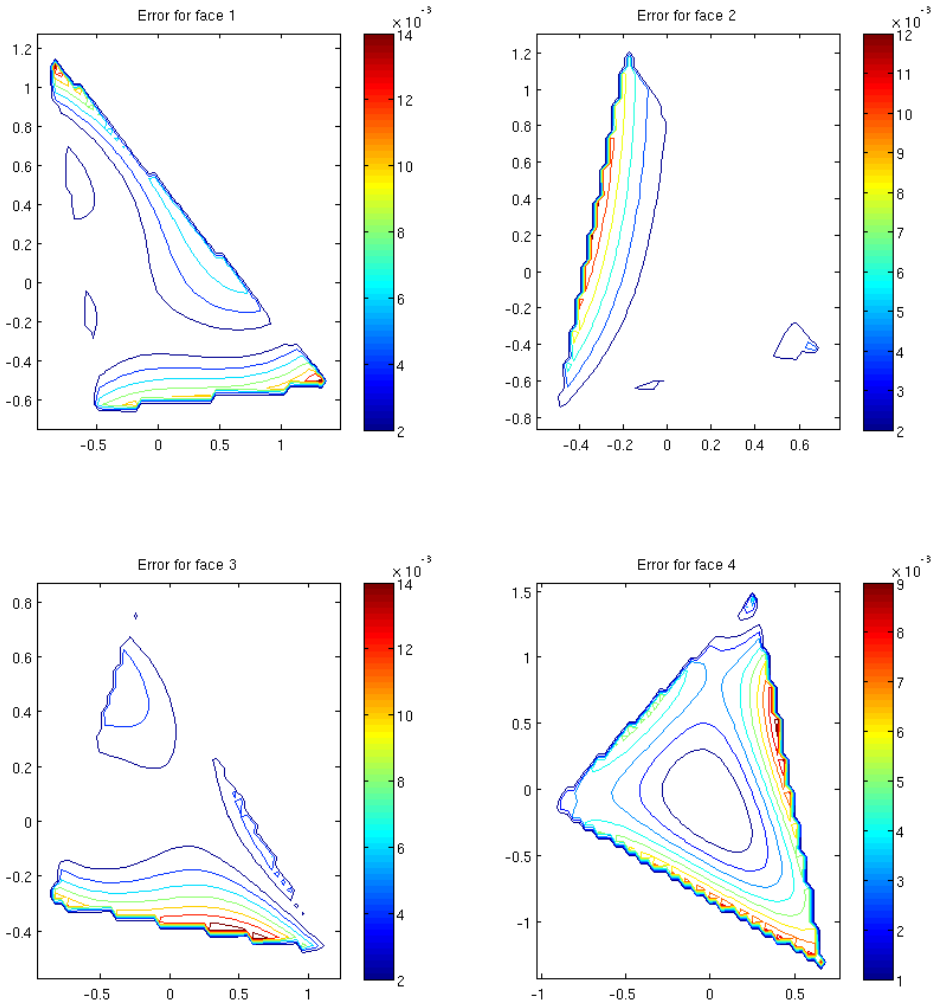


Figure A.1: Errors for the pyramid, for the Laplace problem.

