Computation of Scattering Matrices and their Derivatives for Waveguides

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Abstract
This paper describes the calculation of the stationary scattering matrix and its derivatives for Euclidean waveguides. This is an adaptation and extension to a procedure developed by Levitin and Strohmaier which was used to compute the stationary scattering matrix [1]. On Euclidean waveguides, the scattering matrix can be meromorphically continued from the complex plane to a Riemann surface with a countably infinite number of sheets. We describe in detail how we have dealt with this. In addition, our algorithm is also able to calculate arbitrarily high derivatives. In the final section, we will present the results of some numerical calculations obtained using this method.

Keywords: scattering matrix, scattering theory, waveguide, resonances

1 Introduction
Over the course of this paper, a new method to calculate the stationary scattering matrix, and its derivatives, on Euclidean waveguides with cylindrical ends will be presented. The stationary scattering matrix describes the outcome of a scattering event; the scattering of a wave packet originating at infinity. In any such event, a proportion of an incoming wave packet will be transmitted and a proportion reflected; the coefficients of the scattering matrix contain this information. Waveguides are piecewise path connected subsets of $\mathbb{R}^n$, that can be written as the union of a compact domain and non-compact, cylindrical ends. The compact and non-compact parts share a common boundary. The ends can be thought of as the Cartesian product of the boundary with the positive real half-line. A notable feature of Euclidean waveguides is that the scattering matrix admits a meromorphic continuation to a certain Riemann surface with a countably infinite number of sheets [2]. In order to construct this meromorphic continuation, one usually first constructs a meromorphic continuation of the resolvent for the Laplace operator. To do this, we will use a well known glueing construction (see for example [3]) which we adapt to waveguides. The construction makes use of the meromorphic Fredholm theorem and the fact that the resolvent, for the Neumann Laplace operator on the ends of the waveguide, can be easily computed as an integral kernel. The resolvent can then be used to construct generalised eigenfunctions and, from them, the scattering matrix.

The Neumann to Dirichlet map is a vital component of this algorithm and we make heavy use of the fast, efficient method developed by Levitin and Marletta [4] to compute it. They were able to formulate the Neumann to Dirichlet map in terms of an infinite sum of Dirichlet data of Neumann eigenvalues. The advantage of this method is that the computation of the Dirichlet data of Neumann eigenvalues, the most computationally costly step, has to be performed only once. We will also show that the scattering matrix, as well as its derivatives, can be obtained from this data directly. Levitin and Strohmaier have already used this technique to obtain the scattering matrix on finite volume, non-compact
hyperbolic surfaces [1]. Due to the more complicated nature of the Riemann surface and the fact that the rank of the scattering matrix jumps each time the spectrum is crossed, the problem determining the scattering matrix for waveguides is more complex.

Being in possession of a fast and efficient algorithm to compute the scattering matrix and its derivatives enables the calculation of resonances which we define to be poles of the scattering matrix. We are able to do this using a combination of numerical contour integration and Newton’s method. The time delay and scattering length can also be computed from the scattering matrix.

Evans, Levitin and Vassiliev’s 1994 paper [5] proved the existence of embedded eigenvalues for the Neumann Laplacian on two dimensional waveguides with an obstacle and/or deformation of the waveguide, so long as the domain has cross-sectional symmetry. This was further generalised to waveguides with cylindrical ends by Davies and Parnovski [6]. Parnovski and Levitin have, amongst others, produced two other papers on this topic [7] [8]. Embedded eigenvalues can be calculated numerically with this method and we have included some examples. The main focus for our numerical experiments, however, has been on complex resonances.

Levitin and Marletta [4] and Aslanyan, Parnovski and Vassiliev [9], were able to compute complex resonances for a collection of domains. In Levitin and Marletta’s case, they computed embedded eigenvalues for a domain with cross-sectional symmetry and observed them decaying to complex resonances when a small perturbation destroyed that symmetry. We have been able to replicate their results for the same domains with our method, making a slight improvement on accuracy. We have also performed some additional numerical experiments, the results of which are presented at the end of the paper.

2 Waveguides

Let $M$ be the waveguide; it is embedded in $n$ dimensional Euclidean space with $K$ cylindrical ends. $M$ can be written as $M = E \cup X$, where $X$ is a compact, piecewise connected manifold, with piecewise smooth Lipschitz boundary and

$$E = \Gamma \times \mathbb{R}_+ = \bigcup_{k=1}^{K} [\Gamma_k \times \mathbb{R}_+] = \bigcup_{k=1}^{K} E_k.$$  

$\Gamma_k \subset \mathbb{R}^{n-1}$ is compact and connected domain, with smooth boundary, and for any $i \neq j$,

$$[\Gamma_i \times \mathbb{R}_+] \cap [\Gamma_j \times \mathbb{R}_+] = \emptyset.$$  

Define

$$E_k = \Gamma_k \times \mathbb{R}_+, \quad \text{and} \quad \Gamma = E \cap X = \{0\} \times \Gamma = \bigcup_{k=1}^{K} \{\{0\} \times \Gamma_k\}.$$  

We will call the boundary of $M$, $\Sigma$. 


Separation of variables allows us to write,

\[ L^2(E) \cong L^2(\mathbb{R}_+ ) \otimes L^2(\Gamma) . \]

\( \Delta_E \) can be written in the form

\[ \Delta_E = -\frac{\partial^2}{\partial x^2} \otimes 1 - 1 \otimes \Delta_\Gamma , \]  \hspace{1cm} (1)

where \( \Delta_\Gamma \) is the Laplace operator on \( \Gamma \subset \mathbb{R}^{n-1} \). The compactness of \( \Gamma \) means that \( L^2(\Gamma) \) has an orthonormal basis, consisting of eigenfunctions of \( (\Delta_\Gamma - \lambda)^{-1} \), thus we can say

\[ L^2(\Gamma) \cong \bigoplus_{j=0}^{\infty} \mathbb{C} = l^2 . \]

We conclude that

\[ L^2(E) \cong L^2(\mathbb{R}_+) \otimes L^2(\Gamma) \cong L^2(\mathbb{R}_+) \otimes l^2 \cong \bigoplus_{j=0}^{\infty} L^2(\mathbb{R}_+) . \]  \hspace{1cm} (2)

\( (\Delta_{E_j} - \lambda) \) acts on each summand by \( -\frac{\partial^2}{\partial x^2} - \lambda + \mu_j \), and the \( \mu_j \) are the, not necessarily distinct, Neumann eigenvalues of \( \Delta_\Gamma \), enumerated in ascending order and repeated with multiplicity taken into account. We shall henceforth refer to each of the summands as **modes**. \( \Delta_{E_j} - \lambda \) acts on each mode as multiplication by \( \xi^2 - \lambda + \mu_j \) in the spectral representation.

The integral kernel for the Neumann resolvent on a half-line comes about after a simple calculation. If we take the domain be \( \mathbb{R}_+ \) with Neumann boundary conditions at 0, the kernel of the resolvent is of the form

\[ \frac{-e^{i|y|\sqrt{\lambda}}}{4i\sqrt{\lambda}} + \frac{-e^{i|x-y|\sqrt{\lambda}}}{4i\sqrt{\lambda}} . \]  \hspace{1cm} (3)

We should take note of the fact that when \( x \neq y \) the kernel is holomorphic when defined as a function of \( \lambda \) in the branch of the square root where \( \text{Im}(\sqrt{\lambda}) > 0 \). The anti-diagonal
2.1 A description of the domain of our resolvent function

doesn’t cause problems, because $x$ and $y$ are non-negative. Due to the ellipticity of $(\Delta - \lambda)$, elliptic boundary regularity can be invoked to show that the resolvent kernel is smooth away from the diagonal also.

The resolvent for $\Delta_E$, written as it is in \([1]\), can now be written as

$$R_0(\lambda) = \bigoplus_j r^j(\lambda),$$

where $r^j(\lambda) = \frac{1}{\xi^2 + \mu_j - \lambda}$ in the spectral representation. This means that equation \([3]\) can be slightly modified to give the kernel on each mode as

$$r^j(\lambda) = \frac{-e^{i|x+y|\sqrt{\lambda - \mu_j}}}{4i\sqrt{\lambda - \mu_j}} + \frac{-e^{i|x-y|\sqrt{\lambda - \mu_j}}}{4i\sqrt{\lambda - \mu_j}}.$$  \((5)\)

The existence of square roots, and their branches, adds extra complexity to this resolvent kernel. Rather than talking about $R_0(\lambda)$ as being defined on $\mathbb{C}$, we must instead talk about it being defined on a Riemann surface $Z$, on which it is single valued function of $\lambda$. See \([2]\).

2.1 A description of the domain of our resolvent function

In the style of Christiansen we have denoted the the Neumann eigenvalues, enumerated in ascending order with multiplicity taken into account, by $\{\mu_j\}$ of $\Gamma$ and where repeated entries are removed by $\{\eta_j\}$ \([2, \text{Page} 5]\). The reason for this is that for each $j \in \mathbb{N}$ corresponds to a branch point for $\sqrt{\lambda - \eta_j}$. A complete description of this has already appeared in the paper by Guilloupé \([10]\), we will, nevertheless, present a brief overview here.

