NUMERICAL ANALYSIS OF THE SPECTRA OF DISSIPATIVE SCHRÖDINGER-TYPE AND RELATED OPERATORS

A Thesis
Submitted in partial fulfilment of the requirements for the degree of
DOCTOR OF PHILOSOPHY

by

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February 2022

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Preface

Spectral problems of band-gap structure appear in various applications such as elasticity theory, electromagnetic waves, and photonic crystals. In the numerical approximation of these problems an important phenomenon known as spectral pollution arises due to the discretisation process. In this thesis we focus on two different techniques to calculate eigenvalues in spectral gaps of Schrödinger-type operators which are free of spectral pollution. The original material in this thesis is based on papers [7], [8], and [6]. The material in these papers is explained in details in Chapter 4, Chapter 5, and Chapter 6 with summaries presented in Chapter 2 and Chapter 3, respectively.

In Chapter 4, we investigate approximation of eigenvalues in spectral gaps of Schrödinger operators with matrix coefficients. We employ the dissipative barrier technique and domain truncation and analyse spectral properties of the resulting operators. Our theoretical foundations are based on the notions of Floquet theory and Dirichlet-to-Neumann maps. The effectiveness of this technique is illustrated through different numerical examples including a model in optics.

In Chapter 5, we study approximation of isolated eigenvalues in spectral gaps of elliptic partial differential operators for models of semi-infinite waveguides. The approximation is obtained using the interaction of the dissipative technique and domain truncation of the operators. Our theoretical results are based on the error estimate of the Dirichlet-to-Neumann maps on the cross-section of the waveguides and perturbation determinants. Some numerical examples on waveguides are indicated to show the effectiveness of the presented technique.

In Chapter 6, we propose a numerical algorithm to calculate eigenvalues of the perturbed periodic matrix-valued Schrödinger operators which are located in spectral gaps. The spectral-pollution-free algorithm is based on combining shooting with Floquet theory, as well as Atkinson $\Theta-$matrices, to avoid the associated stiffness problems and allow eigenvalue counting. We derive interesting new oscillation results. As far as we know these are the first oscillation theory results for matrix Schrödinger operators for λ in a spectral gap above the first spectral band. Numerical examples show that this method gives more accurate results and requires less time than those obtained from the finite difference methods, which are coupled with contour integral $\lambda-$nonlinear eigenvalue problems. In addition, the proposed method gives better results than the dissipative barrier scheme with domain truncation which lead to $\lambda-$linear eigenvalue problems.

Acknowledgements

Contents

List of Figures

List of Tables

"My feeling is, nevertheless, that the mathematical theory of the periodic Schrödinger equation is far from complete at present."

-M. S. P. Eastham [1]

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[1][47]

1 Introduction

1.1 Problem statement and general background

Spectral theory is an old field in mathematics which acquires its importance from the fact that spectrum appears in different scientific concepts such as atoms, algebras, and operators. Spectral theory of differential operators concerns the theory of determining eigenvalues and eigenfunctions and essential spectrum of the corresponding operators. The general feature of studying spectral properties of a differential operator is that they give some understanding of the physical phenomena which the operator describes. The Schrödinger operator is one of the most significant differential operators studied in spectral theory. In fact, due to advances in physics, there is a great need to deal with many problems related to this operator which is considered as the fundamental operator of quantum mechanics. Moreover, it appears in many applications, depending on the accompanying model, as a second order ordinary differential equation or as an elliptic partial differential equation.

There are two main branches to the spectral theory of Schrödinger operators. The first branch studies regular differential operators which are divided into regular ordinary differential operators and regular partial differential operators. The regular ordinary differential operators are associated with problems on finite intervals with integrable coefficients. Regular PDEs are generally posed on bounded domains with piecewise smooth boundaries and bounded coefficients. For these problems, determining eigenvalues is equivalent to determining eigenvalues of compact operators. Therefore, according to the spectral theorem of compact operators in Hilbert space, there are infinitely many non-zero, real for the self-adjoint case, eigenvalues and the spectrum is purely discrete. Regular spectral problems have been studied extensively, see e.g., [38, 75] and references therein.

The other interesting, and more complicated, branch of spectral theory of Schrödinger operators is the singular case. This happens when at least one of the regularity conditions does not hold. Moreover, many other cases of singularity can be considered for the PDE, such as boundary conditions which are singular at one point, boundaries which are fractal, potentials which contain a Dirac delta function, and many others. However, in this thesis we focus only on the case when the differential operator associated with either ODE or PDE is singular at ∞. Spectral theory of singular problems has its origin in a remarkable study of Hermann Weyl who expanded the spectral theory of regular problems to include singularities [110]. This leads to the limit-circle and limit-point classification of the singular ordinary differential operators. When one endpoint, or both, of the interval, possibly semi-

infinite or infinite, of the associated operator is singular in the limit point case, then, unlike the regular case, the spectrum need not be discrete. In general, it consists of eigenvalues and essential spectrum.

In this thesis we study the spectral properties of certain types of Schrödinger equations of the form:

$$- \Delta u + Q u = \lambda u \quad \text{in} \quad \Omega, \tag{1}$$

acting in the Hilbert space $L^2(\Omega); \Omega \subseteq \mathbb{R}^d; d \geq 1$. We consider Ω to be $[0, \infty)$ for the ODE case. For the PDE case we let $\mathcal{C}$ be a smooth bounded domain in $\mathbb{R}^{d-1}; d > 1$ and take the semi-infinite waveguide $\Omega = (0, \infty) \times \mathcal{C}$. Here Q is a scalar, bounded and real-valued potential or an $n \times n$, periodic and Hermitian matrix-valued potential which is assumed to be locally integrable over any compact subset of Ω, and $\lambda \in \mathbb{C}$ is a spectral parameter. We assume that it is sufficient to impose a boundary condition at the regular boundary and no boundary condition is required at the singular boundary, see e.g., [38] for the ODE case and [17] for the PDE case. In this study, we consider the Dirichlet boundary condition on the regular boundaries of Ω. Furthermore, since Q is real valued, or Hermitian for the matrix case, then (1) leads to a self-adjoint operator when imposing self-adjoint-type boundary conditions.

1.2 Spectrum and essential spectrum of operators

Before we explain our main focus, we introduce basic definitions for the spectrum and other elements related to our study. Let $T : D(T) \to \mathcal{H}$ be an operator defined on a dense domain $D(T)$ contained in a Hilbert space $\mathcal{H}$.

Definition 1.1. The spectrum of T, denoted by $Spec(T)$, is the set of all complex numbers λ such that $T - \lambda$ is not boundedly invertible.

The complement of the spectrum of T is known as the resolvent set.

Definition 1.2. The resolvent set of T, denoted by $\varrho(T)$, is the set of all complex numbers λ such that $T - \lambda$ is boundedly invertible.

Two important types of spectra are of interest in this study; discrete spectrum and essential spectrum.

Definition 1.3. The discrete spectrum of T, $Spec_{dis}(T)$, is the set of all complex numbers λ which are isolated points of $Spec(T)$, i.e., there exists a ball with centre λ and radius ϵ, $B(\lambda; \epsilon)$, such that $B(\lambda; \epsilon) \cap Spec(T) = \{\lambda\}$. In addition, λ is of finite algebraic multiplicity, i.e., the dimension of $\ker(T - \lambda)$ is finite.

In general, there are several definitions of the notion of the essential spectrum, which are identical for self-adjoint operators. However, our study includes non-selfadjoint operators, thus we are going to consider the following definition below. We first introduce the definition of the so-called *Weyl singular sequence*.

Definition 1.4. A Weyl singular sequence $\{u_n\}_{n=1}^\infty$ in $D(T)$ associated to λ is a sequence with the following properties:

$$\|u_n\| = 1, \quad (n \in \mathbb{N}) \quad u_n \rightharpoonup 0, \quad \text{and} \quad \|(T - \lambda)u_n\| \to 0 \quad \text{in} \quad \mathcal{H}.$$

The symbol $u_n \rightharpoonup 0$ means that $\langle u_n, v \rangle \to 0$ for all $v \in \mathcal{H}$.

Definition 1.5. The essential spectrum of an operator $T, Spec_{ess}(T)$, is the set of all complex numbers λ for which there exists a Weyl singular sequence.

Remark 1.6. This definition is equivalent to $\sigma_{e,2}$ in [49].

The following two definitions provide enclosures to the spectrum and the essential spectrum, respectively, see [22], provided that the resolvent set of T is non-empty.[2]

Definition 1.7. The numerical range is the set of complex numbers

$$W(T) = \{\langle Tu, u \rangle \mid u \in D(T), \|u\| = 1\}.$$

Definition 1.8. [22] The essential numerical range, $W_{ess}(T)$, is the set of all complex numbers λ for which there exists a sequence $\{u_n\}_{n=1}^\infty$ in $D(T)$ with

$$\|u_n\| = 1, \ u_n \rightharpoonup 0, \quad \text{and} \quad \langle Tu_n, u_n \rangle \to \lambda \quad \text{in} \quad \mathcal{H}.$$

The spectrum of the self-adjoint operator associated with equation (1) consists of a finite or countable number of closed intervals of $\mathbb{R}$ [38, 75] which are known as *spectral bands* together with eigenvalues which may lie inside the spectral bands or in the *spectral gaps* between the bands. Band-gap structure of essential spectrum of Schrödinger operators associated with equation (1) arises when the potential is periodic on a relatively compact perturbation. This structure is characterised by the Floquet theory [47, 69] which is the main tool in studying the spectral properties of periodic differential operators.

Meanwhile, when a compactly supported perturbation term is added to the potential Q associated with the self-adjoint operator (1), two main effects may arise.

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[2]If the operator has an empty resolvent set, then the spectrum might be strictly greater than the essential numerical range.

Firstly, according to Weyl's theorem [98] the essential spectrum of the operator remains the same. This property is known as the stability of the essential spectrum under a relatively compact perturbation. Secondly, discrete eigenvalues may appear below the essential spectrum of the operator and in spectral gaps. In other words, discrete eigenvalues move under the compact perturbation.

In addition, a significant part of this thesis focuses on the *dissipative* Schrödinger operator. This operator is obtained from the self-adjoint operator associated with (1) when a complex compactly supported function is added to the potential Q. Discrete eigenvalues and their approximations of self-adjoint Schrödinger operators associated with (1), as well as, spectral properties of the corresponding dissipative Schrödinger operators are our major concerns in this thesis.

1.3   Two types of Schrödinger operators

In this study, we particularly focus on two main differential operators which are already indicated in the form of equation (1):

- Matrix-valued Schrödinger operator on the half line.

  This operator arises naturally in many mathematical processes. For example, from linear PDE in several space dimensions when the equation is separable in some coordinate system, such as cylindrical or spherical coordinates.

- Elliptic PDE on a semi-infinite waveguide.

We introduce the following example to illustrate how a problem from an elliptic PDE on a semi-infinite waveguide can lead to a matrix-valued Schrödinger equation.

Example 1.9. Let us consider the PDE problem:

$$-\Delta u(x,y) + Q(x,y)u(x,y) = \lambda u(x,y),$$

on a waveguide $\Omega := (0,\infty) \times (0,\delta); \delta \in \mathbb{R}^+$ with Dirichlet boundary conditions $u(x,y)_{|\partial\Omega} = 0$, see Figure 1.1. Here, we assume that Q is a real-valued, bounded and measurable function.
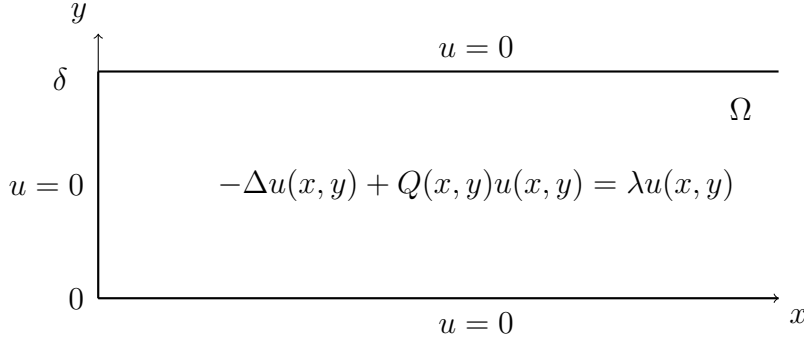
Figure 1.1: The domain of the semi-infinite waveguide problem of Example 1.9.

By applying standard separation of variables and considering the geometry of the domain as well as the given boundary conditions we obtain the ansatz:

$$u(x,y) = \sum_{n=1}^{\infty} u_n(x) \sqrt{\frac{2}{\delta}} \sin(\frac{n\pi}{\delta}y).$$

This leads to the following sequence of equations:

$$-u_n''(x) + \frac{n^2\pi^2}{\delta^2}u_n(x) + \frac{2}{\delta}u_n(x)\sum_{m=1}^{\infty}\int_0^{\delta} Q(x,y)\sin(\frac{n\pi}{\delta}y)\sin(\frac{m\pi}{\delta}y)dy = \lambda u_n(x),$$

provided that the sum is convergent, in particular for sufficiently smooth Q. This system can be written formally in a matrix form, where $\hat{Q}$ is a doubly infinite matrix given by this formula:

$$-\underline{u}''(x) + \hat{Q}(x)\underline{u}(x) = \lambda \underline{u}(x),$$

where

$$\hat{Q}_{n,m}(x) = \begin{cases} \frac{n^2\pi^2}{\delta^2} + \frac{2}{\delta}\sum_{m=1}^{\infty}\int_0^{\delta} Q(x,y)\sin(\frac{n\pi}{\delta}y)\sin(\frac{m\pi}{\delta}y)dy, & \text{if } n = m, \\ \\ \frac{2}{\delta}\sum_{m=1}^{\infty}\int_0^{\delta} Q(x,y)\sin(\frac{n\pi}{\delta}y)\sin(\frac{m\pi}{\delta}y)dy, & \text{if } n \neq m. \end{cases}$$

A standard semi-discretisation technique for the waveguide problem is to replace $\hat{Q}$ by a finite matrix, see e.g., [81].

1.4   Band-gap Schrödinger operators in different studies

Problems involving band-gap spectrum and eigenvalues in spectral gaps of differential operators have been intensively studied in the literature. We refer to Eastham [47]

and Kuchment [69] for a review of the most significant results on spectral properties and differences between them in terms of operators. A well known result related to the existence of spectral gaps is that spectral bands of the second order ordinary differential operators can not overlap but they may touch. Meanwhile, for two dimensional operators, i.e., partial differential operators, spectral bands frequently do overlap. Another result is that there are infinitely many spectral gaps for the ordinary differential operators while there are only finitely many spectral gaps for the periodic elliptic PDEs, see e.g., [93].

Eastham [46, 45] and Eastham and Everitt [48] estimated the length of spectral gaps of the essential spectrum for the scalar case of the Schrödinger operator associated with (1) when Q is real-valued and periodic or generally bounded as well as for higher order case of the operator. Stolz [106] studied the spectrum of the scalar case with different classes of potential including a perturbed periodic potential. For the operator associated with the elliptic PDE (1), counting the number of eigenvalues in spectral gaps for this operator on $L^2(\mathbb{R}^d)$ when Q is real and bounded was discussed by Alama, Deift, and Hempel [5]. Kuchment [73] considered absence of embedded eigenvalues in the essential spectrum of this operator on $L^2(\mathbb{R}^d)$; $d = 2, 3$ when Q is real, periodic and bounded and is perturbed by a fast decaying potential.

Numerous investigations of spectral properties of elliptic PDEs on waveguide-type domains have been conducted. For instance, Nazarov and his co-authors [89, 90, 33] and Figotin and Kuchment ([52] and many references therein) in which they detected sufficient conditions for the existence of spectral gaps of periodic and non-periodic perturbed waveguides. The negative discrete spectrum of elliptic PDE (1) on a waveguide $\Omega \subseteq \mathbb{R}^d$ which is unbounded and periodic along one direction with a real-valued and decaying potential was presented by Birman and Solomyak in [20]. Moreover, other works have been devoted to the numerical approaches and calculations of band-gaps spectra and isolated eigenvalues for different differential operators, see e.g., [53, 113, 25, 2, 105, 66].

In addition to self-adjoint operators, non-selfadjoint Schrödinger operators have received a lot of attention. For example, Naimark [88] investigated the spectrum of the scalar non-selfadjoint operator on $[0, \infty)$ when Q is a complex-valued function and proved that spectrum contains essential spectrum, isolated eigenvalues and spectral singularities. Keldysh [65] considered the case of non-selfadjoint elliptic partial differential operators. Bounds of complex eigenvalues for the elliptic PDE on $L^2(\mathbb{R}^N)$, when Q is a bounded complex potential, were discussed in [1]. Eigenvalue bounds for non-selfadjoint Schrödinger operators were considered in articles such as [42, 27, 56]. Other studies investigated eigenvalues of non-selfadjoint Schrödinger operators when obtained from self-adjoint operators, e.g., [83, 84, 82]. In relation to our study, the

latter papers will be discussed briefly in Chapter 2.

1.5 Dirichlet-to-Neumann maps for Schrödinger operators

The Dirichlet-to-Neumann map (D-to-N) from the theory of Schrödinger equations is a natural analogue of the Weyl-Titchmarsh function. This is because the Weyl-Titchmarsh function $m(\lambda)$, $\Im(\lambda) \neq 0$, is given by $m((\lambda) = -\frac{u'(0;\lambda)}{u(0;\lambda)}$, where u is, in the limit-point case at infinity, the unique square integrable solution (up to scalar multiples) of the scalar case of (1) when $\Omega = (0, \infty)$. The latter map plays an important role in the spectral analysis of ordinary differential operators due to the result that spectral data can be retrieved from the knowledge of the Weyl-Titchmarsh function.

There are many significant contributions devoted to the analysis of Schrödinger-type equations with matrix-valued coefficients on the half-line such as [37, 36, 61], and references therein, in which the Weyl-Titchmarch theory was investigated to the underlying operators. Throughout our analysis, we employ D-to-N maps for the matrix-case operators. We introduce the following definition for the D-to-N map for the matrix Schrödinger operator on the half line.

Definition 1.10. For the self-adjoint matrix Schrödinger problem (1) on $\Omega = [0, \infty)$ with eventually periodic[3] and Hermitian matrix-valued potential Q that is assumed to be locally integrable over any compact subset of Ω, and a boundary condition $\underline{u}(0) = \underline{h} \in \mathbb{C}^n \setminus \{\underline{0}\}$, the corresponding D-to-N map can be given by

$$\Lambda(\lambda)\underline{h} := \underline{u}'(0),$$

where $\underline{u}$ is the unique[4] solution corresponding to λ that is not in the spectrum of the corresponding Dirichlet Schrödinger operator.

Our study involves two types of D-to-N maps for matrix Schrödinger operators. We consider the D-to-N map for the dissipative Schrödinger operator when $\Omega = [0, R]$ for some $R > 0$. In addition, we employ the D-to-N map for the self-adjoint matrix Schrödinger operator associated with (1) on the interval $\Omega = [R, \infty)$. Therefore, we derive error bounds and convergence results which are based on these maps after applying the domain truncation. See Section 4.3 for more details.

For D-to-N maps for spectral problems of elliptic PDEs, we mention some contributions such as [9, 17] and [16] for more abstract context. We introduce the following definition.

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[3]It is decomposed into a periodic function and a compactly supported perturbation.

[4]The solution is unique because, if we had two distinct solutions, their difference would be a Dirichlet Schrödinger eigenfunction.

Definition 1.11. Consider the self-adjoint elliptic problem (1) on the semi-infinite waveguide $\Omega = (0, \infty) \times \mathcal{C} \subseteq \mathbb{R}^d; d \geq 1$ where $\mathcal{C}$ is a smooth bounded domain in $\mathbb{R}^{d-1}; d > 1$ with a bounded and real-valued potential Q which is locally integrable over any compact subset of Ω and a boundary condition $u|_{\Sigma_{(0,\infty)}} = 0$; $\Sigma_{(0,\infty)}$ is the portion of the boundaries of Ω which intersects with the sides of $(0, \infty) \times \partial \mathcal{C}$. Suppose that $f \in L^2(\mathcal{C})$ be a non-zero function and that $u|_{\mathcal{C}} = f$. Then the D-to-N map is given by

$$\Lambda(\lambda)f := \frac{\partial u}{\partial \nu}|_{\mathcal{C}},$$

where $\frac{\partial u}{\partial \nu}|_{\mathcal{C}}$ is the normal derivative of u on $\mathcal{C}$, and u is the unique solution corresponding to λ that is not in the spectrum of the corresponding Dirichlet Schrödinger operator.

In our analysis, the D-to-N map is for the dissipative version of Schrödinger operator associated with (1) when $\Omega = (0, R) \times \mathcal{C}$; for some $R > 0$. It is applied as well to the self-adjoint elliptic PDE (1) with the semi-infinite waveguide $\Omega = (R, \infty) \times \mathcal{C}$, see Section 5.2. We estimate error bounds of these maps after applying the domain truncation and investigate spectral properties of the resulting operators. The use of D-to-N operators is far from new in the context of elliptic PDEs on waveguides. For example, Joly et al. [63] and Fliss [54] considered an approach of D-to-N maps for the cross-section of waveguides. A brief discussion about these studies from the numerical point of view will be presented in Section 1.8.

1.6 Motivation and structure of the thesis

There is a strong connection between analysis and numerical calculation of eigenvalues of differential operators. Bailey, Everitt and Zettl in [13] described this connection in the following quote: "Their numerical calculation is of considerable importance in numerical analysis and is a meeting ground for analysis, numerical analysis and applied mathematics." Consequently, in this thesis we focus on the analysis and the numerical computation of eigenvalues of the Schrödinger-type operator associated with (1).

Since most of the eigenvalue problems, particularly eigenvalues in spectral gaps, encountered in applications can not be determined exactly except for some problems, a variety of methods have been developed to obtain such approximations. Moreover, an important issue associated with these methods, known as *spectral pollution*, has been reported. In Section 1.8, we mention some of these methods briefly and present the spectral pollution in some details.

Our main contribution, firstly, is to investigate the spectral analysis of the dissipative versions of Schrödinger operators associated with (1). Moreover, we study the effect of the dissipative technique and its role in avoidance of spectral pollution. We are motivated by [83] and [84] in which dissipative Schrödinger operators on exterior domains and the scalar ODE case on infinite intervals were considered. In Chapter 2, we give a summary of these studies as well as our results for spectral analysis of the dissipative technique for both matrix-valued Schrödinger operators on infinite intervals and elliptic PDEs on semi-infinite waveguides. The latter studies are presented in detail in Chapter 4 and Chapter 5, respectively.

Secondly, we consider the oscillation theory and shooting for the numerical calculation for eigenvalues in spectral gaps especially for the matrix case problem. In Chapter 3, we present some oscillation results and shooting algorithms done in the literature for scalar and matrix Schrödinger problems. Moreover, we give a summary of our analytical results for the oscillation theory in spectral gaps for the ODE (1). In addition, we present a shooting algorithm to calculate eigenvalues in spectral gaps of Schrödinger operators associated with (1) which can handle scalar and matrix ODEs as well as some elliptic PDEs on waveguides. This study is explained in more details in Chapter 6.

1.7 Applications of band-gap spectrum and Schrödinger operators

Spectral problems of band-gap structure of the differential operator associated with (1) have attracted great attention due to their numerous applications in science. Band-gap spectrum of the underlying operator take place in photonic crystals, metamaterials, fluid dynamics, carbon nanostructures, inverse scattering method of solving integrable systems, and topological insulators, see e.g. [70, 104]. In particular, media that have band-gap structure have many applications such as in filters, lasers, microwaves and optical communications. From a physical point of view, in order to produce, for example, lasers or waveguides, in optics, one should allow modes "eigenfunctions" in the band gaps. These modes are obtained from creating localised defects in the periodic structure and, mathematically, correspond to isolated eigenvalues of finite multiplicity inside the spectral gaps which are known as impurity eigenvalues. The concept of local defects relates to a perturbation with compact support that is introduced to the periodic structure of the underlying operator.

On the other hand, the Schrödinger operator associated with (1) appears in physical models in elasticity theory, electromagnetic waves, and nuclear structure, see [94, 51] and references therein. Moreover, it arises in many models in quan-

9

tum mechanics such as quantum graphs [67] and quantum wires [71]. In contrast to the latter applications of the self-adjoint Schrödinger operator, spectral problems of the non-selfadjoint operator are specifically encountered in hydrodynamics [35] and magnetohydrodynamics [79].

1.8   Spectral pollution and different approaches

Even though most of the essential spectra of self-adjoint operators arising in applications can be determined analytically from Weyl's theorem and Floquet theory and other analytical tools, discrete eigenvalues are often difficult to find explicitly. Thus, a major problem in the numerical computation of band-gap spectrum of self-adjoint operators is calculating isolated eigenvalues in spectral gaps. In the classical variational methods, such as finite element methods, eigenvalues of the discretised problem can appear in the spectral gaps, see e.g., [80, 97], and some of these eigenvalues, called *spurious eigenvalues*, may not converge to spectrum of the original problem. This phenomenon is called *spectral pollution.* Spurious eigenvalues can only occur in the spectral gaps between two successive spectral bands. Moreover, if there are infinitely many isolated eigenvalues, then they accumulate at the ends of the boundaries of the spectral gaps [101], see Figure 1.2. This leads to the difficulty of distinguishing eigenvalues from spectral pollution. For eigenvalues below the essential spectrum, spectral pollution can not happen due to the min-max principle. To see this, suppose that the essential spectrum is bounded below and that the eigenvalues are also bounded below. If there are eigenvalues below the essential spectrum, then there is a lowest eigenvalue λ_0. Suppose λ_k, $k = 0, 1, \ldots$, are the eigenvalues below the essential spectrum. There may be finitely many or infinitely many such eigenvalues. If these are approximated using a Galerkin method, or using domain truncation with Dirichlet boundary conditions, then the corresponding approximating eigenvalues $\lambda_k^{(n)}$, $k = 0, 1, \ldots$, $n \in \mathbb{N}$, satisfy

$$\lambda_k \leq \lambda_k^{(n)} \leq \lambda_k^{(n+1)}, \quad n \in \mathbb{N}.$$

The monotonicity of the convergence of the $\lambda_k^{(n)}$ ensures that spectral pollution is impossible; if some $\lambda_j^{(n)}$ sequence converged to a number strictly above λ_j, then λ_j would not be approximated to full multiplicity, contradicting (an enhanced version of) spectral inclusion.
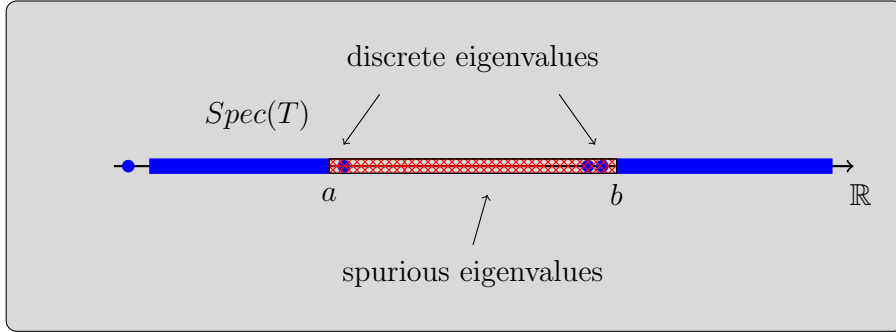
Figure 1.2: Spectral pollution of an operator T can appear in the whole spectral gap (a, b), see [78].

Many studies have been dedicated to overcome the phenomenon of spectral pollution. For example, Mertins and Zimmermann [113], Davies [41], and Davies and Plum [43] obtained enclosures to eigenvalues in spectral gaps which are based on the min-max principle. Levitin and Shargorodsky [77] and Boulton and Levitin [25] applied the quadratic projection method or second order relative spectra to the case of perturbed periodic Schrödinger operators and computed upper and lower bounds of the discretised eigenvalues. Away from the classical technique of determining the approximate eigenvalues, Lewin and Séré [78] characterised, analytically, the spectral pollution under special conditions on the projection method and applied their results to the perturbed periodic Schrödinger operators using some specific basis that is free of spectral pollution. A more general framework for spectral pollution in the projection method was followed by Boulton, Boussaid, and Lewin [24]. However, these approaches are applied to general abstract self-adjoint operators in Hilbert spaces and their applications always require a priori information about the spectrum and choices of the subspaces.

Other studies consider the supercell method. This method turns the problem into a problem on a large-sized bounded domain with periodic boundary conditions. A Fourier method is then used to discretise the problem and leads to an eigenvalue problem on a bounded domain. Analysis of convergence of this method for two-dimensional problems, in particular, Maxwell's equation, was studied by Soussi [105]. Cances et al. [31] proved that for a perturbed periodic Schrödinger operator the supercell method with Fourier bases is free from spectral pollution. Moreover, a rate of convergence and error estimates are derived for this method, including the error of the numerical integration [32]. The main disadvantage of this method is that the size of the supercell needs to be larger in order to obtain an eigenfunction that is decaying slowly, as it corresponds to an eigenvalue that is close to the essential spectrum. Thus

increasing the size of the supercell leads to an increase of the computational cost.

Another method was proposed by Joly et al. [63] and Fliss [54] in which they considered an approach that is based on Dirichlet-to-Neumann maps for photonic crystal waveguides. By introducing these maps on the cross-section of the waveguide together with the Floquet theory, the problem is reduced to local problems on a single periodicity cell. This leads to a nonlinear eigenvalue problem and it is considered as an exact method which can not generate spectral pollution. However, solving a nonlinear eigenvalue problem is known to cost more computational time compared to a linear eigenvalue problem.

Spectral pollution is also a well known issue in the context of differential operators with infinite domains, as it is induced by domain truncation, see [12, 107]. Consequently, it can be avoided by suitable choices of the boundary conditions on the boundary of the truncated domain.

The essential numerical range $W_{ess}(T)$ is a useful tool in the context of spectral pollution. This is because it includes spurious eigenvalues. In particular, for projection or domain truncation methods, the essential numerical range is the smallest set which contains all possible spurious eigenvalues, see [22].

2 Dissipative Schrödinger operators

This chapter is devoted to describing the dissipative barrier approach to approximate eigenvalues in spectral gaps of self-adjoint Schrödinger problems, to avoid spectral pollution. In Section 2.1 we introduce the dissipative barrier approach, and we discuss the previous literature on this approach to approximate eigenvalues in spectral gaps of different operators in Section 2.2. Main analytical results of Chapter 4 and Chapter 5 are presented in Section 2.3 and Section 2.4 respectively. Numerical results of Chapter 4 and Chapter 5 are discussed briefly in Section 2.5.

2.1 Dissipative barrier approach

The *dissipative barrier technique* is based on using a non-selfadjoint perturbation of the self-adjoint operator associated with (1) in order to "move" the eigenvalues from the spectral gaps of the essential spectrum to the complex plane. In particular, it depends on introducing a dissipative perturbation term, $i\gamma S$; γ is a positive real parameter and S is a compactly supported function, to the associated real-valued bounded potential Q. Hence the new problem becomes a non-selfadjoint operator even when equipped with self-adjoint boundary conditions. Since the potential is perturbed by a compactly supported function, then, according to Weyl's theorem [98], the essential spectrum of the original problem is invariant. Moreover, eigenvalues which lie in a spectral gap of the self-adjoint problem are perturbed approximately by the complex shift γ, see Theorem 2.1 in Section 2.3 and Figure 2.1. Thus they move to the complex plane where spectral pollution does not occur, see Theorem 2.4 in Section 2.3 and Theorem 2.6 in Section 2.4. Hence they can be determined easily.
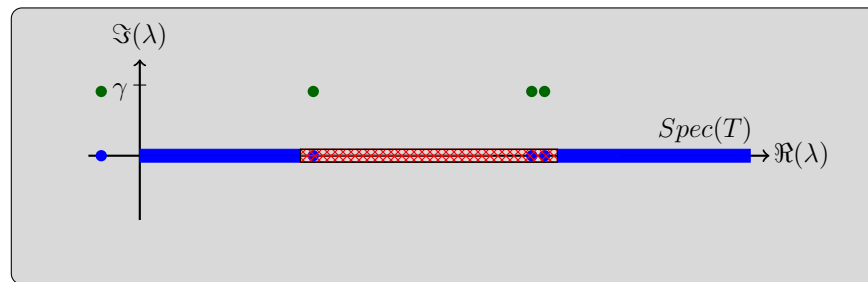
Figure 2.1: The effect of the dissipative perturbation term $i\gamma S$ on the spectrum of the self-adjoint operator T. Discrete eigenvalues (dots) move to the complex plane.

2.2 Previous studies

In the following we present studies done in the literature which consider the dissipative barrier technique on different Schrödinger operators.

Elliptic PDEs on exterior domains

In [82] Marletta studied approximation of non-real isolated eigenvalues of the elliptic PDE (1) on exterior domains with a Dirichlet-to-Neumann map on the inner boundary [5] when Q is a complex-valued potential and has a limit at ∞. This study considers the domain truncation as an approximation method and analyses the convergence of the Dirichlet-to-Neumann maps. It deduces results on the approximation of the spectrum of the original problem by the spectra of the approximating problems. The study shows that spurious eigenvalues can not be generated for this problem using the given procedure.

Marletta generalised this result in [83] to work for the non-selfadjoint operator with suitable boundary conditions when $\Re(Q)$ is bounded below and $\Im(Q)$ satisfies a uniform slow decay condition. The main result implies that the Dirichlet-to-Neumann maps and domain truncation can only generate spectral pollution on the real axis. Thus, the author suggested the "trick" of the compactly supported complex shift to the self-adjoint operator in order to obtain isolated eigenvalues free of spectral pollution. However, error bounds are not investigated for this problem.

Scalar Schrödinger operators on the half-line

In another study [84], the authors adopted the same techniques in the context of the 1-dimensional Schrödinger operator associated with equation (1) on the half line and extensively analysed properties of the resulting approximation. We now summarise the main results.