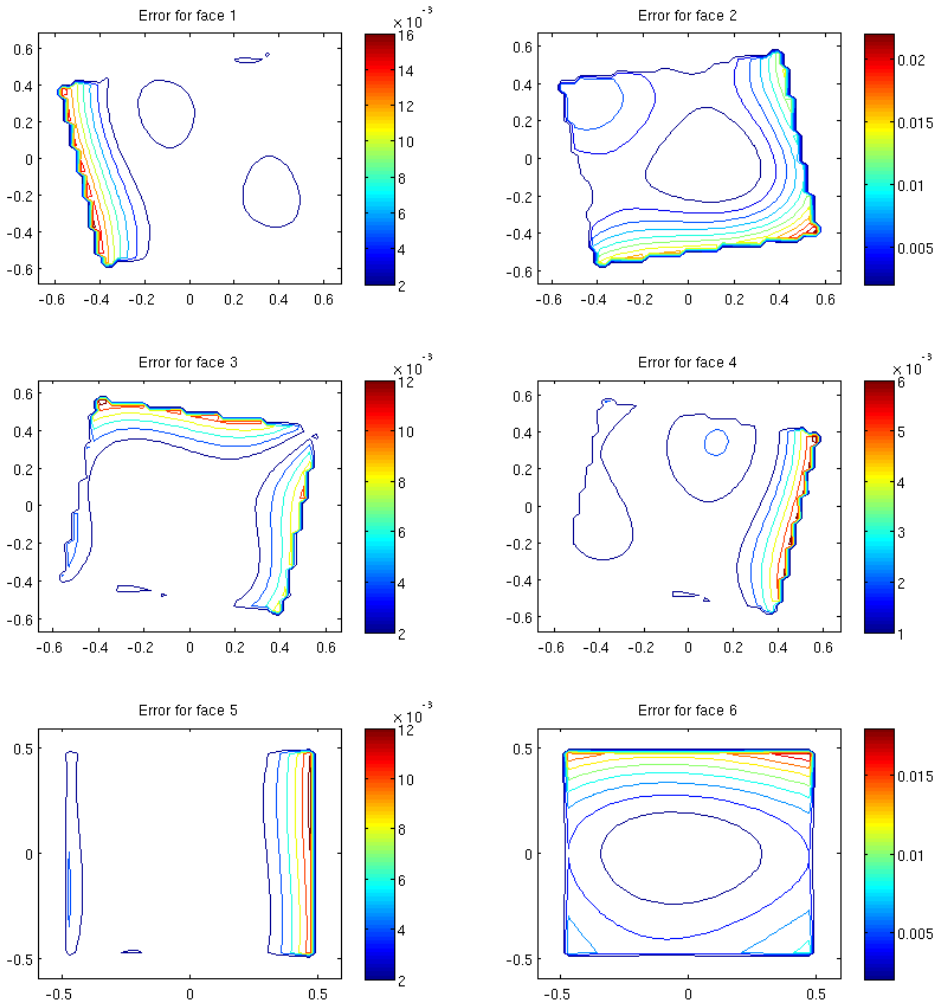


Figure A.2: Errors for the cube, for the Laplace problem.