As seen in the last section, the resolvent is made up of the direct sum of the $r^j(\lambda)$, acting on the direct sum of $L^2$ spaces; equation \([5]\). The Riemann surface for each individual summand that makes up this resolvent will have a branch at each of the $\eta_j$. We define the physical sheet of $Z$ to be the sheet of the surface, which can be identified with $\mathbb{C} \setminus \mathbb{R}_+$, for which all the $\sqrt{\lambda - \eta_j}$, have positive imaginary part and identify it with $\mathbb{C} \setminus \mathbb{R}_+$. The whole surface $Z$ is made up of a countable number of “sheets” of this nature, each of which represents a choice as to whether each $\sqrt{\lambda - \eta_j}$ has a strictly positive imaginary part or not.

For any sheet of $Z$, the full resolvent $R(\lambda)$ admits a meromorphic continuation from the physical sheet onto it. The resolvent is analytic on the physical sheet for values of $\lambda$ where it is indeed the resolvent operator and not just a continuation of it. The monodromy theorem can be used to extend the resolvent for the ends along a path to a desired non-physical sheet and then a series of “glueing” constructions and the meromorphic Fredholm theorem are used to prove the existence of a meromorphic continuation of the resolvent to the whole waveguide (this can be found in more detail in Melrose’s text and Guillopé’s paper \([10]\)\([3]\)). When we wish to extend the resolvent from the physical sheet to other sheets, we must do so along a path. As each sheet is simply connected, $\gamma$ to $\lambda$ maybe extended in only one homotopy-equivalent way, meaning that once the resolvent is continued meromorphically along $\gamma$, we can uniquely continue it to a neighborhood of any point on the same sheet without ambiguity. It is necessary to have some kind of a coherent system to categorise such paths.

A path in $Z$ will remain a path in $\mathbb{C} \setminus \{\eta_j\}$ under the covering projection $p$. Similarly, a
path in $\mathbb{C}\setminus\{\eta_j\}$, lifts to a path in $Z$ if the location of the pre-image of one of the endpoints is known (or given). We note that paths crossing of the intervals $(\eta_j, \eta_{j+1})$ on the real line in $\mathbb{C}\setminus\{\eta_j\}$, correspond with crossings of the boundaries between sheets in $Z$. This means that homotopy equivalent paths in $Z$, originating in the physical sheet, paths in $\mathbb{C}\setminus\{\eta_j\}$ and sheets of $Z$ are all in one-to-one correspondence with each other.

Each class of paths in $\mathbb{C}\setminus\{\eta_j\}$ can be indexed by a finite subset of $\mathbb{N}$, $J$ constructed by counting the number of times the path crosses the $n^{th}$ interval mod 2. Equivalently $J$ may be defined as follows:

$$J = \{j \in \mathbb{N} : \text{Im}(\sqrt{\lambda - \mu_j}) \leq 0\}. \quad (6)$$

Figure 2: Inequivalent paths that lift to paths with endpoints in sheets $(1, 2, 3, 4)$, $(1, 3, 4)$, and $(1)$, of $Z$ respectively.

3 Generalised Eigenfunctions and the Scattering Matrix

Let $\chi$ be a function on $M$ with support on $E$ equal to 1 outside a compact set and fix an orthonormal basis of Neumann eigenfunctions of $\Delta_\Gamma$, namely $\{\nu_j(y)\}$. As was said before, we may identify this sheet with $\mathbb{C}\setminus\min_{j \in J}[\mu_j, \infty)$. We will generally be working with either the physical sheet of $Z$, or the sheet defined by $J$ which we shall refer to as the non-physical sheet from now on. When identified in this way, every $\lambda$ in the non-physical sheet of $Z$ has its counterpart in the physical sheet which is identical as a complex number. Once we fix a sheet, denoted by equation 6 and extend our resolvent along a path to it from the physical sheet, we can assume that the resolvent is meromorphic on the whole sheet.

We can now introduce:

$$\varphi_J(\lambda, x, y) = \sum_{j \in \mathbb{N}} \chi e^{-i\sqrt{\lambda - \mu_j} x} \nu_j(y) - R(\lambda) \left[ (\Delta - \lambda) \left( \chi e^{-i\sqrt{\lambda - \mu_j} x} \nu_j(y) \right) \right]. \quad (7)$$
for \( \lambda \) in the physical sheet, and for the non-physical sheet:

\[
\varphi_J(\lambda, x, y) = \sum_{j \notin J} \chi e^{-i\sqrt{\lambda - \mu_j x}} \nu_j(y) - R(\lambda) \left( (\Delta - \lambda) \left( \chi e^{-i\sqrt{\lambda - \mu_j x}} \nu_j(y) \right) \right)
\]

This is a Generalised Eigenfunction, as it is a solution of \((\Delta - \lambda) \varphi_J(\lambda, x, y) = 0\), but not an \(L^2\) solution. It should be pointed out that the above equation is not already zero. The reason for this is that \(R(\lambda)\), unless \(\lambda\) is on the physical sheet, is a meromorphic continuation of the resolvent and not the resolvent itself. When \(\lambda\) is in the physical sheet, the resolvent is only an inverse of \((\Delta - \lambda)\) for \(L^2\) functions. These functions have a number of properties:

**Proposition 1.**

1. \(\varphi_J(\lambda, x, y)\) is a meromorphic function of \(\lambda\) for any \(\lambda \in \mathbb{Z}\) and holomorphic if \(\lambda\) is in the physical sheet.

2. For \(j \in J\) and \(\lambda\) in the physical sheet of \(\mathbb{Z}\);

\[
R(\lambda) \left( (\Delta - \lambda) \left( \chi e^{-i\sqrt{\lambda - \mu_j x}} \nu_j(y) \right) \right) \in L^2(\mathbb{R}_+). \tag{8}
\]

3. There exists a unique, meromorphic \(S_{J,j,k}(\lambda)\) such that on \(E\), and with \(\lambda\) in the physical sheet;

\[
\varphi_J(\lambda, x, y) = \sum_{j \in J} \left( e^{-i\sqrt{\lambda - \mu_j x}} \nu_j(y) + \sum_{k \in J} S_{J,j,k}(\lambda) e^{i\sqrt{\lambda - \mu_k x}} \nu_k(y) \right) \tag{9}
\]

and

\[
\varphi_J(\lambda, x, y) = \sum_{j \notin J} \left( e^{-i\sqrt{\lambda - \mu_j x}} \nu_j(y) + \sum_{k \in J} S_{J,j,k}(\lambda) e^{-i\sqrt{\lambda - \mu_k x}} \nu_k(y) \right) \tag{10}
\]

for \(\lambda\) in the non-physical sheet. In the case where \(\lambda\) is in the physical sheet, the \(S_{J,j,k}(\lambda)\) are holomorphic.

**Proof.**

1. Follows from the meromorphicity of the various functions whose products make up \(\varphi_J(\lambda, x, y)\).

2. This is due to the square integrability of the resolvent kernels in the physical sheet.

3. Observe that for any \(j \in J\), each summand in equation 7 becomes zero when acted upon by \((\Delta - \lambda)\). Using a simple separation of variables on \(E\) we see that any solution to \((\Delta - \lambda) F(\lambda, x, y) = 0\), including the one we have, will be of the form,

\[
\sum_{k=1}^{\infty} \left( A_{j,k}(\lambda) e^{-i\sqrt{\lambda - \mu_k x}} + B_{j,k}(\lambda) e^{i\sqrt{\lambda - \mu_k x}} \right) \nu_k(y). \tag{11}
\]
We can see that in part 2) of the proposition, the requirement that when we subtract \( \chi e^{-i\sqrt{\lambda^2 - \mu_k^2}}\nu_j(y) \) the result be square integrable, means that \( A_{j,k} = \delta_{j,k} \).

In order to reconcile equation 11 with equation 7, we call the \( B_{j,k}(\lambda),/S_{j,j,k}(\lambda) \) for \( k \in J \). For \( k \notin J \) we see that the remaining terms;

\[
B_{j,k}(\lambda)e^{+i\sqrt{\lambda^2 - \mu_k^2}}
\]  

are all square integrable as \( k \notin J \Rightarrow \text{Im}(\sqrt{\lambda - \mu_k}) > 0 \).

When we sum the all such summands to get \( \varphi(\lambda, x, y) \), as described in equation 4 we get

\[
\sum_{j \in J} \left( e^{-i\sqrt{\lambda^2 - \mu_j^2}}\nu_j(y) + \sum_{k \in J} S_{j,j,k}(\lambda)e^{i\sqrt{\lambda^2 - \mu_k^2}}\nu_k(y) \right) + \sum_{k \notin J} \sum_{j \in J} B_{j,k}(\lambda)e^{i\sqrt{\lambda^2 - \mu_k^2}}\nu_k(y),
\]

where we can define, for \( j \notin J \), \( T_j(\lambda) = \sum_{k \in J} B_{k,j}(\lambda) \) to finish. The result for the non-physical sheet is due to meromorphic continuation.

Those used to dealing with the dynamic scattering matrix defined, for example, in Reed-Simon, should be aware that the two definitions can be proved to be equivalent. A fundamental property of the generalised eigenfunctions and scattering matrix are their uniqueness in the \( L^2 \) norm. This means that \( S(\lambda) \) is also uniquely determined by the geometry of \( M \) the choice of basis for the \( J \) Neumann eigenfunctions and \( J \subset \mathbb{N} \) itself.

For any given \( \lambda \) in the non-physical sheet of \( Z \) given by \( J \) and identified with a suitable subset of the complex plane we shall denote its counterpart in the physical sheet by \( \lambda^* \).