The study implies, in particular, that if Q is a real-valued locally integrable potential on $[0, \infty)$ and an eigenvalue λ lies outside the essential spectrum and has an exponentially decaying eigenfunction, then choosing the barrier $i\gamma S$, where $\gamma > 0$ is fixed and $S = \chi_{[0,R]}$ is the characteristic function of $[0, R]$, then the dissipative problem has, for sufficiently large R, an eigenvalue λ_R whose real part is exponentially close to λ in the precise sense that there exist positive constants C_1 and C_2 independent of R such that $|\Re(\lambda_R) - \lambda| < C_1 \exp(-C_2 R)$.

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[5]In this study, the Dirichlet-to-Neumann map was not included in the boundary conditions, but it was used as a tool.

Moreover, the study derives approximations to the non-real isolated eigenvalues of the singular non-selfadjoint problem. It shows that truncating the shifted problem to some intervals $[0, X]; X > R$ can generate "good" eigenvalues, that converge to an eigenvalue of the non-truncated shifted problem, with an error bound that is exponentially small with respect to $X - R$.

Additionally, a spurious eigenvalue or as the authors referred to it, a "bad" eigenvalue of the truncated shifted problem has imaginary part that is exponentially small with respect to $X - R$. Thus, spectral pollution only occurs on the real axis for this operator.

The study considers the behaviour of eigenvalues λ_γ of the non-truncated shifted problems as functions of γ. An important result indicates that one possible behaviour of λ_γ is that there exists $\gamma_{crit} > 0$ such that, as $\gamma \searrow \gamma_{crit}$, λ_γ converges to an interior point of spectral bands of the underlying 1-dimensional Schrödinger operator. This result is of particular interest for the matrix Schrödinger operators which we will discuss later.

In fact, these studies, [83] and [84], provide some numerical examples to illustrate the theoretical results. The numerical calculations are obtained using a finite element method and finite difference methods, respectively, to discretise the shifted truncated boundary value problems. Numerical results show that the dissipative procedure gives good approximation for many problems and can be considered as a successful method to approximate isolated eigenvalues for these types of operators.

2.3   Matrix Schrödinger operators on the half-line

In this section, we summaries the main results of Chapter 4. We consider the dissipative matrix Schrödinger equation on $\Omega = [0, \infty)$,

$$- \underline{u}'' + (Q + i\gamma S)\underline{u} = \lambda \underline{u}, \tag{2}$$

with a boundary condition:

$$\cos(\alpha)\underline{u}(0) - \sin(\alpha)\underline{u}'(0) = \underline{0}, \tag{3}$$

where $\alpha \in [0, \pi)$. Here $\underline{u}$ is a vector-valued function in a subspace of $L^2([0, \infty))^n$, the parameter γ is a nonzero real, and the coefficients Q, S satisfy the following hypotheses:

(A1): $Q(x)$ is a Hermitian-valued function, integrable over compact subsets of $[0, \infty)$, and is eventually periodic with period $a > 0$ i.e, there exists $R_0 \geq 0$ such that

$$Q(x + a) = Q(x), \quad \forall x \geq R_0. \tag{4}$$

(A2): S is a cutoff function with support in $[0, R]$ for some $R \geq R_0$: there exists $0 < c < 1$ such that

$$S(x) = \begin{cases} I, & x < cR; \\ 0, & x \geq R. \end{cases} \tag{5}$$

When $x \in (cR, R)$, we assume that $0 \leq S(x) \leq I$.

We define an operator L_0 by:

$$L_0 \underline{u} = -\underline{u}'' + Q\underline{u}, \tag{6}$$

with domain:

$$D(L_0) = \{\, \underline{u} \in L^2(0, \infty) | -\underline{u}'' + Q\underline{u} \in L^2(0, \infty),$$
$$\cos(\alpha)\underline{u}(0) - \sin(\alpha)\underline{u}'(0) = \underline{0} \,\}. \tag{7}$$

Motivated by the study [84], summarised in the later section, we employ the domain truncation and investigate the behaviour of eigenvalues λ_γ of the underlying problem (2)-(3). First of all, we show the following result for an isolated eigenvalue λ of the original problem (6)-(7) which is associated with an exponentially decaying eigenfunction.

Theorem 2.1. *Suppose that assumption (A2) holds — see (5). Let λ be an isolated eigenvalue of L_0 with multiplicity ν, where $1 \leq \nu \leq n$, and normalised eigenvectors u_j, $j = 1, \ldots, \nu$. For each sufficiently small $\gamma > 0$, let $\lambda_{\gamma,j}; j = 1, \ldots, \nu$, be eigenvalues of the non-selfadjoint operator $L_0 + i\gamma S$ defined in (6)-(7) with eigenvectors $u_{\gamma,j}$, $j = 1, \ldots, \nu$, and suppose $\lambda_{\gamma,j} \to \lambda$ as $\gamma \to 0$. Then for each $1 \leq j \leq \nu$, the projection of $u_{\gamma,j}$ onto $\mathrm{Span}\{u_1, \ldots, u_\nu\}$ remains bounded away from zero, uniformly with respect to R and γ for sufficiently small γ.*

If, additionally, the assumption
(A1'):

$$\|u_j(x)\| \leq C \exp(-C_4 x), \quad x \in [0, \infty), \quad j = 1, \ldots, \nu,$$

holds for some positive constants C and C_4, then there exists $C_3 > 0$, such that for all $R > 0$,

$$|\lambda + i\gamma - \lambda_{\gamma,j}| \leq C_3 \gamma \exp(-cC_4 R), \tag{8}$$

where $c \in (0, 1)$ is the constant appearing in assumption (A2).

Remark 2.2. Note that $\lambda_{\gamma,j}$ in (8) depends on R.

Another result is specified for the approximation of the non-real isolated eigen-value λ_γ of the non-selfadjoint, or the shifted, problem (2)-(3) when the domain is truncated to some intervals $[0, X]$ for some $X > R$. At $x = X$ we impose, for some $\beta \in \mathbb{R}$, a self-adjoint artificial boundary condition:

$$\cos(\beta)\underline{u}(X) - \sin(\beta)\underline{u}'(X) = \underline{0}.$$

The operator L_0 is replaced by $L_{0,X}$ defined by:

$$L_{0,X}\underline{u} = -\underline{u}'' + Q\underline{u}, \tag{9}$$

with domain:

$$D(L_{0,X}) = \{\, \underline{u} \in L^2(0, X)| - \underline{u}'' + Q\underline{u} \in L^2(0, X),$$
$$\cos(\alpha)\underline{u}(0) - \sin(\alpha)\underline{u}'(0) = \underline{0} = \cos(\beta)\underline{u}(X) - \sin(\beta)\underline{u}'(X) \,\}. \tag{10}$$

Theorem 2.3. *Suppose that assumptions (A1) and (A2) hold. For $\gamma > 0$, let λ_γ be an eigenvalue of the non-self-adjoint Schrödinger operator $L_0 + i\gamma S$ defined in (6)-(7). Then for all sufficiently large $X \geq R + a$, there exist approximations $\lambda_{\gamma,X,good}$ to λ_γ, whose total algebraic multiplicity is equal to the algebraic multiplicity of λ_γ, obtained as eigenvalues of the operator $L_{0,X} + i\gamma S$ defined in (9)-(10), which satisfy*

$$|\lambda_\gamma - \lambda_{\gamma,X,good}| \leq C_5 \exp\left(-C_6(X - R)\right).$$

Here C_5 and C_6 are positive constants which depend on λ_γ.

We establish a special characterisation to the polluting eigenvalue $\lambda_{\gamma,X,bad}$ of the truncated non-selfadjoint problem.

Theorem 2.4. *Suppose that assumptions (A1) and (A2) hold. For $\gamma > 0$, let $\lambda_{\gamma,X,bad}$ be an eigenvalue of the non-self-adjoint Schrödinger operator $L_{0,X} + i\gamma S$ defined in (9)-(10) which converges, as $X \to +\infty$, to a point which is not in the spectrum of $L_0 + i\gamma S$. Then for some positive constants C_7 and C_8:*

$$|\Im(\lambda_{\gamma,X,bad})| \leq C_7 \exp(-C_8(X - R)).$$

These results are in agreement with those in the scalar case established in [84], see Section 2.2.

A particular result which is established for the scalar case proves the existence of $\gamma_{crit} > 0$ for which, as $\gamma \searrow \gamma_{crit}$, λ_γ merges into the essential spectrum. However this result is not generally true for the matrix coefficients operators, as it occurs simply when $\gamma = 0$ for some specific problems. We indicate the following example.

Example 2.5. Consider the matrix Schrödinger problem:

$$-\underline{u}''(x) + (Q(x) + i\gamma S(x))\underline{u}(x) = \lambda\underline{u}(x), \quad \underline{u}(0) = \underline{0},$$

with $Q(x) = \begin{pmatrix} 0 & 0 \\ 0 & \frac{-40}{1+x^2} + \sin(x) \end{pmatrix}$ and $S(x) = \begin{cases} I_2 & in & [0,50], \\ 0 & in & (50,\infty). \end{cases}$

The system can be seen as two scalar problems with $q_1(x) = 0$ and $q_2(x) = \frac{-40}{1+x^2} + \sin(x)$. The problem with potential q_2 and $\gamma = 0$ has a spectral gap which is approximately $(-0.340363, 0.595942)$, with infinitely many eigenvalues accumulating from below at the top end of the gap [101]. However these eigenvalues all lie in the essential spectrum $[0,\infty)$ for the problem with potential q_1 and hence also lie in the essential spectrum of the matrix Schrödinger system. Nevertheless, they emerge from the real axis with positive speed, into the upper half-plane, as soon as γ is increased from zero following the estimate in Theorem 2.1.

2.4 Elliptic PDEs on semi-infinite waveguides

We now turn our attention to Chapter 5 in which we consider the elliptic PDE:

$$-\Delta u + (Q + i\gamma S)u = \lambda u, \tag{11}$$

on a semi-infinite waveguide $\Omega = (0,\infty) \times \mathcal{C} \subseteq \mathbb{R}^d; d \geq 1$ where $\mathcal{C}$ is a smooth bounded domain in $\mathbb{R}^{d-1}; d > 1$ with a boundary condition $u|_{\partial\Omega} = 0$. The coefficients Q and S satisfy the following hypotheses:

(A1): Q is bounded, real-valued, and integrable over compact subsets of Ω.

(A2): S is a cut-off function with support in $[0,R]$ for some $R > 0$: there exists $0 < c < 1$ such that if $x \in [0,\infty)$ and $y \in \mathcal{C}$ then

$$S(x,y) = \begin{cases} 1, & x < cR; \\ 0, & x \geq R. \end{cases} \tag{12}$$

When $x \in (cR, R)$, we assume that S is measurable and takes values in $[0,1]$. We define an operator L_0 by:

$$L_0 u = (-\Delta + Q)u, \tag{13}$$

with domain:

$$D(L_0) = \{ u \in H^2_{loc}(\Omega) \cap H^1_0(\Omega), |\ (-\Delta + Q)u \in L^2(\Omega)\}. \tag{14}$$

We aim to investigate the behaviour of isolated eigenvalues λ_γ of the problem when employing the technique of the complex shift $i\gamma S$ and the domain truncation

over some waveguides $\Omega_{(0,X)} = (0,X) \times \mathcal{C}$ for some $X > R$. At $x = X$, we can impose a Dirichlet condition $u|_X = 0$. The operator L_0 is replaced by L_X:

$$L_X u = (-\Delta + Q)u, \tag{15}$$

with domain:

$$D(L_X) = \{u \in H^2_{loc}(\Omega_{(0,X)}) \cap H^1_0(\Omega_{(0,X)}) \mid (-\Delta + Q)u \in L^2(\Omega_{(0,X)})\}. \tag{16}$$

The following result indicates that the dissipative barrier technique with domain truncation does not generate any spectral pollution in the upper half plane for this problem.

Theorem 2.6. *For $\gamma > 0$, suppose $\lambda_{\gamma,X}$ be in the spectrum of $L_X + i\gamma S$ with $\lambda_{\gamma,X} \to \lambda_\gamma$, as $X \to \infty$ with $\Im(\lambda_\gamma) > 0$. Then λ_γ is in the spectrum of $L_0 + i\gamma S$.*

This result agrees with that in Theorem 2.4 for the matrix case in the previous section. Moreover, our main result establishes approximation of isolated non-real eigenvalues to the non-selfadjoint operator, and it gives an estimate for the error.

Theorem 2.7. *Suppose that Assumptions (A1) and (A2) hold. For $\gamma > 0$, let λ_γ be an eigenvalue of the non-self-adjoint Schrödinger operator $L_0 + i\gamma S$ defined in (13)-(14). Then there exists an approximation $\lambda_{\gamma,X}$ to λ_γ, given by an eigenvalue of the operator $L_X + i\gamma S$ defined in (15)-(16) which satisfies*

$$|\lambda_\gamma - \lambda_{\gamma,X}| \leq C_9 \exp(-C_{10}(X - R)),$$

where C_9 and C_{10} are positive constants which depend on λ_γ.

This result is in agreement with that in Theorem 2.3 for the matrix case in the previous section.

2.5 Numerical results

In Chapter 4 and Chapter 5, we illustrate our theoretical results on different numerical examples. Numerical results for matrix Schrödinger problems are obtained using the finite difference scheme in order to discretise the BVPs which lead to $\lambda-$linear problems. For the elliptic PDEs on waveguides, a finite element method is applied to discretise the resulting shifted eigenvalue problem, see Figure 2.3 for the main procedure of the dissipative barrier scheme on the general self-adjoint Schrödinger equation (1). Numerical results indicate the effectiveness of this approach to calculate isolated eigenvalues to these operators. The approach gives accurate results and

can be easily implemented. In addition, the approach can be considered as a successful tool to obtain approximation to eigenvalues to the non-selfadjoint case which is not covered by the methods of Mertins and Zimmermann, Boulton and Levitin or Soussi mentioned in Section 1.8.

One major difficulty we encounter when using the discretisation in the BVP resulting from the dissipative barrier technique and domain truncation is that it requires adaptive meshing. Figure 2.2 shows the corresponding adaptive mesh we use to do the calculation for one of the elliptic PDEs on waveguides discussed in Example 5.26 in Section 5.5. Accuracy of discretising BVPs is limited by the rate of decay of eigenfunctions. In particular, when calculating eigenfunctions corresponding to eigenvalues that are close to spectral bands, the decay of the eigenfunctions can be slow, hence the associated domain truncations require larger domains. This can affect the adaptive meshing and lead to more computational cost in order to obtain the approximations.
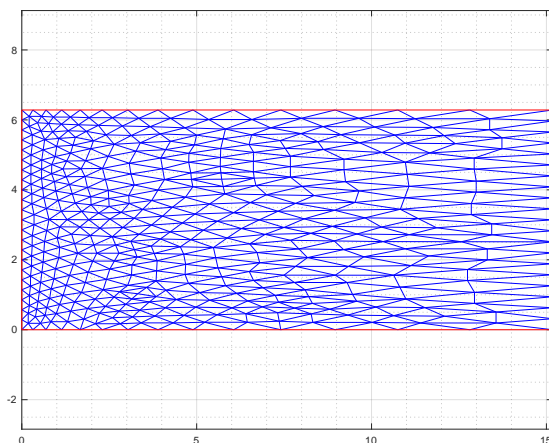
Figure 2.2: Adaptive mesh of Example 5.26 in Section 5.5

Another difficulty is that some of the eigenvalues can be missed. This is because the dissipative barrier technique lifts eigenvalues away from the spectral gaps and hence out of the essential numerical range of the underlying operator. Thus, Arnoldi method, see [100, Chapter 6], must then be used, as the problem becomes non-self-adjoint. This generally performs well, but the subspace iterations may fail to converge, see Figure 5.14 in Section 5.5.

To obtain eigenvalues λ in spectral gaps of the self-adjoint problem:

$$-\Delta u + Qu = \lambda u \quad \text{in} \quad \Omega$$

Add $i\gamma S$ with support on $\Omega_R; R > 0$ to the potential Q and the problem becomes:

$$-\Delta u + \big(Q + i\gamma S\big)u = \lambda u \quad \text{in} \quad \Omega$$

Reduce the problem to a finite domain $\Omega_X; X > R$:

$$-\Delta u + \big(Q + i\gamma S\big)u = \lambda u,$$

with Dirichlet condition $u_{|\partial\Omega_X} = 0$.

Discretise the BVP on the truncated domain Ω_X

Solve the resulting eigenproblem:

$$AU = \lambda BU$$

Eigenvalues of the original problems are those in spectral gaps whose imaginary part is close to γ.

Figure 2.3: Dissipative barrier technique with domain truncation for eigenvalues in spectral gaps of Schrödinger problems.

3 Generalised oscillation theory and shooting for eigenvalues of Schrödinger operators

This chapter presents an approach based on oscillation theory to approximate eigenvalues in spectral gaps of the self-adjoint Schrödinger problem (1). In Section 3.1, we introduce oscillation and shooting approach. In Section 3.2 we discuss previous literature on calculating eigenvalues of Schrödinger operators. A summary of the proposed approach and main analytical results of Chapter 6 are presented in Section 3.3. Numerical results of Chapter 6 are discussed briefly in Section 3.4.

3.1 Oscillation and shooting approach

There are two main standard approaches to the numerical approximation of eigenvalues of boundary value problems, namely reduction to a matrix eigenvalue problem using methods such as finite difference methods and finite element methods, and shooting. This chapter considers shooting. Shooting has played a major role in the development of automatic software for numerical solution of Schrödinger differential equations for over 50 years. The basic idea of shooting methods is to solve the differential equation as an initial value problem over a certain interval. At the same time, a sequence of trial values of λ is chosen which are adjusted until the boundary conditions at the both ends are satisfied at which point we have an eigenvalue to the problem. The shooting process requires using a suitable *miss-distance* function on the resulting solutions. This function has a zero when λ is an eigenvalue for the original problem, i.e., when the boundary conditions are satisfied. However, there are various problems associated with this standard approach of the root-finding process. We indicate the following example.

Example 3.1. Consider the scalar Schrödinger problem:

$$-u'' + \left(-(2\pi - \min(x, 2\pi))^2 + \sin(x)\right) u = \lambda u,$$

on $[0, \infty)$ with $u(0) = 0$. This problem has a spectral gap given in Example 2.5 in Section 2.3. We solve the problem using the shooting method on the truncated interval $[0, X]; X = 6\pi$. In addition, the boundary conditions on the right hand side of the truncated interval are determined by the Floquet solutions $\Psi(.)$ and their derivatives $\Psi'(.)$ and are $\lambda-$dependent. Figure 3.1 shows the graph of the corresponding miss-distance function $N(\lambda)$ for the problem on the given gap. Here $N(\lambda)$ is given by:

$$N(\lambda) = \det \begin{pmatrix} u(X, \lambda) & \Psi(\lambda) \\ u'(X, \lambda) & \Psi'(\lambda) \end{pmatrix}.$$

This function has a zero approximately at 0.479210. In addition, the graph of the corresponding eigenfunction is indicated in Figure 3.2. It can be seen that the derivative of $N(\lambda)$ is small close to the zero of $N(\lambda)$. This makes accurate determination of the location of the zeros difficult.
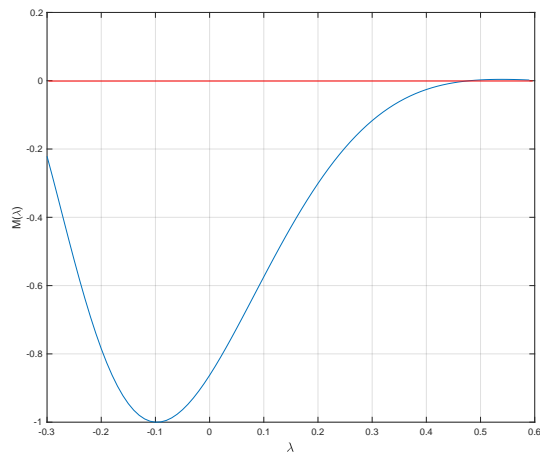
Figure 3.1: Miss-distance function of Example 3.1.
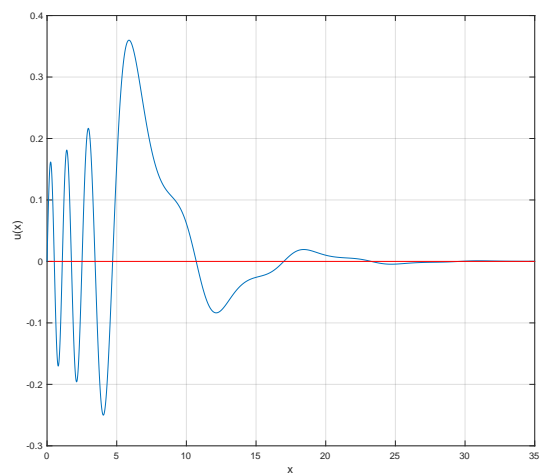
Figure 3.2: Eigenfunction of the eigenvalue $\lambda = 0.479210$ of Example 3.1.

To avoid this difficulty, one can instead count the zeros of the eigenfunction corresponding to the desired eigenvalue. However, this oscillation theory is not valid in the case of eigenfunctions which have infinitely many zeros. Before addressing this

23

difficulty, we introduce a reformulation of oscillation theory using the so-called *Prüfer transformation*. The idea of this transformation is to use the polar coordinate (r, θ) in the phase plane (u, u').

Definition 3.2. [38, Chapter 8] Let u be the real-valued nontrivial solution of the scalar Schrödinger equation:

$$-u'' + qu = \lambda u \ \text{ on } \ [0, \infty)$$

with initial conditions $u(0) = \sin \alpha$ and $u'(0) = \cos \alpha$. The Prüfer transformation takes the form

$$u = r \sin \theta \quad \text{and} \quad u' = r \cos \theta.$$

Then $\theta : [0, \infty) \to \mathbb{R}$ is known as the Prüfer angle and $r : [0, \infty) \to (0, \infty)$ is the Prüfer radius and satisfy the differential equations:

$$\theta' = \cos^2 \theta + (\lambda - q) \sin^2 \theta,$$

$$(\log r)' = (q - \lambda + 1) \sin \theta \cos \theta,$$

with initial conditions $\theta(0, \lambda) = \alpha \in \mathbb{R}$ and $r(0, \lambda) = 1$.

One main advantage of the Prufer θ-angle is that it allows one to define a monotone increasing miss-distance $f(\lambda)$ with the property that $f(\lambda_k) = k\pi$, $k = 0, 1, 2, \ldots$; eigenvalues can even be calculated with the correct index!

3.2   Previous studies

The Prüfer transformation and miss-distance functions form the basis of various methods proposed in the literature. For example, Bailey, Gordon, and Shampine [14] and Bailey, Everitt and Zettl [13] proposed a shooting algorithm and used the Prüfer transformation of the differential equation in order to localise and calculate eigenvalues and eigenfunctions to the 1-dimensional self-adjoint regular and singular differential operators with separated and coupled boundary conditions. To overcome some other associated stiffness problems, which generally appear when using the initial value solver, Pruess and Fulton [96] used the Prüfer-based shooting methods together with the piecewise constant approximation of coefficients of the differential equations and designed an algorithm to obtain the approximations. In these studies, approximations to the desired eigenvalues of the singular differential problems on $[0, \infty)$ are obtained using interval truncation.

For eigenvalues of Schrödinger problems with matrix coefficients, one may face two main difficulties. Firstly, the Prüfer transformation does not extend to this type

of problem. Secondly, matrix problems can often encounter stiffness issues. Thus, Atkinson and his team, in [11], introduced a new algorithm which depends on a replacement for the Prüfer $\theta-$angle to calculate eigenvalues for these problems and avoid associated stiffness problems. The algorithm is based on unitary matrices, introduced first by Atkinson in [10], constructed from the original Schrödinger problem. Moreover, it provides a search procedure, to find the desired eigenvalue to the problem, that is based on tracking eigenvalues of the generated unitary matrix on the unit circle. Hence, if 1 is an eigenvalue to this unitary matrix, then the corresponding λ is an eigenvalue to the original problem. In addition, a miss-distance function is calculated which uses the phase angles of the eigenvalues of the unitary matrix and allows one to compute the counting function $M(\lambda)$

$$M(\lambda) = \text{number of Schrödinger eigenvalues of} < \lambda. \tag{17}$$

Marletta [81] followed the same idea of considering unitary matrices and improved and generalised the miss-distance function (17). The idea is to use the function $M(\lambda)$ to find the eigenvalues of the original problem by finding the points where $M(\lambda)$ is discontinuous. Moreover, it provides a natural indexing to the desired eigenvalues, see Definition 3.16 in Section 3.3. However, this study, [81], considers eigenvalues of the regular case as well as eigenvalues below the essential spectrum to the vector-valued Schrödinger problems. In addition, numerical results are obtained using constant coefficients approximation.

For the context of spectral gaps of the underlying problems and the phenomenon of spectral pollution, shooting can be considered as a "safe" method that is free of spectral pollution. This is not a trivial process as it requires a suitable choice to the truncated boundary conditions. To the best of our knowledge, there is a lack of studies done in the literature in the direction of shooting methods and eigenvalues in spectral gaps of Schrödinger operators, particularly, with matrix coefficients. One of the existing works is devoted to the approximation of eigenvalues in spectral gaps to the scalar case of such operators. Aceto, Ghelardoni, and Marletta [2] provided an algorithm which is based on combining a shooting method with Floquet theory which allows computation to be done on smaller domains. To approximate the problem, the authors suggested truncating the perturbation function, i.e., considering the rapid decay of the perturbed potential instead of the classical way of the rapid decay of eigenfunctions. Thus the original problem then needs a boundary condition on the right hand side. This step is done by solving the unperturbed, periodic, problem using the Floquet theory hence the boundary condition, on the right hand side, becomes of $\lambda-$dependent. The resulting boundary value problem is then solved using shooting. Boundary value methods are used to discretise the initial value problem.

We are inspired by the latter study, [2], as well as the special treatment to the matrix differential equations, [11] and [81]. In the following sections we introduce and discuss a new algorithm to calculate eigenvalues in spectral gaps to matrix-valued Schrödinger operators.

3.3 Oscillation and shooting for eigenvalues in spectral gaps of Schrödinger operators

In this section we describe the main analytical results of Chapter 6. In this study we aim to calculate isolated eigenvalues of the singular self-adjoint Schrödinger equation on $[0, \infty)$:

$$- \underline{u}'' + Q\underline{u} = \lambda\underline{u}, \tag{18}$$

Recall that Q is an n by n Hermitian matrix-valued potential, and that it can be decomposed into an a-periodic function Q_p and a perturbed function R that is compactly supported with support on $[0, X]$, for some $X > 0$. We assume that our problem (18) is supplemented by a boundary condition:

$$A\underline{u}(0) - B\underline{u}'(0) = \underline{0}, \tag{19}$$

where A and B are $n \times n$ matrices such that (A, B) has full rank n and $AB^* - BA^* = 0$.

Compared to the works in [11] and [81], the new features here are:

1. We can deal with matrix coefficients.

2. We still have a monotone increasing integer-valued function whose discontinuity is the eigenvalue which was not previously known.

3. This allows for reliable computation of eigenvalues with no eigenvalue being missed compared to other methods. We saw that using the dissipative barrier method can miss some eigenvalues for the reason that the numerical linear algebra does not have globally guaranteed convergence, see Section 2.5.

In general, the main procedure of the proposed algorithm is similar to the one in [2] in terms of truncating the compactly supported function to R_N with $\mathrm{supp}(R_N) \subseteq [0, Na]$ for some $N \in \mathbb{N}$ and identifying the boundary condition at $x = Na$. The latter is obtained using the Floquet theory, see Section 4.3 for more details. For λ outside the union of spectral bands of (18), let $\Psi(\cdot, \lambda)$ be the $n \times n$ matrix whose columns are the Floquet solutions $\underline{u}_1(x, \lambda), \ldots, \underline{u}_n(x, \lambda)$. These Floquet solutions are obtained from solving the unperturbed periodic Schrödinger equation

$$- \underline{u}'' + Q_p\underline{u} = \lambda\underline{u}, \tag{20}$$

and corresponding to the Floquet multipliers $\rho_j(\lambda) \in \mathbb{C}; j = 1, \ldots, n$ with $|\rho_j(\lambda)| < 1$. This allows us to define the Atkinson Θ-matrix associated with Ψ which we call Θ_F.

Definition 3.3. The *Atkinson Θ-matrix* associated with Ψ is the matrix

$$\Theta_F(x, \lambda) := (\Psi'(x, \lambda) + i\Psi(x, \lambda))(\Psi'(x, \lambda) - i\Psi(x, \lambda))^{-1}.$$

The following proposition collects some important properties of Θ_F. we derive an important monotonicity result, which is new even for the scalar case $n = 1$ which describes the behaviour as a function of λ of the Prüfer $\theta-$ angles of the square integrable Floquet solutions.

Proposition 3.4. For λ in a fixed spectral gap, the following are true.

1. $\Theta_F(x, \lambda)$ is a well-defined unitary matrix.

2. $\Theta_F(x + a, \lambda) = \Theta_F(x, \lambda)$.

3. For each fixed x, the eigenvalues of $\Theta_F(x, \lambda)$ move strictly monotonically round the unit circle in $\mathbb{C}$, in a negative direction with increasing λ.

Let $\Psi_R(\cdot, \lambda)$ be the unique $n \times n$ matrix which satisfies the initial value problem

$$-\Psi_R''(x, \lambda) + (Q_p(x) + R(x))\Psi_R(x, \lambda) = \lambda\Psi_R(x, \lambda),$$

$$\Psi_R(X, \lambda) = \Psi(X, \lambda), \quad \Psi_R'(X, \lambda) = \Psi'(X, \lambda).$$

This leads to the definition of the Θ_R matrix.

Definition 3.5. The Atkinson Θ-matrix associated with Ψ_R is defined by

$$\Theta_R(x, \lambda) = (\Psi_R'(x, \lambda) + i\Psi_R(x, \lambda))(\Psi_R'(x, \lambda) - i\Psi_R(x, \lambda))^{-1}.$$

Note that by unique continuation, since $R(x) = 0$ for $x > X$, we have $\Psi(x, \lambda) = \Psi_R(x, \lambda)$ for $x \geq X$. This means, in turn, that

$$\Theta_R(x, \lambda) = \Theta_F(x, \lambda) \quad \forall x \geq X. \tag{21}$$

We derive the following properties for Θ_R.

Proposition 3.6. For λ in a fixed spectral gap, the following are true.

1. $\Theta_R(x, \lambda)$ is a well defined and unitary matrix.

27

2. the eigenvalues of $\Theta_R(x, \lambda)$ move negatively round the unit circle for all $x \geq 0$, for increasing λ.

Moreover, $\Theta_R(x, \lambda)$ is the solution of the following differential equation.

Proposition 3.7. Suppose that $N \in \mathbb{N}$ is such that $Na \geq X$. Then $\Theta_R(x, \lambda)$ is the unique solution of the initial value problem

$$\frac{d}{dx}\Theta_R(x, \lambda) = i\Theta_R(x, \lambda)\Omega(x, \lambda, \Theta_R), \quad \Theta_R(Na, \lambda) = \Theta_F(0, \lambda), \qquad (22)$$

in which $\Omega(x, \lambda, \bullet)$ is defined by the formula

$$\Omega(x, \lambda, \Theta) = \frac{1}{2}((\Theta^{-1} + I)(\Theta + I) - (\Theta^{-1} - I)(Q(x) - \lambda I)(\Theta - I)). \qquad (23)$$

Similarly, let $\Psi_L(\cdot, \lambda)$ be the unique $n \times n$ matrix which satisfies the initial value problem

$$-\Psi_L''(x, \lambda) + (Q_p(x) + R(x))\Psi_L(x, \lambda) = \lambda\Psi_L(x, \lambda),$$

$$\Psi_L(0, \lambda) = B^*, \quad \Psi_L'(0, \lambda) = A^*; \qquad (24)$$

where A and B are given in the boundary condition (19). Thus, we define Θ_L as the following.

Definition 3.8. The Atkinson Θ-matrix associated with Ψ_L is defined by

$$\Theta_L(x, \lambda) := (\Psi_L'(x, \lambda) + i\Psi_L(x, \lambda))(\Psi_L'(x, \lambda) - i\Psi_L(x, \lambda))^{-1}.$$

Properties of $\Theta_L(x, \lambda)$ are already known, see [81].

Proposition 3.9. For each $x \geq 0$, and every $\lambda \in \mathbb{R}$,

1. $\Theta_L(x, \lambda)$ is a unitary matrix.

2. for $x > 0$, eigenvalues of $\Theta_L(x, \lambda)$ move positively round the unit circle with increasing λ.

Proposition 3.10. $\Theta_L(x, \lambda)$ is the unique solution of the initial value problem

$$\frac{d}{dx}\Theta_L(x, \lambda) = i\Theta_L(x, \lambda)\Omega(x, \lambda, \Theta_L), \quad \Theta_L(0, \lambda) = (A^* + iB^*)(A^* - iB^*)^{-1}, \qquad (25)$$

in which $\Omega(x, \lambda, \bullet)$ is given by (23).

3.3 Oscillation and shooting for eigenvalues in spectral gaps of Schrödinger operators

From these results, we are able to obtain a unitary matrix $\Theta_R^*(c, \lambda)\Theta_L(c, \lambda)$, for some $c \in [0, \infty)$ which we use as the basis for our shooting procedure. This matrix allows us to derive the following important result.