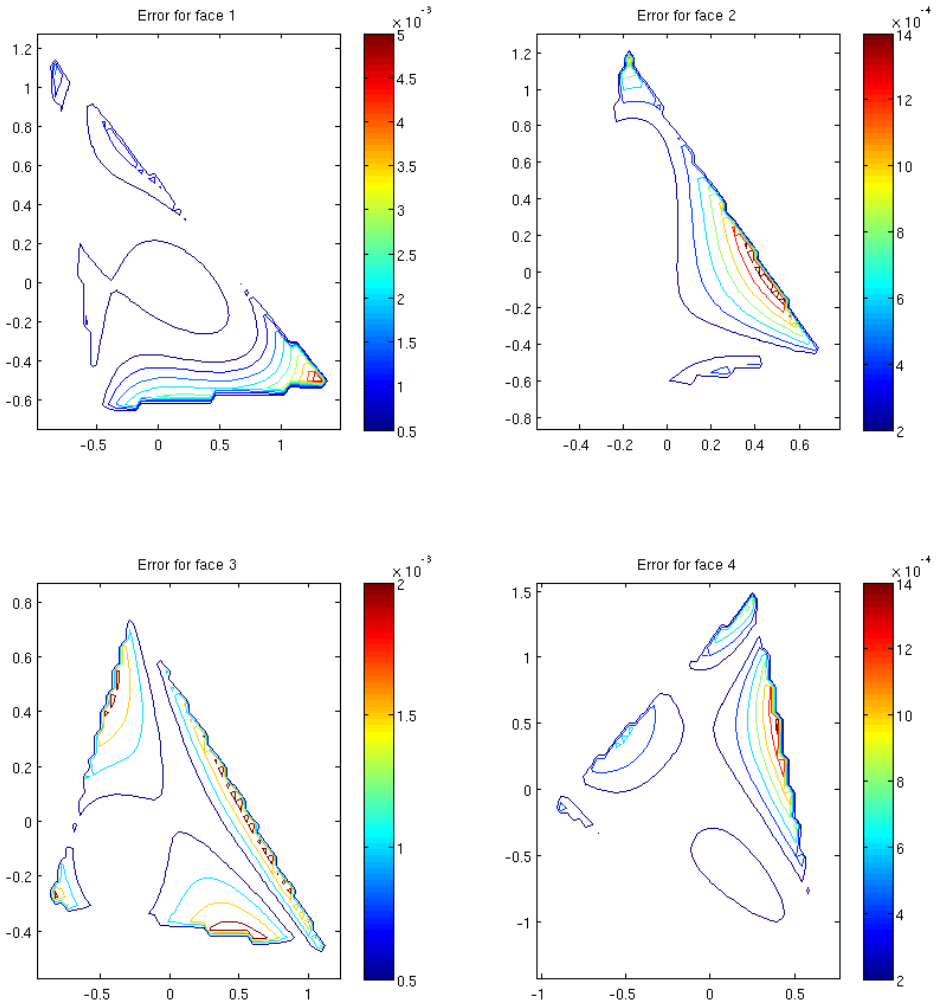


Figure A.3: Errors for the pyramid, for the Helmholtz problem.

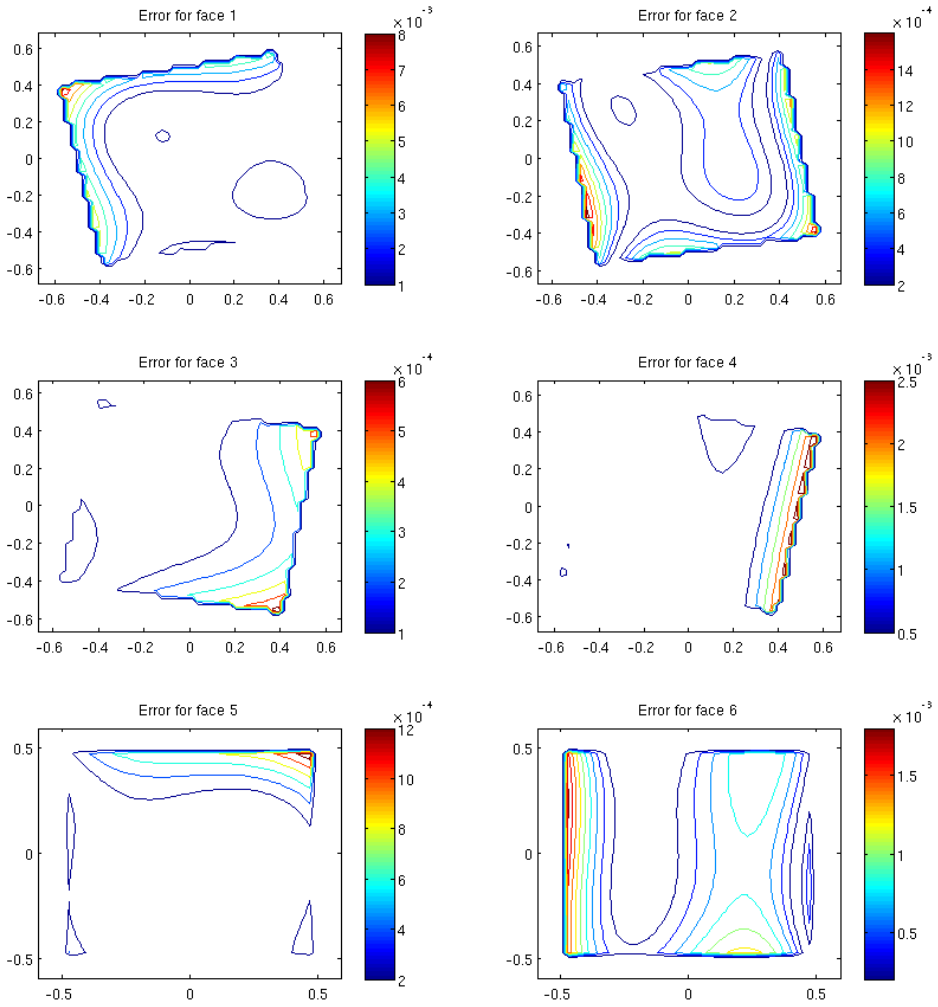


Figure A.4: Errors for the cube, for the Helmholtz problem.