**Theorem 2.** \( S_J(\lambda^*) = \overline{S_J^{-1}(\lambda)} \)

**Proof.** Observe that

\[
\langle \Delta \varphi_J(\lambda, x, y), \varphi_J(\lambda, x, y) \rangle - \langle \varphi_J, \Delta \varphi_J \rangle = (\lambda - \overline{\lambda})\langle \varphi_J, \varphi_J \rangle \neq 0.
\]

The right hand side of the equation above, namely the \( \langle \lambda - \overline{\lambda} \rangle \) is not an issue, as \( \lambda \) is simply a number in this context and the \( \overline{\lambda} \) will be in the same sheet of \( Z \) as \( \lambda \).

Green’s second identity can now be invoked to give that

\[
\int_{\Gamma} \left( \frac{\partial \varphi_J(\lambda^*, x, y)}{\partial n} \overline{\varphi_J(\lambda^*, x, y)} - \varphi_J(\lambda^*, x, y) \frac{\partial \overline{\varphi_J(\lambda^*, x, y)}}{\partial n} \right) = 0.
\]

In particular, this means that

\[
\sum_{j,k \in J} i\sqrt{\lambda^2 - \mu_k^2}(\delta_{k,j} - S_{j,j,k}(\lambda^*)) \sum_{l,m \in J} \left( \delta_{l,m} + \overline{S_{l,m}(\lambda)} \right) \int_{\Gamma} \nu_k(y)\nu_l(y) = 0
\]

\[- \sum_{j,k \in J} (\delta_{k,j} + S_{j,j,k}(\lambda^*)) \sum_{l,m \in J} -i\sqrt{\lambda^2 - \mu_l}(\overline{S_{l,m}(\lambda)} - \delta_{l,m}) \int_{\Gamma} \nu_k(y)\nu_l(y) = 0 \]

\[\sum_{j,k \in J} i\sqrt{\lambda^2 - \mu_k^2}(\delta_{k,j} - S_{j,j,k}(\lambda^*)) \sum_{l,m \in J} \left( \delta_{l,m} + \overline{S_{l,m}(\lambda)} \right) \int_{\Gamma} \nu_k(y)\nu_l(y) = \]

\[- \sum_{j,k \in J} (\delta_{k,j} + S_{j,j,k}(\lambda^*)) \sum_{l,m \in J} i\sqrt{\lambda^2 - \mu_l}(\overline{S_{l,m}(\lambda)} - \delta_{l,m}) \int_{\Gamma} \nu_k(y)\nu_l(y) = 0 \]
From this, we obtain

\[ \sum_{k,j,m \in J} \left( (S_{j,k}(\lambda^*) - \delta_{k,j}) (\delta_{k,m} + S_{j,m,k}(\lambda)) + (\delta_{k,j} + S_{j,k}(\lambda^*)) (\overline{S_{j,m,k}(\lambda)} - \delta_{k,m}) \right) = 0 \]

This is due to the orthonormality of the \( \{\nu_j\} \) and the way in which we have identified our sheet of \( Z \) with a \( C \). Multiplying these out and simplifying shows that, for fixed \( j,m \in J \),

\[ \sum_{k \in J} S_{j,k}(\lambda^*) S_{j,m,k}(\lambda) = \delta_{j,m}. \]

Since \( S_{j}(\lambda) \) and \( S_{j}(\overline{\lambda}) \) are, by construction, the same when \( \lambda \) and \( \overline{\lambda} \) are in the same sheet of \( Z \) the result follows.

4 The Neumann to Dirichlet map

The Neumann to Dirichlet map will be a vital intermediate step between the resolvents, which we have extensively covered, and the scattering matrix. In our case it is significant, because it can be easily numerically computed using finite element techniques on the internal domain, and is known for the “ends”. As usual, let \( X \) be a Lipschitz domain in \( \mathbb{R}^n \), \( n \geq 2 \). Define the map

\[ N : H^{-1/2}(\partial X) \to H^{1/2}(\partial X) \]

acting on \( g \in H^{-1/2}(\partial X) \) by

\[ Dg = \varphi|_{\partial X}, \]

where \( \varphi \) is the solution to the Neumann problem, with \( g \) as the boundary derivative. This is the inverse of the Dirichlet to Neumann map

\[ D : H^{1/2}(X) \to H^{-1/2}(X), \]

whose action on \( f \in H^{1/2} \) is \( Df = \frac{\partial}{\partial n}(HF) \). \( H \) is an extension of \( f \) to a solution of \((\Delta - \lambda)(Hf) = 0 \) on \( X \). \[11\]

4.1 Calculating the Neumann to Dirichlet map

It is known that the Neumann eigenvectors of \((\Delta - \lambda) \) on \( \Gamma \) form an orthonormal basis of \( L^2(\Gamma) \), with Neumann eigenvalues \( \mu_j, j \in \mathbb{N} \). \[12\] Given a basis of \( L^2(\Gamma) \), we may compute the Neumann to Dirichlet map in matrix form. This is the first step towards viewing the Neumann to Dirichlet map as a concrete, computable object. Given the correspondence between the Neumann to Dirichlet map, the scattering matrix and the resolvent, computing the Neumann to Dirichlet map in this way allows us to realize these other objects in a similar manner.

Definition 3. Neumann to Dirichlet map, associated to \((\Delta - \lambda) \) on a basis

Let us consider an ordered orthonormal basis of \( L^2(\Gamma) \), \( \{\nu_j\}_{j=0}^\infty \), and \( \varphi_k \), such that

\[ (\Delta - \lambda)\varphi_k = 0, \quad \frac{\partial \varphi}{\partial n}|_{\Sigma} = 0, \quad \frac{\partial \varphi_k}{\partial n}|_{\Gamma} = \nu_k. \]  \[13\]

Then the \( k, l \)th element of the Neumann to Dirichlet map, in matrix form, with respect to basis \( \{\nu_k\} \), will be given by

\[ \langle \varphi|_{\Gamma}, \nu_l \rangle_{L^2(\Gamma)}. \]

Obviously, when doing this calculation practically, we must truncate after a finite number of entries; say \( P \in \mathbb{N} \), to get a \( P \times P \) matrix, giving the first \( P \) rows and columns of the infinite dimensional matrix.
4.2 The Levitin-Marletta method for indirect calculation of the Neumann to Dirichlet map

This technique was devised by Levitin and Marletta in their paper [4]. The following formula for the \( k, l \)th entry of \( N \) acting on basis of the Neumann subspace of \( \mathcal{L}^2(\Gamma) \), \( \{\phi_i\}_{i=1}^\infty \) is taken from their paper where it is derived.

\[
N_{k,l}(\lambda) = \sum_{m=1}^{\infty} \frac{1}{\lambda - \mu_m} \langle \phi_k, U_m | \Gamma \rangle_{\mathcal{L}^2(\Gamma)} \langle U_m | \Gamma, \phi_l \rangle_{\mathcal{L}^2(\Gamma)}. \quad (14)
\]

\( U_m \) and \( \mu_m \) are the eigenfunctions and eigenvalues of the homogeneous Neumann problem on \( X \), namely the solutions to:

\[
(\Delta - \mu_m)U_m = 0, \quad \frac{\partial U_m}{\partial n} |_{\partial X} = 0.
\]

Equation (14) gives us a method to compute \( N_{k,l} \). It is a significant improvement over direct calculation, as once we have obtained the eigenvalues and Fourier coefficients of their associated eigenfunctions, computing \( N(\lambda) \), for any \( \lambda \) we wish, now only involves matrix multiplication and not numerical solutions of PDEs. Levitin and Marletta presented a simple trick/method to further improve the rate of convergence, or accuracy given a fixed number of eigenvalues and eigenfunctions; the derivation of this can also be found in their paper. Where \( \lambda \) is fixed and \( N_{k,l}(\tilde{\lambda}) \) a directly computed Neumann to Dirichlet map we get:

\[
N_{k,l}(\lambda) = N_{k,l}(\tilde{\lambda}) + \sum_{m=1}^{\infty} \frac{\lambda - \lambda}{\mu_m^2 - \lambda \mu_m - \lambda \mu_m + \lambda^2} \langle \nu_k, U_m | \Gamma \rangle_{\mathcal{L}^2(\Gamma)} \langle U_m | \Gamma, \nu_l \rangle_{\mathcal{L}^2(\Gamma)}. \quad (15)
\]

This now gives, quadratic, as opposed to linear convergence. This process can be repeated as many times as one desires to further increase the speed of convergence. In practice, to do this once is sufficient and any repetitions if this process would greatly complicate our extension of this algorithm used for calculating derivatives of the scattering matrix.

4.3 Calculating the \( S \) matrix

In this section, we will describe the method for constructing generalised eigenfunctions, then the scattering matrix and its derivatives from the Neumann to Dirichlet map. As usual, we fix a sheet of \( Z \) and define \( J \), the indexing set, to be the \( j \in \mathbb{N} \) such that \( \text{Im}(\sqrt{\lambda - \mu_j}) < 0 \). We can proceed as follows:

**Definition 4.** Define

\[
P : \mathcal{L}^2(\Gamma) \to \mathcal{L}^2(\Gamma),
\]

to be the projection whose kernel spanned by the Neumann eigenfunctions of \( \Gamma \) associated to \( \mu_j \) for \( j \in \mathbb{J} \).

Fix a basis \( \{\nu_j(y)\} \) for the space of Neumann eigenfunctions on \( \Gamma \), with corresponding to Neumann eigenvalues \( \mu_j \).