Theorem 3.11. *Fix $c \in [0, \infty)$ and fix a spectral gap $\mathcal{J}$ of the essential spectrum associated with the Schrödinger equation (18)-(19). Then the following are true.*

1. *A real value $\lambda \in \mathcal{J}$ is an eigenvalue for the original problem (18)-(19) if and only if 1 is an eigenvalue of the matrix $\Theta_R^*(c, \lambda)\Theta_L(c, \lambda)$.*

2. *The multiplicity of λ as an eigenvalue of the original problem (18)-(19) is equal to the multiplicity of 1 is an eigenvalue of the matrix $\Theta_R^*(c, \lambda)\Theta_L(c, \lambda)$.*

3. *The eigenvalues of $\Theta_R^*(c, \lambda)\Theta_L(c, \lambda)$ move positively round the unit circle as λ increases in $\mathcal{J}$.*

In fact, this theorem generalises the key result in [10] and [81] which works only for regular problems and problems of eigenvalues below the essential spectrum. Figure 3.3 illustrates the behaviour of eigenvalues of the generated Atkinson Θ-matrices for the underlying problem.
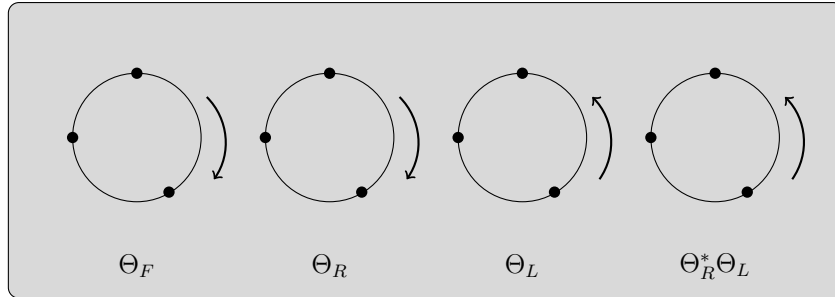
Figure 3.3: Behaviour of eigenvalues (dots) of the generated Atkinson Θ-matrices around the unit circle as λ increases.

In order to locate the eigenvalues of the original problem effectively from the resulting matrix $\Theta_R^*(c, \lambda)\Theta_L(c, \lambda)$, we need to introduce some important functions. Let the eigenvalues of $\Theta_L(x, \lambda)$ be $\exp(i\phi_j^L(x))$, $j = 1, \ldots, n$. The *phase angles* $\phi_j^L(x, \lambda)$ are continuous functions of x and λ. Moreover, they can be determined uniquely by the normalisation condition

$$0 \leq \phi_j^L(0, \lambda) < 2\pi.$$

In addition, let the eigenvalues of $\Theta_R(x, \lambda)$ be $\exp(i\phi_j^R(x))$, $j = 1, \ldots, n$. The phase angles $\phi_j^R(x, \lambda)$ are continuous functions of x and λ. Moreover, they can be determined uniquely by the normalisation condition

$$0 < \phi_j^R(0, \lambda) < 2\pi. \tag{26}$$

Since the initial condition for Θ_R is of λ-dependent and in order to ensure that $\phi_j^R(x, \lambda)$ are continuous with respect to λ we introduce the following hypothesis.

Proposition 3.12. If the pure-periodic problem (20) has pure a.c. spectrum [99, Chapter VII], then 1 cannot be an eigenvalue of the unitary matrix $\Theta_F(0, \lambda)$. Consequently, the phase angles of $\Theta_F(0, \lambda)$ may be chosen as continuous functions of λ with values in $(0, 2\pi)$, in each spectral gap.

Thus, we can introduce the following continuous functions.

Remark 3.13. The sum of the functions $\phi_j^L(x, \lambda)$ is given by

$$\arg \det(\Theta_L(x, \lambda)) = \sum_{j=1}^{n} \phi_j^L(x, \lambda).$$

Similarly, the sum of the $\phi_j^R(x, \lambda)$ is given by

$$\arg \det(\Theta_R(x, \lambda)) = \sum_{j=1}^{n} \phi_j^R(x, \lambda).$$

These functions are solutions to the differential equations.

Proposition 3.14. The function $\arg \det(\Theta_L(x))$ is the unique solution of the initial value problem:

$$\left. \begin{array}{l} \dfrac{d}{dx} \arg \det(\Theta_L(x)) = \mathrm{trace}(\Omega(x)), \\[2mm] \arg \det(\Theta_L(0)) = \arg \det((A^* + iB^*)(A^* - iB^*)^{-1}), \end{array} \right\} \tag{27}$$

in which $\Omega(x)$ is given by (23).

Proposition 3.15. The function $\arg \det(\Theta_R(x))$ is the unique solution of the initial value problem:

$$\left. \begin{array}{l} \dfrac{d}{dx} \arg \det(\Theta_R(x)) = \mathrm{trace}(\Omega(x)), \\[2mm] \arg \det(\Theta_R(Na)) = \arg \det(\Theta_F(0)), \end{array} \right\} \tag{28}$$

in which $\Omega(x)$ is given by (23).

30

On the other hand, let the eigenvalues of the unitary matrix $\Theta_R^*(c)\Theta_L(c)$ be $\exp(i\omega_j)$, $j = 1, \ldots, n$, where

$$0 \leq \omega_j < 2\pi. \tag{29}$$

The phase angles ω_j are not generally continuous functions of λ. This follows from the normalisation condition (29) as they have jump discontinuities whenever an eigenvalue $\exp(i\omega_j)$ passes through the point 1 on the unit circle. Now we define an integer-valued function $M(\lambda)$ which is introduced in [81].

Definition 3.16. The miss-distance function associated with $\Theta_R^*(c)\Theta_L(c)$ is given by

$$M(\lambda) = \frac{1}{2\pi}\left\{\arg\det(\Theta_L(c)) - \arg\det(\Theta_R(c)) - \sum_{j=1}^{n}\omega_j\right\}.$$

The following theorem indicates important properties of $M(\lambda)$.

Theorem 3.17. *Suppose that the pure periodic problem has pure a.c. spectrum [99, Chapter VII]. Fix $c \in [0, \infty)$. For each spectral gap $\mathcal{J}$ of the essential spectrum associated with the Schrödinger equation (18)-(19), let $\Theta_R^*(c)\Theta_L(c)$ be the unitary matrix in Theorem 3.11. Then the following are true.*

1. *$M(\lambda)$ is an integer-valued function.*

2. *$M(\lambda)$ is a monotonically increasing function inside the spectral gap $\mathcal{J}$ whose points of increase are the eigenvalues of the problem (18)-(19).*

From this result we can locate eigenvalues of the original problem by observing discontinuities to this function. This function can be considered as a reliable tool to calculate and locate all the possible eigenvalues of the problem and no eigenvalues can be missed, see Figure 6.3 in Section 6.4 and discussion of Problem (30) in Section 3.4.

The proposed algorithm is illustrated in Figure 3.6 which describes briefly the general steps for the numerical implementation. First of all, an initial range of values of a spectral gap must be given. This is followed by the first ingredient which is calculating the Floquet solutions Ψ from the unperturbed periodic problem (20) over a single period $[0, a]$ and defining the Θ_F matrix. Then, a matching point c must be chosen in the interior of $[0, X]$. The second ingredient involves the forward and backward numerical integrations to the initial valued differential equations (25)-(27) and (22)-(28) to obtain $\Theta_L(c, \lambda)$ and $\Theta_R(c, \lambda)$ respectively. The last ingredient includes calculating the unitary matrix $\Theta_R^*(c, \lambda)\Theta_L(c, \lambda)$ and its corresponding eigenvalues. This is followed by calculating the miss-distance function $M(\lambda)$ and employing a bisection procedure to locate and calculate the isolated eigenvalues of the original problem (18)-(19) effectively.

3.4   Numerical results

Numerical integrations of the IVPs (25)-(27) and (22)-(28) are done using two integrators: the Magnus integrator [34] and the projection integrator [44]. These are chosen to guarantee unitary solutions. Figure 3.4 shows the norm of the resulting solution when a non-unitary integrator is used to solve the IVP (25). Clearly, the solution is non-unitary since the norm is greater than 1.
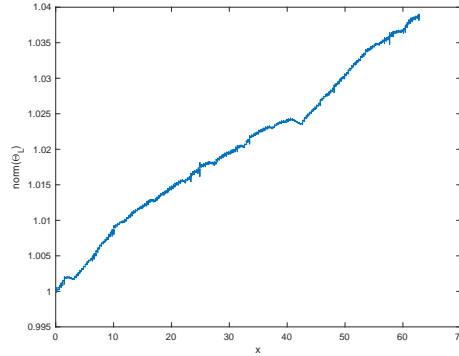
Figure 3.4: norm of non-unitary solution of the IVP (25) for one of the eigenvalues above the essential spectrum of Example 6.22 in Section 6.4.

We apply the proposed algorithm to various numerical examples. The algorithm obtains more accurate results and consumes much less time comparing to the often-used finite difference methods that are combined with contour integral methods to solve the resulting $\lambda-$nonlinear eigenvalue problems.

For PDEs on waveguides, the proposed algorithm can be applied after transforming the PDE into a matrix Schrödinger equation using a semi-discretisation method. Comparing to the dissipative barrier algorithm, discussed in Chapter 2, the proposed algorithm achieves higher accuracy with lower cost. In addition, the shooting method with $M(\lambda)$ guarantees observing all the eigenvalues of the underlying problem. Figure 3.5 shows eigenvalues of the problem

$$- \Delta u + \big(\cos(x + \epsilon y) - 25 \exp(-x)\big)u = \lambda u \tag{30}$$

on a waveguide $[0, \infty) \times [0, 2\pi]$ when $\epsilon = 1$ on two different spectral gaps. These eigenvalues are missed when employing the dissipative barrier technique, see Figure 5.14 in Section 5.5. Here, results are obtained on matrix Schrödinger equation of

size 5 which transformed from the PDE after using the semi discretisation method. The shooting is applied to a truncated interval $[0, 4\pi]$ and a matching point $c = 2\pi$.
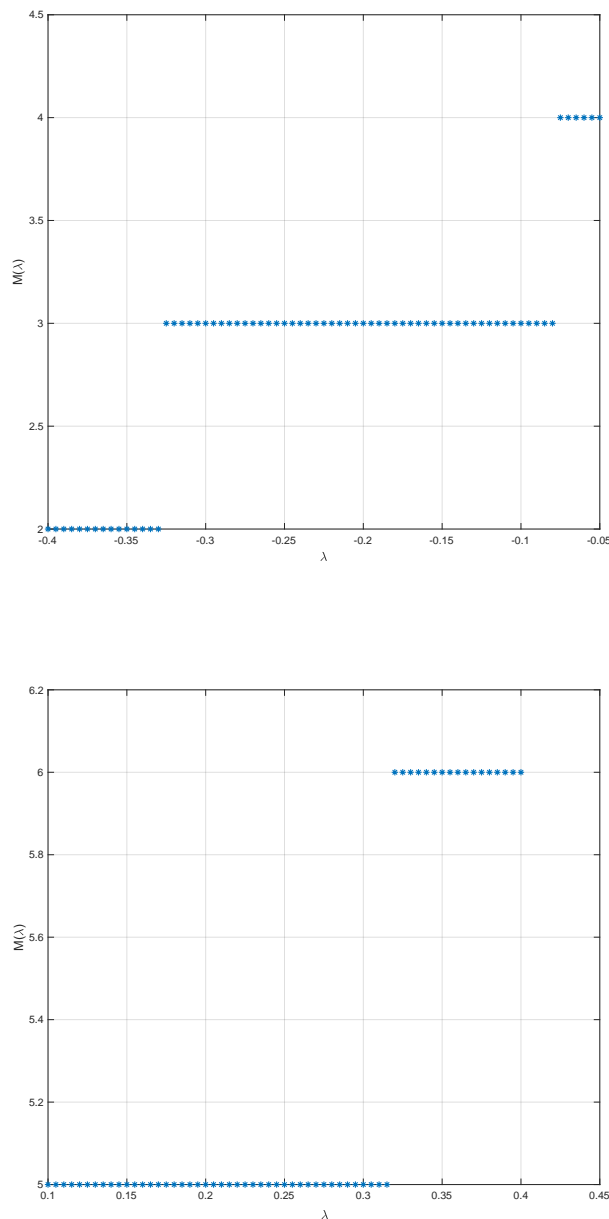
Figure 3.5: Eigenvalues (discontinuities of $M(\lambda)$) of Problem (30) on two different spectral gaps.
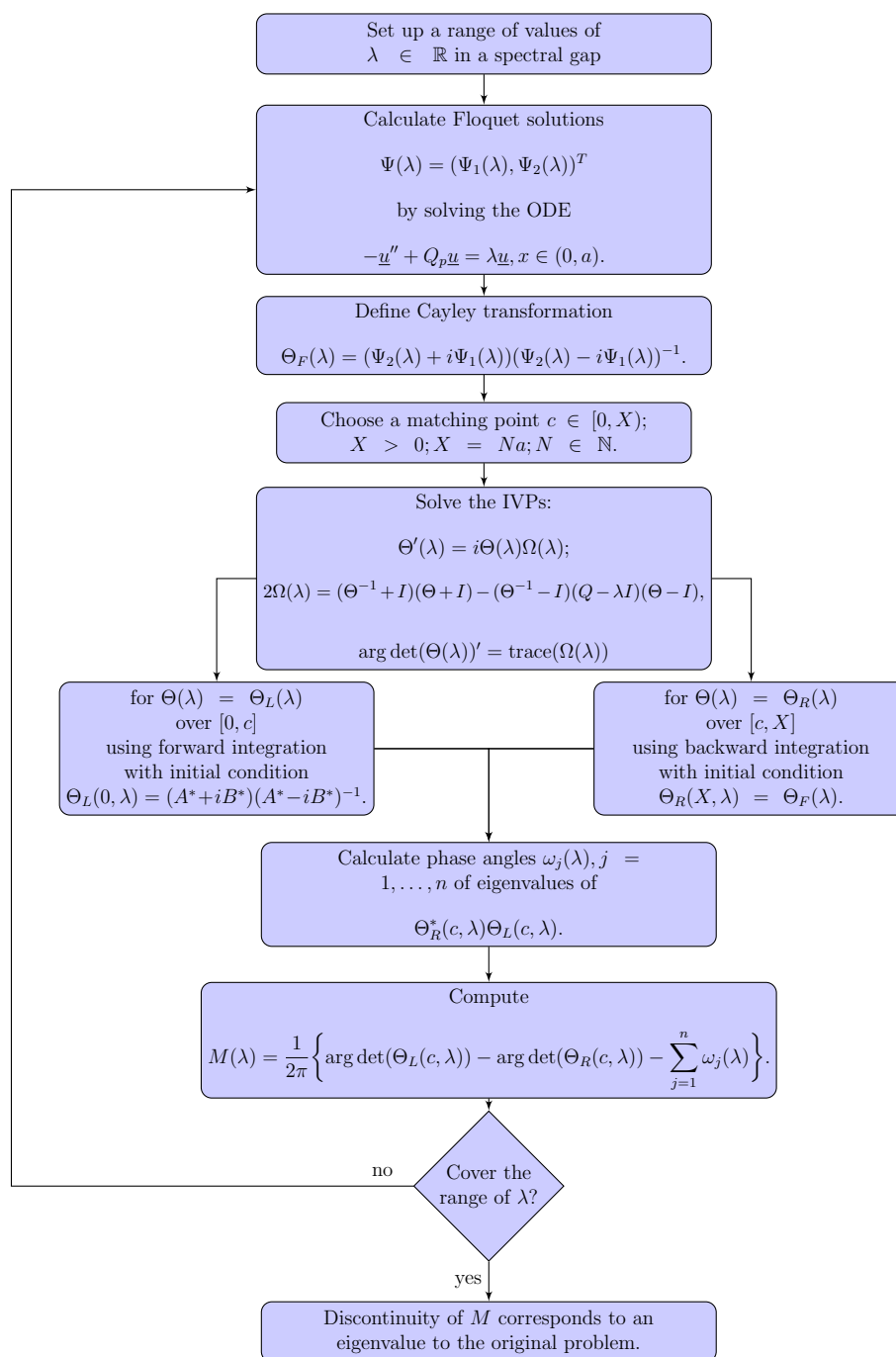
Figure 3.6: Shooting algorithm for eigenvalues in spectral gaps of Schrödinger problems.

4 On the eigenvalues of spectral gaps of matrix-valued Schrödinger operators

4.1 Introduction

This chapter is a sequel to two studies, written over a period of more than twenty-five years. The first, [81], presents numerical methods for selfadjoint Sturm-Liouville type equations with matrix coeffiecients, while the second, [84], analyses the application of a dissipative barrier scheme to a Schrödinger equation on a half-line. In the years since [81] appeared there has been a lot of activity on Schrödinger-type equations with matrix-valued coefficients - see, e.g., Clark and Gesztesy [36] and Clark, Gesztesy, Holden and Levitan [37], together with the substantial bibliographies therein. Some results from the scalar case carry across to the matrix case in a straightforward way; some require new proofs; and some are simply no longer true. As a simple example, the usual spectral data only determines the Titchmarsh-Weyl coefficient, and hence the matrix-valued potential, up to unitary equivalence. Our concern in this chapter is to examine which of the results in [84] are still true in the case of a matrix-valued potential, and which not.

To fix notation, we consider the dissipative matrix Schrödinger equation on the half-line $[0, \infty)$,

$$- \underline{u}'' + (Q + i\gamma S)\underline{u} = \lambda \underline{u}, \tag{31}$$

with a regular selfadjoint-type boundary condition at the origin. The precise form of this condition is not important for our results, so we shall use

$$\cos(\alpha)\underline{u}(0) - \sin(\alpha)\underline{u}'(0) = \underline{0}, \tag{32}$$

where $\alpha \in [0, \pi)$, even though this is not the most general form. Here $\underline{u}$ is a vector-valued function in a subspace of $L^2([0, \infty))^n$, the parameter γ is a nonzero real, and the coefficients Q, S satisfy the following hypotheses:

(A1): $Q(x)$ is a Hermitian-valued function, integrable over compact subsets of $[0, \infty)$, and is eventually periodic with period $a > 0$ i.e, there exists $R_0 \geq 0$ such that

$$Q(x + a) = Q(x), \quad \forall x \geq R_0. \tag{33}$$

(A2): S is a cutoff function with support in $[0, R]$ for some $R \geq R_0$: there exists $0 < c < 1$ such that

$$S(x) = \begin{cases} I, & x < cR; \\ 0, & x \geq R. \end{cases} \tag{34}$$

When $x \in (cR, R)$, we assume that $0 \leq S(x) \leq I$.

The hypothesis (A2) in particular is stronger than is really needed for most of our results, but sufficient to analyse most dissipative barrier schemes.

We define an operator L_0 by:

$$L_0 \underline{u} = -\underline{u}'' + Q\underline{u}, \tag{35}$$

with domain:

$$D(L_0) = \{ \underline{u} \in L^2(0, \infty)| -\underline{u}'' + Q\underline{u} \in L^2(0, \infty), \\ \cos(\alpha)\underline{u}(0) - \sin(\alpha)\underline{u}'(0) = \underline{0} \}. \tag{36}$$

Our aim is to present a substantial analysis of the interaction between the dissipative barrier approach to the problem of numerical approximation of the spectrum of L_0, and interval truncation methods. Our methods will be based on Floquet theory and Weyl-Titchmarsh functions.

4.2 Summary of results

We investigate the following results for an eigenvalue λ_γ of our problem with the dissipative term $i\gamma S(\cdot)$ which develops from the eigenvalue λ when $\gamma = 0$:

1. For our non-truncated problem, if λ is an isolated eigenvalue of multiplicity ν, where $1 \leq \nu \leq n$, Q is a compactly supported perturbation of a Hermitian periodic function, and for a sufficiently small $\gamma > 0$, the approximation $\lambda_{\gamma,j}$ for each $j = 1, \ldots, \nu$ satisfies the bound:

$$|\lambda + i\gamma - \lambda_{\gamma,j}| \leq C_1\gamma \exp(-cC_2R),$$

   where C_1 and C_2 are positive constants.

2. If our problem is truncated to some interval $[0, X]$, $X > R$, then by imposing a boundary condition at $x = X$, any eigenvalue $\lambda_{\gamma,X,good}$ of the truncated problem which converges to λ_γ as $X \to \infty$ satisfies:

$$|\lambda_\gamma - \lambda_{\gamma,X,good}| \leq C_3 \exp\left(-C_4(X - R)\right),$$

   where C_3 and C_4 are positive constants and depend on λ_γ. Moreover, the total algebraic multiplicities of all $\lambda_{\gamma,X,good}$ converging to λ_γ is equal to the algebraic multiplicity of λ_γ.

3. If our problem is truncated to some interval $[0, X]$, $X > R$, then by imposing a boundary condition at $x = X$, then any eigenvalue $\lambda_{\gamma, X, bad}$ of the truncated problem which converges as $X \to \infty$ to a point which is not in the spectrum of $L_0 + i\gamma S$ satisfies

$$|\Im(\lambda_{\gamma, X, bad})| \leq C_5 \exp(-C_6(X - R)),$$

   where C_5 and C_6 are positive constants.

4. One crucial difference between the operators considered here and the scalar-coefficient operators in [84] concerns the behaviour of eigenvalues of $L_0 + i\gamma S$ as $\gamma \searrow 0$. In [84] it is shown that if an eigenvalue λ_γ of $L_0 + i\gamma S$ evolves continuously to become an interior point of a spectral band of $L_0 + i\gamma S$ when $\gamma = 0$ then a threshold effect occurs: there exists $\gamma_{crit} > 0$ such that as $\gamma \searrow \gamma_{crit}$, λ_γ converges to the interior point of the spectral band. We give an example to show that this is not generally true for the operators considered in the present article.

This chapter is organised as follows. Section 4.3 is devoted to the representation of the Floquet theory and Glazman decomposition for the main equation. Section 4.4 and Section 4.5 contain the analysis of the method for the truncated and non-truncated problem respectively. Finally, Section 4.6 represents some numerical experiments to illustrate our results.

4.3   Floquet theory and Glazman decomposition for matrix Schrödinger operators

The essential spectrum of L_0 can be described using Floquet theory, studying the solutions of the differential equation (31) over just one period. We shall review the elements of Floquet theory below, primarily to introduce the notation which we require for an analysis of the domain truncation technique.

For the point spectrum of $L_0 + i\gamma S$, we shall apply the Glazman decomposition technique [3, Appendix 2].

Recall the parameter $R > 0$ from hypothesis (A2). For a fixed $\lambda \in \mathbb{C}$ and any non-zero constant vector $\underline{h}$, consider the following two boundary value problems:

$$P_{left} : \begin{cases} -\underline{v}'' + (Q + i\gamma S)\underline{v} = \lambda\underline{v}, & x \in (0, R); \\ \cos(\alpha)\underline{v}(0) - \sin(\alpha)\underline{v}'(0) = \underline{0} \in \mathbb{C}^n; \\ \underline{v}(R) = \underline{h} \in \mathbb{C}^n; \end{cases} \tag{37}$$

$$P_{right} : \begin{cases} -\underline{w}'' + Q\underline{w} = \lambda\underline{w}, & x \in (R, \infty); \\ \underline{w}(R) = \underline{h} \in \mathbb{C}^n; \\ \underline{w} \in L^2(R, \infty). \end{cases} \tag{38}$$

If these problems can be solved uniquely for every $\underline{h}$ [6] then the maps $\underline{v}(R) \longmapsto \underline{v}'(R) \in \mathbb{C}^n$ and $\underline{w}(R) \longmapsto -\underline{w}'(R) \in \mathbb{C}^n$ are linear operators (Weyl-Titchmarsh operators or Dirichlet-to-Neumann maps) which admit representations by $n \times n$ matrices:

$$M_{left}(\lambda)\underline{v}(R) = \underline{v}'(R); \qquad M_{right}(\lambda)\underline{w}(R) = -\underline{w}'(R).$$

The matrices $M_{left}(\lambda)$ and $M_{right}(\lambda)$ are analytic functions of λ on suitable subsets of $\mathbb{C}$. In particular M_{left} is meromorphic with poles in $\mathbb{C}^+$ when $\gamma > 0$, and on the real axis when $\gamma = 0$; the function M_{right} is analytic outside $Spec_{ess}(L_0)$ except at a set of poles, see [61, 36].

If λ is an eigenvalue of $L_0 + i\gamma S$ then there exists an eigenfunction $\underline{u}$; we can take $\underline{v}(x) = \underline{u}(x), x \in [0, R]$, and $\underline{w}(x) = \underline{u}(x), x \in [R, \infty)$ so that:

$$[M_{left}(\lambda) + M_{right}(\lambda)]\underline{u}(R) = \underline{u}'(R) + (-\underline{u}'(R)) = \underline{0}.$$

Assuming that $\underline{u}(R)$ is not zero, this leads to the condition that $\ker(M_{left}(\lambda) + M_{right}(\lambda))$ is not trivial. In fact if $\underline{u}(R)$ were zero then both $M_{left}(\cdot)$ and $M_{right}(\cdot)$ would be undefined at λ, so the condition that $\underline{u}(R)$ be non-zero is satisfied automatically if $M_{left}(\lambda)$ and $M_{right}(\lambda)$ are well defined.

Conversely, suppose there exists $\mu \in \mathbb{C}$ such that

$$\ker(M_{left}(\mu) + M_{right}(\mu)) \neq \{0\}. \tag{39}$$

Take $\underline{h} \in \ker(M_{left}(\mu) + M_{right}(\mu))$ and define a nontrivial vector $\underline{u}$ by:

$$\underline{u}(x) = \begin{cases} \underline{v}(x), & x \leq R, \\ \underline{w}(x), & x \geq R, \end{cases} \tag{40}$$

where $\underline{v}$ and $\underline{w}$ are the solutions of P_{left} and P_{right} respectively for the case $\lambda = \mu$. Then $\underline{u}$ is a solution for the differential equation $-\underline{u}'' + (Q + i\gamma S)\underline{u} = \mu\underline{u}$ on both the intervals $(0, R)$ and (R, ∞), which is continuous. Moreover, it has a continuous first derivative at $x = R$ which follows from (39) since $\underline{h} \in \ker(M_{left}(\mu) + M_{right}(\mu))$ and

---

[6]It may happen (for a countable nowhere-accumulating set of $\mathbb{R}$) that, e.g., P_{left} is not uniquely solvable when $\lambda \in Spec(L_0 + i\gamma S)$ with Dirichlet Schrödinger operators on $[0, R]$. In this case one would replace the Dirichlet conditions $\underline{v}(R) = \underline{h}, \underline{w}(R) = \underline{h}$ by Robin conditions, and work with Robin-to-Neumann maps. Issues such as this are well known to numerical analysts who use Riccati methods for boundary value problems.

using the definitions of $M_{left}(\mu)$ and $M_{right}(\mu)$. This means that $\underline{u}$ is an eigenfunction of $L_0 + i\gamma S$ with eigenvalue μ.

We have proved the following result.

Lemma 4.1. *Suppose that $M_{left}(\lambda)$ and $M_{right}(\lambda)$ are well defined at $\lambda = \mu$. Then μ is an eigenvalue of $L_0 + i\gamma S$ if and only if the kernel of $M_{left}(\mu) + M_{right}(\mu)$ is non-trivial.*

We now describe how to calculate M_{left} and M_{right}. For M_{left} the procedure is (at least in principle) straightforward:

$$M_{left}(\lambda) = U'(R)U(R)^{-1}, \tag{41}$$

where U is the $n \times n$ matrix-valued solution of the initial value problem

$$\begin{aligned} -U'' + (Q + i\gamma S)U &= \lambda U, \\ U(0) &= I \sin \alpha \in \mathbb{C}^{n \times n}, \\ U'(0) &= I \cos \alpha \in \mathbb{C}^{n \times n}. \end{aligned}$$

In order to find M_{right} we bear in mind that the $Q(x)$ is periodic for $x \geq R_0$ and hence for $x \geq R \geq R_0$; also the dissipative perturbation $S(x) = 0$ for $x \geq R$. Therefore we can apply Floquet Theory [47] for the system of differential equations. We rewrite (31) as a first order differential system:

$$\left(\begin{array}{c} \underline{u}(x) \\ \underline{u}'(x) \end{array} \right)' = \left(\begin{array}{cc} 0 & I \\ \lambda I - Q & 0 \end{array} \right) \left(\begin{array}{c} \underline{u}(x) \\ \underline{u}'(x) \end{array} \right). \tag{42}$$

Let $\Phi(x, \lambda)$ be the fundamental matrix of this equation, i.e.

$$\Phi'(x, \lambda) = \left(\begin{array}{cc} 0 & I \\ \lambda I - Q & 0 \end{array} \right) \Phi(x, \lambda), \quad \Phi(0, \lambda) = I_{2n \times 2n}, \tag{43}$$

where $I_{2n \times 2n}$ is the $2n \times 2n$ identity. Define a non-singular matrix $A(\lambda)$ by

$$A(\lambda) = \Phi(R, \lambda)^{-1} \Phi(R + a, \lambda), \tag{44}$$

Then we can find the eigenvalues of $A(\lambda)$, say $\varrho_1(\lambda), \varrho_2(\lambda), \ldots, \varrho_{2n}(\lambda)$. These eigenvalues are called **Floquet multipliers**. Suppose that $A(\lambda)$ has a canonical Jordan form, i.e.

$$A(\lambda) = F(\lambda)J(\lambda)F(\lambda)^{-1} \tag{45}$$

where $J(\lambda)$ is a Jordan matrix and $F(\lambda)$ is a non-singular matrix. Note that $\Phi(x + a, \lambda)$ satisfies the same differential equation as $\Phi(x, \lambda)$:

$$\Phi'(x + a, \lambda) = H(x + a, \lambda)\Phi(x + a, \lambda),$$

where $H(x + a, \lambda) = \begin{pmatrix} 0 & I \\ \lambda I - Q(x + a) & 0 \end{pmatrix}$. Thus, since Q is periodic, it follows that $H(x + a, \lambda) = H(x, \lambda)$ and that $\Phi(x + a, \lambda)$ and $\Phi(x, \lambda)$ give a matrix solution to the same differential equation (42). This tells us that the column of $\Phi(x + a, \lambda)$ and $\Phi(x, \lambda)$ span the same solution and

$$\Phi(x + a, \lambda) = \Phi(x, \lambda)C(\lambda), \tag{46}$$

where $C(\lambda)$ is some constant non-singular matrix. In fact, $C(\lambda)$ is just $A(\lambda)$ introduced in (44) and from (46) and (45) we have:

$$\Phi(x + a, \lambda) = \Phi(x, \lambda)F(\lambda)J(\lambda)F(\lambda)^{-1},$$

so $\Phi(x+a, \lambda)F(\lambda) = \Phi(x, \lambda)F(\lambda)J(\lambda)$. In fact, the columns of $\Phi(\cdot, \lambda)F(\lambda)$ are called **Floquet solutions** of (42).

The following Lemma summarises some standard facts; for more information about the Floquet theory for Hamiltonian systems see [37, 112]:

Lemma 4.2.

1. *The Floquet multipliers $\varrho_1(\lambda), \ldots, \varrho_{2n}(\lambda)$ satisfy $\varrho_1(\lambda) \ldots \varrho_{2n}(\lambda) = 1$.*

2. *For $\lambda \notin Spec_{ess}(L_0)$, there exist precisely n of the $\varrho_j(\lambda)$; say $\varrho_1(\lambda), \ldots, \varrho_n(\lambda)$, such that $|\varrho_j(\lambda)| < 1$.*

Proof.

1. This statement holds because $\det(A(\lambda)) = 1$, which follows from the fact that $\det(\Phi(x, \lambda))$ is a non-zero constant (the coefficient matrix on the right hand side of (43) having zero trace).

2. The equation (31) is in the limit-point case at infinity, see [37], and hence for λ outside the essential spectrum it has precisely an n-dimensional space of solutions in $L^2(0, \infty)$. None of the Floquet multipliers $\varrho_1(\lambda), \ldots, \varrho_{2n}(\lambda)$ has absolute value 1, for otherwise it is possible to construct a Weyl singular sequence of oscillatory solutions from the corresponding Floquet solution; this is impossible as λ lies outside the essential spectrum. Thus precisely n of the Floquet multipliers must have absolute value strictly less than 1, precisely n have absolute value strictly greater than 1, and we can order them so that $|\varrho_1(\lambda)|, \ldots, |\varrho_n(\lambda)| < 1$ and $|\varrho_{n+1}(\lambda)|, \ldots, |\varrho_{2n}(\lambda)| > 1$.

□

It follows from Lemma 4.2 that if λ lies outside the essential spectrum then the Jordan matrix $J(\lambda)$ in (45) decomposes into $n \times n$ blocks as

$$J(\lambda) = \begin{pmatrix} J_1(\lambda) & 0 \\ 0 & J_2(\lambda) \end{pmatrix}, \tag{47}$$

where $J_1(\lambda)$ corresponds to $\varrho_1(\lambda), \ldots, \varrho_n(\lambda)$ and $J_2(\lambda)$ corresponds to $\varrho_{n+1}(\lambda)$, ..., $\varrho_{2n}(\lambda)$. In this case the matrix

$$\Gamma(x, \lambda) = \Phi(x, \lambda) F(\lambda) \begin{pmatrix} J_1(\lambda) \\ 0 \end{pmatrix},$$

has columns which span the n-dimensional space of square-integrable solutions; moreover, for $N \in \mathbb{N}$:

$$\Gamma(x + Na, \lambda) = \Gamma(x, \lambda) J_1(\lambda)^N. \tag{48}$$

We can partition $\Gamma(x, \lambda)$ as

$$\Gamma(x, \lambda) = \begin{pmatrix} \Psi(x, \lambda) \\ \Psi'(x, \lambda) \end{pmatrix}, \tag{49}$$

where $\Psi(x, \lambda)$ is an $n \times n$ solution of

$$-\Psi'' + Q\Psi = \lambda\Psi, \tag{50}$$

whose columns (as we mentioned above) span the space of all square integrable solutions of (31).

Hence, by direct verification, if $\Psi(R, \lambda)$ is invertible [7] then the function

$$\underline{w}(x) = \Psi(x, \lambda) \Psi(R, \lambda)^{-1} \underline{h}$$

is the solution of the problem P_{right}. A simple calculation now shows that $-\underline{w}'(R) = M_{right}(\lambda)\underline{w}(R)$, where

$$M_{right}(\lambda) = -\Psi'(R, \lambda)\Psi(R, \lambda)^{-1}. \tag{51}$$

We immediately have the following corollary to Lemma 4.1.