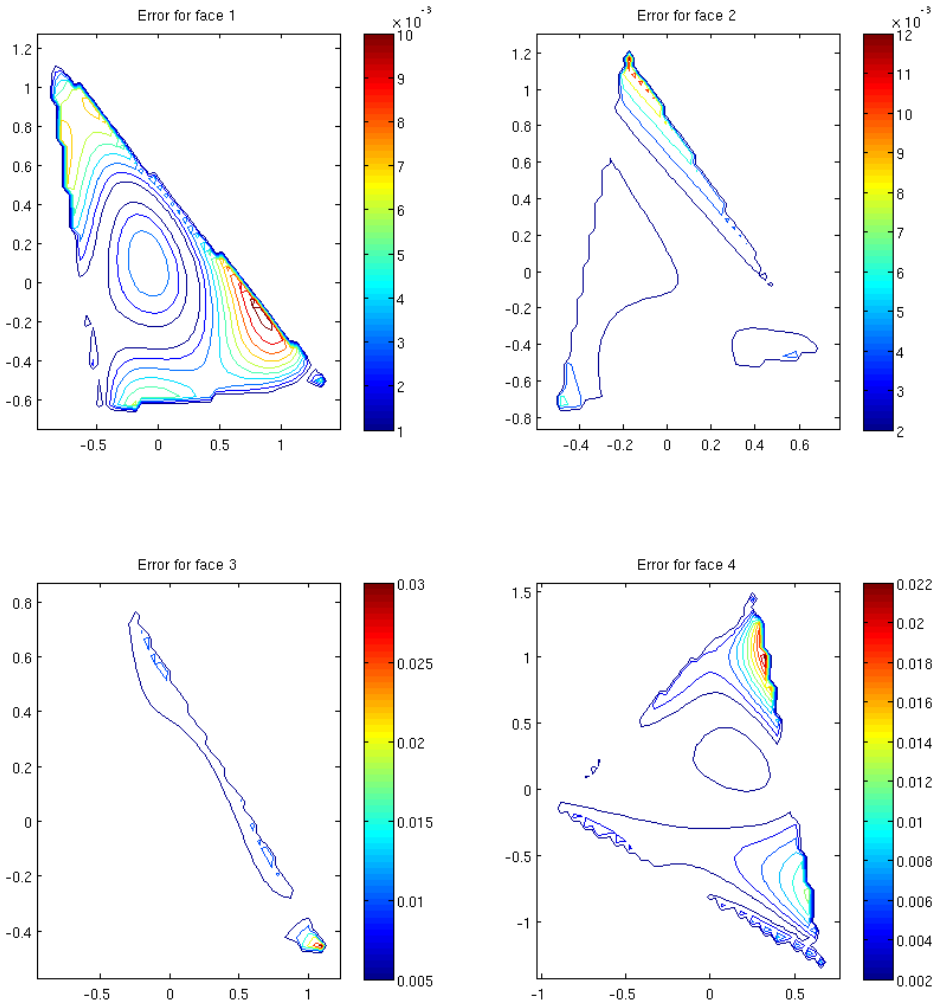


Figure A.5: Errors for the pyramid, for the modified-Helmholtz problem.