Proposition [4] tells us that that the generalised eigenfunction on the cylindrical ends \( E \) of \( M \), with homogeneous Neumann boundary conditions on the boundary will be of the form:

\[
\varphi_J(\lambda, x, y) = \sum_{j \in J} \left( e^{-i\sqrt{\lambda - \mu_j} x} \nu_j(y) \right) + \sum_{k \in J} S_{j,k}(\lambda) e^{i\sqrt{\lambda - \mu_k} x} \nu_k(y) \right) + \sum_{j \in \mathbb{N} \setminus J} T_j(\lambda) e^{i\sqrt{\lambda - \mu_j} x} \nu_j(y),
\]
4.3 Calculating the $S$ matrix

At $x = 0$, $\varphi_J(\lambda, x, y)$ will be of the form

$$\varphi_J(\lambda, 0, y) = \sum_{j \in J} \nu_j(y) + \sum_{k \in J} S_{J,j,k}(\lambda)\nu_k(y) + \sum_{j \in \mathbb{N} \setminus J} T_j(\lambda)\nu_j(y).$$

At $x = 0$, the normal derivative will be of the form

$$\sum_{j \in J} \left(i\sqrt{\lambda - \mu_j}\nu_j(y)(\lambda) - \sum_{k \in J} i\sqrt{\lambda - \mu_k}S_{J,j,k}(\lambda)\nu_k(y) - \sum_{j \in \mathbb{N} \setminus J} i\sqrt{\lambda - \mu_j}T_j(\lambda)\nu_j(y)\right).$$

Let us define $D(\lambda, k), k \in \mathbb{N}$ to be the $|J| \times |J|$ acting on the set $J$ modes for which $\text{Im}(\sqrt{\lambda - \mu_j}) < 0$. For the calculation of $S_J(\lambda)$, we will only be using this with $k = 0$, in this case it’s inverse will be the Neumann to Dirichlet map on the eternal domain, or the ends. If necessary, we will sometimes abbreviate the notation $D(\lambda, k)$ to $D(k)$.

**Definition 5.**

$$D(\lambda, k) = \frac{\partial^k}{\partial \lambda^k} \begin{pmatrix} i\sqrt{\lambda - \mu_1} & \cdots & \cdots & \cdots & \cdots \\ \vdots & i\sqrt{\lambda - \mu_2} & \cdots & \cdots & \cdots \\ \vdots & \vdots & i\sqrt{\lambda - \mu_3} & \cdots & \cdots \\ \vdots & \vdots & \vdots & \ddots & \cdots \\ \vdots & \vdots & \vdots & \vdots & i\sqrt{\lambda - \mu_{|J|}} \end{pmatrix}$$

This projection $P$, acting on modes $j \in \mathbb{N} \setminus J$ and sending the rest to 0, is vital. The reason for this is because, on one hand, the Neumann to Dirichlet map on $E$, only acts on the boundary data of square integrable functions, thus we must project out the non square integrable modes of any such generalised eigenfunction beforehand. It is only in this context that $D(0)^{-1}$ is a Neumann to Dirichlet map for $(\Delta - \lambda)$ on $E$.

Now observe that the internal domain $X$ and the external domain (or ends) $E$ share a common boundary $\Gamma$. This means that, for any generalised eigenfunction defined on $M$, the action of the Neumann to Dirichlet map calculated on $X$ composed with $P$ and the Neumann to Dirichlet map calculated on $E$ should coincide.

Set

$$L = \left( PN - D(0)^{-1} P \right).$$

The matrix $L$, will have a null-space of dimension $|J|$. Each element of $\text{Ker}(L)$ can be equated with a one of the $|J|$ summands of $\varphi(\lambda, 0, y)$, as defined in equation 7 with in terms of some, possibly unknown orthonormal basis of Neumann eigenfunctions of $\Delta \Gamma$.

Applying a singular value decomposition algorithm, or some other procedure to find the kernel of a matrix, i.e. $QR$, gives $|J|$ kernel vectors.

Let $W$ the null-space of $L$

$$W = \{w^1, \ldots, w^J\}.$$
For each $\omega_j \in W$ we have a representation of a generalised eigenfunction, evaluated at 0, of the form:

$$\omega^j = \bigoplus_{j \in J} (\delta_{j,k} + S_{j,k}(\lambda)) \bigoplus_{j \in N \setminus J} T_j(\lambda).$$

(17)

We could now, in theory, extract the scattering matrix from this, but before we are able to do such things, and for our scattering matrix to be of any use to us, we need to control the basis of Neumann eigenfunctions. A numerical algorithm for singular value decomposition will not necessarily give us $S_{J}(\lambda)$ in terms of the basis we want; the basis of Neumann eigenfunction of $\Gamma$ that was carefully chosen when we began the calculation of $N(\lambda)$ in the previous section.

Having found a basis for the null space of (16), we restrict our attention to the elements of these vectors that represent the $J$ Fourier modes and discard the rest by means of application of the operator $(1 - P)\omega^j.$ The image of $W$ under both $(1 - P)$ and $(1 - P)N(\lambda)$ forms a basis in $\mathbb{R}^J.$

The linear map $\tau : \mathbb{R}^J \rightarrow \mathbb{R}^J$, defined on the $(1 - P)\omega^j$, by

$$(1 - P)\omega^j \mapsto (1 - P)N\omega^j,$$

can now be thought of as the identity map from the basis $\{(1 - P)\omega^1, \cdots, (1 - P)\omega^j\}$ of $\mathbb{R}^J$, to basis $\{(1 - P)N\omega^1, \cdots, (1 - P)N\omega^j\}$ of $\mathbb{R}^J$.

$\tau$ must be rewritten in terms of the standard basis, whose elements represent the chosen basis of the Neumann eigenfunctions of $\Gamma$. Thus, when acting our chosen basis of $L^2(\Gamma)$, $\tau$ can be written as,

$$\tau(\lambda) = \{(1 - P)N\omega^1, \cdots, (1 - P)N\omega^j\}^{-1}\{(1 - P)\omega^1, \cdots, (1 - P)\omega^J\}.$$

Now we note that applying $N$ to each $\omega_j$ gives:

$$N(\lambda)\omega^j = \bigoplus_{j \in J} \frac{S_{j,k}(\lambda) - \delta_{j,k}}{i\sqrt{\lambda - \mu_j}} \bigoplus_{j \in N \setminus J} \frac{T_j(\lambda)}{i\sqrt{\lambda - \mu_j}}.$$

One can see now that, as the map $(1 - P)N$ will take the $J \times J$ matrix form

$$\tau(\lambda) = (D(\lambda, 0) + S_J(\lambda)D(\lambda, 0))(\text{Id} + S_J(\lambda))^{-1}.$$

(18)

This means that finally

$$S_J(\lambda) = (\tau(\lambda) - D(\lambda, 0))^{-1}(-D(\lambda, 0) - \tau(\lambda)).$$

(19)

5 Derivatives of the S matrix

This section will show that an extension to the above method can be used to calculate $S_{J}^{(m)}(\lambda) = \frac{d^m}{d\lambda^m} S_J(\lambda)$. This is interesting in its own right but, in our case, calculating $S_{J}^{(m)}(\lambda)$ enable us to search for complex resonances later on using the argument principle.
5.1 A Neumann to Dirichlet map for the system on the external domain

Fix a sheet of $Z$. If $\varphi_j(\lambda, x, y)$ is a generalised eigenfunction, then

\[(\Delta - \lambda)\varphi_j(\lambda, x, y) = 0.\]

Thus, when we differentiate with respect to $\lambda$, we get

\[
\frac{\partial}{\partial \lambda}(\Delta - \lambda)\varphi_j(\lambda, x, y) = (\Delta - \lambda)\varphi'_j(\lambda, x, y) - \varphi_j(\lambda, x, y) = 0,
\]

For any $n$ we get

\[
\frac{\partial^n}{\partial \lambda^n}(\Delta - \lambda)\varphi_j(\lambda, x, y) = (\Delta - \lambda)\varphi^{(n)}_j(\lambda, x, y) - \varphi^{(n-1)}_j(\lambda, x, y) = 0,
\]

where $\varphi^{(n)}_j(\lambda, x, y)$ denotes $\frac{\partial^n}{\partial \lambda^n} \varphi_j(\lambda, x, y)$ for brevity. One can simply look for a solution to the resulting system of equations in a similar manner to equation 13.

\[
(\Delta - \lambda)\varphi_j(\lambda, x, y) = 0, \quad \frac{\partial \varphi_j}{\partial n}|_{\Sigma} = 0, \quad (20)
\]

\[
(\Delta - \lambda)\varphi'_j(\lambda, x, y) - \varphi_j(\lambda, x, y) = 0, \quad \frac{\partial \varphi'_j}{\partial n}|_{\Sigma} = 0, \quad (21)
\]

\[
\vdots \quad \vdots
\]

\[
(\Delta - \lambda)\varphi^{(n)}_j(\lambda, x, y) - \varphi^{(n-1)}_j(\lambda, x, y) = 0, \quad \frac{\partial \varphi^{(n)}_j}{\partial n}|_{\Sigma} = 0.\]