Corollary 4.3. *Suppose that $M_{left}(\lambda)$ is well defined and that $\Psi(R, \lambda)^{-1}$ exists. Then λ is an eigenvalue of $L_0 + i\gamma S$ if and only if*

$$\ker \left(M_{left}(\lambda) - \Psi'(R, \lambda)\Psi(R, \lambda)^{-1} \right) \neq \{0\}. \tag{52}$$

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[7]In fact $\Psi(R, \lambda)$ is always invertible when $\Im(\lambda) > 0$, see Lemma 4.6.

4.4 Approximation of spectral-gap eigenvalues using truncated problems

In this section, we truncate the problem over $[0, \infty)$ to a problem on $[0, X]$ for some $X > R$. At $x = X$ we impose, for some $\beta \in \mathbb{R}$, a self-adjoint artificial boundary condition

$$\cos(\beta)\underline{u}(X) - \sin(\beta)\underline{u}'(X) = \underline{0}. \tag{53}$$

The operator L_0 is replaced by $L_{0,X}$ defined by:

$$L_{0,X}\underline{u} = -\underline{u}'' + Q\underline{u}, \tag{54}$$

with domain:

$$D(L_{0,X}) = \{ \underline{u} \in L^2(0, X) | -\underline{u}'' + Q\underline{u} \in L^2(0, X), \\ \cos(\alpha)\underline{u}(0) - \sin(\alpha)\underline{u}'(0) = \underline{0} = \cos(\beta)\underline{u}(X) - \sin(\beta)\underline{u}'(X) \}. \tag{55}$$

In this case, the spectra of $L_{0,X}$ (and hence $L_{0,X} + i\gamma S$ since S is bounded) is purely discrete, see e.g., [38]. To characterize the eigenvalues of $L_{0,X} + i\gamma S$, we replace P_{right} in (38) by:

$$P_{right,X} : \quad \begin{cases} -\underline{w}'' + Q\underline{w} = \lambda \underline{w}, & x \in (R, X); \\ \underline{w}(R) = \underline{h}; \\ \cos(\beta)\underline{w}(X) - \sin(\beta)\underline{w}'(X) = \underline{0}. \end{cases} \tag{56}$$

Let $\Lambda(x, \lambda)$ be a $2n \times n$ matrix of non-$L^2(0, \infty)$ solutions corresponding to the eigenvalues $\varrho_{n+1}, \ldots, \varrho_{2n}$ of (44), thus,

$$\Lambda(x, \lambda) = \Phi(x, \lambda)F(\lambda) \begin{pmatrix} 0 \\ J_2(\lambda) \end{pmatrix},$$

where $J_2(\lambda)$ is the corresponding Jordan matrix introduced in (47). Moreover, for $N \in \mathbb{N}$:

$$\Lambda(x + Na, \lambda) = \Lambda(x, \lambda)J_2(\lambda)^N. \tag{57}$$

We may partition $\Lambda(\lambda, x)$ as

$$\Lambda(x, \lambda) = \begin{pmatrix} \Theta(x, \lambda) \\ \Theta'(x, \lambda) \end{pmatrix}; \tag{58}$$

construct the matrix:

$$\Psi_X(x, \lambda) = \Psi(x, \lambda) - \Theta(x, \lambda)C_X(\lambda), \tag{59}$$

choosing $C_X(\lambda)$ so that $\cos(\beta)\Psi_X(X) - \sin(\beta)\Psi'_X(X) = 0$:

$$C_X(\lambda) = (\cos(\beta)\Theta(X,\lambda) - \sin(\beta)\Theta'(X,\lambda))^{-1}(\cos(\beta)\Psi(X,\lambda) - \sin(\beta)\Psi'(X,\lambda)). \quad (60)$$

Note that the matrix $\cos(\beta)\Theta(X,\lambda) - \sin(\beta)\Theta'(X,\lambda)$ is always invertible when β is real and $\Im(\lambda) \neq 0$. This is because the columns of $\Theta(\cdot,\lambda)$ span the space of solutions which are in $L^2(-\infty, X]$, extending the potential Q as a periodic Hermitian function to the whole real axis. Any λ for which $\cos(\beta)\Theta(X,\lambda) - \sin(\beta)\Theta'(X,\lambda)$ is not invertible is necessarily an eigenvalue of a selfadjoint problem on $(-\infty, X]$ with the boundary condition $\cos(\beta)u(X)\sin(\beta)u'(X) = 0$. Such λ are necessarily real. We seek eigenvalues of $L_0 + i\gamma S$, which all have strictly positive imaginary parts.

Hence, the solution $\underline{w}$ of the boundary value problem (56) exists if the corresponding $\Psi_X(R,\lambda)^{-1}$ exists and:

$$\underline{w}(x) = \Psi_X(x,\lambda)\Psi_X(R,\lambda)^{-1}\underline{h},$$

Thus the eigenvalues of $L_{0,X} + i\gamma S$ may be characterised by an analogue of Lemma 4.1 if we replace M_{right} by

$$M_{right,X}(\lambda) := -\Psi'_X(R,\lambda)\Psi_X(R,\lambda)^{-1}. \quad (61)$$

Corollary 4.3 also has the following analogue.

Lemma 4.4. *Suppose that $M_{left}(\lambda)$ and $\Psi_X(R,\lambda)^{-1}$ exist. Then λ is an eigenvalue of $L_{0,X} + i\gamma S$ if and only if*

$$\ker\left(M_{left}(\lambda) - \Psi'_X(R,\lambda)\Psi_X(R,\lambda)^{-1}\right) \neq \{0\}. \quad (62)$$

We analyse the effect of interval truncation through a sequence of intermediate results and technical lemmas.

Proposition 4.5. *If $X = R + Na$ where $N \in \mathbb{N}$, and $J_1(\lambda)$ and $J_2(\lambda)$ are defined as in (47) then*

$$\Psi(R + Na, \lambda) = \Psi(R,\lambda)J_1(\lambda)^N; \quad \Theta(R + Na, \lambda) = \Theta(R,\lambda)J_2(\lambda)^N. \quad (63)$$

Furthermore,

$$C_X(\lambda) = J_2(\lambda)^{-N}C_R(\lambda)J_1(\lambda)^N; \quad (64)$$

in particular,

$$\|C_X(\lambda)\| \leq C \|C_R(\lambda)\| \left(\frac{\varrho(\lambda)}{\tilde{\varrho}(\lambda)}\right)^N \left(N^2\frac{\tilde{\varrho}(\lambda)}{\varrho(\lambda)}\right)^{n-1}, \quad (65)$$

where C is a positive constant, $\varrho(\lambda) = \max(|\varrho_1(\lambda)|, \ldots, |\varrho_n(\lambda)|)$ and $\tilde{\varrho}(\lambda) = \min(|\varrho_{n+1}(\lambda)|, \ldots, |\varrho_{2n}(\lambda)|)$.

Proof. Equation (63) follows directly from (48,57) upon using the definitions (49,58). Substituting (63) into (60) yields (64). In order to estimate the norm of $C_X(\lambda)$ we need to find the norm of $J_1(\lambda)^N$. The expression for the norm of $J_1(\lambda)^N$ may have terms, of worst case scenario, like:

$$\varrho(\lambda)^N, N\varrho(\lambda)^{N-1}, \ldots, N(N-1)\ldots(N-n+2)\varrho(\lambda)^{N-n+1},$$

where $\varrho(\lambda) = \max(|\varrho_1(\lambda)|, \ldots, |\varrho_n(\lambda)|)$. Thus,

$$\|J_1(\lambda)^N\| \leq c_1 n\sqrt{n}\varrho(\lambda)^N\left(\frac{N}{\varrho(\lambda)}\right)^{n-1},$$

where we have used the inequality $\|A\| \leq \sqrt{n}\|A\|_1 \leq n\sqrt{n}\max_{i,j}|a_{i,j}|$ for any matrix $A = (a_{ij})$. A similar approach would be followed to estimate the norm of $J_2(\lambda)^{-N}$. Therefore,

$$\|J_2(\lambda)^{-N}\| \leq c_2 n\sqrt{n}\left(\frac{1}{\tilde{\varrho}(\lambda)}\right)^N\left(N\tilde{\varrho}(\lambda)\right)^{n-1},$$

where $\tilde{\varrho}(\lambda) = \min(|\varrho_{n+1}(\lambda)|, \ldots, |\varrho_{2n}(\lambda)|)$. Finally, (65) follows from the above estimates for the norms of $J_1(\lambda)^N$ and $J_2(\lambda)^{-N}$. $\qquad\square$

Lemma 4.6. *Let $\Psi(x,\lambda)$ be defined as in (50) and suppose $\Im(\lambda) > 0$. Then $\Psi(R,\lambda)$ is invertible.*

Proof. Assume that $\Psi(R,\cdot)$ is not invertible: then we can find a non-zero vector $\underline{c} \in \mathbb{C}^n$ such that

$$\Psi(R,\lambda)\underline{c} = \underline{0}.$$

Define a function $\underline{u}(x,\lambda) = \Psi(x,\lambda)\underline{c}$, which satisfies the differential equation for all x. Also, $\underline{u}(R,\lambda) = \underline{0}$. However, the fact that $|\varrho_j(\lambda)| < 1$ for $j = 1, \ldots, n$, means that $\underline{u}(\cdot,\lambda) \in L^2(R,\infty)$. Hence $\underline{u}(x,\lambda)$ is an eigenfunction for the problem $-\underline{u}'' + Q\underline{u} = \lambda\underline{u}$, on $[R,\infty)$ with Dirichlet condition at R. This problem is self-adjoint, so $\Im(\lambda) = 0$, which is a contradiction. $\qquad\square$

Lemma 4.7. *Let $\Psi_X(x,\lambda)$ be defined as in (59) and suppose $\Im(\lambda) > 0$. Then $\Psi_X(R,\lambda)$ is invertible.*

Proof. Assume $\Psi_X(R,\lambda)$ is not invertible. Then $\exists$ a non-zero $\underline{c} \in \mathbb{C}^n$ such that

$$\Psi_X(R,\lambda)\underline{c} = \underline{0}.$$

Define a function $\underline{u}_X(x, \lambda) = \Psi_X(x, \lambda)\underline{c}$, so that $\underline{u}_X(R, \lambda) = \underline{0}$. Hence $\underline{u}_X(x, \lambda)$ is an eigenfunction of the problem on $[R, X]$ with Dirichlet condition at R and the boundary condition (53) at X with $\beta \in \mathbb{R}$. This is also a self-adjoint problem, so again we have the contradiction $\Im(\lambda) = 0$. $\square$

Finally, we have a quantitative lemma on continuity of determinants, which will be needed in the proof of Theorem 4.9. We shall use this lemma with $X = R + Na$ and large N.

Lemma 4.8. *Suppose that $A, A_X \in \mathbb{M}_n(\mathbb{C})$ have the property:*

$$\|A - A_X\| \le b\tau^X (X^2 \frac{1}{\tau})^{n-1},$$

where b is a positive constant and $0 < \tau < 1$. Then

$$|\det(A) - \det(A_X)| \le \tilde{b}\tau^X (X^2 \frac{1}{\tau})^{n-1},$$

where $\tilde{b}$ is a positive constant.

Proof. The proof follows directly from [57], by letting $\tilde{b} = nb[\|A\| + b\tau]^{n-1}$. $\square$

Theorem 4.9. *Suppose that assumptions (A1) and (A2) hold. For $\gamma > 0$, let λ_γ be an eigenvalue of the non-self-adjoint Schrödinger operator $L_0 + i\gamma S$ defined in (35)-(36). Then for all sufficiently large $X \ge R + a$, there exist approximations $\lambda_{\gamma, X, good}$ to λ_γ, whose total algebraic multiplicity is equal to the algebraic multiplicity of λ_γ, obtained as eigenvalues of the operator $L_{0,X} + i\gamma S$ defined in (54)-(55), which satisfy*

$$|\lambda_\gamma - \lambda_{\gamma, X, good}| \le C_3 \exp\left(-C_4(X - R)\right). \tag{66}$$

Here C_3 and C_4 are positive constants which depend on λ_γ.

Proof. Without loss of generality, it is sufficient to check the cases $X = R + Na$ where $N \in \mathbb{N}$ is sufficiently large. The other cases follow by exploiting the freedom in the choice of the constants c and R in (34). For example, if $X = R + Na + b$, with $0 < b < a$, then we can replace R by $R + b$ and use a smaller constant c in (34). First we observe that for $\gamma > 0$, λ_γ has strictly positive imaginary part. If $\underline{u}_\gamma$ is the corresponding normalised eigenfunction then a standard integration by parts yields:

$$\Im(\lambda_\gamma) = \gamma \int_0^R \underline{u}_\gamma^*(x) S(x) \underline{u}_\gamma(x) dx$$
$$\ge \gamma \int_0^{cR} \underline{u}_\gamma^*(x) \underline{u}_\gamma(x) dx > 0,$$

45

where $\underline{u}_\gamma^*(x)$ is the Hermitian conjugate of $\underline{u}_\gamma(x)$. Next, we observe consequently from Lemma 4.6 and Lemma 4.7, $\Psi(R, \cdot)$ and $\Psi_X(R, \cdot)$ are invertible for all λ in a neighbourhood of λ_γ. It follows that $M_{right}(\cdot)$ and $M_{right,X}(\cdot)$ are well defined in a neighbourhood of λ_γ.

If $M_{left}(\lambda_\gamma)$ is well defined then from Corollary 4.3,

$$\ker\left(M_{left}(\lambda_\gamma) + M_{right}(\lambda_\gamma)\right) \neq \{0\}; \tag{67}$$

from Lemma 4.4, we seek points $\lambda_{\gamma,X,good}$ which satisfy (66) together with the truncated problem eigenvalue condition:

$$\ker\left(M_{left}(\lambda_{\gamma,X,good}) + M_{right,X}(\lambda_{\gamma,X,good})\right) \neq \{0\}. \tag{68}$$

Using (59) and the definitions of M_{right} and $M_{right,X}$ for a fixed λ, we obtain

$$\begin{aligned} M_{right,X}(\lambda) &= (M_{right}(\lambda) + \Theta'(R,\lambda)C_X(\lambda)\Psi(R,\lambda)^{-1}) \\ &\quad \times (I - \Theta(R,\lambda)C_X(\lambda)\Psi(R,\lambda)^{-1})^{-1}. \end{aligned} \tag{69}$$

Now we exploit the fact that $X = R + Na$, which allows us to use Proposition 4.5 (eqn. (65)). By Lemma 4.2 part 2, since λ is outside the essential spectrum, and since the Floquet multipliers may be chosen to be continuous functions of λ, there exist constants $c_- < 1$ and $c_+ > 1$ such that $\max(|\varrho_1(\lambda)|, \ldots, |\varrho_n(\lambda)|) < c_- < 1$ and $\min(|\varrho_{n+1}(\lambda)|, \ldots, |\varrho_{2n}(\lambda)|) = (\max(|\varrho_1(\lambda)|, \ldots, |\varrho_n(\lambda)|))^{-1} > c_+ > 1$ uniformly with respect to λ in a neighbourhood of λ_γ which does not intersect in a spectral band. Thus, in addition to (67), we have from (65) and (69),

$$\|M_{right}(\lambda) - M_{right,X}(\lambda)\| \leq b\left(\frac{c_-}{c_+}\right)^N \left(N^2 \frac{c_+}{c_-}\right)^{n-1}, \tag{70}$$

uniformly with respect to λ in a neighbourhood of λ_γ, where b is a positive constant. Using Lemma 4.8 and since $0 < \left(\frac{c_-}{c_+}\right) < 1$,

$$|\det(M_{left}(\lambda) + M_{right}(\lambda)) - \det(M_{left}(\lambda) + M_{right,X}(\lambda))| \leq \tilde{b}\left(\frac{c_-}{c_+}\right)^N \left(N^2 \frac{c_+}{c_-}\right)^{n-1},$$

uniformly with respect to λ in a neighbourhood of λ_γ, where $\tilde{b}$ is a positive constant. It follows by a standard zero-counting argument for analytic functions (Lemma 3 in [84]) that there exist points $\lambda_{\gamma,X,good}$ which satisfy (68) and are such that

$$|\lambda_\gamma - \lambda_{\gamma,X,good}| \leq C\left(\frac{c_-}{c_+}\right)^{N/\nu} \left(N^2 \frac{c_+}{c_-}\right)^{(n-1)/\nu}, \tag{71}$$

where $C > 0$ and ν is the order of the zero of $\det(M_{left}(\cdot) + M_{right}(\cdot))$ at λ_γ. Moreover, the total order of the $\lambda_{\gamma,X,good}$ as zeros of $\det(M_{left}(\cdot) + M_{right,X}(\cdot)) = 0$ in a neighbourhood of λ_γ, is ν.

To complete the proof of the result, we need to eliminate the term $(N^2)^{(n-1)/\nu}$ on the right hand side of (71). Since $0 < \frac{c_-}{c_+} < 1$, we may choose $\epsilon > 0$ such that $(1+\epsilon)\frac{c_-}{c_+} < 1$. For all sufficiently large N we also have $(1+\epsilon)^{N/\nu} > (N^2)^{(n-1)/\nu}$, and hence (71) implies

$$|\lambda_\gamma - \lambda_{\gamma,X,good}| \leq C\left((1+\epsilon)\frac{c_-}{c_+}\right)^{N/\nu}; \tag{72}$$

furthermore, any solutions of (68) which converge to λ_γ must satisfy (72). This completes the proof. $\qquad\square$

Remark 4.10. When $M_{left}(\lambda)$ has a pole at λ, it is still possible for λ to be an eigenvalue of $L_0 + i\gamma S$. However, $M_{right}(\lambda)$ and $M_{right,X}(\lambda)$ cannot have poles off the real axis, as Lemma 4.6 and Lemma 4.7 show that $\Psi(R,\lambda)$ and $\Psi_X(R,\lambda)$ are invertible for $\Im(\lambda) \neq 0$.

Theorem 4.11. *Suppose that assumptions (A1) and (A2) hold. For $\gamma > 0$, let $\lambda_{\gamma,X,bad}$ be an eigenvalue of the non-self-adjoint Schrödinger operator $L_{0,X} + i\gamma S$ defined in (35)-(36) which converges, as $X \to +\infty$, to a point which is not in the spectrum of $L_0 + i\gamma S$. Then for some positive constants C_5 and C_6:*

$$|\Im(\lambda_{\gamma,X,bad})| \leq C_5 \exp(-C_6(X - R)). \tag{73}$$

Proof. Similarly to the proof of Theorem 4.9, it is sufficient to consider the case $X = R + Na$ where $N \in \mathbb{N}$. Since $\lambda_{\gamma,X,bad}$ has the property:

$$\ker\left(M_{left}(\lambda_{\gamma,X,bad}) + M_{right,X}(\lambda_{\gamma,X,bad})\right) \neq \{0\},$$

in particular $M_{left}(\lambda_{\gamma,X,bad}) + M_{right,X}(\lambda_{\gamma,X,bad})$ has an eigenvalue 0. It is known (see, e.g., [22]) that spectral pollution must lie on the real axis, since $L_0 + i\gamma S$ is a relatively compact perturbation of the semi-bounded selfadjoint operator L_0: thus $\lambda_{\gamma,X,bad} \to \mu \in \mathbb{R} \cap \{$Spectral Gap$\}$ as $X \to \infty$. Additionally, since μ is not in the spectrum of $L_0 + i\gamma S$, the matrix $M_{left}(\mu) + M_{right}(\mu)$ is invertible if it is well defined, i.e. if $\Psi(R,\mu)$ and $U(R,\mu)$ are invertible, see (41,51). We may use a greater value of R in the Glazman decomposition (37)-(38).

Hence, there is a compact neighbourhood of μ, say $\overline{B(\mu,r)}; r > 0$ such that $M_{left}(\lambda) + M_{right}(\lambda)$ is invertible $\forall \lambda \in \overline{B(\mu,r)}$. Following the reasoning which led to (70), we deduce that provided $C_R(\mu)$ is well defined, then $M_{right,X}$ will converge locally uniformly to M_{right} in a neighbourhood of μ. Since such a uniform convergence

excludes spectral pollution, see [29], it follows that $C_R(\mu)$ must not be well defined, i.e.

$$\cos(\beta)\Theta(R,\mu) - \sin(\beta)\Theta'(R,\mu) \text{ is not invertible.}$$

Observe that by exploiting periodicity to extend the coefficient $Q(\cdot)$ to the whole real axis, the columns of the matrix $\Theta(\cdot,\lambda)$ may be seen to span the space of solutions of the formally self-adjoint matrix Schrödinger equation which lie in $L^2((-\infty,R])$. This basis for the $L^2((-R,\infty))$ solution space may be chosen so that the matrix $\begin{pmatrix} \Theta(\cdot,\lambda) \\ \Theta'(\cdot,\lambda) \end{pmatrix}$ is analytic outside the essential spectrum, except possibly at a set of isolated poles, see e.g. Marletta-Zettl [85], or the abstract construction of 'solution operators' in Brown et al. [28]. In fact for every point μ outside the essential spectrum, we may choose a basis of the $L^2((-\infty,R])$ solution space which is analytic at that point, by choosing a self-adjoint boundary condition at $x = R$ such that μ is not an eigenvalue of the associated problem on $(-\infty,R]$. Thus we may assume without loss of generality that $\lambda \mapsto \begin{pmatrix} \Theta(R,\lambda) \\ \Theta'(R,\lambda) \end{pmatrix}$ is analytic at $\lambda = \mu$. It then follows that

$$\lambda \mapsto \det(\cos(\beta)\Theta(R,\lambda) - \sin(\beta)\Theta'(R,\lambda))$$

is analytic at $\lambda = \mu$, with a zero of some finite order at μ. It follows that for some $C > 0$ and $\nu \in \mathbb{N}$,

$$\|(\cos(\beta)\Theta(R,\lambda) - \sin(\beta)\Theta'(R,\lambda))^{-1}\| \leq \frac{C}{(\lambda - \mu)^\nu}.$$

for some $C, \nu > 0$, in a neighbourhood of $\lambda = \mu$. Combining this with (65) and using the notation of (70) we see that, for $X = R + Na$,

$$\|C_X(\lambda_{\gamma,X,bad})\| \leq \frac{C}{|\lambda_{\gamma,X,bad} - \mu|^\nu}\left(\frac{c_-}{c_+}\right)^N \left(N^2\frac{c_+}{c_-}\right)^{n-1}.$$

The fact that the eigenvalues $\lambda_{\gamma,X,bad}$ form a polluting sequence means that $M_{right,X}(\lambda_{\gamma,X,bad})$ cannot converge to $M_{right}(\mu)$ as $X \to \infty$, so in view of (69) the norms $\|C_X(\lambda_{\gamma,X,bad})\|$ cannot converge to zero. This implies a bound

$$|\Im(\lambda_{\gamma,X,bad})| \leq |\lambda_{\gamma,X,bad} - \mu| \leq C\left(\frac{c_-}{c_+}\right)^{N/\nu}\left(N^2\frac{c_+}{c_-}\right)^{(n-1)/\nu},$$

and the required result follows since the exponential decay of $\left(\frac{c_-}{c_+}\right)^{N/\nu}$ overcomes the power $N^{2(n-1)/\nu}$. This completes the proof.

$\square$

4.5 Eigenvalues in spectral gaps for non-truncated problems

The purpose of this section is to study the evolution of the point spectrum of $L_0 + i\gamma S$ with respect to the coupling constant γ. Throughout this section, we drop the assumption of eventual periodicity (A1).

Theorem 4.12. *Suppose that assumption (A2) holds — see (34). Let λ be an isolated eigenvalue of L_0 with multiplicity ν, where $1 \leq \nu \leq n$, and normalised eigenvectors u_j, $j = 1, \ldots, \nu$. For each sufficiently small $\gamma > 0$, let $\lambda_{\gamma,j}; j = 1, \ldots, \nu$, be eigenvalues of the non-selfadjoint operator $L_0 + i\gamma S$ defined in (35)-(36) with eigenvectors $u_{\gamma,j}$, $j = 1, \ldots, \nu$, and suppose $\lambda_{\gamma,j} \to \lambda$ as $\gamma \to 0$. Then for each $1 \leq j \leq \nu$, the projection of $u_{\gamma,j}$ onto $Span\{u_1, \ldots, u_\nu\}$ remains bounded away from zero, uniformly with respect to R and γ for sufficiently small γ.*
If, additionally, the assumption
(A1'):
$$\|u_j(x)\| \leq C \exp(-C_2 x), \quad x \in [0, \infty), \quad j = 1, \ldots, \nu, \tag{74}$$

holds for some positive constants C and C_2, then there exists $C_1 > 0$, such that for all $R > 0$,
$$|\lambda + i\gamma - \lambda_{\gamma,j}| \leq C_1 \gamma \exp(-cC_2 R), \tag{75}$$

where $c \in (0, 1)$ is the constant appearing in assumption (A2).

Proof. The existence of $\lambda_{\gamma,j}$ with $|\lambda_{\gamma,j} - \lambda| \to 0$ as $\gamma \to 0$ is a consequence of results in [64] on analytic families. Since γ is sufficiently small, let Γ be a contour which encloses the spectral point λ of L_0 and suppose that $\lambda_{\gamma,j}$, $j = 1, \ldots, \nu$ are the only spectral points of $L_0 + i\gamma S$ inside Γ. Clearly, $\|S\| = 1$ independently of R and since L_0 is a self-adjoint operator then $|\lambda - \lambda_{\gamma,j}| \leq \gamma$ independently of R; thus the contour Γ can be chosen independently of R. Suppose $u_{\gamma,j}$, $j = 1, \ldots, \nu$ are eigenvectors of $L_0 + i\gamma S$, linearly independent with $\|u_{\gamma,j}\| = 1$. Following Kato [64, VII,§3], let $P(\gamma)$ be the projection onto the eigenspace of $L_0 + i\gamma S$ spanned by the $u_{\gamma,j}$, $j = 1, \ldots, \nu$, and $P(0)$ be the projection onto the eigenspace of L_0 associated with λ; the projection $P(\gamma)$ is analytic as a function of γ, so that

$$\|P(\gamma) - P(0)\| \leq O(\gamma). \tag{76}$$

Since

$$P(0)u_{\gamma,j} = u_{\gamma,j} + (P(0) - P(\gamma))u_{\gamma,j}, \tag{77}$$

taking the norm of (77) and using (76) we conclude that $P(0)u_{\gamma,j}$ is bounded away from zero uniformly with respect to R and γ for sufficiently small γ.

Now, since $(L_0 + i\gamma S)u_{\gamma,j} = \lambda_{\gamma,j}u_{\gamma,j}$ and $(L_0 - i\gamma I)u_k = (\lambda - i\gamma)u_k$, using the inner product for the first equation with u_k we obtain:

$$\langle (L_0 + i\gamma S)u_{\gamma,j}, u_k \rangle = \lambda_{\gamma,j}\langle u_{\gamma,j}, u_k \rangle. \tag{78}$$

Similarly, using the inner product for the second equation with $u_{\gamma,j}$ we obtain:

$$\langle (L_0 - i\gamma I)u_k, u_{\gamma,j} \rangle = (\lambda - i\gamma)\langle u_k, u_{\gamma,j} \rangle. \tag{79}$$

Because L_0 and S are self-adjoint and u_k and $u_{\gamma,j}$ are in the domain of L_0 and it is contained in the domain of S then from (79) we have:

$$\langle (L_0 + i\gamma I)u_{\gamma,j}, u_k \rangle = (\lambda + i\gamma)\langle u_{\gamma,j}, u_k \rangle. \tag{80}$$

From (78) and (80), we obtain:

$$|\lambda + i\gamma - \lambda_{\gamma,j}| \, \langle u_{\gamma,j}, u_k \rangle = i\gamma\langle (I - S)u_{\gamma,j}, u_k \rangle = i\gamma\langle u_{\gamma,j}, (I - S)u_k \rangle.$$

We know that $P(0)u_{\gamma,j}$ is bounded away from zero and

$$P(0)u_{\gamma,j} = \sum_{k=1}^{\nu} \langle u_{\gamma,j}, u_k \rangle u_k.$$

In addition

$$\|P(0)u_{\gamma,j}\|^2 = \sum_{k=1}^{\nu} |\langle u_{\gamma,j}, u_k \rangle|^2.$$

We know that $\|P(0)u_{\gamma,j}\|^2$ is bounded away from zero uniformly with respect to R and γ as γ tends to zero; say $\|P(0)u_{\gamma,j}\|^2 > 1/2$. Hence $\sum_{k=1}^{\nu} |\langle u_{\gamma,j}, u_k \rangle|^2$ is also similarly bounded away from zero; the largest term in the sum has to be at least $1/(2k)$, and so for each $\gamma > 0$ we may choose k such that $|\langle u_{\gamma,j}, u_k \rangle|^2 > 1/(2k)$. Thus, we may choose k (possibly depending on γ) such that $\langle u_{\gamma,j}, u_k \rangle$ is bounded away from zero for small γ, uniformly with respect to R; furthermore, from the assumption (74) and (A2) we deduce

$$\|(I - S)u_k\| \le C \exp(-cC_2 R),$$

for some positive constants C and C_2. The result is proved. $\qquad\square$

Remark 4.13. In fact, the proof gives a slightly stronger statement: only the estimate (76) depends on (A2); the rest of the theorem requires only that S to be bounded independently of R as a multiplication operator.

Remark 4.14. We may also ask what happens when an eigenvalue λ_γ merges into the essential spectrum with decreasing γ. For the scalar problem, Theorem 5 in [84] states that in this situation, there is a strictly positive value $\gamma_{crit} > 0$ of the the coupling constant at which λ_γ merges into the essential spectrum.

In our current setup, this is false. Consider the following system:

$$-\underline{u}''(x) + (Q(x) + i\gamma S(x))\underline{u}(x) = \lambda\underline{u}(x), \quad \underline{u}(0) = \underline{0},$$

with $Q(x) = \begin{pmatrix} 0 & 0 \\ 0 & \frac{-40}{1+x^2}\chi_{[0,40]}(x) + \sin(x) \end{pmatrix}$ and $S(x) = \begin{cases} I_2 & in \quad [0, 50], \\ 0 & in \quad (50, \infty). \end{cases}$

The system can be seen as two scalar problems with $q_1(x) = 0$ and $q_2(x) = \frac{-40}{1+x^2}\chi_{[0,40]}(x) + \sin(x)$. The problem with potential q_2 and $\gamma = 0$ has a spectral gap which is approximately $(-0.340363, 0.595942)$, with infinitely many eigenvalues accumulating from below at the top end of the gap [101]. However these eigenvalues all lie in the essential spectrum $[0, \infty)$ for the problem with potential q_1 and hence also lie in the essential spectrum of the matrix Schrödinger system. Nevertheless they emerge from the real axis with positive speed, into the upper half-plane, as soon as γ is increased from zero, following the estimate in Theorem 4.12, eqn. (75).

4.6   Numerical examples

In this section we present some numerical examples to demonstrate our theoretical results. We generally apply the 3-point finite difference scheme to our system; the number of steps-per-period is fixed when the number of periods increases. The main advantage of using 'low tech' finite differences rather than a spectral method or Galerkin method is that there exists a Floquet theory for periodic Jacobi matrices, so the theorems of the previous section may be expected to have analogues for the (infinite) discretised system.

Example 4.15. Consider the following matrix Schrödinger systems:

(P):

$$-\underline{u}''(x) + \left(\frac{-40}{1+x^2}\chi_{[0,40]}(x)I_3 + Q(x)\right)\underline{u}(x) = \lambda\underline{u}(x), \quad \underline{u}(0) = \underline{0};$$

(P'):

$$-\underline{u}''(x) + \left(\frac{-40}{1+x^2}I_3 + Q(x)\right)\underline{u}(x) = \lambda\underline{u}(x), \quad \underline{u}(0) = \underline{0};$$

problem P satisfies hypothesis (A1) while problem P' satisfies (A1'). The fact that P' satisfies (A1') can be proved by an ODE version of the Agmon-type results in Janas, J. et al [62]. In both these equations we use:

$$Q(x) = \begin{pmatrix} \frac{\sin(x)+\cos(x)}{6} & \frac{\sin(x)-\cos(x)}{2\sqrt{3}} & -\frac{\sin(x)+\cos(x)}{3\sqrt{2}} \\ \frac{\sin(x)-\cos(x)}{2\sqrt{3}} & \frac{\sin(x)+\cos(x)}{2} & \frac{\cos(x)-\sin(x)}{\sqrt{2}\sqrt{3}} \\ -\frac{\sin(x)+\cos(x)}{3\sqrt{2}} & \frac{\cos(x)-\sin(x)}{\sqrt{2}\sqrt{3}} & \frac{\sin(x)+\cos(x)}{3} \end{pmatrix}.$$

Both problems have exactly the same essential spectrum, though their point spectra are slightly different due to the compactly supported potential well in P. The first two spectral bands are approximately [84]:

$$[-0.378514, -0.340363], [0.595942, 0.912391].$$

For problem P', we expect an eigenvalue close to $\lambda \approx -0.1076$ in the spectral gap $(-0.340363, 0.595942)$, and an eigenvalue embedded in the spectral band $[0.595942, 0.912391]$ near $\lambda \approx 0.6336$. For both problems we use the perturbation:

$$Q(x) \mapsto Q(x) + i\gamma S(x); \quad S(x) = \begin{cases} I_3 & in \quad [0, R], \\ 0 & in \quad (R, \infty), \end{cases}$$

and observe the resulting eigenvalues with $\gamma = 1/4$. Figure 4.1 shows eigenvalue computations for both P and P'. They show that our estimate (75) holds with $C_1' \approx 1293.6$ and $C_2' \approx 0.5386$ for (P'), and $C_1 \approx 1291.9$ and $C_2 \approx 0.5384$ for (P). These figures were calculated using $X = 100$ and a step-size $h = 0.1$, both of which were chosen to ensure that the effects of discretisation error would not be seen in the estimated constants.
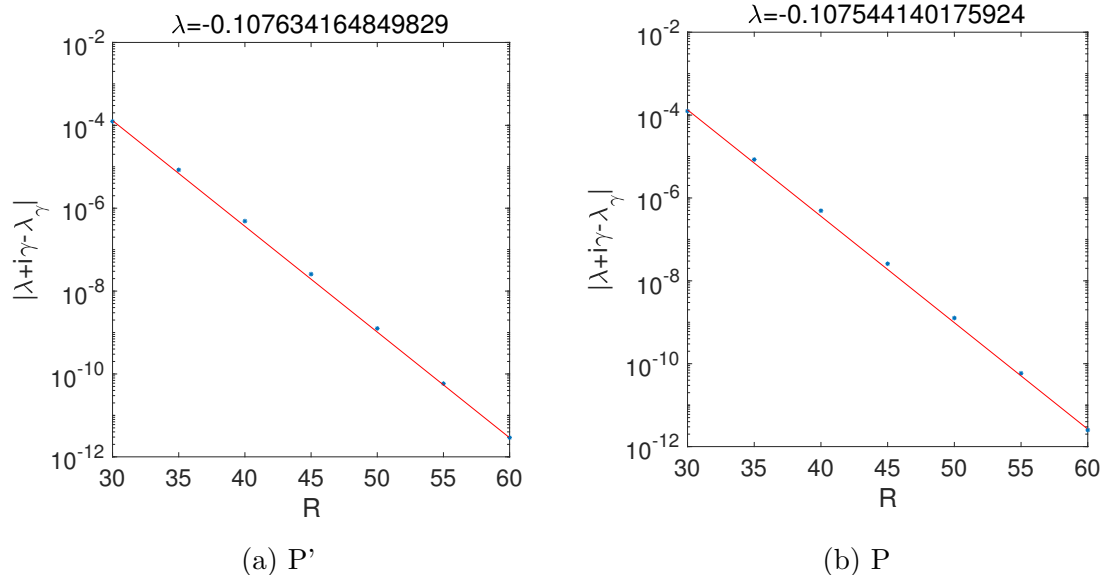
Figure 4.1: Logarithmic plot of $|\lambda + i\gamma - \lambda_\gamma|$ against R.