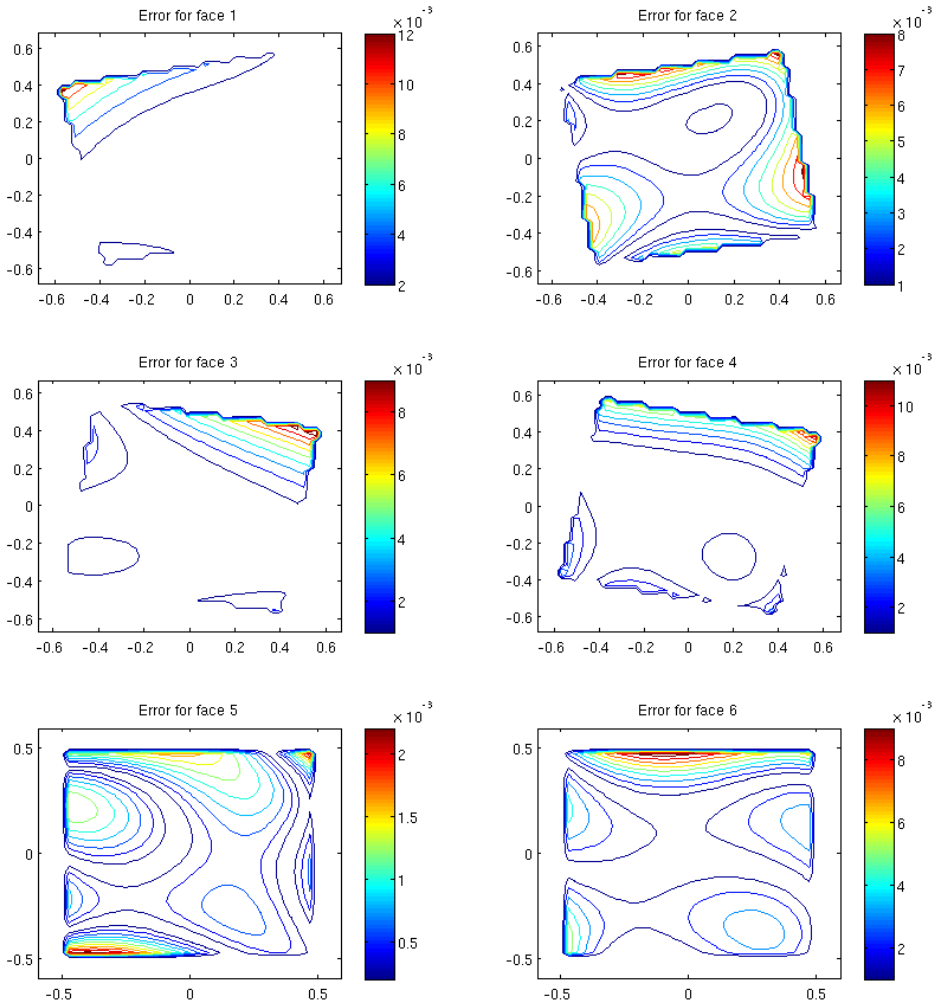


Figure A.6: Errors for the cube, for the modified-Helmholtz problem.

APPENDIX B

Paley–Wiener spaces

The properties of the Paley–Wiener spaces were crucial in our analysis of the operator equations for the two-dimensional and three-dimensional PDEs. Some of the relevant results were quoted above, and we include here some further important properties of these spaces. Knowledge of the exponential growth bounds for Paley–Wiener functions were used to provide an integral representation for $e^{i\sigma_j\lambda}\Phi_j(\lambda)$ - as the bound ensures decay in $\mathbb{C}^+$. Other pointwise bounds which were merely stated above are also given here in their proper context. The Paley–Wiener spaces are generally denoted PW^p_π, where p indicates the L^p space which the functions lie in; and the lower number is the size of support (typically equal to π)[1]. The important classical Theorems that we present here are the Plancherel–Pólya; Phragmén–Lindelöf and Paley–Wiener Theorems that can be found in [Boa54, Lev96].

Recall that a function f is in $L^p(\mathbb{R})$ if the following norm is finite:

$$\|f\|_p := \int_{-\infty}^{\infty} |f(x)|^p \, \mathrm{d}x < \infty.$$

For $p \geq 1$, the Paley–Wiener space, PW^p_π, is defined as the Fourier transform of functions with specific support, such that this Fourier transform lies in an L^p space:[2]

$$PW^p_\pi := \{f : \mathbb{C} \to \mathbb{C} \text{ entire } : \|f\|_p < \infty \text{ and } |f(z)| \lesssim e^{\pi|\Im z|} \text{ for all } z \in \mathbb{C}\}.$$

In view of Plancherel's theorem, for $p = 2$ this space coincides with our definition 2.3.1, where $PW = \mathcal{F}L^2(K)$, for some compact set K. However, because of the Paley–Wiener Theorem, these spaces have an alternative classification in terms of growth properties.

Definition B.0.1. *A function has exponential type (less than or equal to) τ if for suffi-*

[1] We used $p = 2$ only, so it was convenient to write PW^σ in place of PW^2_σ.