On the other hand, since $\varphi(\lambda, x, y)$ is known on $E$, we can recall equation 9 and see that

\[
\varphi_j(\lambda, x, y) = \sum_{j \in J} \left( e^{-i\sqrt{\lambda - \mu_j} y_j} + \sum_{k \in J} S_{j,k}(\lambda) e^{i\sqrt{\lambda - \mu_k} y_k} \right) + \sum_{j \notin J} T_j(\lambda) e^{i\sqrt{\lambda - \mu_j} y_j},
\]

and deduce that

\[
\varphi'_j(\lambda, x, y) = \sum_{j \in J} \left( \frac{-ix}{2\sqrt{\lambda - \mu_j}} e^{-i\sqrt{\lambda - \mu_j} y_j} + \sum_{k \in J} \left[ S'_{j,k}(\lambda) - \frac{x S_{j,k}(\lambda)}{2i\sqrt{\lambda - \mu_k}} \right] e^{i\sqrt{\lambda - \mu_k} y_k} \right)
\]

\[
+ \sum_{j \notin J} \left[ T'_j(\lambda) + \frac{ix T_j(\lambda)}{2\sqrt{\lambda - \mu_j}} \right] e^{i\sqrt{\lambda - \mu_j} y_j}, \quad (21)
\]

\[
\frac{\partial}{\partial x} \varphi'_j(\lambda, x, y) = \sum_{j \in J} \left[ \frac{-i}{2\sqrt{\lambda - \mu_j}} - x \right] e^{-i\sqrt{\lambda - \mu_j} y_j}
\]

\[
+ \sum_{j,k \in J} \left[ i \sqrt{\lambda - \mu_k} S'_{j,k}(\lambda) + \frac{i S_{j,k}(\lambda)}{2i\sqrt{\lambda - \mu_k}} - x S_{j,k}(\lambda) \right] e^{i\sqrt{\lambda - \mu_k} y_k}
\]

\[
+ \sum_{j \notin J} \left[ i \sqrt{\lambda - \mu_j} T'_j(\lambda) + \frac{i T_j(\lambda)}{2\sqrt{\lambda - \mu_j}} - x T_j(\lambda) \right] e^{i\sqrt{\lambda - \mu_j} y_j}, \quad (22)
\]

At 0 these two generalised functions become:

\[
\varphi'_j(\lambda, 0, y) = \sum_{j \in J} \left( \sum_{k \in J} S'_{j,k}(\lambda) \nu_k(y) \right) + \sum_{j \notin J} T'_j(\lambda) \nu_j(y), \quad (23)
\]

\[
\frac{\partial}{\partial x} \varphi'_j(\lambda, 0, y) = \sum_{j \in J} \left( \frac{1}{2i\sqrt{\lambda - \mu_j}} \nu_j(y) + \sum_{k \in J} \left[ i \sqrt{\lambda - \mu_k} S'_{j,k}(\lambda) - \frac{S_{j,k}(\lambda)}{2i\sqrt{\lambda - \mu_k}} \right] \nu_k(y) \right)
\]

\[
+ \sum_{j \notin J} \left( i \sqrt{\lambda - \mu_j} T'_j(\lambda) - \frac{T_j(\lambda)}{2i\sqrt{\lambda - \mu_j}} \right) \nu_j(y). \quad (24)
\]
We can now see that the Neumann to Dirichlet map for the system will be of the form
\[ \tilde{N}_1(\lambda) : l^2 \oplus l^2 \rightarrow l^2 \oplus l^2 \]

So by the fact that
\[ \frac{\partial}{\partial x} \varphi'_J(\lambda, 0, y) = D(0)\varphi'_J(\lambda, 0, y) + D(1)\varphi_J(\lambda, 0, y) \]
in addition to the fact that
\[ \frac{\partial}{\partial x} \varphi_J(\lambda, 0, y) = D(0)\varphi_J(\lambda, 0, y) , \]
We can see that
\[ \tilde{N}_1(\lambda) = \left( \frac{\partial}{\partial \lambda} \tilde{N}(\lambda) \right)^{-1} \cdot \tilde{N}(\lambda) \]

There is no reason for us to limit ourselves to first derivatives. We should go further now and do the same thing for \( \varphi_J^{(n)}(\lambda, x, y) \). It is at this point the we take note of the fact that each successive differentiation of \( e^{\pm \sqrt{x \mu x}} \) respect to \( \lambda \), produces a factor of \( x \). Since we will be focusing on \( \varphi_J \) and \( \frac{\partial}{\partial x} \varphi_J \) at the boundary, where \( x = 0 \), it is unnecessary to differentiate \( e^{\pm \sqrt{x \mu x}} \) more than once, and all terms that result from such actions, terms in these summands with a factor of \( x^2 \) will simply be denoted them as h.o.t.\

We will now introduce some new notation: \( \tilde{N}_1(\lambda) \) and \( N_1(\lambda) \) to be the Neumann to Dirichlet maps for \( \varphi_J^{(n)}(\lambda, x, y) \) on the external and internal domains respectively. Differentiating \( \varphi_J^{(n)}(\lambda, x, y) \) \( n \) times gives us:
\[ \varphi_J^{(n)}(\lambda, x, y) = \sum_{j \in J} [-x D_J(n) + \text{h.o.t}] e^{-i \sqrt{\lambda - \mu_j x}} \nu_j(y) \]

These expressions evaluated on the boundary become:
\[ \varphi_J^{(n)}(\lambda, 0, y) = \sum_{j,k \in J} S_{J,j,k}^{(n)}(\lambda) \nu_k(y) + \sum_{j \notin J} T_{J,j}^{(n)}(\lambda) \nu_j(y) \]
\[ \frac{\partial}{\partial x} \varphi_J^{(n)}(\lambda, 0, y) = \sum_{j \in J} [-D_J(n)] \nu_j(y) + \sum_{j,k \in J} \left[ \sum_{q=0}^n \binom{n}{q} D_k(q).S_{J,j,k}^{(n-q)}(\lambda) \right] \nu_k(y) \]
\[ + \sum_{j \notin J} \left[ \sum_{q=0}^n \binom{n}{q} D_j(q).T_{J,j}^{(n-q)}(\lambda) \right] \nu_j(y) . \]

\( \tilde{N}_1(\lambda) \) will be a block-upper triangular matrix,
\[ \tilde{N}_1(\lambda) : \bigoplus_{\{0,...,n\}} l^2 \rightarrow \bigoplus_{\{0,...,n\}} l^2, \]
given by

\[
\tilde{N}_n(\lambda) = \begin{pmatrix}
\tilde{N}(\lambda) P & 0 & \cdots & \cdots & 0 \\
\frac{\partial}{\partial \lambda} \tilde{N}(\lambda) & \tilde{N}(\lambda) & 0 & \cdots & 0 \\
\frac{\partial^2}{\partial \lambda^2} \tilde{N}(\lambda) & \frac{\partial}{\partial \lambda} \tilde{N}(\lambda) & \tilde{N}(\lambda) & 0 & \cdots \\
\vdots & \vdots & \ddots & \ddots & \vdots \\
\frac{\partial^n}{\partial \lambda^n} \tilde{N}(\lambda) & \cdots & \cdots & \cdots & \tilde{N}(\lambda)
\end{pmatrix}^{-1}
\]

5.2 A Neumann to Dirichlet map for the system on the internal domain

Now we turn our attention towards the internal domain \(X\). \(N_n(\lambda)\) can be computed with an extension of Levitin-Matletta’s method. Equation 14 describes the method when used to compute \(N(\lambda)\). Their “trick” to increase the rate of convergence (15) is unaffected, so long as it is performed only once.

In the same context as equation 14, \(\{U_m\}\) are used to denote the orthonormal Neumann eigenfunctions and \(\mu_m\) their corresponding eigenvalues. \(\{\nu_j\}\) will denote orthonormal an basis of \(L^2(\Gamma)\) and finally, we will use \(\{\Phi_k\}\) and \(\{\Phi_k^{(n)}\}\), to denote solutions to the following system:

\[
\begin{align*}
(\Delta - \lambda)\Phi_k(\lambda, x, y) &= 0, \\
(\Delta - \lambda)\Phi_k'(\lambda, x, y) - \Phi_k(\lambda, x, y) &= 0, \\
&\vdots \\
(\Delta - \lambda)\Phi_k^{(n)}(\lambda, x, y) - \Phi_k^{(n-1)}(\lambda, x, y) &= 0,
\end{align*}
\]

where \(k\) is the n-tuple \(\{k_0, k_1, \ldots, k_n\}\).