For the embedded eigenvalues, Figure 4.2 shows the effects of interval truncation. In particular we observe that for P the prediction of Theorem 4.9 holds with $C_3 \approx 0.0039$ and $C_4 \approx 0.3842$. Theorem 4.9 has not been proved for P', which does not have an eventually periodic Q. However, the experiments indicate that the result still hold, with $C_3' \approx 0.0047$ and $C_4' \approx 0.3842$. For these experiments the step-size was $h = 0.1$.

(a) P'

(b) P
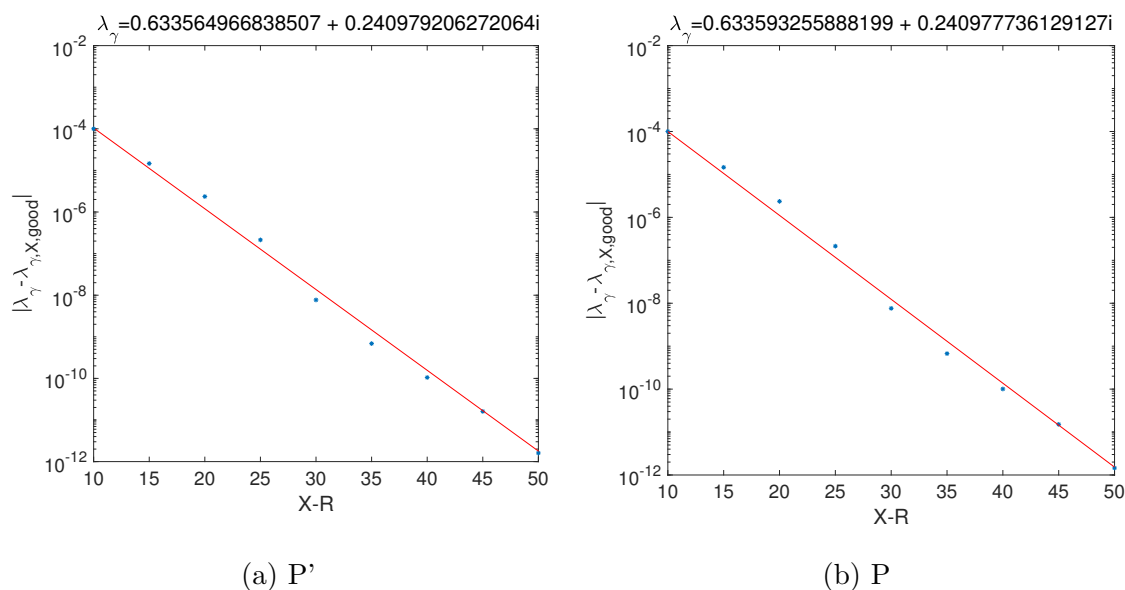
Figure 4.2: Logarithmic plot of $|\lambda_\gamma - \lambda_{\gamma,X,good}|$ against $X - R$.

Finally, we shall show that the prediction of Theorem 4.11 for a spurious eigenvalue also holds; in fact, Figure 4.3 indicates that it holds not only for P, but also for P', for which it is not proved. In these figures we consider the value $\lambda_{bad} \approx -0.1847$, which lies in a spectral gap but is not an eigenvalue of either problem. We fixed $X = 55$ and varied R from 19 to 43 in steps of 4. The value of h was again chosen small enough to suppress effects of discretisation error. The constants C_5 and C_6 predicted by Theorem 4.11 are $C_5 \approx 0.0017$ and $C_6 \approx 0.5345$; it seems also that $C_5' \approx 0.0017$ and $C_6' \approx 0.5345$ for P'.

(a) P' (b) P
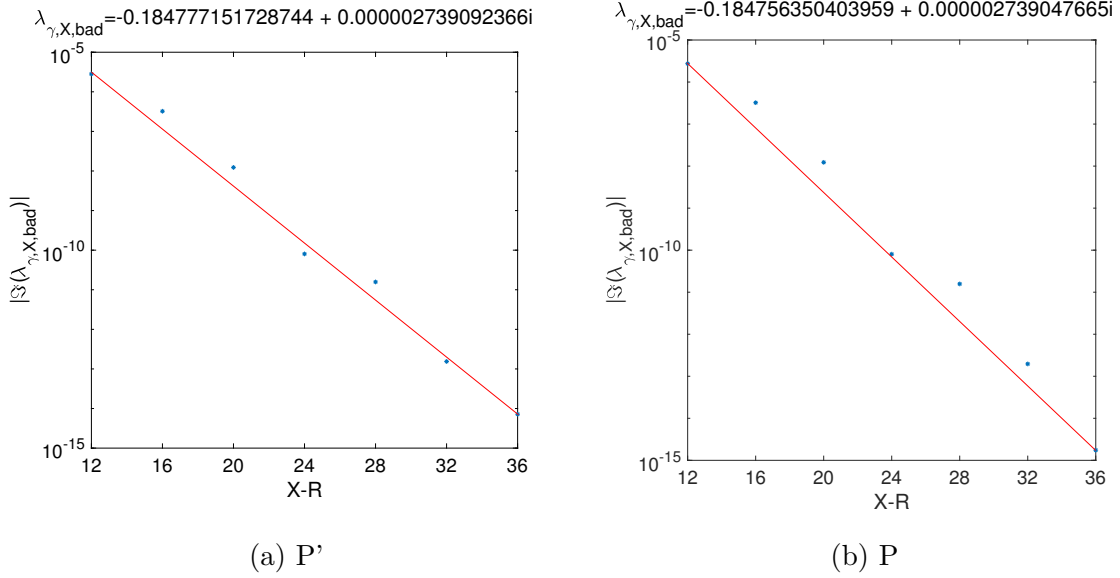
Figure 4.3: Logarithmic plot of $|\Im(\lambda_{\gamma,X,bad})|$ against $X - R$.

Example 4.16. Consider the system:

$$-\underline{u}''(x) + Q(x)\underline{u}(x) = \lambda\underline{u}(x), \quad \underline{u}(0) = \underline{0},$$

with the following perturbed periodic potential:

$$Q(x) = \begin{pmatrix} 4.8876 - 5.9996k(x) & -1.8348 \times 10^{-4}k(x) - 1.5641 & 3.1428 \times 10^{-4}k(x) - 8.05947 \times 10^{-3} & 2.2452 \times 10^{-4}k(x) - 1.3334 & 2.2686 \times 10^{-4}k(x) + 0.4743 \\ -1.8348 \times 10^{-4}k(x) - 1.5641 & 3.1766 - 5.9993k(x) & 8.562 \times 10^{-5}k(x) - 0.0318 & 0.0905 - 1.6524 \times 10^{-4}k(x) & 1.5527 - 2.5128 \times 10^{-4}k(x) \\ 3.143 \times 10^{-4}k(x) - 8.06 \times 10^{-3} & 8.562 \times 10^{-5}k(x) - 0.0318 & 0.7789 - 5.9997k(x) & 0.13405 - 1.8348 \times 10^{-4}k(x) & 3.711 \times 10^{-4}k(x) + 0.5288 \\ 2.2452 \times 10^{-4}k(x) - 1.3334 & 0.0905 - 1.6524 \times 10^{-4}k(x) & 0.13405 - 1.8348 \times 10^{-4}k(x) & 2.8067 - 5.9999k(x) & 5.358 \times 10^{-5}k(x) - 0.1412 \\ 2.2686 \times 10^{-4}k(x) + 0.4743 & 1.5527 - 2.5128 \times 10^{-4}k(x) & 3.711 \times 10^{-4}k(x) + 0.5288 & 5.358 \times 10^{-5}k(x) - 0.1412 & 2.1111 - 6.0001k(x) \end{pmatrix},$$

in which $k(x) = \text{sech}^2(x)\chi_{[0,5]}(x)$.

This rather unwieldy formula was obtained by an expression

$$Q(x) = T\tilde{Q}(x)T^*,$$

in which $\tilde{Q}(x) = -6k(x)I_5 + \text{diag}(n^2/4, n = 1, \ldots, 5)$ and T is the matrix of orthonormal eigenvectors of a randomly chosen real, symmetric 5×5 matrix. According to [18], one eigenvalue for the scalar problem with $q(x) = -6k(x)$ is -1; from this we know that one of the eigenvalues of our differential operator is 1.25 which is an embedded eigenvalue in the essential spectrum $[1/4, \infty)$ of this multi-channel problem. We expect that if the dissipative barrier method is working well then we should see

an eigenvalue close to $1.25 + 0.25i$ when $\gamma = 1/4$. Figure 4.4 shows the plot of the corresponding eigenfunction, for which the calculated eigenvalue was approximately $1.24998 + 0.24993i$. This illustrates the usefulness of the dissipative barrier method for lifting embedded eigenvalues out of the essential spectrum and making them easier to calculate, even bearing in mind Remark 4.14.
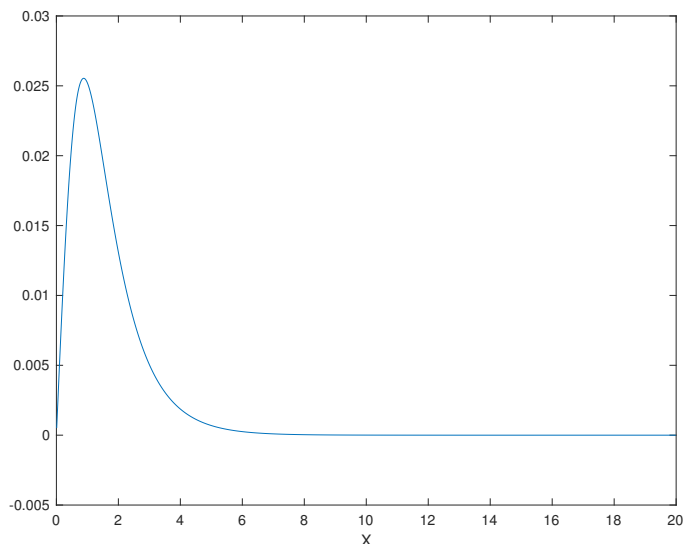
Figure 4.4: Plot of a finite difference approximation of a genuine eigenfunction.

Example 4.17. We consider an equation of the form

$$-\underline{u}'' + D\underline{u} = \lambda(W(x) - iS(x))\underline{u}, ; \quad x \in (0, \infty),$$

$$\underline{u}(0) = \mathbf{0}.$$

Here W is a continuous, periodic matrix, strictly positive definite, so that the corresponding weighted L^2 space is equivalent to $L^2(0, \infty)$. The matrix $S(x)$ was chosen to be compactly supported and bounded. The matrix D is a diagonal matrix with

$$D(j, j) = j^2, \quad j = 1, \ldots, n;$$

qualitatively this is a truncated Fourier representation of a second order derivative operator.

The main differences compared to the cases considered in our theorems are, firstly, the weight $W(x)$ is no longer the identity; and secondly, the compactly supported

dissipative barrier $S(x)$ is now also multiplied by the spectral parameter. The form of this problem is inspired by work in optics with complex index of refraction, see, e.g., [55].

It is not difficult to show that the Floquet theory still holds for the problem on $[R, \infty)$, and so $M_{right,X}(\lambda)$ still converges exponentially fast to $M_{right}(\lambda)$ as $X \to \infty$. For the problem on $[0, R]$, there is now an additional λ-dependence of the barrier term, but $M_{left}(\lambda)$ is still meromorphic. We therefore expect to see fast convergence of the eigenvalues lying well away from the real axis.

Figure 4.5 shows the results of computations in the purely diagonal case

$$W(x) = (2 + \sin(x))I, \quad S(x) = I\chi_{[0,1]}(x), \tag{81}$$

with all matrices being of dimension 5×5. These results were computed using the Numerov discretisation [92], with a uniform mesh of 80 intervals per period (mesh size $2\pi/80$). Because the values of λ in Figure 4.5 are not large, this mesh size is sufficient to ensure that the points plotted in Figure 4.5 will not move in the 'eyeball norm' if the mesh size is halved.

In Figure 4.5 we see that the asterisks (shorter interval approximations) and circles (longer interval approximations) are essentially coincident for the eigenvalues well away from the real axis. We expected this, due to the exponentially small error which interval truncation causes. The more interesting parts are the 'loops' in the upper half plane, one of which starts at approximately $\lambda = 1.75$ and returns to the real axis around $\lambda = 2.6$. Here the asterisk loop (approximating interval $[0, 20\pi]$) is approximately twice as far from the real axis as the circle loop (approximating interval $[0, 40\pi]$). These loops are approximations to a spectral band. Though we have not proved this, they appear to converge at a rate $1/X$, as the interval $[0, X]$ goes to infinity. Note that there are also other approximations to (parts of) spectral bands, due to the fact that the spectral multiplicity of the higher bands can be greater than 1. It seems that, in this picture, only the bands near 0.5, and from 0.75 to just below 1, are simple.
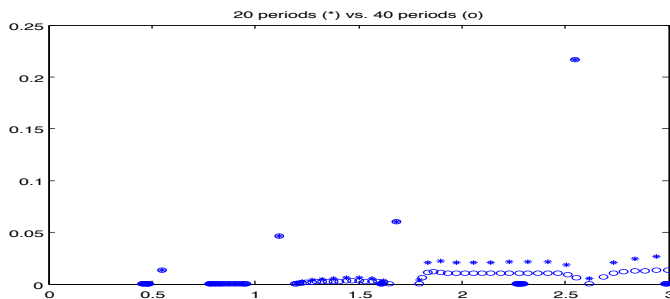
Figure 4.5: Eigenvalue approximations for coefficients in eqn. (81) computed using $[0, 20\pi]$ and $[0, 40\pi]$ as approximations to $[0, \infty)$. Eigenvalues are marked with asterisks for $[0, 20\pi]$ and circles for $[0, 40\pi]$.

In Figure 4.6 we repeated the experiments using non-diagonal $W(x)$ given by

$$W_{j,k}(x) = 2I + \frac{j+k}{2n} \sin(x). \tag{82}$$

The same phenomena are noted as in the diagonal coefficient case, though the different scale on the vertical axis makes the slow convergence to the essential spectrum more stark.
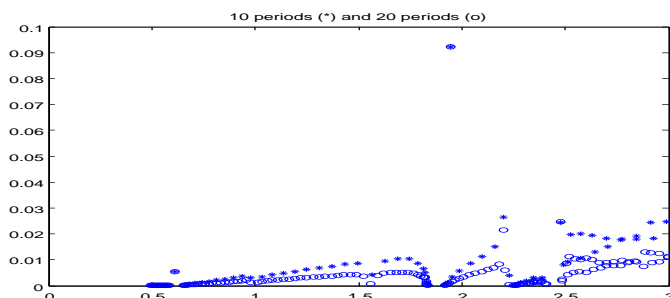
Figure 4.6: Eigenvalue approximations for coefficients in eqn. (82) computed using $[0, 20\pi]$ and $[0, 40\pi]$ as approximations to $[0, \infty)$. Eigenvalues are marked with asterisks for $[0, 20\pi]$ and circles for $[0, 40\pi]$.

4.7 Conclusion

We have introduced a method to calculate eigenvalues in gaps of matrix-valued Schrödinger operators. Theoretically, we have shown that the relatively compact

dissipative perturbation technique together with domain truncation obtain approximations of isolated eigenvalues close to the ones of the original problem. Moreover, spurious eigenvalues can be predicted using this method and are characterised by exponentially small imaginary parts. These approximations have been computed using finite difference schemes for some numerical examples and have shown excellent agreement with the theoretical part. An additional remark on this procedure is that the approximating results of the implementations of both fast decaying periodic potentials and compactly supported periodic potentials see e.g., Example 4.15 are mostly the same.

We have also observed the effectiveness of the presented method when the weighted matrix is different from the identity and the dissipative barrier is multiplied by the spectral parameter as in Example 4.17. The only caveat for these cases is that the approximations to the spectral bands do not converge fast, so if very high accuracy is required then one should use λ-dependent non-reflecting boundary conditions [55].

One of the main sources of Hamiltonian eigenvalue problems is the use of semi-discretisation for PDE problems on waveguides. In the next chapter, we will consider the PDE:

$$- \Delta u + Q(x,y)u = \lambda u, \tag{83}$$

on a semi-infinte waveguide. These give rise to a Hamiltonian system in which $Q(x)$ in our problem is an operator in $l^2(\mathbb{N})$; they can also be studied directly in a PDE form.

5 On the eigenvalues of spectral gaps of elliptic PDEs on waveguides

5.1 Introduction

Elliptic PDEs on waveguides occupy a significant role in many applications related to physics and quantum mechanics such as photonic crystals and metamaterials, see e.g. [70, 104]. There is therefore a keen interest in the study of spectral problems of band-gap structure of the differential operators on waveguides.

There are a number of different approaches to these problems. For the self-adjoint case, for instance, the articles [63, 54, 108] are devoted to calculation of the band-gap spectrum of elliptic PDEs on periodic waveguides by using Dirichlet-to-Neumann operators on the interfaces of subdomains, coupled with the Floquet-Bloch theory in which the problem is reduced to a nonlinear eigenvalue problem. Other studies concern the spectra of non-self-adjoint differential operators in the underlying model. In particular, [68, 91] studied the essential spectrum of the Laplacian operator equipped with complex Robin boundary conditions, on waveguides, and derived sufficient conditions for the existence or absence of isolated eigenvalues. For more information on the spectral gaps of elliptic PDEs, we refer the reader to [72] and many references therein.

In this chapter, we concentrate on isolated eigenvalues of the elliptic differential operator $-\Delta + Q$, in which Q is any real, bounded potential; we assume that with appropriate boundary conditions this operator is self-adjoint. In order to obtain spectral approximations, we change the operator to a non-self-adjoint version using a *dissipative barrier* and employ domain truncation. Our main results are proved by the use of Dirichlet-to-Neumann maps on the cross-section and establish convergence that is exponentially fast with respect to the size of the truncated domain - see Theorem 5.13 for the approximation of the Dirichlet-to-Neumann maps, Theorem 5.16 for absence of spectral pollution in the upper half plane, and Theorem 5.25 for the rate-of-convergence estimate for isolated eigenvalues of finite multiplicity. We also consider a dissipative pencil problem; our theorems can be adapted to this case too. The key to proving exponential accuracy of the truncated domain eigenvalue approximations is the exponential decay of the eigenfunctions, Lemma 5.10, which is established using an adaptation of a result of Janas, Naboko and Stolz [62], itself based on a technique of Barbaroux, Combes and Hislop [15]. In [84], exponential decay was also used, but it was proved using Floquet theory and hence depended on periodicity in an essential way. The method in [15, 62] is so adaptable to different situations that we believe it could also be used to provide exponentially small error

bounds for the domain truncation methods in [23, 83] where, as here, the hypotheses on the potential are reasonably general.

This chapter is organised as follows. In Section 5.2, we present the original and truncated problems and introduce Dirichlet-to-Neumann maps and derive standard lemmas. We also deal with some regularity questions. Section 5.3 establishes error bounds for truncated-domain approximations to the Dirichlet-to-Neumann maps. The main theorem is proved in Section 5.4. Finally, Section 5.5 represents some numerical examples to illustrate our results.

5.2 Preliminary and background theory

We consider the dissipative Schrödinger equation:

$$-\Delta u + (Q + i\gamma S)u = \lambda u, \tag{84}$$

on a semi-infinite waveguide $\Omega = (0, \infty) \times \mathcal{C}$; the cross-section $\mathcal{C}$ is a smooth, bounded domain in $\mathbb{R}^d, d \geq 1$, or a $d-$dimensional smooth compact manifold. Boundary conditions are imposed as illustrated schematically in Figure 5.1.
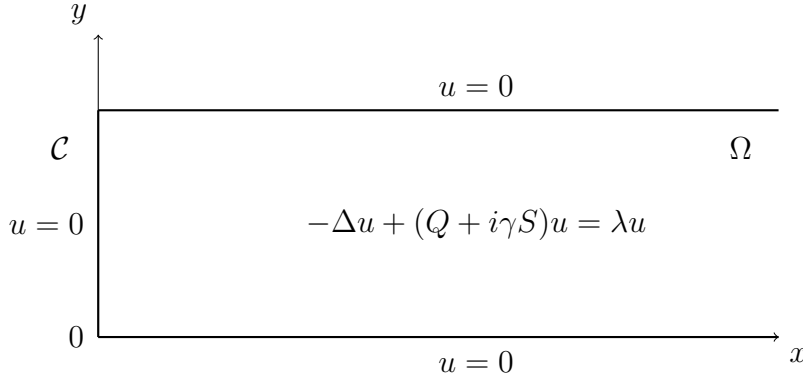
Figure 5.1: The domain of the semi-infinite waveguide problem.

In eqn. (84) we require u to lie in the domain $D(L_0)$ of an operator L_0; this will be described below. The parameter γ appearing in (84) is nonzero real, while the coefficients Q and S satisfy the following hypotheses:

(A1): Q is bounded, real-valued, and integrable over compact subsets of Ω.

(A2): S is a cut-off function with support in $[0, R]$ for some $R > 0$: there exists

$0 < c < 1$ such that if $x \in [0, \infty)$ and $y \in \mathcal{C}$ then

$$S(x, y) = \begin{cases} 1, & x < cR; \\ 0, & x \geq R. \end{cases} \tag{85}$$

When $x \in (cR, R)$, we assume that S is measurable and takes values in $[0, 1]$. We define an operator L_0 by:

$$L_0 u = (-\Delta + Q)u, \tag{86}$$

with domain[8]:

$$D(L_0) = \{\, u \in H_{loc}^2(\Omega) \cap H_0^1(\Omega), \mid (-\Delta + Q)u \in L^2(\Omega)\}. \tag{87}$$

We now give an informal description of the Glazman decomposition method [3] for this problem, and the associated Dirichlet-to-Neumann maps. Denote by $\Omega_{(R,\infty)}$ the domain $(R, \infty) \times \mathcal{C}$ and by $\Omega_{(0,R)}$ the domain $(0, R) \times \mathcal{C}$; we use the notation $\Sigma_{(R,\infty)}$ and $\Sigma_{(0,R)}$ to denote the portion of the boundaries of these domains which intersects with the 'sides' of the waveguide, $(0, \infty) \times \partial\mathcal{C}$. The Glazman decomposition method divides the waveguide into two components, $\Omega_{(0,R)}$ and $\Omega_{(R,\infty)}$, for $R > 0$ as in A2, with matching conditions on the cross-section $\mathcal{C}_R = \{(R, y) \mid y \in \mathcal{C}\}$. For a fixed $\lambda \in \mathbb{C}$ and a suitable nonzero function f defined on $\mathcal{C}_R$ we consider the two boundary value problems P_{left} and P_{right} described schematically in Figure 5.2.
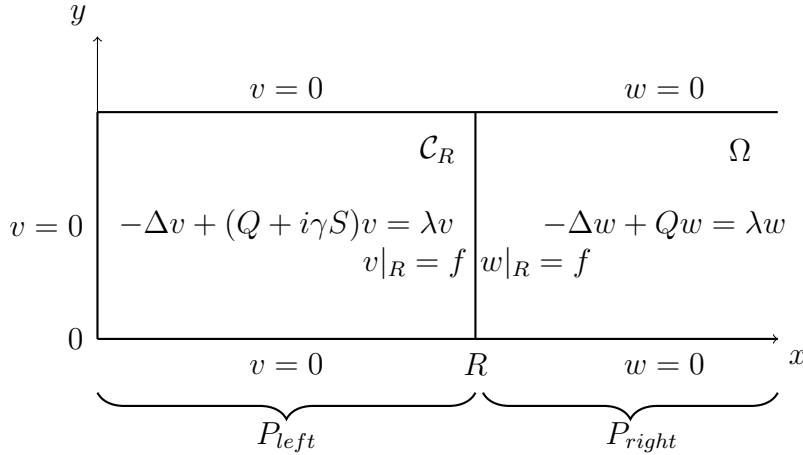
Figure 5.2: Glazman decomposition for the infinite waveguide problem.

[8]The reason that the functions may not lie in $H^2 \cap H_0^1$ is due to the corners. In some earlier papers (e.g. [76]) the second author neglected to take account of this; it was pointed out post-publication by E.B. Davies [41].

Note that P_{left} can be assumed uniquely solvable without loss of generality (if necessary, R can be increased slightly to ensure this and move the spectrrum). In fact, P_{left} is uniquely solvable if and only if λ is not an eigenvalue of the underlying Dirichlet operator and changing R changes the eigenvalues of this operator. The same is true for P_{right} provided $\lambda \notin Spec(-\Delta_D + Q)$, where $-\Delta_D$ is the Dirichlet Laplacian in $\Omega_{(R,\infty)}$. Under these assumptions the mappings

$$f = v|_{\mathcal{C}_R} \mapsto \frac{\partial v}{\partial x}|_{\mathcal{C}_R}, \quad f = w|_{\mathcal{C}_R} \mapsto -\frac{\partial w}{\partial x}|_{\mathcal{C}_R},$$

define linear *Dirichlet-to-Neumann* operators, which we denote $M_{left}(\lambda)$ and $M_{right}(\lambda)$. In the exterior domain situation described in [83], and in [16], these maps are pseudodifferential operators of order 1 mapping a scale of Sobolev spaces on the boundary, e.g. H^s to H^{s-1}. In order to establish such results here we need to be a little more careful, as the function f in Figure 5.2 need not itself satisfy the boundary conditions on the sides of the waveguide. However we shall shortly show that, for this problem, M_{left} and M_{right} map $L^2(\mathcal{C}_R)$ to $H^{-1}(\mathcal{C}_R)$; furthermore, since their principal symbols are independent of λ, elliptic bootstrapping arguments will enable us to show that differences of such Dirichlet-to-Neumann maps, e.g. $M_{left}(\lambda) - M_{left}(\mu)$, are actually smoothing operators, mapping $L^2(\mathcal{C}_R)$ into $H^{1/2}(\mathcal{C}_R)$.

Lemma 5.1. *Let*

$$N_{left} = \{u \in L^2(\Omega_{(0,R)}) \mid \Delta u = 0, \ \ u|_{\Sigma_{(0,R)}} = 0\},$$

$$N_{right} = \{u \in L^2(\Omega_{(R,\infty)}) \mid \Delta u = 0, \ \ u|_{\Sigma_{(R,\infty)}} = 0\}.$$

Then there exist bounded harmonic extension operators S_{left} and S_{right} mapping $L^2(\mathcal{C}_R)$ into N_{left} and N_{right} respectively. Furthermore, the 'normal derivative' operators Γ_{left} and Γ_{right} on $\mathcal{C}_R$ from the left and right respectively, may be defined on the ranges $Ran(S_{left})$ and $Ran(S_{right})$, in such a way that that

$$\Gamma_{left}S_{left} : L^2(\mathcal{C}_R) \to H^{-1}(\mathcal{C}_R), \quad \Gamma_{right}S_{right} : L^2(\mathcal{C}_R) \to H^{-1}(\mathcal{C}_R)$$

are bounded in the natural operator norms.

Proof. The proof is by direct calculation; we give the details for S_{right} and Γ_{right} only. We use the decomposition

$$\Delta = \frac{\partial^2}{\partial x^2} + \Delta_{\mathcal{C}},$$

63

where $\Delta_{\mathcal{C}}$ is the Laplace (or Laplace-Beltrami) operator on $\mathcal{C}$. Denote the eigenvalues and normalized eigenfunctions of $-\Delta_{\mathcal{C}}$ by μ_n and ψ_n, $n \in \mathbb{N}$, bearing in mind that the $H_0^1(\mathcal{C})$-norm is given up to equivalence by

$$\|u\|_{H_0^1(\mathcal{C})}^2 = \sum_{n=1}^{\infty} \mu_n |\langle u, \psi_n \rangle|^2,$$

in which $\langle \cdot, \cdot \rangle$ denotes the inner product in $L^2(\mathcal{C})$. Any function $f \in L^2(\mathcal{C}_R) = L^2(\mathcal{C})$ has an expansion

$$f = \sum_{n=1}^{\infty} \langle f, \psi_n \rangle \psi_n$$

and hence a harmonic extension into N_{right} is given by

$$(S_{right}f)(x, y) = \sum_{n=1}^{\infty} \langle f, \psi_n \rangle \psi_n(y) \exp(-\sqrt{\mu_n}(x - R)). \tag{88}$$

A direct calculation shows that $\|S_{right}\|^2 = 1/(2\sqrt{\mu_1})$. This is because

$$\|S_{right}\|^2 = \int_R^{\infty} \exp(-2\sqrt{\mu_n}(x - R))dx = \frac{1}{2\sqrt{\mu_n}} \Big[\exp(-2\sqrt{\mu_n}(R - R)) \Big] \leq \frac{1}{2\sqrt{\mu_1}},$$

where $\mu_1 = \min(\mu_n); n \in \mathbb{N}$. Now a formal calculation yields the normal derivative

$$\Gamma_{right} S_{right}f = - \left.\frac{\partial(S_{right}f)}{\partial x}\right|_{x=R} = \sum_{n=1}^{\infty} \langle f, \psi_n \rangle \psi_n \sqrt{\mu_n};$$

hence, for any $u = \sum_{n=1}^{\infty} \langle u, \psi_n \rangle \psi_n$ in $H_0^1(\mathcal{C}_R)$,

$$\left| \left\langle - \left.\frac{\partial(S_{right}f)}{\partial x}\right|_{x=R}, u \right\rangle \right| = \left| \sum_{n=1}^{\infty} \langle f, \psi_n \rangle \sqrt{\mu_n} \overline{\langle u, \psi_n \rangle} \right|$$

$$\leq \left(\sum_{n=1}^{\infty} |\langle f, \psi_n \rangle|^2 \right)^{1/2} \left(\sum_{n=1}^{\infty} \mu_n |\langle u, \psi_n \rangle|^2 \right)^{1/2} = \|f\|_{L^2(\mathcal{C}_R)} \|u\|_{H_0^1(\mathcal{C}_R)}.$$

Since $H^{-1}(\mathcal{C}_R)$ is the dual space of $H_0^1(\mathcal{C}_R)$, this establishes that required result. $\square$

While Lemma 5.1 deals with harmonic extensions, for later use it will be convenient to use a compactly supported extension. The following lemma guarantees this.

Lemma 5.2. *For any $f \in L^2(\mathcal{C}_R)$, there exists a compactly supported function $F \in L^2(\Omega_{(R,\infty)})$ such that $F|_{\mathcal{C}_R} = f$, with $F|_{\Sigma_{(R,\infty)}} = 0$, and $\Delta F \in L^2(\Omega_{(R,\infty)})$. Moreover, $\|F\|_{L^2(\Omega_{(R,\infty)})} \leq C\|f\|_{L^2(\mathcal{C}_R)}$, in which the constant C depends only on the geometry of the domain $\Omega_{(R,\infty)}$. In addition, if $G_\lambda = -(-\Delta + Q - \lambda)F$, then $\|G_\lambda\|_{L^2(\Omega_{(R,\infty)})} \leq \tilde{C}\|f\|_{L^2(\mathcal{C}_R)}$, where $\tilde{C}$ depends on the geometry of the domain $\Omega_{(R,\infty)}$.*

Proof. Let $\tilde{F} = S_{right}f$; from Lemma 5.1, $\tilde{F}$ has all the properties required for F apart from compact support. We therefore introduce a smooth cut-off function χ satisfying

$$\chi(x,y) = \begin{cases} 1, & 0 \leq x \leq R + \delta, y \in \mathcal{C}; \\ 0, & R+1 \leq x, y \in \mathcal{C}_R; \end{cases}$$

χ can be chosen with trivial dependence on y; formally $\chi(x,y) = \chi(x)$. We may choose $\delta > 0$ such that $\nabla\chi(x,y) = 0$ in $(R, R+\delta) \times \mathcal{C}_R$. We set $F := \chi\tilde{F}$, and observe that F satisfies the boundary conditions illustrated in Figure 5.3:
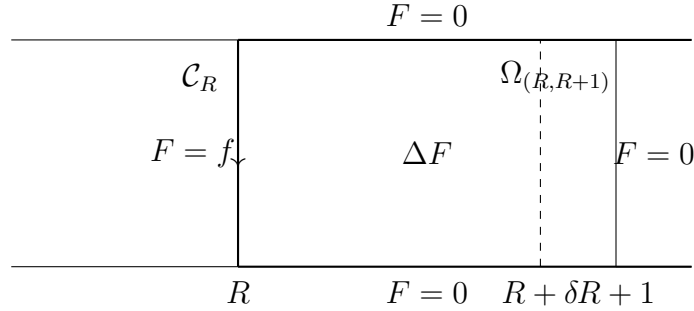
Figure 5.3: The constructed function F on a truncated waveguide $\Omega_{(R,R+1)}$.