[2] For $0 < p < 1$, this is still defined, though $\|\cdot\|_p$ is a pseudo-norm as it does not obey the triangle inequality.

ciently large values of r [3],

$$\sup_{|z|=r} |f(z)| \lesssim e^{\tau r}.$$

If f *is entire, then it is called an entire function of exponential type-*τ *(EFET-*τ*).*

Let us provide some more background for the Paley–Wiener results used in this thesis: firstly we note a result by Plancherel and Pólya, which gives bounds on the norm of Paley–Wiener functions along lines parallel to $\mathbb{R}$. In particular this Theorem tells us that the Paley–Wiener spaces are nested: $PW_\pi^p \subset PW_\pi^q$ for any $q > p$.

Theorem B.0.2 (Plancherel and Pólya, [Boa54])**.** *Let* f *be entire, and of exponential type* τ*. If also* $\|f\|_p < \infty$ *then*

$$\int_{-\infty}^{\infty} |f(x + \mathrm{i}y)|^p \, \mathrm{d}x \leq e^{p\tau|y|} \|f\|_p^p. \tag{B.0.1}$$

Furthermore, $|f(x)| \to 0$ *as* $|x| \to \infty$*. Thus* $\|f\|_q < \infty$ *for any* $q > p$*.*

Another important class of results for Paley–Wiener functions are the Phragmén–Lindelöf Theorems. These give boundedness properties in regions where a function has known estimates on the boundary. For the first result, we consider a wedge domain $D := \{z = \rho e^{\mathrm{i}\theta} \in \mathbb{C} : \alpha < \theta < \beta\}$, and given an analytic function $f : D \to \mathbb{C}$ let us define

$$M(r) \equiv M_f(r) := \sup_{re^{i\theta} \in D} |f(re^{i\theta})|.$$

Then the following Phragmén–Lindelöf Theorems hold, and are given in [Lev96, pp. 38-39]:

Theorem B.0.3 (Phragmén–Lindelöf version 1)**.** *Suppose* D *has angle* π/λ *and* $M(r) \overset{as}{<} r^\rho$ *for some* $\rho < \lambda$*, where this inequality means that as* $r \to \infty$*,* $\frac{M(r)}{r^\rho} \to 0$*. If* $|f| \leq M$ *on* ∂D*, then* $|f| \leq M$ *on* D*.*

Theorem B.0.4 (Phragmén–Lindelöf version 2)**.** *Suppose* D *is symmetric about the positive real axis with opening angle* π/ρ *(i.e.* $\pi/(2\rho)$ *in each half-plane), and* $f \leq M$ *on* ∂D *satisfies*

$$M(r) \overset{as}{<} e^{(\tau+\epsilon)r^\rho}$$

for all $\epsilon > 0$*. Then setting* $z = re^{i\theta}$*, we have*

$$|f(z)| \leq Me^{\tau r^\rho \cos\rho\theta}, \quad \forall\, z \in D.$$

Theorem B.0.5 (Phragmén–Lindelöf version 3)**.** *Suppose* D *is the upper half plane and* $|f| \leq M$ *on* $\mathbb{R}$ *satisfies*

$$M(r) \overset{as}{<} e^{(\tau+\epsilon)r^\rho}$$

[3] Because of the special properties of Paley–Wiener functions, it will be equivalent to say that $f(z) = O(e^{(\tau+\epsilon)|z|})$ for any $\epsilon > 0$.

for all $\epsilon > 0$. *Then*

$$|f(z)| \leq Me^{\tau(\Im z)}, \quad \forall\, z \in D.$$

By symmetry, if $|f| \leq M$ is an EFET-τ, then it satisfies the bound

$$|f(z)| \leq Me^{\tau|\Im z|}, \quad \forall\, z \in \mathbb{C}. \tag{B.0.2}$$

These theorems allow us to prove the inequality (B.0.1) as follows:

Proof of Theorem B.0.2. Let $u_N(z) := \int_{-N}^{N} |f(z+t)|^p dt$. Then using that f is EFET-τ, and for fixed N,

$$u_N(z) \overset{as}{<} e^{p(\tau+\epsilon)|z|} \quad \text{for all } \epsilon > 0.$$

Thus u_N is an EFET-$(p\tau)$, and $u_N \leq \|f\|_p$ on $\mathbb{R}$, so by Phragmén–Lindelöf,

$$|u_N(x+iy)| \leq \|f\|_p^p e^{p\tau|y|}.$$

We may now take $N \to \infty$ obtaining

$$\int_{-\infty}^{\infty} |f(z+t)|^p \,\mathrm{d}t \leq \|f\|_p^p e^{p\tau|\Im z|}.$$