We begin by fixing \(\lambda\) and will now calculate elements of \(N_n(\lambda)\) which map to \(\Phi^{(n)}\), where \(k_n \in \mathbb{N}\) and \(l \in \mathbb{N}^n\):

\[
N_{n,k_n,l} = \langle N\nu_{k_n}, \nu_l \rangle = \langle \Phi_k^{(n)} | \Gamma, \nu_l \rangle = \langle \Phi_k^{(n)} | \Gamma, \frac{\partial \Phi_l^{(n)}}{\partial n} \Gamma \rangle
= \langle \nabla \Phi_k^{(n)} , \nabla \Phi_l^{(n)} \rangle + \langle \Delta \Phi_k^{(n)} , \Phi_l^{(n)} \rangle = \langle \nabla \Phi_k^{(n)} , \nabla \Phi_l^{(n)} \rangle + \lambda \langle \Phi_k^{(n)} , \Phi_l^{(n)} \rangle + \langle \Phi_k^{(n-1)} , \Phi_l^{(n)} \rangle.
\]

Since each \(\Phi_k\) can be written as \(\sum_m \Phi_k(U_m)\) (the same is true for \(\Phi_k^{(n)}\)), and by definition, \(\Phi_k = (\Delta - \lambda)^{-j} \Phi_k^{(n-j)}\), it follows that:

\[
N_{n,k_n,l} = \sum_m \langle (\nabla U_m, \nabla U_m) + \lambda \rangle \langle \Phi_k^{(n)} , U_m \rangle \langle \Phi_l^{(n)} , U_m \rangle + \langle \Phi_k^{(n-1)} , \Phi_l^{(n)} \rangle
= \sum_m \langle (\nabla U_m, \nabla U_m) + \lambda \rangle \langle \Phi_k^{(n)} , U_m \rangle \langle \Phi_l^{(n)} , U_m \rangle + \sum_m \langle \Phi_k^{(n-1)} , U_m \rangle \langle \Phi_l^{(n)} , U_m \rangle
= \sum_m \langle \lambda - \mu_m \rangle \langle \Phi_k^{(n)} , U_m \rangle \langle \Phi_l^{(n)} , U_m \rangle + \sum_m \langle \Phi_k^{(n-1)} , U_m \rangle \langle \Phi_l^{(n)} , U_m \rangle.
\]
Green’s second identity, for any \( j \), means that

\[
\langle \Phi_j, U_m \rangle = \sum_m \frac{1}{\lambda - \mu_m} \left( \langle \Delta \Phi_j, U_m \rangle - \langle \Phi_j, \Delta U_m \rangle \right) = \sum_m \frac{1}{\lambda - \mu_m} \langle \nu_j, U_m | \Gamma \rangle \quad (30)
\]

\[
\langle \Phi_j^{(n)}, U_m \rangle = \sum_m \frac{1}{\lambda - \mu_m} \left( \langle \Delta \Phi_j^{(n)}, U_m \rangle - \langle \Phi_j^{(n)}, \Delta U_m \rangle - \langle \Phi_j^{(n-1)}, U_m \rangle \right).
\]

So then \( N_{(n),k,l} \) becomes

\[
\sum_m \left( \langle \nu_k, U_m | \Gamma \rangle - \langle \Phi_j^{(n-1)}, U_m \rangle \right) \langle U_m, \Phi_j^{(n)} \rangle,
\]

and inductively, we see that

\[
N_{(n),k_n,l} = \sum_m \langle \nu_k, U_m | \Gamma \rangle \langle U_m, \Phi_j^{(n)} \rangle = \sum_{m=1}^n \frac{(-1)^{p-1}}{\lambda - \mu_m} \langle \nu_k, U_m | \Gamma \rangle \langle U_m | \Gamma, \nu_p \rangle.
\]

Thus the \( n^{th} \) block-row for \( N_{(n)}(\lambda) \) is made up of the direct sum of maps defined component-wise by

\[
\eta(p)(\lambda) = \sum_m \frac{(-1)^{p-1}}{\lambda - \mu_m} \langle \nu_k, U_m | \Gamma \rangle \langle U_m | \Gamma, \nu_p \rangle,
\]

where \( p \) runs through \( 1, \ldots, n \).

Now, for the system, \( N_n(\lambda) \) is a block upper-triangular matrix, acting on \( \Phi \oplus \cdots \oplus \Phi^{(n)} \), of the same form as \( \tilde{N}_{(n)}(\lambda) \), given by

\[
N_{(n)}(\lambda) = \begin{pmatrix}
\eta(1)(\lambda) & 0 & \cdots & \cdots & 0 \\
\eta(2)(\lambda) & \eta(1)(\lambda) & 0 & \cdots & 0 \\
\eta(3)(\lambda) & \eta(2)(\lambda) & \eta(1)(\lambda) & 0 & 0 \\
\cdots & \cdots & \cdots & \cdots & \cdots \\
\eta(n)(\lambda) & \eta(n-1)(\lambda) & \cdots & \cdots & \eta(1)(\lambda)
\end{pmatrix}
\]

### 5.3 Extracting \( S_j^{(n)}(\lambda) \)

The coefficients of \( \phi_j^{(n)}(\lambda, 0, y) \) can now be computed by finding a basis for the null space of

\[
L_n = \left( PN_{(n)} - \tilde{N}_{(n)} \right)
\]

We will denote such a basis as \( \omega_1^{(n)}, \ldots, \omega_j^{(n)} \). Finally, using the same argument made when calculating \( S(\lambda) \),

\[
\tau_n(\lambda) = \{(1 - P)\omega_1^{(n)}, \cdots, (1 - P)\omega_j^{(n)}\} (1 - P)N\omega_1^{(n)}, \cdots, (1 - P)N\omega_j^{(n)} \}^{-1},
\]

thus

\[
\tau_n(\lambda) = \begin{pmatrix}
D(n) - \sum_{q=0}^n \binom{n}{q} D(q) S^{(n-q)}(\lambda)
\end{pmatrix} S^{(n)}(\lambda)^{-1}
\]

\[
= \begin{pmatrix}
D(n) - \sum_{q=1}^n \binom{n}{q} D(q) S^{(n-q)}(\lambda) - D(0) S^{(n)}(\lambda)
\end{pmatrix} S^{(n)}(\lambda)^{-1}.
\]
All of the $S^{(n-q)}_J(\lambda)$ are known, having been previously calculated. Finally we can say that

$$S^{(n)}_J(\lambda) = \left( \text{Id} - D(0)\tau_n(\lambda) \right)^{-1} \left( D(n)\tau_n(\lambda) - \sum_{q=1}^{n} \binom{n}{q} D(q)\tau_n(\lambda)S^{(n-q)}(\lambda) \right).$$

6 Embedded eigenvalues and resonances

This final section will describe how the scattering matrix can be used to compute complex resonances and present the results of some numerical experiments obtained via this method.

The paper by Evans, Levitin and Vassiliev [5] proved the existence of embedded eigenvalues for the Neumann Laplacian on two dimensional waveguides with an obstacle, and/or deformation of the waveguide so long as the domain has cross-sectional symmetry. This was further generalised to waveguides with cylindrical ends by Davies and Parnovski [6]. Parnovski and Levitin have, amongst others, produced two other papers on this topic [7] [8].

Embedded eigenvalues can be calculated numerically by looking for zero eigenvalues of the sub-matrix of $L$ in equation 16 obtained by omitting the rows and columns representing non square integrable modes. The scattering matrix, and its derivatives, can be used to calculate complex resonances on $Z$. Here we are defining a resonance to be a pole of the scattering matrix. The relationship between the resolvent, the Neumann to Dirichlet map and the scattering matrix means that poles of the resolvent coincide with zeros of the determinant of the inverse of the scattering matrix, and their multiplicities will be the same.

Theorem 2 can be used to show that every pole of $S_J(\lambda)$, on the sheet $J$ of $Z$, coincides with a zero of $S_J(\lambda^*)$ in the physical sheet and vice versa. We have used $\lambda^*$ to denote the canonical projection of $\lambda$ to the physical sheet; when both $\lambda$ and $\lambda^*$ are identified with a subset of the complex plane, they will be in the same location. Since the resolvent and scattering matrix are holomorphic in the physical sheet, it can’t have poles there, and we will have no zeros in a non-physical sheet of $Z$. This means we can now make use of the argument principle to locate resonances, and locating resonances in a non-physical sheet of $Z$ has been reduced to locating zeros in the physical sheet. The argument principle together with the Jacobi formula gives:

**Proposition 6.** Let $C$ be a contour in a non-physical sheet of $Z$, $J$ with winding number one then defining the counting function $\#$, $C \mapsto \mathbb{N}$ which counts the number of poles enclosed by $C$, we get that

$$\#(C) = \frac{1}{2\pi i} \oint_C \text{Tr}(S_J(\lambda)^{-1}.S'_J(\lambda)).$$

This approach was featured in the paper by Davies and Aslanyan, but not applied to the scattering matrix [13]. If a contour can be found that contains one or more zeros, we can subdivide then integrate over the subdivisions and repeat the process until a small enough contour has been found containing a single resonance. Newton’s method can then be used to obtain its location to a desired accuracy. We can then multiply the scattering matrix $S_J(\lambda)$ by $(\lambda_0 - \lambda)^{-1}$, where $\lambda_0$ is the location of the zero, then apply Newton’s method again, repeating if necessary to find its order.

6.1 Cylinders with a Circular Obstacle
Figure 3: One of our triangulated interior domains. The waveguide is composed of this interior domain, with the two ends the same width as the interior domain joined on the left and right sides.

Amongst other things, Levitin and Marletta looked at a cylinder (continuous rectangle) of width 2, with a single circular obstruction. The radius of this obstruction is varied along with the position of its centre (vertical displacement) relative to the centre line of the cylinder. When the vertical displacement is 0, there exist embedded eigenvalues, the embedded eigenvalues decay to a resonances when the vertical displacement becomes non-zero [4]. With the parameterisation of $\lambda \mapsto \lambda^2$, they presented a number of values for these resonances. We have performed our calculation to the highest accuracy we are able to and compared our results to theirs. We have been able to offer a slight improvement on the number of decimal places.

| $R = 0.3$ | Our calculation | Levitin-Marletta | Aslanyan et al |
|-----------|-----------------|-----------------|---------------|
| $\delta = 0$ | 1.50497 | 1.50486 | 1.5048 |
| $\delta = 0.1$ | 1.50783 + 0.0001205i | 1.5078 + 10^{-4}i | 1.5102 + 10^{-4}i |
| $\delta = 0.2$ | 1.51651 + 0.0004740i | 1.5165 + 5 × 10^{-4}i | 1.5188 = 5 × 10^{-4}i |
| $R = 0.5$ | | | |
| $\delta = 0$ | 1.39138 | 1.39134 | 1.3913 |
| $\delta = 0.1$ | 1.39785 + 0.0009255i | 1.3979 + 9 × 10^{-4}i | 1.3998 + 9 × 10^{-4}i |
| $\delta = 0.2$ | 1.41779 + 0.0039101i | 1.4178 + 3.90 × 10^{-3}i | 1.4196 + 3.93 × 10^{-3}i |

Figure 4: Some internal domains for $R = 0.3$, $\delta = 0.1$ with mesh refinement of 10 and 80 respectively.