Note that $F|_{\mathcal{C}_R} = f$, and $F|_{\Sigma_{(R,\infty)}} = 0$. Because $\tilde{F}$ is harmonic,

$$\Delta F = \Delta(\chi\tilde{F}) = (\Delta\chi)\tilde{F} + 2\nabla\chi \cdot \nabla\tilde{F}, \tag{89}$$

and

$$\|\Delta F\|_{L^2(\Omega_{(R,\infty)})} \leq \|\Delta\chi\|_{L^\infty(\Omega)}\|\tilde{F}\|_{L^2(\Omega_{(R,\infty)})} + 2\|\nabla\chi \cdot \nabla\tilde{F}\|_{L^2(\Omega_{(R,\infty)})} \tag{90}$$

To estimate the L^2-norm of ΔF we estimate the L^2-norm of each term in (90). For the term $\|\nabla\chi \cdot \nabla\tilde{F}\|_{L^2(\Omega_{(R,\infty)})}$, we use the fact that $\nabla\chi(x,\cdot)$ is non-trivial only for

$x \in (R + \delta, R + 1)$, and thus

$$\|\nabla \chi \cdot \nabla \tilde{F}\|^2_{L^2(\Omega_{(R,\infty)})} \leq \|\nabla \chi\|^2_{L^\infty(\Omega)} \int_{\mathcal{C}_R} \mathrm{d}y \int_{R+\delta}^\infty \left(\left| \frac{\partial \tilde{F}}{\partial x} \right|^2 + |\nabla_y \tilde{F}|^2 \right) \mathrm{d}x.$$

Using the explicit expression for $F = S_{right} f$ in (88) we have

$$
\begin{aligned}
\int_{\mathcal{C}_R} \mathrm{d}y \int_{R+\delta}^\infty \left| \frac{\partial \tilde{F}}{\partial x} \right|^2 \mathrm{d}x &= \sum_{n=1}^\infty |\langle f, \psi_n \rangle|^2 \mu_n \int_{R+\delta}^\infty \exp(-2\sqrt{\mu_n}(x - R))\mathrm{d}x \\
&\leq \sum_{n=1}^\infty |\langle f, \psi_n \rangle|^2 \frac{1}{4\delta} 2\delta\sqrt{\mu_n} \exp(-2\sqrt{\mu_n}\delta) \\
&\leq \frac{1}{4\mathrm{e}\delta} \sum_{n=1}^\infty |\langle f, \psi_n \rangle|^2 = \frac{1}{4\mathrm{e}\delta} \|f\|^2_{L^2(\mathcal{C}_R)}.
\end{aligned}
$$

Since the ψ_n are the Dirichlet eigenfunctions of $\Delta_{\mathcal{C}_R}$, their gradients are orthogonal and $\int_{\mathcal{C}_R} |\nabla \psi_n(y)|^2 \mathrm{d}y = \mu_n$. Thus

$$\int_{\mathcal{C}_R} \mathrm{d}y \int_{R+\delta}^\infty |\nabla_y \tilde{F}|^2 \mathrm{d}x = \sum_{n=1}^\infty |\langle f, \psi_n \rangle|^2 \mu_n \int_{R+\delta}^\infty \exp(-2\sqrt{\mu_n}(x - R))\mathrm{d}x,$$

from which we see that

$$\int_{\mathcal{C}_R} \mathrm{d}y \int_{R+\delta}^\infty \left| \nabla_y \tilde{F} \right|^2 \mathrm{d}x = \int_{\mathcal{C}_R} \mathrm{d}y \int_{R+\delta}^\infty \left| \frac{\partial \tilde{F}}{\partial x} \right|^2 \mathrm{d}x$$

and hence

$$\|\nabla \chi \cdot \nabla \tilde{F}\|^2_{L^2(\Omega_{(R,\infty)})} \leq \frac{1}{2\mathrm{e}\delta} \|\nabla \chi\|^2_{L^\infty(\Omega)} \|f\|^2_{L^2(\mathcal{C}_R)}.$$

Using this in conjunction with (90) and bearing in mind that $\|\Delta \chi\|_{L^\infty(\Omega)}$ is bounded, we see that ΔF admits a bound $\|\Delta F\|_{L^2(\Omega_{(R,\infty)})} \leq C\|f\|_{L^2(\mathcal{C}_R)}$, as required. The other result follows from the latter and the fact that $Q \in L^\infty(\Omega_{(R,\infty)})$. $\qquad\square$

Lemma 5.3. *The Dirichlet-to-Neumann maps $M_{left}(\lambda)$ and $M_{right}(\lambda)$, defined initially for smooth functions defined on $\mathcal{C}_R$, admit extensions as bounded linear maps from $L^2(\mathcal{C}_R)$ to $H^{-1}(\mathcal{C}_R)$.*

Proof. As in the proof of Lemma 5.1, we consider just the case of M_{right}; the case of M_{left} is similar: one has to replace Q by $Q + i\gamma S$ and note that M_{left} depends also on γ. Given $f \in L^2(\mathcal{C}_R)$ we seek the solution w of problem P_{right} in Figure 5.1 in the form $w = S_{right}f + v$, in which $v \in L^2(\Omega_{(R,\infty)})$ must satisfy the Schrödinger equation

$$(-\Delta + Q - \lambda)v = -(-\Delta + Q - \lambda)S_{right}f = (\lambda - Q)S_{right}f,$$

the second equality holding because $S_{right}f$ is a harmonic extension of f. The boundary conditions satisfied by v are now homogeneous Dirichlet on the entire boundary of Ω_R and hence

$$v = (-\Delta_D + Q - \lambda)^{-1}(\lambda - Q)S_{right}f,$$

in which we have exploited the boundedness of Q and in which $-\Delta_D$ is the Dirichlet Laplacian in $\Omega_{(R,\infty)}$. It follows that the normal derivative of w on $\mathcal{C}_R$ is

$$\Gamma_{right}w = \Gamma_{right}S_{right}f + \Gamma_{right}(-\Delta_D + Q - \lambda)^{-1}(\lambda - Q)S_{right}f;$$

in other words,

$$M_{right}(\lambda) = \Gamma_{right}S_{right} + \Gamma_{right}(-\Delta_D + Q - \lambda)^{-1}(\lambda - Q)S_{right}. \qquad (91)$$

Because Q is bounded, $(-\Delta_D + Q - \lambda)^{-1}$ is a bounded map from $L^2(\Omega_{(R,\infty)})$ to $H_0^1(\Omega_{(R,\infty)}) \cap H^2(\Omega_{(R,\infty)})$. Applying standard trace theorems it therefore follows that $\Gamma_{right}(-\Delta_D + Q - \lambda)^{-1}$ is a bounded linear map from $L^2(\Omega_{(R,\infty)})$ to $H^{1/2}(\mathcal{C}_R)$, which is compactly embedded in $H^{-1}(\mathcal{C}_R)$. The result now follows from Lemma 5.1. $\qquad \square$

Remark 5.4. Following the abstract results in [28], the unbounded part of $M_{right}(\lambda)$ is $\Gamma_{right}S_{right}$; the remaining term in (91), which is the only $\lambda-$dependent term, is bounded, as long as λ lies in the resolvent set of $-\Delta_D + Q$.

The following lemma is standard; we include a proof for completeness.

Lemma 5.5. *Suppose that $M_{left}(\lambda)$ and $M_{right}(\lambda)$ are well-defined at $\lambda = \mu$. Then μ is an eigenvalue of $L_0 + i\gamma S$ if and only if $\ker\{ M_{left}(\mu) + M_{right}(\mu) \} \neq \{0\}$.*

Proof. If μ is an eigenvalue of $L_0 + i\gamma S$, illustrated as in Figure 5.2, then there exists an eigenfunction u; we may take $v = u$ on $\Omega_{(0,R)}$ and $w = u$ on $\Omega_{(R,\infty)}$. Hence

$$\{M_{left}(\mu) + M_{right}(\mu)\}u|_{\mathcal{C}_R} = \frac{\partial u}{\partial \nu}|_{\mathcal{C}_R} + \left(-\frac{\partial u}{\partial \nu}|_{\mathcal{C}_R}\right) = 0.$$

Assuming that $u|_{\mathcal{C}_R}$ is not zero, this leads to the condition that $\ker\{\ M_{left}(\mu) + M_{right}(\mu)\}$ is not trivial.

Conversely, suppose that $\mu \in \mathbb{C}$ such that

$$\ker\{\ M_{left}(\mu) + M_{right}(\mu)\} \neq \{0\}. \tag{92}$$

Let $f \in \ker\{\ M_{left}(\mu) + M_{right}(\mu)\}$ and define a nontrivial function u by:

$$u = \begin{cases} v, & \Omega_{(0,R)}; \\ w, & \Omega_{(R,\infty)}. \end{cases}$$

where v and w are the solutions of P_{left} and P_{right} in Figure 5.2 respectively when $\lambda = \mu$. Then u is a solution for the differential equation $-\Delta u + (Q + i\gamma S)u = \mu u$, on $\Omega_{(0,R)}$ and $\Omega_{(R,\infty)}$, whose trace and normal derivative (interpreted in the usual weak sense) match across $\mathcal{C}_R$. These establish that u satisfies all the weak characterisation of an eigenfunction, and so μ is an eigenvalue. $\qquad \square$

Remark 5.6. If $u|_R$ is zero, then both $M_{left}(\cdot)$ and $M_{right}(\cdot)$ are undefined at the eigenvalue λ. Hence the condition $u|_R$ is nonzero follows immediately when $M_{left}(\cdot)$ and $M_{right}(\cdot)$ are well-defined.

We now truncate our semi-infinite waveguide problem (84) to a finite one on a domain $\Omega_{(0,X)} = (0, X) \times \mathcal{C}$ for some $X > R$. At $x = X$, we can impose a Dirichlet condition $u|_X = 0$. The truncated problem is shown schematically in Figure 5.4:
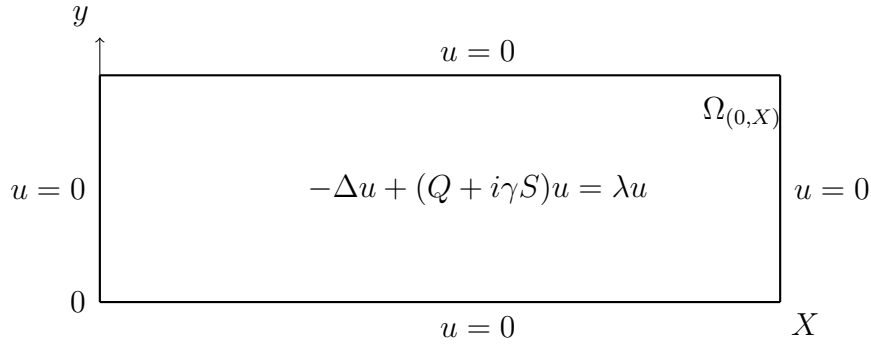
Figure 5.4: The domain of the truncated waveguide problem.

The operator L_0 is replaced by L_X:

$$L_X u = (-\Delta + Q)u, \tag{93}$$

with domain:

$$D(L_X) = \{u \in H^2_{loc}(\Omega_{(0,X)}) \cap H^1_0(\Omega_{(0,X)}) \mid (-\Delta + Q)u \in L^2(\Omega_{(0,X)})\}. \qquad (94)$$

Remark 5.7. Other boundary conditions are possible apart from $u|_X = 0$; the study of non-reflecting boundary conditions is a very active area of research, see e.g., [50] and references therein. Our objective here is to study the approximation properties of the simplest approach, whose computational implementation is straightforward.

The characterisation of the eigenvalues of $L_X + i\gamma S$ can be obtained by replacing P_{right} by $P_{right,X}$ in Figure 5.2 and consequently Glazman decomposition becomes:

Figure 5.5: Glazman decomposition for the truncated waveguide problem.

Again if these problems can be solved uniquely for f, then we may define a map $M_{right,X}(\lambda)$ informally as follows

$$M_{right,X}(\lambda)w|_{\mathcal{C}_R} = -\frac{\partial w}{\partial \nu}|_{\mathcal{C}_R}. \qquad (95)$$

Following the ideas in Lemma 5.1 it is straightforward to prove that $M_{right,X}(\lambda)$ is, like $M_{right}(\lambda)$, a bounded linear map from $L^2(\mathcal{C}_R)$ to $H^{-1}(\mathcal{C}_R)$, with the same λ-independent principal symbol as $\Gamma_{right}S_{right}$. The following result is proved in the same way as Lemma 5.5, replacing M_{right} by $M_{right,X}$.

Corollary 5.8. *Suppose that $M_{left}(\lambda)$ and $M_{right,X}(\lambda)$ are well-defined at $\lambda = \mu$. Then μ is an eigenvalue of $L_X + i\gamma S$ if and only if* $\ker\{M_{left}(\mu) + M_{right,X}(\mu)\} \neq \{0\}$.

The following technical result will be useful in the sequel.

Lemma 5.9. *On all the domains Ω, $\Omega_{(0,X)}$, the norms $\|u\|_{H^2}$ for functions in $H_0^1 \cap H^2$ are equivalent to $\|u\|_{L^2} + \|\Delta u\|_{L^2}$, with constants independent of X :*

$$c_1 \left(\|u\|_{L^2} + \|\Delta u\|_{L^2} \right) \leq \|u\|_{H^2} \leq c_2 \left(\|u\|_{L^2} + \|\Delta u\|_{L^2} \right). \tag{96}$$

Proof. We prove Inequality (96) when $\Omega_{(0,X)}$. The other case is similar. Note that the inequality

$$\|u\|_{L^2}^2 + \|\Delta u\|_{L^2}^2 \leq \|u\|_{H^2}^2$$

always holds. Also, since $(a+b)^2 \leq 2(a^2 + b^2)$; $a, b \in \mathbb{R}$, it follows that

$$\frac{1}{\sqrt{2}} (\|u\|_{L^2} + \|\Delta u\|_{L^2}) \leq \sqrt{\|u\|_{L^2}^2 + \|\Delta u\|_{L^2}^2} \leq \|u\|_{H^2}.$$

Hence, we take $c_1 = \frac{1}{\sqrt{2}}$.

For the other side of Inequality (96), we define

$$\phi_n(x) = \sqrt{\frac{2}{X}} \sin \left(\frac{n\pi(x - X)}{X} \right);$$

for sufficiently large X, also let $-\Delta_y \Psi_m = \mu_m \Psi_m$ on $\mathcal{C}$ and $\|\Psi_m\|_{L^2(\mathcal{C})} = 1$. Observe that $\|\nabla_y \Psi_m\|^2 = \mu_m \|\Psi_m\|^2$, so $\|\nabla_y \Psi_m\| = \sqrt{\mu_m}$. Given $u \in H_0^1(\Omega_{(0,X)}) \cap H^2(\Omega_{(0,X)})$ expand u as

$$u(x, y) = \sum_{n,m=1}^{\infty} c_{n,m} \phi_n(x) \Psi_m(y)$$

so that $\|u\|^2 = \sum_{n,m=1}^{\infty} |c_{n,m}|^2$. Observe that

$$-\Delta u(x, y) = \sum_{n,m=1}^{\infty} \left(\frac{n^2 \pi^2}{X^2} + \mu_m \right) c_{n,m} \phi_n(x) \Psi_m(y)$$

and so

$$\|u\|^2 + \|\Delta u\|^2 = \sum_{n,m=1}^{\infty} |c_{n,m}|^2 \left(1 + \left(\frac{n^2 \pi^2}{X^2} + \mu_m \right)^2 \right).$$

We wish to show that there exists $c_2 > 0$, independent of X, such that $\|u\|_{H^2} \leq c_2 \left(\|u\|_{L^2} + \|\Delta u\|_{L^2} \right)$, for which it is sufficient to show that

$$\|u\|_{H^2}^2 \leq c_2^2 \left(\|u\|_{L^2}^2 + \|\Delta u\|_{L^2}^2 \right) = \tilde{c} (\|u\|_{L^2}^2 + \|\Delta u\|_{L^2}^2).$$

Observe that

$$\|\frac{\partial u}{\partial x}\|_{L^2}^2 = \sum_{n,m=1}^{\infty} \frac{n^2\pi^2}{X^2}|c_{n,m}|^2$$

$$\leq \frac{1}{2}\sum_{n,m=1}^{\infty}\left(1 + \left(\frac{n^2\pi^2}{X^2} + \mu_m\right)^2\right)|c_{n,m}|^2$$

$$\leq \frac{1}{2}\left(\|u\|_{L^2}^2 + \|\Delta u\|_{L^2}^2\right),$$

$$\|\frac{\partial^2 u}{\partial x^2}\|_{L^2}^2 = \sum_{n,m=1}^{\infty}\left(\frac{n^2\pi^2}{X^2}\right)^2|c_{n,m}|^2$$

$$\leq \|\Delta u\|_{L^2}^2;$$

and

$$\|\nabla_y u\|_{L^2}^2 = \sum_{n,m=1}^{\infty}|c_{n,m}|^2\|\nabla_y \Psi_m\|^2$$

$$= \sum_{n,m=1}^{\infty}|c_{n,m}|^2\mu_m$$

$$\leq \frac{1}{2}\sum_{n,m=1}^{\infty}(1 + \mu_m^2)|c_{n,m}|^2$$

$$\leq \frac{1}{2}\left(\|u\|_{L^2}^2 + \|\Delta u\|_{L^2}^2\right).$$

In addition,

$$\|\frac{\partial}{\partial x}\nabla_y u\|_{L^2}^2 = \sum_{n,m=1}^{\infty}\frac{n^2\pi^2}{X^2}|c_{n,m}|^2\|\nabla_y \Psi_m\|^2$$

$$= \sum_{n,m=1}^{\infty}\frac{n^2\pi^2}{X^2}|c_{n,m}|^2\mu_m$$

$$\leq \frac{1}{2}\sum_{n,m=1}^{\infty}|c_{n,m}|^2\left(\left(\frac{n^2\pi^2}{X^2}\right)^2 + \mu_m^2\right) \leq \frac{1}{2}\|\Delta u\|_{L^2}^2.$$

It remains only to deal with the terms involving cross-derivatives of second order between different $y-$variables. These will be controlled if and only if the cross-sectional eigenfunctions $\Psi_m(y)$ satisfy bounds of the form:

$$\|\Psi_m\|^2_{H^2(\mathcal{C})} \leq c\left(\|\Psi_m\|^2_{L^2(\mathcal{C})} + \|\Delta\Psi_m\|^2_{L^2(\mathcal{C})}\right).$$

This is true when $\mathcal{C}$ is a compact manifold without boundary, with a lower bound on its Ricci curvature; also when $\mathcal{C}$ is a domain with $\mathcal{C}^2-$boundary in a Riemannian manifold with a lower bound on its Ricci curvature; see [39, 95] and the references therein. □

5.3 Error bound of Dirichlet-to-Neumann maps

The following lemma provides an exponential decay result based on a modification of the Agmon-type result of Janas et al [62]. In particular, [62] establishes that all eigenfunctions of a bounded self-adjoint Jacobi matrix whose eigenvalues lie in a spectral gap are exponentially decaying. In this section we assume that Q is a bounded real-valued potential.

Lemma 5.10. *If v solves the boundary value problem in Figure 5.6:*
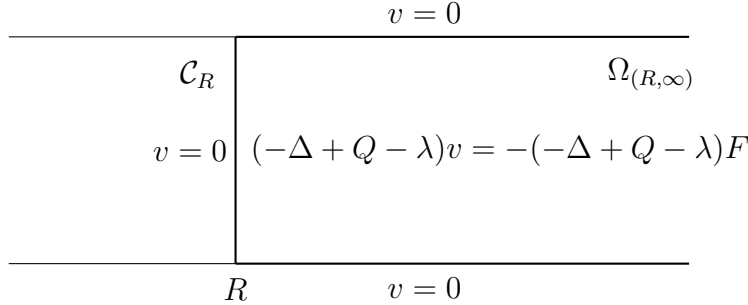
Figure 5.6: Schrödinger equation with a compactly supported function F on a waveguide.

where F is constructed as in Lemma 5.2 (in particular, $\operatorname{supp}(F) \subseteq \Omega_{(R,R+1)}$), and if $\operatorname{dist}(\lambda, Spec((-\Delta_D + Q)|_{\Omega_{(R,\infty)}})) > 0$, then v admits a representation $v(x,\cdot) = e^{-\alpha x}\tilde{v}(x,\cdot)$, where $\tilde{v} \in H^2_{loc}(\Omega_{(R,\infty)}) \cap H^1_0(\Omega_{(R,\infty)})$ and satisfies:

$$\|\tilde{v}\|_{H^2(\Omega_{(R,\infty)})} \leq C(\alpha, \lambda, R, \|Q\|_{L^\infty(\Omega)})\|f\|_{L^2(\mathcal{C}_R)},$$

and $\alpha < c\operatorname{dist}(\lambda, Spec((-\Delta_D + Q)|_{\Omega_{(R,\infty)}}))$, for some fixed $0 < c < 1$.

Proof. A formal calculation gives, for suitable $\tilde{v}$,

$$
e^{\alpha x}(-\Delta + Q - \lambda)e^{-\alpha x}\tilde{v} = e^{\alpha x}\left(-\alpha^2 e^{-\alpha x}\tilde{v} + 2\alpha e^{-\alpha x}\frac{\partial \tilde{v}}{\partial x} + e^{-\alpha x}(-\Delta + Q - \lambda)\tilde{v}\right)
$$
$$
= (-\Delta + Q - \lambda - \alpha^2)\tilde{v} + 2\alpha\frac{\partial \tilde{v}}{\partial x}
$$
$$
= (T - \lambda - \alpha^2 + 2\alpha S)\tilde{v},
$$

provided $\tilde{v} \in D(T) \subset D(S)$, where $T := -\Delta + Q$ and $S := \frac{\partial}{\partial x}$.
We start by solving the problem:

$$
e^{\alpha x}(-\Delta + Q - \lambda)e^{-\alpha x}\tilde{v} = e^{\alpha x}G_\lambda \quad \text{in } \Omega_{(R,\infty)}, \tag{97}
$$
$$
\tilde{v} = 0 \quad \text{on } \partial\Omega_{(R,\infty)}; \tag{98}
$$

where $-(-\Delta + Q - \lambda)F = G_\lambda$. Recall that F is constructed as in Lemma 5.2; we deduce that $e^{\alpha x}F$ is a compactly supported function with support contained in $\Omega_{(R,R+1)}$. Moreover, $e^{\alpha x}F|_{\Sigma_R} = 0$, $\Delta(e^{\alpha x}F) \in L^2(\Omega_{(R,\infty)})$, and $e^{\alpha x}F \in L^2(\Omega_{(R,\infty)})$ with a bound

$$
\|e^{\alpha x}G_\lambda\|_{L^2(\Omega_{(R,\infty)})} \leq e^{\alpha(R+1)}\|G_\lambda\|_{L^2(\Omega_{(R,\infty)})}. \tag{99}
$$

Solving (97)-(98) is equivalent to solving the operator equation

$$
(T - \lambda - \alpha^2 + 2\alpha S)\tilde{v} = e^{\alpha x}G_\lambda. \tag{100}
$$

Thus our problem is uniquely solvable provided

$$
\text{dist}(\lambda, Spec(T - \alpha^2)) = \min(|\lambda + \alpha^2 - r|, |s - \lambda - \alpha^2|) > 0,
$$

and

$$
2\alpha\|S(T - \lambda - \alpha^2)^{-1}\|_{L^2(\Omega_{(R,\infty)}) \to H^1(\Omega_{(R,\infty)})} < 1. \tag{101}
$$

Suppose that $(T - \lambda - \alpha^2)\omega = h$. Then since T is a self-adjoint operator and $(T - \lambda - \alpha^2)$ is invertible,

$$
\|\omega\|_{L^2(\Omega_{(R,\infty)})} \leq \|h\|_{L^2(\Omega_{(R,\infty)})}/\min(|\lambda + \alpha^2 - r|, |s - \lambda - \alpha^2|). \tag{102}
$$

Moreover,

$$
\int_{\Omega_{(R,\infty)}} (|\nabla\omega|^2 + (Q - \lambda - \alpha^2)|\omega|^2) = \int_{\Omega_{(R,\infty)}} h\overline{\omega},
$$

whence

$$\int_{\Omega_{(R,\infty)}} |\frac{\partial \omega}{\partial x}|^2 \leq \int_{\Omega_{(R,\infty)}} |\nabla \omega|^2$$

$$\leq \int_{\Omega_{(R,\infty)}} |(Q - \lambda - \alpha^2)||\omega|^2 + \epsilon \|\omega\|^2_{L^2(\Omega_{(R,\infty)})} + \frac{1}{4\epsilon} \|h\|^2_{L^2(\Omega_{(R,\infty)})}$$

$$\leq \left(|\lambda + \alpha^2| + \|Q\|_{L^\infty(\Omega)} + \epsilon \right) \|\omega\|^2_{L^2(\Omega_{(R,\infty)})} + \frac{1}{4\epsilon} \|h\|^2_{L^2(\Omega_{(R,\infty)})}$$

$$\leq \left[\frac{|\lambda + \alpha^2| + \|Q\|_{L^\infty(\Omega)} + \epsilon}{\min^2(|\lambda + \alpha^2 - r|, |s - \lambda - \alpha^2|)} + \frac{1}{4\epsilon} \right] \|h\|^2_{L^2(\Omega_{(R,\infty)})},$$

in which the last inequality follows by (102). However by definition of S and ω we know that $\int_{\Omega_{(R,\infty)}} |\frac{\partial \omega}{\partial x}|^2 = \|S(T - \lambda - \alpha^2)^{-1}h\|^2$, thus the condition (101) holds whenever α is small enough to ensure that

$$2\alpha \left[\frac{|\lambda + \alpha^2| + \|Q\|_{L^\infty(\Omega)} + \epsilon}{\min^2(|\lambda + \alpha^2 - r|, |s - \lambda - \alpha^2|)} + \frac{1}{4\epsilon} \right]^{1/2} < 1. \tag{103}$$

With all these calculations done, the solution $\tilde{v}$ of (100) exists and is unique. In addition, since

$$\int_{\Omega_{(R,\infty)}} |\nabla \tilde{v}|^2 + \int_{\Omega_{(R,\infty)}} (Q - \lambda - \alpha^2)|\tilde{v}|^2 + 2\alpha \int_{\Omega_{(R,\infty)}} \frac{\partial \tilde{v}}{\partial x}\overline{\tilde{v}} = \int_{\Omega_{(R,\infty)}} e^{\alpha x} G_\lambda \overline{\tilde{v}} \quad (104)$$

then taking the imaginary parts of (104) and using Young's inequality for $0 < \delta < |\Im(\lambda)|$ yields

$$\|\tilde{v}\|^2_{L^2(\Omega_{(R,\infty)})} \leq \frac{1}{|\Im(\lambda)| - \delta} \left[\frac{1}{4\delta} \|e^{\alpha x} G_\lambda\|^2_{L^2(\Omega_{(R,\infty)})} + \left(\delta + \frac{|\alpha|}{2\delta} \right) \|\tilde{v}\|^2_{H^1(\Omega_{(R,\infty)})} \right]. \quad (105)$$

Moreover, (104) can be written as:

$$\int_{\Omega_{(R,\infty)}} |\nabla \tilde{v}|^2 + \int_{\Omega_{(R,\infty)}} |\tilde{v}|^2 = \int_{\Omega_{(R,\infty)}} e^{\alpha x} G_\lambda \overline{\tilde{v}} + \int_{\Omega_{(R,\infty)}} (\lambda - Q + \alpha^2 + 1)|\tilde{v}|^2$$

$$+ 2\alpha \int_{\Omega_{(R,\infty)}} \tilde{v} \overline{\frac{\partial \tilde{v}}{\partial x}}. \tag{106}$$

Since $\|Q\|_{L^\infty(\Omega_{(R,\infty)})} < +\infty$ then $\|\lambda - Q + \alpha^2 + 1\|_{L^\infty(\Omega_{(R,\infty)})} \leq c$ for some $c > 0$. Hence

taking the real parts of (106) with $\Re(\lambda - Q + \alpha^2 + 1) \leq c$ we obtain:

$$\int_{\Omega_{(R,\infty)}} |\nabla \tilde{v}|^2 + \int_{\Omega_{(R,\infty)}} |\tilde{v}|^2 \leq \frac{1}{2}\|e^{\alpha x}G_\lambda\|^2_{L^2(\Omega_{(R,\infty)})} + (\frac{1}{2} + c + |\alpha|)\|\tilde{v}\|^2_{L^2(\Omega_{(R,\infty)})}$$
$$+ \frac{1}{2}\|\tilde{v}\|^2_{H^1(\Omega_{(R,\infty)})}.$$

Together with (105), and since $\tilde{v} = 0$ on $\partial\Omega_{(R,\infty)}$, we deduce that $\tilde{v}$ lies in $H^1_0(\Omega_{(R,\infty)})$ and has a bound:

$$\|\tilde{v}\|^2_{H^1_0(\Omega_{(R,\infty)})} \leq \tilde{C}\|G_\lambda\|^2_{L^2(\Omega_{(R,\infty)})} \tag{107}$$

in which $\tilde{C}$ depends on λ, α, R, and $\|Q\|_{L^\infty(\Omega_{(R,\infty)})}$. Furthermore, from (100) we have

$$-\Delta\tilde{v} = (\lambda - Q + \alpha^2)\tilde{v} - 2\alpha\frac{\partial\tilde{v}}{\partial x} + e^{\alpha x}G_\lambda.$$

Again from the boundedness of Q on Ω we have $\|\lambda - Q + \alpha^2\|_{L^\infty(\Omega_{(R,\infty)})} \leq c$ for some $c > 0$, and from (99)

$$\|\Delta\tilde{v}\|_{L^2(\Omega_{(R,\infty)})} \leq c\|\tilde{v}\|_{L^2(\Omega_{(R,\infty)})} + 2\alpha\|\frac{\partial\tilde{v}}{\partial x}\|_{L^2(\Omega_{(R,\infty)})} + \|e^{\alpha x}G_\lambda\|_{L^2(\Omega_{(R,\infty)})}$$
$$\leq c\|\tilde{v}\|_{L^2(\Omega_{(R,\infty)})} + 2\alpha\|\tilde{v}\|_{H^1_0(\Omega_{(R,\infty)})} + e^{\alpha(R+1)}\|G_\lambda\|_{L^2(\Omega_{(R,\infty)})}.$$

Thus, from (107)

$$\|\Delta\tilde{v}\|_{L^2(\Omega_{(R,\infty)})} \leq C\|G_\lambda\|_{L^2(\Omega_{(R,\infty)})}, \tag{108}$$

in which the constant C depends on λ, α, R, and $\|Q\|_{L^\infty(\Omega_{(R,\infty)})}$. We have shown that

$$\|\tilde{v}\|_{L^2(\Omega_{(R,\infty)})} \leq C\|G_\lambda\|_{L^2(\Omega_{(R,\infty)})},$$

but

$$\|G_\lambda\|_{L^2(\Omega_{(R,\infty)})} \leq C\|f\|_{L^2(\mathcal{C}_R)},$$

thus

$$\|\tilde{v}\|_{L^2(\Omega_{(R,\infty)})} \leq C\|f\|_{L^2(\mathcal{C}_R)},$$

in which the constant C depends on λ, α, R, and $\|Q\|_{L^\infty(\Omega_{(R,\infty)})}$. However, $v = e^{-\alpha x}\tilde{v}$ is the solution of the original problem in Figure 5.6 and using (107) we obtain a bound:

$$\|v\|_{L^2(\Omega_{(R,\infty)})} \leq C\|G_\lambda\|_{L^2(\Omega_{(R,\infty)})},$$

in which C depends on λ, α, R, and $\|Q\|_{L^\infty(\Omega_{(R,\infty)})}$. Furthermore, Since

$$\Delta v = \Delta(e^{-\alpha x}\tilde{v}) = \alpha^2 e^{-\alpha x}\tilde{v} - 2\alpha e^{-\alpha x}\nabla\tilde{v} + e^{-\alpha x}\Delta\tilde{v}$$

then

$$\|\Delta v\|_{L^2(\Omega_{(R,\infty)})} \leq \alpha^2 e^{-\alpha R}\|\tilde{v}\|_{L^2(\Omega_{(R,\infty)})} + 2\alpha e^{-\alpha R}\|\nabla\tilde{v}\|_{L^2(\Omega_{(R,\infty)})}$$
$$+ e^{-\alpha R}\|\Delta\tilde{v}\|_{L^2(\Omega_{(R,\infty)})}.$$

Inserting the estimates (107) and (108) in this inequality gives

$$\|\Delta v\|_{L^2(\Omega_{(R,\infty)})} \leq C\|G_\lambda\|_{L^2(\Omega_{(R,\infty)})} \leq C\|f\|_{L^2(\mathcal{C}_R)},$$

again with C depending on λ, α, R, and $\|Q\|_{L^\infty(\Omega_{(R,\infty)})}$. From Lemma 5.9 we conclude that $v \in H^2(\Omega_{(R,\infty)})$. $\qquad\square$

Remark 5.11. The condition that appears in the proof, namely

$$\min(|\lambda + \alpha^2 - r|, |s - \lambda - \alpha^2|) = \text{dist}(\lambda + \alpha^2, Spec(T)),$$
$$\geq \text{dist}(\lambda, Spec(T)) - \alpha^2,$$
$$\geq (1 - c)^2\text{dist}(\lambda, Spec(T)).$$

holds when $\alpha^2 < c \text{ dist}(\lambda, Spec(T))$ for some $0 < c < 1$. However, Eq. (103) is satisfied if

$$2\alpha\left[\frac{|\lambda + \alpha^2| + \|Q\|_{L^\infty(\Omega)} + \epsilon}{(1 - c)^4\text{dist}^2(\lambda, Spec(T))} + \frac{1}{4\epsilon}\right]^{1/2} < 1. \qquad (109)$$

This needs $\alpha = \mathcal{O}\big(\text{dist}(\lambda, Spec(T))\big)$ when λ is close to $Spec(T)$, which is more strict than $\alpha^2 < c \text{ dist}(\lambda, Spec(T))$.