(Here the $|y|$ comes from considering the upper/lower half planes separately). □

In addition, these Paley–Wiener spaces are complete with respect to the L^p norm:

Theorem B.0.6 (PW_π^p is complete, [Lev96])**.** *Let* $f \in PW_\pi^p$, *then the estimate*

$$|f(z)| \leq \|f\|_p \left[\frac{1}{p\pi^2}(e^{p\pi} - 1)\right]^{1/p} e^{\pi|y|}$$

holds, and in particular $(PW_\pi^p, \|\cdot\|_p)$ *is complete.*

Proof. Since $|f|^p$ is subharmonic (see [Lev96]), it satisfies a Mean Value Property: For $x \in \mathbb{R}$, using Plancherel–Pólya for $z = iy$, and integrating along a strip containing $\mathbb{R}$ we have

$$\begin{aligned} |f(x)|^p &\leq \frac{1}{\pi} \int_{|Im\xi|<1} |f(x+\xi)|^p dA_\xi \\ &\leq \frac{1}{\pi} \int_{-1}^{1} \|f\|_p^p e^{p\pi|y|} dy \\ &= \frac{2\|f\|_p^p}{p\pi^2}\,(e^{p\pi} - 1) =: M, \end{aligned}$$

so by Phragmén–Lindelöf, $|f| \leq M^{1/p} e^{\pi|y|}$.

Therefore if $f_n \in PW_\pi^p$ is Cauchy with respect to the L^p norm, then on compact sets since $|y|$ is bounded, $f_n \to f$ uniformly (where f is pointwise defined). This function satisfies $|f(z)| \leq Ce^{\pi|z|}$ and therefore $f \in PW_\pi^p$. □

Since in fact $|f|$ is bounded on $\mathbb{R}$, the norm $\|f\|_{B_\pi} := \sup_{\mathbb{R}} |f(x)|$ (after Bernstein) is sometimes used, which also makes PW_π^p a Banach space ([Lev96, p. 150]).

The Plancherel–Pólya result B.0.2 is a bound on the integral of a Paley–Wiener function in terms of its norm. A similar result holds in the discrete case, which will lead to the natural sinc basis for Paley–Wiener spaces.

Theorem B.0.7 (Plancherel–Pólya version 2, [Lev96, p. 152]). *Let $f \in PW_\pi^p$, then*

$$\sum_{n=-\infty}^{\infty} |f(n)|^p \leq C_p \|f\|_p^p.$$

If $1 < p < \infty$ then

$$\|f\|_p \leq C_p \left(\sum_{n=-\infty}^{\infty} |f(n)|^p \right)^{1/p}.$$

Conversely, given $\{c_n\} \in l^p$, the series

$$f(z) := \sum_{n=-\infty}^{\infty} (-1)^n c_n \frac{\sin \pi z}{\pi(z-n)}$$

converges in L^p, and satisfies $f(n) = c_n$.

As a result, we have a representation Theorem for PW_π^p; such that any function can be written in a sinc basis:

Corollary B.0.8 (Representation of PW_π^p for $1 < p < \infty$). *The map $L : l^p \to PW_\pi^p$ defined by*

$$\{c_n\} \mapsto \sum_{n=-\infty}^{\infty} (-1)^n c_n \frac{\sin \pi z}{\pi(z-n)}$$

is an isomorphism of l^p and PW_π^p.

Another way of phrasing this result is noting that a function in PW_π^p is uniquely determined by it's values at the integers[4].

Let us now look at the Fourier transform representation of PW_π^p as highlighted by the classical theorem of Paley and Wiener. In view of our discussion here, the following two characterisations are equivalent. The latter in [Rud91] uses the space of distributions. We recall that the Fourier transform of any compactly supported distribution is an analytic function, and that if $g \in L^2(\mathbb{R})$ then the *a-priori* distribution $\mathcal{F}^{-1}g$, is also in $L^2(\mathbb{R})$.

[4]The cases where $0 < p \leq 1$ are considered in [Eof95], and are given in terms of the discrete Hardy Spaces, and indeed $PW_\pi^p \cong H^p(\mathbb{Z})$.