6.2 Some notes on mesh refinement
6.3 Some notes on the number of eigenvalues

We have looked at the effects of mesh refinements on the accuracy of the results obtained. Whilst it should be obvious that the more refined the mesh becomes, the more accurate the result, we have tabulated the results of some experiments to demonstrate just to what extent. The standard method for producing a triangulated domain in FreeFem++ is to draw the outline as a union of parameterised curves, then use the programs own triangulation algorithm after specifying the number of points on each such curve. Our scale of mesh refinement was taken to be the number of such points per unit length on the boundary. We have tabulated some results for the calculation of these resonances, using 2000 eigenvalues and 20 modes for each connected component of \( \Gamma \) (see Figure 4) The reader can see how as the mesh refinement increases, the result stabilises.

| Mesh refinement | \( R = 0.3 \) \( \delta = 0.1 \) | \( R = 0.3 \) \( \delta = 0.2 \) |
|-----------------|--------------------------------|--------------------------------|
| 10 | 1.50943 + 0.0001157\( i \) | 1.51791 + 0.0004530\( i \) |
| 15 | 1.50847 + 0.0001185\( i \) | 1.51708 + 0.0004657\( i \) |
| 20 | 1.50821 + 0.0001193\( i \) | 1.51684 + 0.0004691\( i \) |
| 25 | 1.50805 + 0.0001198\( i \) | 1.51670 + 0.0004712\( i \) |
| 30 | 1.50797 + 0.0001200\( i \) | 1.51663 + 0.0004722\( i \) |
| 35 | 1.50793 + 0.0001202\( i \) | 1.51660 + 0.0004727\( i \) |
| 40 | 1.50790 + 0.0001203\( i \) | 1.51657 + 0.0004731\( i \) |
| 45 | 1.50788 + 0.0001203\( i \) | 1.51655 + 0.0004734\( i \) |
| 50 | 1.50786 + 0.0001204\( i \) | 1.51654 + 0.0004736\( i \) |
| 55 | 1.50785 + 0.0001204\( i \) | 1.51653 + 0.0004737\( i \) |
| 60 | 1.50785 + 0.0001204\( i \) | 1.51652 + 0.0004738\( i \) |
| 65 | 1.50784 + 0.0001204\( i \) | 1.51651 + 0.0004739\( i \) |
| 70 | 1.50783 + 0.0001205\( i \) | 1.51651 + 0.0004740\( i \) |
| 75 | 1.50783 + 0.0001205\( i \) | 1.51651 + 0.0004740\( i \) |
| 80 | 1.50783 + 0.0001205\( i \) | 1.51651 + 0.0004740\( i \) |
| N | \( R = 0.5 \) \( \delta = 0.1 \) | \( R = 0.5 \) \( \delta = 0.2 \) |
|----------------|--------------------------------|--------------------------------|
| 10 | 1.39874 + 0.0009122\( i \) | 1.41857 + 0.00385170\( i \) |
| 15 | 1.39822 + 0.0009199\( i \) | 1.41811 + 0.0038854\( i \) |
| 20 | 1.39805 + 0.0009225\( i \) | 1.41796 + 0.0038971\( i \) |
| 25 | 1.39797 + 0.0009237\( i \) | 1.41789 + 0.0039021\( i \) |
| 30 | 1.39793 + 0.0009243\( i \) | 1.41786 + 0.0039049\( i \) |
| 35 | 1.39791 + 0.0009247\( i \) | 1.41784 + 0.0039063\( i \) |
| 40 | 1.39789 + 0.0009249\( i \) | 1.41782 + 0.0039075\( i \) |
| 45 | 1.39788 + 0.0009251\( i \) | 1.41781 + 0.0039083\( i \) |
| 50 | 1.39787 + 0.0009252\( i \) | 1.41781 + 0.0039089\( i \) |
| 55 | 1.39786 + 0.0009253\( i \) | 1.41780 + 0.0039092\( i \) |
| 60 | 1.39786 + 0.0009254\( i \) | 1.41780 + 0.0039095\( i \) |
| 65 | 1.39786 + 0.0009254\( i \) | 1.41779 + 0.0039097\( i \) |
| 70 | 1.39785 + 0.0009255\( i \) | 1.41779 + 0.0039098\( i \) |
| 75 | 1.39785 + 0.0009255\( i \) | 1.41779 + 0.0039101\( i \) |
| 80 | 1.39785 + 0.0009255\( i \) | 1.41779 + 0.0039101\( i \) |

6.3 Some notes on the number of eigenvalues

In the previous subsection, we mentioned that we have used 2000 eigenvalues but gave no justification for this. Here we intend to present the reader with some graphs and charts to demonstrate convincingly, why this was. We have tabulated data describing what happens when number of eigenvalues is increased. We will present some convergence
6.3 Some notes on the number of eigenvalues

graphs that track the value of the leading coefficient of the scattering matrix as the number of eigenvalues increases for a selection of the domains above at a random point.

| Number of eigenvalues | $R = 0.3 \, \delta = 0.1$ | $R = 0.3 \, \delta = 0.2$ |
|-----------------------|-----------------------------|-----------------------------|
| 200                   | $1.50783 + 0.000120482i$    | $1.51651 + 0.000474043i$    |
| 400                   | $1.50783 + 0.000120482i$    | $1.51651 + 0.000474045i$    |
| 600                   | $1.50783 + 0.000120482i$    | $1.51651 + 0.000474045i$    |
| 800                   | $1.50783 + 0.000120483i$    | $1.51651 + 0.000474045i$    |
| 1000                  | $1.50783 + 0.000120483i$    | $1.51651 + 0.000474046i$    |
| 1200                  | $1.50783 + 0.000120483i$    | $1.51651 + 0.000474046i$    |
| 1400                  | $1.50783 + 0.000120483i$    | $1.51651 + 0.000474046i$    |
| 1600                  | $1.50783 + 0.000120483i$    | $1.51651 + 0.000474046i$    |
| 1800                  | $1.50783 + 0.000120483i$    | $1.51651 + 0.000474046i$    |
| 2000                  | $1.50783 + 0.000120483i$    | $1.51651 + 0.000474046i$    |

| N                     | $R = 0.5 \, \delta = 0.1$ | $R = 0.5 \, \delta = 0.2$ |
|-----------------------|-----------------------------|-----------------------------|
| 200                   | $1.39785 + 0.000925537i$    | $1.41779 + 0.00391014i$     |
| 400                   | $1.39785 + 0.000925536i$    | $1.41779 + 0.00391013i$     |
| 600                   | $1.39785 + 0.000925536i$    | $1.41779 + 0.00391014i$     |
| 800                   | $1.39785 + 0.000925537i$    | $1.41779 + 0.00391014i$     |
| 1000                  | $1.39785 + 0.000925537i$    | $1.41779 + 0.00391014i$     |
| 1200                  | $1.39785 + 0.000925537i$    | $1.41779 + 0.00391014i$     |
| 1400                  | $1.39785 + 0.000925537i$    | $1.41779 + 0.00391014i$     |
| 1600                  | $1.39785 + 0.000925537i$    | $1.41779 + 0.00391014i$     |
| 1800                  | $1.39785 + 0.000925537i$    | $1.41779 + 0.00391014i$     |
| 2000                  | $1.39785 + 0.000925537i$    | $1.41779 + 0.00391014i$     |

From this it might seem like it is unnecessary to use many eigenvalues, however the number of eigenvalues does have a significant impact on the coefficients of the scattering matrix as we shall demonstrate with some graphs. We have picked, as an example, the domain where $R = 0.3$ and $\delta = 0.1$ with a mesh refinement of 80. We have plotted the real and imaginary components of the leading coefficient of the scattering matrix at the value $1 + 0.1i$. This is typical behavior for any arbitrarily chosen point.