In the remainder of this section, we aim to prove that $M_{right,X}(\cdot)$ converges to $M_{right}(\cdot)$ at a certain rate. In order to avoid cumbersome notation we prove the result when Q is a bounded and real-valued potential on the whole domain $\Omega = \Omega_{(0,\infty)}$. This is equivalent to proving the result on $\Omega_{(R,\infty)}$ since $S(x, \cdot) = 0$ for $x \geq R$. By applying Lemma 5.10 to Dirichlet-to-Neumann maps for the non-dissipative barrier problems with $\lambda \in \mathbb{C}$ with $\Im(\lambda) > 0$ we obtain the following sharp result.

Theorem 5.12. *Let* $\lambda \in \mathbb{C} \setminus \mathbb{R}$ *and suppose* $\Re(\lambda) \in (r, s)$, *where* (r, s) *is a spectral gap of the Dirichlet operator* $-\Delta + Q$; $Q \in L^\infty(\Omega)$. *Consider the boundary value problem in Figure 5.7:*
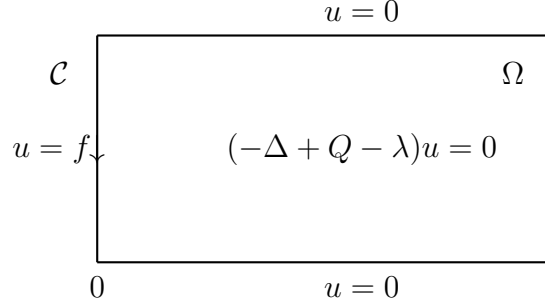
Figure 5.7: Schrödinger equation with nonzero Dirichlet condition on $\mathcal{C}$ of a waveguide.

Then there exist constants c and α_λ, as in Lemma (5.10), such that for all $f \in L^2(\mathcal{C})$ and all sufficiently large X

$$\|M_{right,X}(\lambda)f - M_{right}(\lambda)f\|_{H^{1/2}(\mathcal{C})} \leq c\|f\|_{L^2(\mathcal{C})}\exp(-\alpha_\lambda X).$$

Proof. Fix f. By Lemma 5.2, there exists a function F with $\mathrm{supp}(F) \subset \Omega_{(0,1)}$ such that $F|_{\mathcal{C}} = f, F|_\Sigma = 0, F \in L^2(\Omega), \Delta F \in L^2(\Omega)$, and

$$\|F\|_{L^2(\Omega)} \leq C\|f\|_{L^2(\mathcal{C})}. \tag{110}$$

Define $u := F + v$ and $u_X := F + v_X$ in which v and v_X are the solutions of the boundary value problems in Figures 5.8 and 5.9 respectively.
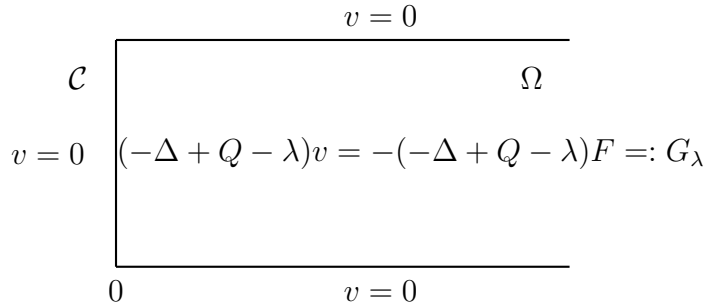
Figure 5.8: The solution v of the given BVP on Ω.

Figure 5.9: The solution v_X of the given BVP on $\Omega_{(0,X)}$.

Then
$$M_{right}(\lambda)f - M_{right,X}(\lambda)f = \left.\frac{\partial u}{\partial \nu}\right|_{\mathcal{C}} - \left.\frac{\partial u_X}{\partial \nu}\right|_{\mathcal{C}} = \left.\frac{\partial(v - v_X)}{\partial \nu}\right|_{\mathcal{C}},$$
and so we proceed to estimate $v - v_X$. Recall from Lemma 5.2 that
$$\|G_\lambda\|_{L^2(\Omega)} \leq C\|f\|_{L^2(\mathcal{C})}.$$

Moreover, G_λ inherits a compactly support from F. We note that since $Q \in L^\infty(\Omega)$, from Lemma 5.10 the solution v has the form $v = e^{-\alpha_\lambda x}\tilde{v}$, where $\tilde{v} \in H^2_{loc}(\Omega) \cap H^1_0(\Omega)$ and α_λ satisfies $\alpha_\lambda < \text{dist}(\lambda, Spec(-\Delta_D + Q)|_\Omega)$. We wish to obtain an estimate for $v - v_X$ in $H^2(\Omega_{(0,X)})$ which is, from Lemma 5.9, equivalent to obtaining an estimate of $\|v - v_X\|_{L^2(\Omega_{(0,X)})} + \|\Delta(v - v_X)\|_{L^2(\Omega_{(0,X)})}$. To do so, let χ_X be a smooth cut-off function with

$$\text{supp}(\chi_X) \subseteq \Omega_{(0,X)}, \quad \text{supp}(\nabla\chi_X) \subseteq \Omega_{(X-1,X)}, \quad \|\nabla\chi_X\|_{L^\infty(\Omega)} \leq 2, \tag{111}$$

and define $w_X := \chi_X v - v_X$ which satisfies the BVP in Figure 5.10:

Figure 5.10: The new problem with $w_X = \chi_X v - v_X$.

Since $(-\Delta + Q - \lambda)(v - v_X) = 0$, the function g_X satisfies

$$g_X := (-\Delta + Q - \lambda)w_X = (-\Delta + Q - \lambda)(\chi_X v - v_X)$$
$$= (-\Delta + Q - \lambda)(\chi_X v - v + v - v_X)$$
$$= (-\Delta + Q - \lambda)(\chi_X - 1)v.$$

Our first task is to estimate $\|g_X\|_{L^2(\Omega_{(0,X)})}$. By elementary differentiation,

$$g_X = -(\partial_x^2 \chi_X)v - 2(\partial_x \chi_X)(\partial_x v) + (\chi_X - 1)(-\Delta v + (Q - \lambda)v). \qquad (112)$$

Note that by (111), the representation of $v = e^{-\alpha_\lambda x}\tilde{v}$ and Lemma 5.10,

$$\|(\partial_x^2 \chi_X)v\|_{L^2(\Omega_{(0,X)})}^2 = \int_{\Omega_{(0,X)}} (\partial_x^2 \chi_X)^2 v^2$$

$$\leq \|(\partial_x^2 \chi_X)\|_{L^\infty(\Omega_{(X-1,X)})}^2 \int_{\mathcal{C}} \int_{X-1}^X \exp(-2\alpha_\lambda x)\tilde{v}^2 \mathrm{d}x\mathrm{d}y,$$

$$\leq \|(\partial_x^2 \chi_X)\|_{L^\infty(\Omega_{(X-1,X)})}^2 \|\tilde{v}\|_{L^2(\Omega_{(0,X)})}^2 \exp(-2\alpha_\lambda X),$$

$$\leq c_1 \|f\|_{L^2(\mathcal{C})} \exp(-2\alpha_\lambda X), \qquad (113)$$

where c_1 is a constant depending on α_λ. Similarly, and since $\tilde{v}$ is in $H_{loc}^2(\Omega) \cap H_0^1(\Omega)$, then $\partial_x \tilde{v}$ is in $L^2(\Omega_{(0,X)})$, so we have:

$$\|(\partial_x \chi_X)(\partial_x v)\|_{L^2(\Omega_{(0,X)})}^2 = \int_{\Omega_{(0,X)}} (\partial_x \chi_X)^2 (\partial_x v)^2,$$

$$\leq \|(\partial_x \chi_X)\|_{L^\infty(\Omega_{(X-1,X)})}^2 \big[[\|\tilde{v}\|_{L^2(\Omega_{(0,X)})}^2 \exp(-2\alpha_\lambda X)]$$

$$+ [\|\partial_x \tilde{v}\|_{L^2(\Omega_{(0,X)})}^2 \exp(-2\alpha_\lambda X)] \big],$$

$$\leq c_2 \|f\|_{L^2(\mathcal{C})} \exp(-2\alpha_\lambda X), \qquad (114)$$

where c_2 is a constant depending on α_λ. To handle the last term of (112), observe that by (111) we know that

$$\|(\chi_X - 1)(-\Delta + Q - \lambda)v\|_{L^2(\Omega_{(0,X)})}^2 = \int_{\Omega_{(0,X)}} (\chi_X - 1)^2 \big[(-\Delta + Q - \lambda)v\big]^2$$

$$\leq \|(\chi_X - 1)\|_{L^\infty(\Omega_{(0,X)})}^2 \int_{\mathcal{C}} \int_{X-1}^X \big[(-\Delta + Q - \lambda)v\big]^2 \mathrm{d}x\mathrm{d}y$$

$$\leq \|(\chi_X - 1)\|_{L^\infty(\Omega_{(0,X)})}^2 \int_{\mathcal{C}} \int_{X-1}^X \exp(-2\alpha_\lambda x)\big[(-\Delta + Q - \lambda)\tilde{v} + 2\alpha_\lambda \partial_x \tilde{v} - \alpha_\lambda^2 \tilde{v}\big]^2 \mathrm{d}x\mathrm{d}y.$$

$$(115)$$

Since we have, from Lemma 5.10, a bound $\|\tilde{v}\|_{H^2(\Omega)} \leq C\|f\|_{L^2(\mathcal{C})}$, and since $\mathrm{supp}(F) \subseteq \Omega_{(0,X)}$ for all sufficiently large X, we may combine (113), (114), and (115) in (112) to obtain the estimate:

$$\|g_X\|_{L^2(\Omega_{(0,X)})} \leq C\|f\|_{L^2(\mathcal{C})} \exp(-\alpha_\lambda X), \tag{116}$$

where C is a constant independent of f.

Having estimated g_X we may now consider the BVP in Figure 5.10. Taking inner products in the usual way gives

$$\int_{\Omega_{(0,X)}} (|\nabla w_X|^2 + (Q - \lambda)|w_X|^2) = \int_{\Omega_{(0,X)}} g_X \overline{w_X}. \tag{117}$$

Taking imaginary parts of (117) and using the fact that Q is real-valued, we obtain

$$\int_{\Omega_{(0,X)}} |\Im(\lambda)||w_X|^2 = \left|\Im\left(\int_{\Omega_{(0,X)}} g_X \overline{w_X}\right)\right| \leq \left|\int_{\Omega_{(0,X)}} g_X \overline{w_X}\right|.$$

Using Young's inequality with $0 < \delta < |\Im(\lambda)|$,

$$|\Im(\lambda)|\|w_X\|^2_{L^2(\Omega_{(0,X)})} \leq \frac{1}{4\delta}\|g_X\|^2_{L^2(\Omega_{(0,X)})} + \delta\|w_X\|^2_{L^2(\Omega_{(0,X)})},$$

we obtain a bound for w_X in $L^2(\Omega_{(0,X)})$:

$$\|w_X\|^2_{L^2(\Omega_{(0,X)})} \leq \frac{1}{4\delta[|\Im(\lambda)| - \delta]}\|g_X\|^2_{L^2(\Omega_{(0,X)})}; \tag{118}$$

upon using (116) we have the bound

$$\|w_X\|_{L^2(\Omega_{(0,X)})} \leq C\|f\|_{L^2(\mathcal{C})} \exp(-\alpha_\lambda X), \tag{119}$$

where C is a constant independent of f. Moreover, from the BVP in Figure 5.10,

$$-\Delta w_X = g_X + (\lambda - Q)w_X.$$

Since $Q \in L^\infty(\Omega)$, and using (116), (119),

$$\|\Delta w_X\|_{L^2(\Omega_{(0,X)})} \leq \|g_X\|_{L^2(\Omega_{(0,X)})} + \|\lambda - Q\|_{L^\infty(\Omega_{(0,X)})}\|w_X\|_{L^2(\Omega_{(0,X)})},$$
$$\leq C\|f\|_{L^2(\mathcal{C})} \exp(-\alpha_\lambda X). \tag{120}$$

Recalling that $w_X = \chi_X v - v_X = v - v_X$, from (119), (120) and Lemma 5.9 we conclude that

$$\|v - v_X\|_{H^2(\Omega_{(0,X)})} \leq c\|f\|_{L^2(\mathcal{C})} \exp(-\alpha_\lambda X);$$

here c is a constant depending on α_λ. A fortiori, therefore, $v - v_X$ admits the bound $\|v - v_X\|_{H^2(\Omega_{(0,1)})} \leq c\|f\|_{L^2(\mathcal{C})} \exp(-\alpha_\lambda X)$, and since the normal derivative is a bounded map from $H^2(\Omega_{(0,1)})$ to $H^{1/2}(\mathcal{C})$, then

$$\|\frac{\partial v}{\partial \nu} - \frac{\partial v_X}{\partial \nu}\|_{H^{1/2}(\mathcal{C})} \leq \|v - v_X\|_{H^2(\Omega)} \leq c\|f\|_{L^2(\mathcal{C})} \exp(-\alpha_\lambda X);$$

but

$$M_{right,X}(\lambda)f - M_{right}(\lambda)f = \frac{\partial}{\partial \nu}(u - u_X)|_{\mathcal{C}} = \frac{\partial}{\partial \nu}(v - v_X)|_{\mathcal{C}}.$$

Thus

$$\|M_{right,X}(\lambda)f - M_{right}(\lambda)f\|_{H^{1/2}(\mathcal{C})} \leq c\|f\|_{L^2(\mathcal{C})} \exp(-\alpha_\lambda X).$$

$\square$

The following theorem is a straightforward consequence of Theorem 5.12.

Theorem 5.13.

$$\|M_{right,X}(\lambda) - M_{right}(\lambda)\|_{L^2(\mathcal{C}) \to H^{1/2}(\mathcal{C})} \leq C \exp(-\alpha_\lambda X),$$

as $X \to \infty$, where C is a constant depending only on α_λ.

Proof. By Lemma 5.2 and Theorem 5.12, we have

$$\|M_{right,X}(\lambda)f - M_{right}(\lambda)f\|_{H^{1/2}(\mathcal{C})} \leq C\|f\|_{L^2(\mathcal{C})} \exp(-\alpha_\lambda X),$$

where C is a constant depending on α_λ and independent of f; the result follows upon taking sup over all $\|f\|_{L^2(\mathcal{C})} = 1$. $\square$

5.4 Application to spectral problems

In order to state and prove our main result, we introduce some notations and technical lemmas.

Lemma 5.14. *If*

$$\|M_{right,X}(\cdot) - M_{right}(\cdot)\|_{L^2(\mathcal{C}) \to H^{1/2}(\mathcal{C})} \to 0 \text{ as } X \to \infty, \tag{121}$$

uniformly in a neighbourhood of $\lambda \in \mathbb{C}$ with $\Im(\lambda) > 0$, then there exists $X_0 > 0$ such that, in this neighbourhood, $M_{left}(\cdot) + M_{right}(\cdot)$ is invertible if and only if $M_{left}(\cdot) + M_{right,X}(\cdot)$ is invertible for all $X \geq X_0$.

Proof. Let $M_{left}(\cdot) + M_{right}(\cdot)$ be invertible in a neighbourhood of λ. We have the identity

$$M_{left}(\cdot) + M_{right,X}(\cdot) = \big(M_{left}(\cdot) + M_{right}(\cdot)\big)$$
$$\times \big[I + \big(M_{left}(\cdot) + M_{right}(\cdot)\big)^{-1}\big(M_{right,X}(\cdot) - M_{right}(\cdot)\big)\big].$$

The result follows immediately using this and the assumption (121), which implies that

$$\big\|\big(M_{left}(\cdot) + M_{right}(\cdot)\big)^{-1}\big(M_{right,X}(\cdot) - M_{right}(\cdot)\big)\big\| < 1,$$

for sufficiently large X. The converse follows by swapping M_{right} and $M_{right,X}$ to obtain the identity

$$M_{left}(\cdot) + M_{right}(\cdot) = \big(M_{left}(\cdot) + M_{right,X}(\cdot)\big)$$
$$\times \big[I + \big(M_{left}(\cdot) + M_{right,X}(\cdot)\big)^{-1}\big(M_{right}(\cdot) - M_{right,X}(\cdot)\big)\big].$$

$$\square$$

Theorem 5.15. *Suppose $\lambda \in Spec(L_0 + i\gamma S)$, $\Im(\lambda) > 0$. Then for sufficiently large $X \geq R$ there exists $\lambda_X \in Spec(L_X + i\gamma S)$ such that $\lambda_X \to \lambda$ as $X \to \infty$.*

Proof. Assume for a contradiction that for some sequence of values of X tending to ∞, there exists a neighbourhood of λ containing no eigenvalues of $L_X + i\gamma S$. Then there exists $r > 0$ such that for the chosen sequence of X tending to ∞, $L_X + i\gamma S$ has no eigenvalues in the closed disc with centre λ and radius r. Let Γ be any simple contour contained in this disc, surrounding λ, see Figure 5.11.
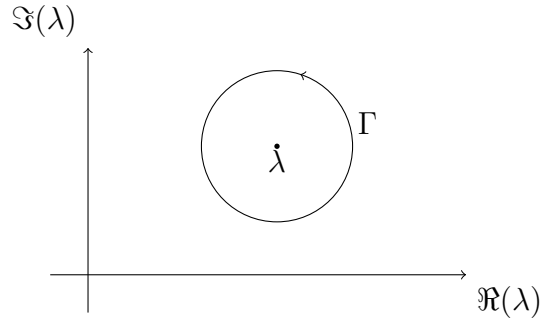
Figure 5.11: A contour Γ surrounding the eigenvalue λ.

This means that $M_{left}(\cdot) + M_{right,X}(\cdot)$ is invertible in a neighbourhood of Γ. From the Cauchy's Theorem (for more information about Cauchy's Theorem for operator-valued analytic functions see e.g., [109, Chapter 5]):

$$\frac{1}{2\pi\imath} \oint_\Gamma \left(M_{left}(\mu) + M_{right,X}(\mu)\right)^{-1}\mathrm{d}\mu = 0.$$

However from Theorem 5.13 and Lemma 5.14, this means that

$$\frac{1}{2\pi\imath} \oint_\Gamma \left(M_{left}(\mu) + M_{right}(\mu)\right)^{-1}\mathrm{d}\mu = 0.$$

Thus $M_{left}(\cdot) + M_{right}(\cdot)$ is analytic inside the contour Γ, and since Γ can be any sufficiently small contour surrounding λ, the map $\mu \mapsto (M_{left}(\mu) + M_{right}(\mu))^{-1}$ is analytic at $\mu = \lambda$. In particular, ker$\left\{ M_{left}(\lambda) + M_{right}(\lambda)\right\} = \{0\}$, so λ is not in $Spec(L_0 + i\gamma S)$ by Lemma 5.5. $\qquad\square$

Theorem 5.16. *Suppose* $\lambda_X \in Spec(L_X + i\gamma S)$; $\lambda_X \to \lambda$, *with* $\Im(\lambda) > 0$. *Then* $\lambda \in Spec(L_0 + i\gamma S)$.

Proof. Assume for a contradiction that $\lambda \notin Spec(L_0 + i\gamma S)$. Hence λ is in the resolvent set of $L_0 + i\gamma S$ and since the resolvent set is an open set, then there exists a neighbourhood of λ that is not in the spectrum of $L_0 + i\gamma S$. It follows that $M_{left}(\cdot) + M_{right}(\cdot)$ is invertible in a neighbourhood of λ by Lemma 5.14. Following Theorem 5.13, we can deduce that the operators $M_{left}(\cdot) + M_{right,X}(\cdot)$ converge locally uniformly to $M_{left}(\cdot) + M_{right}(\cdot)$ in a neighbourhood of λ. Moreover, from Lemma 5.14, the operator $M_{left}(\cdot) + M_{right,X}(\cdot)$ is invertible in a neighbourhood of λ for all sufficiently large X. It follows that from Lemma 5.5 ker$\left\{ M_{left}(\cdot) + M_{right,X}(\cdot)\right\} = \{0\}$ in a neighbourhood of λ. Hence, there is no eigenvalues of $L_X + i\gamma S$ in a neighbourhood of λ. This contradicts the assumption that $\lambda_X \in Spec(L_X + i\gamma S)$ converges to λ. $\quad\square$

Lemma 5.17. *Suppose that* λ *and* $\lambda^\dagger$ *are such that* $M_{left}(\lambda)$ *and* $M_{left}(\lambda^\dagger)$ *are well defined. Then* $M_{left}(\lambda) - M_{left}(\lambda^\dagger)$ *maps* $L^2(\mathcal{C}_R)$ *into* $H^{1/2}(\mathcal{C}_R)$. *Similarly, if* $M_{right}(\lambda)$ *and* $M_{right}(\lambda^\dagger)$ *are well defined then* $M_{right}(\lambda) - M_{right}(\lambda^\dagger)$ *maps* $L^2(\mathcal{C}_R)$ *into* $H^{1/2}(\mathcal{C}_R)$.

Proof. We present the proof for M_{right}; the proof for M_{left} is similar. Using (91) in the proof of Lemma 5.3, the Hilbert resolvent identity yields

$$\frac{M_{right}(\lambda) - M_{right}(\lambda^\dagger)}{\lambda - \lambda^\dagger} = \Gamma_{right}(-\Delta_D + Q - \lambda)^{-1}$$
$$\times \left[I + (-\Delta_D + Q - \lambda^\dagger)^{-1}(\lambda^\dagger - Q)\right] S_{right}.$$

Starting from $L^2(\mathcal{C}_R)$, the operator S_{right} maps into $L^2(\Omega_{(R,\infty)})$. In turn, the resolvent set of $(-\Delta_D + Q - \lambda^\dagger)^{-1}$ maps $L^2(\Omega_{(R,\infty)})$ into $H^1_0(\Omega_{(R,\infty)}) \cap H^2(\Omega_{(R,\infty)})$. Applying the normal derivative operator Γ_{right} loses $3/2$ orders of smoothness (1 order for differentiation and $1/2$ order for the trace), see [111, Theorem 8.1], taking the final image into $H^{1/2}(\mathcal{C}_R)$. $\qquad\square$

Lemma 5.18. *If $M_{left}(\lambda) + M_{right}(\lambda)$ and $M_{left}(\lambda) + M_{right,X}(\lambda)$ have trivial kernel, then they are boundedly invertible with inverses which map $H^{-1}(\mathcal{C}_R)$ to $L^2(\mathcal{C}_R)$.*

Proof. For the case when $Q \equiv 0$ and $S \equiv 0$, an explicit calculation using separation of variables, following the method in the proof of Lemma 5.1, shows that

$$(M_{right}(\lambda, 0) + M_{left}(\lambda, 0))f = \sum_{n=1}^{\infty} \langle f, \psi_n \rangle \psi_n(y) \sqrt{\mu_n - \lambda}(1 + \coth(R\sqrt{\mu_n - \lambda})),$$

with inverse given by

$$(M_{right}(\lambda, 0) + M_{left}(\lambda, 0))^{-1}g = \sum_{n=1}^{\infty} \frac{\langle g, \psi_n \rangle \psi_n(y)}{\sqrt{\mu_n - \lambda}(1 + \coth(R\sqrt{\mu_n - \lambda}))};$$

this inverse maps $H^{-1}(\mathcal{C}_R)$ to $L^2(\mathcal{C}_R)$. By a calculation analogous to the proof of Lemma 5.17, the maps for non-trivial Q and S are related to the zero-coefficient maps by formulae of the form

$$M_{right}(\lambda) = M_{right}(\lambda, 0) + N_Q(\lambda), \quad M_{left}(\lambda) = M_{left}(\lambda, 0) + \tilde{N}_{Q,S}(\lambda),$$

in which $N_Q(\lambda)$ and $\tilde{N}_{Q,S}(\lambda)$ are some perturbations from $L^2(\mathcal{C}_R) \to H^{1/2}(\mathcal{C}_R)$ and are therefore compact. The result for $M_{left}(\lambda) + M_{right}(\lambda)$ now follows by the Analytic Fredholm Theorem, see [58, Section 5.9]. For $M_{left}(\lambda) + M_{right,X}(\lambda)$ the proof is essentially the same, starting from the formula

$$(M_{right,X}(\lambda, 0) + M_{left}(\lambda, 0))f =$$

$$\sum_{n=1}^{\infty} \langle f, \psi_n \rangle \psi_n(y) \sqrt{\mu_n - \lambda} \left(\coth\left((X - R)\sqrt{\mu_n - \lambda}\right) + \coth\left(R\sqrt{\mu_n - \lambda}\right) \right).$$

$\qquad\square$

Fix $\lambda^\dagger$ such that $M_{left}(\lambda^\dagger) + M_{right}(\lambda^\dagger)$ has trivial kernel. For λ in a neighbourhood of $\lambda^\dagger$, define an operator $K(\lambda)$ by:

$$
\begin{aligned}
K(\lambda) =& \left(M_{left}(\lambda^\dagger) + M_{right}(\lambda^\dagger)\right)^{-1} \\
& \times \left(M_{left}(\lambda) - M_{left}(\lambda^\dagger) + M_{right}(\lambda) - M_{right}(\lambda^\dagger)\right),
\end{aligned}
\tag{122}
$$

so that

$$
\left(M_{left}(\lambda^\dagger) + M_{right}(\lambda^\dagger)\right)^{-1}\left(M_{left}(\lambda) + M_{right}(\lambda)\right) = I + K(\lambda).
\tag{123}
$$

Similarly, if

$$
\begin{aligned}
K_X(\lambda) =& \left(M_{left}(\lambda^\dagger) + M_{right,X}(\lambda^\dagger)\right)^{-1} \\
& \times \left(M_{left}(\lambda) - M_{left}(\lambda^\dagger) + M_{right,X}(\lambda) - M_{right,X}(\lambda^\dagger)\right)
\end{aligned}
\tag{124}
$$

then

$$
\begin{aligned}
K(\lambda) - K_X(\lambda) =& (I - (I + Q^{-1}(\lambda^\dagger)E_X(\lambda^\dagger))^{-1})Q^{-1}(\lambda^\dagger)R(\lambda) \\
& - (I + Q^{-1}(\lambda^\dagger)E_X(\lambda^\dagger))^{-1}Q^{-1}(\lambda^\dagger)\tilde{E}_X(\lambda),
\end{aligned}
\tag{125}
$$

in which

$$
\begin{aligned}
& Q(\lambda^\dagger) := M_{left}(\lambda^\dagger) + M_{right}(\lambda^\dagger), Q_X(\lambda^\dagger) := M_{left}(\lambda^\dagger) + M_{right,X}(\lambda^\dagger), \\
& R(\lambda) := M_{left}(\lambda) - M_{left}(\lambda^\dagger) + M_{right}(\lambda) - M_{right}(\lambda^\dagger), \\
& R_X(\lambda) := M_{left}(\lambda) - M_{left}(\lambda^\dagger) + M_{right,X}(\lambda) - M_{right,X}(\lambda^\dagger), \\
& E_X(\lambda^\dagger) := M_{right,X}(\lambda^\dagger) - M_{right}(\lambda^\dagger), \text{and} \\
& \tilde{E}_X(\lambda) := M_{right,X}(\lambda) - M_{right}(\lambda) - M_{right,X}(\lambda^\dagger) + M_{right}(\lambda^\dagger).
\end{aligned}
$$

We observe the following results.

Lemma 5.19. *Let $\lambda^\dagger \in \mathbb{C}\backslash\mathbb{R}$ and $\lambda^\dagger \notin Spec(L_0 + i\gamma S)$. Then for λ in a neighbourhood of $\lambda^\dagger$ we have $\lambda \in Spec(L_0 + i\gamma S)$ if and only if $I + K(\lambda)$ has a nontrivial kernel.*

Proof. Assume that $\lambda \in Spec(L_0 + i\gamma S)$ then from Lemma 5.5 $\ker\{\,M_{left}(\lambda) + M_{right}(\lambda)\,\} \neq \{0\}$. Following the formula of $I + K(\lambda)$ in (123) we derive the desired result; the converse reasoning is analogous. $\qquad\square$

Definition 5.20. For $1 \leq p < \infty$, the Schatten p-class, $\mathfrak{S}_p$, is the class of all compact operators A in a Hilbert space such that

$$\|A\|_p = \big(\sum_{n=1}^{\infty} s_n^p(A) \big)^{1/p} < \infty,$$

where $s_n(A)$ are the singular numbers of A.

$\mathfrak{S}_1$ is called the trace class and $\mathfrak{S}_2$ is the Hilbert-Schmidt class. See e.g., Gohberg et al. [59] for basic properties of Schatten classes.

Lemma 5.21. *If $p > 2\mathrm{dim}(\mathcal{C}_R)$ then $K(\lambda)$ and $K_X(\lambda)$ lie in the Schatten p-class $\mathfrak{S}_p$.*

Proof. We obtain, from (122), (124) and Lemmas 5.17 and 5.18, the following diagrams, in which J_1 and J_2 are imbeddings:

$$K(\lambda) : L^2(\mathcal{C}_R) \xrightarrow{R(\lambda)} H^{1/2}(\mathcal{C}_R) \xhookrightarrow{J_1} L^2(\mathcal{C}_R) \xhookrightarrow{J_2} H^{-1}(\mathcal{C}_R) \xrightarrow{(Q(\lambda^\dagger))^{-1}} L^2(\mathcal{C}_R),$$

$$K_X(\lambda) : L^2(\mathcal{C}_R) \xrightarrow{R_X(\lambda)} H^{1/2}(\mathcal{C}_R) \xhookrightarrow{J_1} L^2(\mathcal{C}_R) \xhookrightarrow{J_2} H^{-1}(\mathcal{C}_R) \xrightarrow{(Q_X(\lambda^\dagger))^{-1}} L^2(\mathcal{C}_R).$$

In fact, since the cross-section $\mathcal{C}_R$ is bounded then the Sobolev imbedding J_1 belongs to Schatten class $\mathfrak{S}_p$ for $p > 2\mathrm{dim}(\mathcal{C}_R)$ (see [86]). Using the standard inequality for Schatten class which states that if A is bounded and $B \in \mathfrak{S}_p$ then AB is in $\mathfrak{S}_p$ and $\|AB\|_p \leq \|A\|\|B\|_p$,

$$\begin{aligned}
\|K(\lambda)\|_p &= \|Q^{-1}(\lambda^\dagger)R(\lambda)\|_p = \|Q^{-1}(\lambda^\dagger)J_2 J_1 R(\lambda)\|_p \\
&\leq \|Q^{-1}(\lambda^\dagger)J_2\|_{L^2(\mathcal{C}_R) \to L^2(\mathcal{C}_R)} \|J_1 R(\lambda)\|_p \\
&\leq C\|Q^{-1}(\lambda^\dagger)J_2\|_{L^2(\mathcal{C}_R) \to L^2(\mathcal{C}_R)} \|R(\lambda)\|_{L^2(\mathcal{C}_R) \to H^{1/2}(\mathcal{C}_R)},
\end{aligned}$$

the last inequality holding for $p > 2\mathrm{dim}(\mathcal{C}_R)$; similar reasoning applies to $K_X(\lambda)$. $\qquad \square$

Lemma 5.22. *Both $\lambda \mapsto K(\lambda)$ and $\lambda \mapsto K_X(\lambda)$ are analytic in $\mathfrak{S}_p$-norm.*

Proof. We have seen that

$$K(\lambda) = Q(\lambda^\dagger)^{-1} J_2 J_1 R(\lambda),$$

where J_1 is $\mathfrak{S}_p$-class, independently of λ, and $R(\lambda)$ is analytic in the natural norm for maps from $L^2(\mathcal{C}_R)$ to $H^{1/2}(\mathcal{C}_R)$. Using the first-principles definition of derivative for an operator-valued analytic function one then proves that

$$K'(\lambda) = Q(\lambda^\dagger)^{-1} J_2 J_1 R'(\lambda),$$

in which $R'(\lambda)$ is an analytic operator-valued map from $L^2(\mathcal{C}_R)$ to $H^{1/2}(\mathcal{C}_R)$. From this the result follows; the proof for $K_X(\lambda)$ is similar.

$\square$

In the following, we shall use the concept of perturbation determinant $\det_p$, see [103, Chapter 12]. A brief summary is included in The Appendix 5.6 at the end of this chapter.

Lemma 5.23. *Let $\lambda^\dagger \in \mathbb{C} \backslash \mathbb{R}$ and $\lambda^\dagger \notin Spec(L_0 + i\gamma S)$. Then for λ in a neighbourhood of $\lambda^\dagger$ we have $\lambda \in Spec(L_0 + i\gamma S)$ if and only if $\det_p(I + K(\lambda)) = 0$.*

Proof. If $\lambda \in Spec(L_0 + i\gamma S)$ then from Lemma 5.19 $I + K(\lambda)$ has nontrivial kernel. It follows that $I + K(\lambda)$ is not invertible and since $K(\lambda) \in \mathfrak{S}_p$ then $\det_p(I + K(\lambda)) = 0$. The converse reasoning is similar. $\square$

Proposition 5.24. *If $p > 2\dim(\mathcal{C}_R)$ then*

$$\|K(\lambda) - K_X(\lambda)\|_p \leq c \exp(-\alpha_\lambda(X - R)); \tag{126}$$

c is a constant depending on α_λ which is chosen as in Lemma 5.10. Moreover,

$$|\det_p(I + K(\lambda)) - \det_p(I + K_X(\lambda))| \leq C \exp(-\alpha_\lambda(X - R)); \tag{127}$$

where C depends on α_λ.