Theorem B.0.9 (Paley–Wiener Theorem, [Lev96]). *A function $g = \hat{\psi}$ for some $\psi \in L^2(a,b)$ if and only if g is EFET $\max\{|a|,|b|\}$ and $g \in L^2(\mathbb{R})$.*

Theorem B.0.10 (Paley–Wiener Theorem, [Rud91]). *Let $\psi \in \mathcal{D}'(\mathbb{R}^n)$ with support in $B_s(0)$ (and of order N). Defining the distribution $g := \hat{\psi}$ to be the extension to the complex space $\mathbb{C}^n$ ([Rud91][p. 199]). Then g is entire, and the estimate*

$$|g(z)| \leq C(1+|z|)^N e^{s|\Im(z)|} \tag{B.0.3}$$

is satisfied.

Conversely, if an entire function g satisfies (B.0.3) for some constants C and N, then $g = \hat{\psi}$ for some $\psi \in \mathcal{D}'(\mathbb{R}^n)$ with support in $B_s(0)$.

For the statement of this Theorem, we have used the following fact from [Rud91, p.164]: that a distribution of compact support has finite order. Therefore it follows that the hypothesis of Theorem B.0.10 is automatically satisfied, when $g = \hat{\psi}$ is a Paley–Wiener function. Also, the estimate (B.0.3) implies that g is of exponential type s. In this thesis, we have used the following one-dimensional statement of this result:

Lemma B.0.11. *If $\psi \in \mathcal{D}'(\mathbb{R}^n)$ with support in $[-\pi,\pi]$. Then*

$$|\hat{\psi}(z)| \leq C(1+|z|)^N e^{\pi|\Im(z)|}.$$

In particular, $|\hat{\psi}(z)| \leq C(1+|z|)^N e^{\pi|z|} \overset{as}{<} e^{(\pi+\epsilon)|z|}$ for all $\epsilon > 0$, and so $\hat{\psi}(z)$ is an EFET-π.

Finally, let us deduce the following equivalent characterisation of the Paley–Wiener space from the Paley–Wiener Theorem:

Theorem B.0.12. *The space PW_π^p is equal to*

$$\mathcal{A} := \{g : \mathbb{C} \to \mathbb{C} : g = \hat{\psi},\ \text{for some } \psi \in \mathcal{D}'(\mathbb{R}) \text{ with support on } [-\pi,\pi],\ \text{and s.t. } g|_{\mathbb{R}} \in L^p(\mathbb{R})\}$$

Proof. By Lemma B.0.11, if $g \in \mathcal{A}$, then it is an EFET-π. As it is the Fourier transform of a distribution, g is an entire function, and the other properties hold.

Conversely, if $g \in PW_\pi^p$, we need to show that the estimate $|g(z)| \leq C(1+|z|)^N e^{\pi|\Im(z)|}$ holds. Indeed, by Theorem B.0.6,

$$|g(z)| \leq Ce^{\pi|\Im(z)|} \leq C(1+|z|)^N e^{\pi|\Im(z)|},$$

and the result follows by B.0.10. □

These characterisation results can be extended to more general Paley–Wiener spaces, and some of these are given in [Boa54]. For this thesis, we have dealt with the reflexive case, $p = 2$, as the regularity for our boundary data. We conclude with two analogues for $p \neq 2$.

Theorem B.0.13 ([Boa54, p. 107]). *Let $1 < p < 2$. Then $g(z) \in PW_\pi^p$ implies that $g = \hat{\psi}$ for some $\psi \in (L^p)^*$, the conjugate space of L^p. Alternatively, if $\psi \in (L^p)^*$ for $2 < p < \infty$ then $g := \hat{\psi} \in PW_\pi^p$.*

Theorem B.0.14 ([Boa54, p.107]). *Fix $p > 1$, then $g \in PW_\pi^p$ if and only if*

$$g(z) = z \int_{-\pi}^{\pi} [\psi(t) - \psi(-t)] e^{izt} \, \mathrm{d}t - 2 \frac{\psi(\pi)}{z} \sin \pi z$$

for some continuous function ψ of period 2π such that $\sum |n\hat{\psi}(n)|^p < \infty$.

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