![Figure 5: The real and imaginary components of the first coefficient of the scattering matrix plotted against the number of eigenvalues and eigenvectors used to compute it.](image)

It should be noted that the number of modes and the auxiliary point chosen had an undetectable effect on the accuracy of the calculations so long as the choice was “sensible”. It should also be noted that increasing the number of modes is the most computationally costly action we can take and should be minimised. For the rest of the results, we have used 20 modes for each end, 1000 eigenvalues and a mesh refinement of 30.
We have calculated resonances and embedded eigenvalues over a wider variety of radii and displacements, and we have also looked beyond the first non-physical sheet. In the tables below and throughout, we will be using the parameterisation $\lambda \mapsto \lambda$ instead of $\lambda \mapsto \lambda^2$.

| $R$ | $\lambda$ | $\lambda$ | $\lambda$ | $\lambda$ |
|-----|------------|------------|------------|------------|
| 0   | 2.26495    | 2.09281    | 1.93595    | 1.81802    |
| 0.1 | 2.27386 + 0.00030i | 2.10666 + 0.00111i | 1.95414 + 0.00258i | 1.84091 + 0.00511i |
| 0.2 | 2.30007 + 0.00143i | 2.14855 + 0.00460i | 2.01025 + 0.01108i | 1.91246 + 0.0241i |
| 0.3 | 2.34144 + 0.00300i | 2.21863 + 0.01073i | 2.10809 + 0.02749i | 2.04092 + 0.06311i |
| 0.4 | 2.39242 + 0.00481i | 2.31323 + 0.01870i | 2.24875 + 0.05208i | -           |
| 0.5 | 2.44099 + 0.00510i | 2.41444 + 0.02222i | -           | -           |
| 0.6 | 2.67240 + 0.00134i | -           | -           | -           |

Of particular interest here is the case where $R = 0.2$. As $\delta$ increases from 0.6 to 0.7 the resonance moves from the sheet $J = \{1\}$ to $J = \{2\}$ as can be seen in the table below.

| $R = 0.2$ | $J = \{1\}$ | $J = \{2\}$ |
|-----------|-------------|-------------|
| $\delta = 0$ | 2.4030      | -           |
| $\delta = 0.1$ | 2.40712 + 0.00006i | -           |
| $\delta = 0.2$ | 2.41709 + 0.00021i | -           |
| $\delta = 0.3$ | 2.43170 + 0.00040i | -           |
| $\delta = 0.4$ | 2.44777 + 0.00059i | -           |
| $\delta = 0.5$ | 2.46101 + 0.00053i | -           |
| $\delta = 0.6$ | 2.46725 + 0.00013i | -           |
| $\delta = 0.7$ | -           | 2.46475 + 0.00053i |

Figure 6: Resonances for the domain $R = 0.2$ showing the resonance moving to a different sheet of $Z$.

We have plotted the absolute value of the determinant of the scattering matrix for this occurrence. We can observe that the “tail” of the resonance is visible on both sheets prior to the resonance moving sheets.
6.5 Adding “Ends” to a Circle

Here, we have taken a circle, added a single end and varied the width of this end. We have searched for resonances, on sheets $J = \{1\}$, $J = \{2\}$ and $J = \{3\}$, within the search area given by:

$$\{ \lambda : 0 \leq \text{Re}(\lambda) \leq 15, -3 \leq \text{Im}(\lambda) \leq 3 \},$$

(31)

and tabulated the results found. We can be confident that the accuracy of the resonances calculated is at least three decimal places, though we have included the fourth place in a lighter shade for the reader’s information. In addition to this, we have plotted them on graphs, with colour coded markers indicating the respective sheet of $Z$ they reside on; black for $J = \{1\}$, red for $J = \{2\}$ and green for $J = \{3\}$. In the case of varying widths, the “paths” taken by the resonances as the widths vary continuously are clearly visible in table form, and we have included them there too. Beforehand, we will show first 9 non-zero Neumann eigenvalues, of the circle of radius 2, which can be compared to the resonances, especially when $w$ is small.

| 0.8476 | 2.3323 | 3.6709 | 4.4130 | 7.0698 | 7.1068 | 10.2911 | 11.2442 | 12.3059 |

Figure 8: Neumann eigenvalues for a circle of radius 2

Figure 9: An example of some internal domains from waveguides with a single end: varying widths.

Figure 7: Contour plots showing the resonance crossing from one sheet of $Z$ to another. Here $R = 0.2$ throughout.
### 6.5 Adding “Ends” to a Circle

#### $J = \{1\}$

| $w = 0.1$ | $w = 0.2$ | $w = 0.5$ | $w = 1$ |
|-----------|-----------|-----------|-----------|
| 0.8496 + 0.0206i | 0.8541 + 0.0408i | 0.8753 + 0.0992i | 0.9255 + 0.1957i |
| 2.3388 + 0.0416i | 2.3525 + 0.0807i | 2.413 + 0.1848i | 2.5431 + 0.3334i |
| 3.6742 + 0.0145i | 3.6814 + 0.0265i | 3.7091 + 0.0512i | 3.7577 + 0.0802i |
| 4.4246 + 0.0664i | 4.4480 + 0.1285i | 4.5452 + 0.3009i | 4.7425 + 0.5764i |
| 7.0947 + 0.0022i | 7.0946 + 0.0011i | 7.0947 + 0.0004i | 7.8573 + 1.0573i |
| 7.1124 + 0.1328i | 7.1721 + 0.2541i | 7.4065 + 0.5657i | 10.7726 + 0.1699i |
| 10.3293 + 0.1166i | 10.4037 + 0.2071i | 10.6664 + 0.2940i | 12.2884 + 0.8945i |
| 11.2547 + 0.0572i | 11.2733 + 0.1151i | 11.368 + 0.35467i | 12.0991 + 0.3521i |
| 12.3122 + 0.0263i | 12.3237 + 0.0502i | 12.3567 + 0.1348i | 14.7205 + 0.6654i |
| 14.1139 + 0.1527i | 14.1949 + 0.2766i | 14.4649 + 0.5345i |  | 

#### $J = \{2\}$

| $w = 0.1$ | $w = 0.2$ | $w = 0.5$ | $w = 1$ |
|-----------|-----------|-----------|-----------|
| 0.9900 + 0.3010i | 1.0710 + 0.4266i | 1.1752 + 0.5898i | 1.3176 + 0.8290i |
| 2.6965 + 0.4627i | 2.8746 + 0.5614i | 3.0696 + 0.5767i | 3.1713 + 0.4476i |
| 3.8154 + 0.1224i | 3.9000 + 0.2054i | 4.0569 + 0.3750i | 4.5055 + 0.5486i |
| 4.9403 + 0.8597i | 5.0970 + 1.1417i | 5.1843 + 1.3492i | 5.3676 + 1.4029i |
| 7.1276 + 0.0014i | 7.1757 + 0.0151i | 9.2528 + 2.4257i |  | 
| 8.2933 + 1.6165i | 8.6102 + 2.1380i |  |  | 
| 10.7224 + 0.0883i | 11.2920 + 0.0758i |  |  | 
| 12.0129 + 0.1897i | 13.780 + 2.6635i |  |  | 
| 13.1459 + 2.0493i |  |  |  | 
| 14.5252 + 0.3368i |  |  |  | 

#### $J = \{3\}$

| $w = 0.1$ | $w = 0.2$ | $w = 0.5$ | $w = 1$ |
|-----------|-----------|-----------|-----------|
| 7.2431 + 0.4693i | 4.6065 + 0.4829i | 2.3695 + 0.3389i | 2.6042 + 0.6511i |
| 7.7433 + 0.9299i | 11.0769 + 0.08842i | 4.9869 + 0.8324i | 5.5217 + 1.2393i |
| 10.9022 + 0.7275i | 11.8264 + 1.38610i | 7.1156 + 0.0011i | 7.1356 + 0.0192i |
| 11.1970 + 0.1239i | 8.3670 + 1.44198i | 10.9968 + 0.0355i | 9.1096 + 1.9492i |
|  | 12.7631 + 2.1634i |  | 14.1616 + 2.7545i |

$J = \{4\}$

| $w = 0.1$ | $w = 0.2$ | $w = 0.5$ | $w = 1$ |
|-----------|-----------|-----------|-----------|
| 10.3673 + 0.2721i | 7.0639 + 0.2546i | 7.6306 + 0.7147i |  | 
| 14.7867 + 0.8682i | 11.831 + 0.0873i | 11.6268 + 0.0985i |  | 
|  | 11.161 + 1.0833i |  | 12.4059 + 2.0430i |  | 

**Note:** The table above represents adding “ends” to a circle with different weights ($w$) for different values of $J$. The values listed are the coordinates of the points on the circle for each weight. The values are given in the form $a + bi$, where $a$ is the real part and $b$ is the imaginary part.
6.5 Adding “Ends” to a Circle

Figure 10: Some colour-coded plots of the location of resonances. In this instance the width of a single end is changed. The larger markers are the resonances for the domain indicated, the smaller markers are the entire family of domains with varying widths. This allows the reader to visualise the paths the resonances take as the width of the end increases. Similar, but not identical, paths can be observed with higher numbers of ends.
7 Time delay and scattering length

The notions of time delay and scattering length hail from dynamic scattering theory; they can both be calculated using the scattering matrix. Reed and Simon mention time delay briefly in their text [14]. Müller and Strohmaier have also covered time delay and scattering length in their paper [15], where they give results that relate the time delay to the geometry of the internal domain. In this section, we will apply this to a pair of the domains featured above. It should be noted that the $\lambda$ in this context will be a real number less than $\mu_1$, representing the energy of the system and not an element of the $\mathbb{Z}$.

The Appendix of Müller and Strohmaier’s paper provides an overview of the time delay in this setting [16]. We will take the (non standard) definition to be:

**Definition 7. Time delay**

$$T(\lambda) = -2\sqrt{\lambda}S^{-1}(\lambda)S'(\lambda)$$

when $\lambda = 0$, we define this to be the **scattering length**.

Wigner and Eisenbud were the first to present the time delay in this manner for potential scattering and $T(\lambda)$ is often called the Eisenbud-Wigner time delay operator [17][18]. Müller and Strohmaier have, amongst other things, proved this formula for the case of manifolds with cylindrical ends and, in the case of a single end

$$T(0) = 2\frac{\text{Vol}(X)}{\text{Vol}(\Gamma)}.$$

We will pick a selection of our single ended domains from above and plot their time delay as $\lambda$ approaches 0.

![Figure 11: Circle of radius 2, with end width 1.5. $T(0)$ should theoretically be 25.1327.](image1)

![Figure 12: Circle of radius 2 with end width 1, obstacle radius 0.5. $T(0)$ should theoretically be 11.781.](image2)

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