Proof. First, we aim to find an estimate of $K(\lambda) - K_X(\lambda)$ in $\mathfrak{S}_p$ norm. Following (125), we start by considering $Q^{-1}(\lambda^\dagger)E_X(\lambda^\dagger)$:

$$Q^{-1}(\lambda^\dagger)E_X(\lambda^\dagger) : L^2(\mathcal{C}_R) \xrightarrow{E_X(\lambda^\dagger)} H^{1/2}(\mathcal{C}_R) \xhookrightarrow{J_1} L^2(\mathcal{C}_R) \xhookrightarrow{J_2} H^{-1}(\mathcal{C}_R) \xrightarrow{Q^{-1}(\lambda^\dagger)} L^2(\mathcal{C}_R).$$

Here we apply the chain of inequalities

$$\|Q^{-1}(\lambda^\dagger)E_X(\lambda^\dagger)\|_p = \|Q^{-1}(\lambda^\dagger)J_2 J_1 E_X(\lambda^\dagger)\|_p$$
$$\leq \|Q^{-1}(\lambda^\dagger)J_2\|_{L^2(\mathcal{C}_R)\to L^2(\mathcal{C}_R)}\|J_1 E_X(\lambda^\dagger)\|_p$$
$$\leq C\|Q^{-1}(\lambda^\dagger)J_2\|_{L^2(\mathcal{C}_R)\to L^2(\mathcal{C}_R)}\|E_X(\lambda^\dagger)\|_{L^2(\mathcal{C}_R)\to H^{1/2}(\mathcal{C}_R)}$$

provided p is such that the imbedding J_1 is Schatten class, i.e, $p > 2\dim(\mathcal{C}_R)$. Hence

$$\|Q^{-1}(\lambda^\dagger)E_X(\lambda^\dagger)\|_p \leq C_1\|E_X(\lambda^\dagger)\|_{L^2(\mathcal{C}_R)\to H^{1/2}(\mathcal{C}_R)}, \tag{128}$$

where C_1 is independent of X. Inserting this estimate into the first term of (125) and using $\|AB\|_p \leq \|A\|_p\|B\|$, for $A \in \mathfrak{S}_p$ and a bounded B, we have:

$$\|I - (I + Q^{-1}(\lambda^\dagger)E_X(\lambda^\dagger))^{-1}Q^{-1}(\lambda^\dagger)R(\lambda)\|_p$$
$$= \|(Q^{-1}(\lambda^\dagger)E_X(\lambda^\dagger))\sum_{n=0}^{\infty}(Q^{-1}(\lambda^\dagger)E_X(\lambda^\dagger))^n Q^{-1}(\lambda^\dagger)R(\lambda)\|_p$$
$$\leq \|Q^{-1}(\lambda^\dagger)E_X(\lambda^\dagger)\|_p\|\sum_{n=1}^{\infty}(Q^{-1}(\lambda^\dagger)E_X(\lambda^\dagger))^n\|\|Q^{-1}(\lambda^\dagger)R(\lambda)\|_{L^2(\mathcal{C}_R)\to L^2(\mathcal{C}_R)}$$

provided $p > 2\dim(\mathcal{C}_R)$. Hence, using (128):

$$\|I - (I + Q^{-1}(\lambda^\dagger)E_X(\lambda^\dagger))^{-1}Q^{-1}(\lambda^\dagger)R(\lambda)\|_p$$
$$\leq \|Q^{-1}(\lambda^\dagger)E_X(\lambda^\dagger)\|_p\frac{1}{1 - \|Q^{-1}(\lambda^\dagger)E_X(\lambda^\dagger)\|}\|Q^{-1}(\lambda^\dagger)R(\lambda)\|_{L^2(\mathcal{C}_R)\to L^2(\mathcal{C}_R)}$$
$$\leq C\|E_X(\lambda^\dagger)\|_{L^2(\mathcal{C}_R)\to H^{1/2}(\mathcal{C}_R)}; \tag{129}$$

where C is a constant independent of X. For the second term of the right hand side of (125) the same ideas can be applied to the term $Q^{-1}(\lambda^\dagger)\tilde{E}_X(\lambda)$ to obtain the $\mathfrak{S}_p$-norm:

$$\|Q^{-1}(\lambda^\dagger)\tilde{E}_X(\lambda)\|_p \leq C_2\|\tilde{E}_X(\lambda)\|_{L^2(\mathcal{C}_R)\to H^{1/2}(\mathcal{C}_R)};$$

again C_2 is independent of X. Therefore, the estimate of the second term of (125) becomes

$$\|(I + Q^{-1}(\lambda^\dagger)\tilde{E}_X(\lambda))^{-1}Q^{-1}(\lambda^\dagger)\tilde{E}_X(\lambda)\|_p \leq \tilde{C}\|\tilde{E}_X(\lambda)\|_p. \tag{130}$$

Inserting the Inequalities (129) and (130) in (125) we derive the following estimate:

$$\|K(\lambda) - K_X(\lambda)\|_p \leq C\|E_X(\lambda)\|_{L^2(\mathcal{C}_R)\to H^{1/2}(\mathcal{C}_R)} + \tilde{C}\|\tilde{E}_X(\lambda)\|_{L^2(\mathcal{C}_R)\to H^{1/2}(\mathcal{C}_R)}.$$

Employing Theorem 5.13 on $E_X(\lambda^\dagger)$ and $\tilde{E}_X(\lambda)$ on the corresponding domain $\Omega_{(R,\infty)}$ leads to the desired estimate (126), locally uniformly with respect to λ, where c is a constant depending on α_λ.

Now in order to obtain (127), we use Theorem 5.31 in the Appendix 5.6 to obtain

$$| \det_p(I + K(\lambda)) - \det_p(I + K_X(\lambda))| \leq C\|K(\lambda) - K_X(\lambda)\|_p, \qquad (131)$$

where C is a constant independent of X. Hence (127) is obtained by inserting (126) into (131). $\qquad\square$

We can now put the previous lemmas together to derive the following key result.

Theorem 5.25. *Suppose that Assumptions (A1) and (A2) hold. For $\gamma > 0$, let λ_γ be an eigenvalue of the non-self-adjoint Schrödinger operator $L_0 + i\gamma S$ defined in (86)-(87). Then there exists an approximation $\lambda_{\gamma,X}$ to λ_γ, given by an eigenvalue of the operator $L_X + i\gamma S$ defined in (93)-(94) which satisfies*

$$|\lambda_\gamma - \lambda_{\gamma,X}| \leq C_1 \exp(-C_2(X - R)), \qquad (132)$$

where C_1 and C_2 are positive constants which depend on λ_γ.

Proof. First, since $\gamma > 0$ we observe that λ_γ has strictly positive imaginary part, since

$$\Im(\lambda_\gamma) = \gamma \int_\Omega S|u_\gamma|^2,$$

where u_γ is the corresponding normalised eigenfunction. Hence, both $M_{right}(\cdot)$ and $M_{right,X}(\cdot)$ are well-defined in a neighbourhood of λ_γ. Moreover, if $M_{left}(\cdot)$ is well-defined in a neighbourhood of λ_γ, then from Lemma 5.5:

$$\ker \{M_{left}(\lambda_\gamma) + M_{right}(\lambda_\gamma)\} \neq \{0\}.$$

Consequently, the existence of the approximating eigenvalues $\lambda_{\gamma,X}$ follows immediately from Theorem 5.15. Next, in order to obtain the estimate (132), observe that is an isolated eigenvalue of some finite algebraic multiplicity $\nu \in \mathbb{N}$, in any neighbourhood of λ_γ we may choose $\lambda^\dagger \neq \lambda_\gamma$ such that both formulae (122) and (123) make sense. Furthermore, the corresponding truncated problem generates $K_X(\lambda)$ which is given by (124). Moreover, from Lemma 5.21 $K(\lambda)$ and $K_X(\lambda)$ lie in Schatten class $\mathfrak{S}_p$ with $p > 2\dim(\mathcal{C}_R)$. We then follow Proposition 5.24 and obtain the estimate

$$| \det_p(I + K(\lambda)) - \det_p(I + K_X(\lambda))| \leq C \exp(-\alpha_{\lambda_\gamma}(X - R));$$

89

locally uniformly with respect to λ in a neighbourhood of λ_γ, where C is a constant depending on α_{λ_γ}. Since $K(\lambda)$ and $K_X(\lambda)$ are analytic with respect to λ, it follows that from Lemma 5.32 in the Appendix 5.6 both $\det_p(I + K(\lambda))$ and $\det_p(I + K_X(\lambda))$ are analytic with respect to λ. Following a zero-counting argument for analytic functions (see, e.g., [84, Lemma 3]), there exist points $\lambda_{\gamma,X}$ which are zeros of $\det_p(I + K_X(\cdot))$ and which satisfy

$$|\lambda_\gamma - \lambda_{\gamma,X}| \leq c \exp\left(-\alpha_{\lambda_\gamma}(X - R)/\nu\right),$$

where ν is the order of the zero of $\det_p(I + K(\cdot))$ at λ_γ. This proves the result.

$\square$

5.5 Numerical Examples

In this section we present several examples of elliptic PDEs on waveguides and study approximations of isolated eigenvalues. Computations are performed using finite element method by PDETOOL of MATLAB.

Example 5.26. We consider the following PDE problem:

$$-\Delta u + \cos(x)u - 25\exp(-x)u = \lambda u, \tag{133}$$

in a waveguide $[0, \infty) \times [0, 2\pi]$, with Dirichlet boundary conditions. We chose this example because a straightforward separation of variables allows one to generate high-accuracy results to compare with the later numerics, by separating the PDE into a family of ODEs

$$-u_n'' + \left(\cos(x) + \frac{n^2}{4} - 25\exp(-x)\right)u_n = \lambda u_n; \quad n = 1, 2, \cdots, \quad \text{on} \quad [0, \infty). \tag{134}$$

The spectral bands of the Mathieu equation are reported to high accuracy in [25]. Shifting these bands by $n^2/4$ for $n = 1, 2, \ldots$, we obtain the spectral bands of (133). Table 5.1 shows the first two spectral bands of (133). The first spectral band I_1 is obtained from the first band of the Mathieu equation which is given by $[-0.378490, -0.34767]$ after shifting this band by $1/4$. The second spectral band I_2 is obtained from the first spectral band of the Mathieu equation when it is shifted by 1. The third spectral band of (133) I_3 would come from shifting the second spectral band of the Mathieu equation, which is given by $[0.595942, 0.912391]$, by $1/4$.

In order to obtain approximations of eigenvalues in the gaps of (133), we first introduce a dissipative barrier to obtain

$$-\Delta u + \cos(x)u - 25\exp(-x)u + iS(x)u = \lambda u, \tag{135}$$

m	I_m
1	[-0.12849,-0.09767]
2	[0.62151,0.65233]
3	[0.84594,1.16239]

Table 5.1: Spectral bands for (133)

where $S(x) = \frac{1}{2}(1-\tanh(x-20))$. Since $S(x)$ decays at infinity the essential spectrum of the modified problem is the same as the original problem. After that, we truncate the waveguide to $[0, X] \times [0, 2\pi]; X > 0$ and solve the problem using the PDETOOL solver with an initial mesh. Since the standard mesh produces very fine elements everywhere on the waveguide and we are mainly interested in eigenfunctions which live on the left hand side of it, we adapt the mesh using the map $x \mapsto \mathcal{M}(x)$, in which

$$\mathcal{M}(x) := \min(x, X^*) \exp(\min(x, X^*)/3) + \max(x - X^*, 0)(1 + X^*/3) \exp(X^*/3), \tag{136}$$

see Figure 5.12.
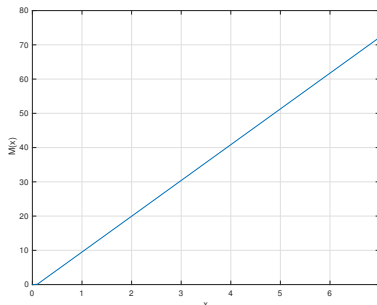
Figure 5.12: Plot of $\mathcal{M}$ on $[0, 7]$.

The parameter $X^* > 0$ is chosen heuristically to give a compromise between good resolution of eigenfunctions concentrated in the left-most part of the waveguide, and sufficient resolution of the periodic structure in the right-most part of the waveguide. In the computations in Table 5.2 we started with a standard three-times-refined MATLAB PDETOOL mesh on $[0, 7] \times [0, 2\pi]$ and mapped it to a mesh on $[0, X] \times [0, 2\pi]$, with $X = \mathcal{M}(7)$, and $X^* = 14/3$.

Table 5.2 shows approximate eigenvalues for the self-adjoint problem (133) and non-self-adjoint problem (135). As we can see, the self adjoint problem generates

91

Self-adjoint	Non-self-adjoint
-0.084962803557113	-0.084961545990299 + 0.999988974782084i
0.065250381213409	
0.075056449171371	
0.075920453707749	
0.082342277041306	
0.094868041295541	
0.395135728508211	0.395135728509314 + 0.999999999980165i

Table 5.2: True and spurious eigenvalues with range of real part between $[-0.08, 0.6]$ for the PDE, note that the spurious eigenvalues disappeared in the non-self-adjoint case.

refinement	eigenvalues		
3	0.39513573		
4	0.37196251	0.36423810	
5	0.36613459	0.36419195	0.36418887

Table 5.3: Richardson extrapolation of order 2, 4, and 6 to a true eigenvalue in a gap with different refinements.

spectral pollution. Spurious eigenvalues did not simply disappear in the non-self-adjoint case, but were discounted because their imaginary parts lay below a chosen threshold (0.9.)

Richardson extrapolation [30] can be used to enhance the accuracy further. Applying this technique to one of the isolated eigenvalues in Table 5.2, with three further mesh refinements, yields the results in Table 5.3. The most accurate of these is probably correct when rounded to four decimal places.

Example 5.27. We consider the following PDE problem:

$$-\Delta u + \left(\cos(x) - 25 \exp(-x)(1 - \epsilon(\pi - y)^2) + \frac{i}{2}(1 - \tanh(x - 5)) \right) u = \lambda u, \quad (137)$$

in a waveguide $[0, \infty) \times [0, 2\pi]$, with Dirichlet boundary conditions. Clearly, Example 5.26 is a special case of this problem when $\epsilon = 0$, and since the perturbation term decays fast as x tends to infinity, the essential spectrum of this problem still the same as in Example 5.26. Moreover, if $\epsilon > \frac{1}{\pi^2}$ then $(1 - \epsilon(\pi - y)^2)$ becomes negative in some layers near the boundaries of the waveguide. As a result, we expect that eigenvalues in the gaps merge into the essential spectrum as ϵ becomes large enough, i.e., larger
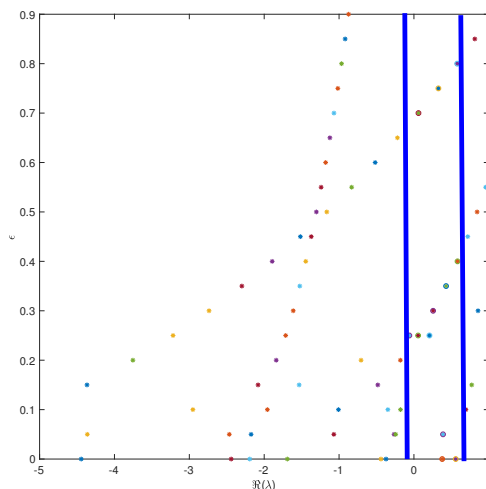
Figure 5.13: Eigenvalues of the PDE (137) with $|\Im(\lambda) - 1| < 0.01$ for different values of ϵ between 0 and 0.9. Isolated eigenvalues of the problem with real part in $[-0.08, 0.59]$, are marked as asterisks surrounded by circles. The blue shaded lines indicate the spectral bands, which are ϵ-independent.

than $\frac{1}{\pi^2}$. Indeed, Figure 5.13 shows the behaviour of the eigenvalues with imaginary parts close to 1 with different values of ϵ. It can be seen that an eigenvalue close to 0 when $\epsilon = 0.25$ starts merging into the spectral band $[0.6, 0.7]$ as ϵ increases to 0.4. Another point is that the effect of the perturbation term is to move eigenvalues from left to right with increasing ϵ, which is clearly observable in this figure. The computation was performed using the same domain, mesh and MATLAB settings as Example 5.26 with four refinements.

Example 5.28. Consider the PDE

$$-\Delta u + \left(\cos(x + \epsilon y) - 25 \exp(-x) + \frac{i}{2}(1 - \tanh(x - 5)) \right) u = \lambda u, \qquad (138)$$

in a waveguide $[0, \infty) \times [0, 2\pi]$, with Dirichlet boundary conditions. This problem was chosen because it does not admit separation of variables; nor is it clear whether the essential spectrum is independent of ϵ or not.

Figure 5.14 appears to show spectral bands which move to the right as ϵ increases from 0 to 1, but these results should be treated with scepticism as we have not proved any approximation results for points of the essential spectrum. The eigenvalues
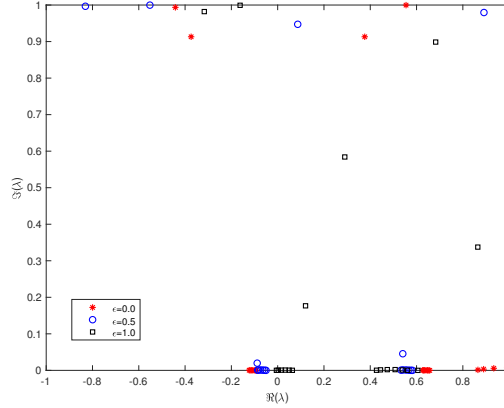
Figure 5.14: True and spurious eigenvalues of the PDE (138) on $[-1, 1]$ for different values of ϵ. True and genuine eigenvalues are with imaginary parts close to 1.

with imaginary part very close to 1 are likely to give good approximations to the eigenvalues of the underlying self adjoint problem; all other eigenvalues should be treated with scepticism, possibly being artefacts of the dissipative barrier or of the domain truncation. Moreover, eigenvalues with imaginary parts not close to 1 but also not close to 0 always require further investigation, for instance by increasing the length of the dissipative barrier. This requires a corresponding increase in the length of the truncated domain, and can become very expensive.

Figure 5.15 zooms in on eigenvalues with imaginary parts close to 1, for values of ϵ between 0 and 1. Unlike in (137), the potential no longer has a real part which is increasing with ϵ, so the non-monotone behaviour of the eigenvalues in Figure 5.15 is not surprising. The computation here was obtained using the same settings as in Example 5.26 with five refinements.

Example 5.29. We consider the following PDE problem:

$$ -\Delta u - 25\exp(-x)u = \lambda(2 + \sin(x) - iS(x))u, \tag{139} $$

in a waveguide $[0, \infty) \times [0, \pi]$, with Dirichlet boundary conditions and $S(x) = \frac{1}{2}(1 - \tanh(x-5))$. Compared to the previous examples, the dissipative term now multiplies the spectral parameter, and the 'weight' $2 + \sin(x)$, though strictly positive, is no longer constant. This problem does not fall within the scope of the analysis which we presented in the earlier sections, though it is likely that elements of that analysis could be generalised to this case.

94
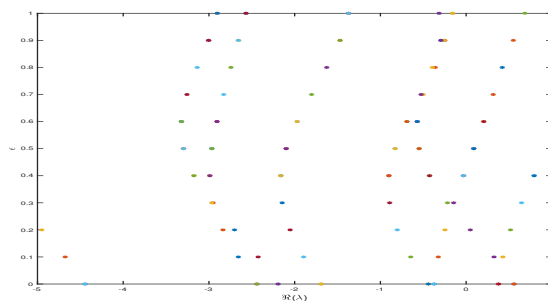
Figure 5.15: Eigenvalues of the PDE (138) on range between $[-5, 1]$ with $|\Im(\lambda) - 1| < 0.02$ for different values of ϵ.

By separation of variable the PDE can be reduced to a Schrödinger equation with an infinite matrix-valued potential, suggesting that in addition to a finite element approach one also perform numerics on the system

$$-\underline{u}'' + (D - 25\exp(-x)I)\underline{u} = \lambda((2 + \sin(x))I - iS(x)I)\underline{u},; \quad x \in (0, \infty), \quad (140)$$

$$\underline{u}(0) = \mathbf{0},$$

where $D(j, j) = j^2, j = 1, \cdots, n$. Figure 4.5 indicates the spectral bands of this ODE system with $n = 5$, as discussed in Example 4.17 in Section 4.6, and computed using the Numerov discretisation [92]. For comparison, Figure 5.16 shows approximating eigenvalues produced by a finite element approach with the same MATLAB settings of Example 5.26. While there are qualitative similarities, the quantitative agreement is poor.
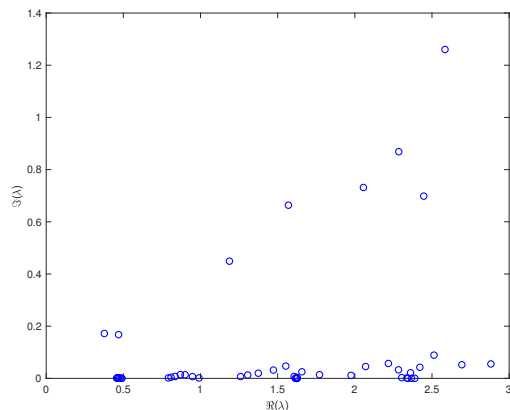
Figure 5.16: Eigenvalues of the PDE (139) with real part of λ in the interval $[0, 3]$, using five refinements.
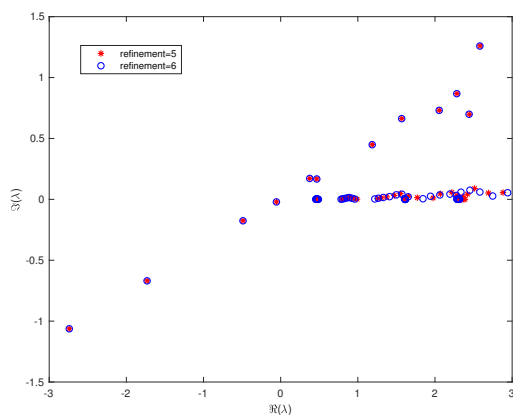
Figure 5.17: Eigenvalues of the PDE (139) with refinements 5 and 6 and real part of λ in the interval $[-3, 3]$.

In order to understand the difficulty of obtaining accurate results for (139), we performed two high-accuracy finite element calculations which are shown in Figure 5.17. The 'refinement' number is the number of times that MATLAB was asked to refine the mesh. We start to see good approximation of eigenvalues which are well removed from the essential spectrum, and there is some evidence of the spectral bands also being approximated. However since the essential spectrum for this pencil

problem is actually a subset of $\mathbb{R}$, see Remark 5.30 below, the error is clearly not very small.

Remark 5.30.   1. The essential spectrum of the PDE pencil (139) is a subset of $\mathbb{R}$. Since $A := -\Delta_D + Q$ is a self-adjoint operator, $B - B_0 := -iS(x)$ is compact relative to A, and $B_0 := w(x) = 2 + \sin(x)$ is strictly positive, then $Spec_{ess}(A, B) \subseteq W_{ess}(A, B) \subseteq W_{ess}(A, B_0) \subseteq Spec_{ess}(A, B_0) \subseteq \mathbb{R}$, see [21, Theorem 2.26] and Lemma 5.33 in the Appendix 5.6.

2. For each eigenvalue λ of the pencil (139):

    (a) The real and imaginary parts have the same sign;

    (b) $|\Re(\lambda)| \geq |\Im(\lambda)|$.

    These follow directly from standard numerical range estimates using integration by parts and the fact that $0 \leq S(x) \leq (2 + \sin(x))$.

3. From Lemma 5.33 in the Appendix 5.6 the essential numerical range of the pencil satisfies that $W_{ess}(A, B) \subseteq \mathbb{R}$.

5.6   APPENDIX

For the convenience of the reader we provide some basic facts about perturbation determinants. If A is a trace-class operator, i.e. $A \in \mathfrak{S}_1$, then the determinant of $I + A$ may be defined as an (infinite) product using the eigenvalues (α_j) of $I + A$:

$$\det(I + A) := \Pi_{j=1}^{\infty}(1 + \alpha_j),$$

which is convergent because $\sum_{j=1}^{\infty} |\alpha_j| < +\infty$.

In order to extend this definition to other Schatten classes, one uses a trick from the infinite product representation of analytic functions in complex analysis. Replacing $1 + \alpha_j$ in the formula above by $(1 + \alpha_j) \exp(-\alpha_j)$, one finds that the infinite product will be convergent under the less stringent hypothesis that $\sum_{j=1}^{\infty} |\alpha_j|^2 < +\infty$. This holds for $A \in \mathfrak{S}_2$, and so we may define, for $A \in \mathfrak{S}_2$,

$$\det_2(I + A) := \Pi_{j=1}^{\infty}(1 + \alpha_j) \exp(-\alpha_j).$$

In the case that $A \in \mathfrak{S}_1 \subset \mathfrak{S}_2$, then one has

$$\det_2(I + A) = \det(I + A) \exp(-\text{trace}(A)).$$

As in the case of infinite product representations of analytic functions, one may further adjust the factors in the infinite product to cope with the case in which one only has $\sum_{j=1}^{\infty} |\alpha_j|^p < +\infty$. Define

$$r_p(\alpha) := (1 + \alpha) \exp\left(\sum_{j=1}^{p-1} (-1)^j \frac{\alpha^j}{j}\right) - 1.$$

Then $A \in \mathfrak{S}_p$ implies that the sequence $(r_p(\alpha_j))$ is absolutely summable, and we may define

$$\det_p(I + A) := \Pi_{j=1}^{\infty}(1 + r_p(\alpha_j)), \quad A \in \mathfrak{S}_p. \tag{141}$$

In every case, $\det_p(I + A)$ is non-zero if and only if $I + A$ is invertible.

Theorem 5.31. *[59, Theorem 2.2] Let $A, B \in \mathfrak{S}_p(1 \leq p < \infty)$. Then there exists a constant C_p such that*

$$|\det_p(I + A)| \leq \exp(C_p \|A\|_p^p) \tag{142}$$

for any operator $A \in \mathfrak{S}_p$. Furthermore,

$$|\det_p(I + A) - \det_p(I + B)| \leq \|A - B\|_p \exp(C_p(\|A\|_p + \|B\|_p + 1)^p). \tag{143}$$

Lemma 5.32. *Suppose $F(\lambda)$ is an analytic operator-valued function in $\mathfrak{S}_p$. Then $\det_p(I + F(\lambda))$ depends analytically on λ.*

Proof. Since $F(\lambda)$ is an analytic operator-valued function in $\mathfrak{S}_p$, it has a Taylor expansion around each λ_0 which converges in the $\mathfrak{S}_p$-norm, see Definition 5.20:

$$F(\lambda) = \sum_{n=0}^{\infty} (\lambda - \lambda_0)^n G_n, \quad \sum_{n=0}^{\infty} |\lambda - \lambda_0|^n \|G_n\|_p < \infty \quad \text{for } |\lambda - \lambda_0| < \rho,$$

for some $\rho > 0$. $F(\lambda)$ can be approximated locally uniformly with respect to λ by finite rank operators, in $\mathfrak{S}_p$:

1. Given $\epsilon > 0$, choose N such that:

$$\left\|F(\lambda) - \sum_{n=0}^{N} (\lambda - \lambda_0)^n G_n\right\|_p < \epsilon \quad \text{for all } |\lambda - \lambda_0| \leq \frac{1}{2}\rho.$$

2. For each $n \in \{0, \cdots, N\}$ choose a finite rank operator $G_{n,\epsilon}$ such that:

$$\|G_n - G_{n,\epsilon}\|_p \leq \frac{\epsilon \cdot 2^{-n}}{\max(1, (\frac{1}{2}\rho)^n)}$$

and define a finite-rank analytic operator-valued function F_ϵ by

$$F_\epsilon = \sum_{n=0}^{N} (\lambda - \lambda_0)^n G_{n,\epsilon}, \quad |\lambda - \lambda_0| \leq \frac{1}{2}\rho.$$

Then

$$\|F(\lambda) - F_\epsilon(\lambda)\|_p < \epsilon + \sum_{n=0}^{\infty} \epsilon \cdot 2^{-n} = 3\epsilon, \quad \text{for all } |\lambda - \lambda_0| \leq \frac{1}{2}\rho.$$

Following Theorem 5.31, we have, for $|\lambda - \lambda_0| \leq \rho/2$,

$$|\det_p(I + F_\epsilon(\lambda)) - \det_p(I + F(\lambda))| \leq C\|F_\epsilon(\lambda) - F(\lambda)\|_p < 3C\epsilon,$$

where C is a positive constant. Since F_ϵ is finite rank, it is not difficult to show that $\det_p(I + F_\epsilon(\lambda))$, see (141), is analytic. As the locally uniform limit of an analytic function is analytic (Hurwitz), then $\det_p(I + F(\lambda))$ is analytic in λ. $\qquad\square$

Lemma 5.33. *Consider the PDE problem $-\Delta u + Qu = \lambda(w - iS)u$ on a semi-infinite waveguide Ω in which Q is bounded and $S(x, y) \to 0$ uniformly with respect to y as $x \to +\infty$. Define the operators A and B by $A := -\Delta_D + Q$ and $B := w - iS$. Then the essential numerical range $W_{ess}(A, B)$ is a subset of $\mathbb{R}$.*

Proof. If S were compactly supported then we would know that $S(A + i)^{-1}$ is compact. However since $S(x, y) \to 0$ uniformly with respect to y as $x \to +\infty$, it follows that $S(A + i)^{-1}$ can be approximated in operator norm to arbitrary accuracy by $\chi(A + i)^{-1}$, where χ is a compactly supported sup-norm approximation to S, and is therefore compact. Since A is semi-bounded, it follows from [21, Theorem 2.26] that $W_{ess}(A, B) = W_{ess}(A, B + iS) = W_{ess}(A, w)$. Since w is real-valued and A is selfadjoint, $W_{ess}(A, w) \subseteq \mathbb{R}$. $\qquad\square$

6 Numerical computation of eigenvalues in spectral gaps of Schrödinger operators

6.1 Introduction

We consider the calculation of eigenvalues in spectral gaps of singular Schrödinger operators of the form

$$- \underline{u}'' + Q\underline{u} = \lambda \underline{u}, \quad (0, \infty), \tag{144}$$

supplemented by a boundary condition:

$$A\underline{u}(0) - B\underline{u}'(0) = \underline{0}, \tag{145}$$

where, for some $n \in \mathbb{N}$, Q is an $n \times n$ Hermitian matrix-valued potential, while A and B are $n \times n$ matrices such that (A, B) has full rank n and $AB^* - BA^* = 0$. The symbol $\underline{u}$ denotes an $n-$vector-valued solution of the differential equation. Recall that one may associate with this problem an operator $\mathcal{L}$ with domain

$$D(\mathcal{L}) = \{\underline{u} \in L^2(0, \infty) \mid \underline{u} \text{ satisfies (145) and } -\underline{u}'' + Q\underline{u} \in L^2(0, \infty)\},$$

acting according to

$$\mathcal{L}\underline{u} = -\underline{u}'' + Q\underline{u}.$$

We shall further assume that Q can be decomposed as:

$$Q(x) = Q_p(x) + R(x), \tag{146}$$

where Q_p is a Hermitian periodic function with period $a > 0$,

$$Q_p(x + a) = Q_p(x), \quad \forall \quad x \geq 0, \tag{147}$$

and $R(x)$ is a compactly supported function with support in $[0, X]$ for some $X > 0$. Our problem is therefore a perturbation of a problem with a periodic background potential, and the operator $\mathcal{L}$ is selfadjoint with non-empty essential spectrum. In general the essential spectrum is a union of disjoint sub-intervals of $\mathbb{R}$, called *spectral bands*; the gaps between these intervals are termed *spectral gaps*, see 1.2 for more details.

Eigenvalues in spectral gaps of Schrödinger operators have attracted some attention due to their appearance in applications including solid state physics and photonic crystals [70]. Some approaches have been considered in the literature in order to obtain such approximations. For example, [84] employed a dissipative barrier

scheme together with domain truncation and obtained approximations for eigenvalues of the scalar Schrödinger operators. In Chapter 4, we considered this procedure to approximate eigenvalues in spectral gaps for matrix Schrödinger operators. This technique allows the BVP to be discretised to a standard λ-linear problem and solved by an appropriate method for matrix eigenproblems. However, its accuracy is limited by the rate of decay of the eigenfunctions; for eigenvalues close to spectral bands, the decay can be slow, and the associated domain truncations require large domains. This poses serious problems for adaptive meshing and/or computational cost. Similar drawbacks were reported using the supercell method, see [105] and [31]. This method performs computations on a large, bounded domain with periodic boundary conditions. The periodicity allows the use of Floquet theory and Fourier analysis to discretise the problem. Even when the non-periodic part of the operator (in our case, the function R appearing in (146) has a small support, the supercell generally needs to be much larger, particularly for eigenvalues close to spectral bands, whose eigenfunctions decay slowly. This increases the computational cost.

For photonic crystal waveguides, therefore, Joly et al. [63] and Fliss [54] considered an approach that is based on using Dirichlet-to-Neumann maps to compute accurate non-reflecting boundary conditions and shorten the computational domains. The D-to-N maps can be calculated at the cost of performing computations on a single periodicity cell, and the required non-reflecting boundary conditions are obtained by solving an appropriate operator quadratic equation. The approach is particularly well adapted to PDEs.

Our approach is similar in spirit; however the fact that we are dealing with a system of ODEs means that we are able to employ stabilised shooting methods over one period, combined with ODE Floquet theory, to determine very accurate non-reflecting boundary conditions. The overall algorithm depends not on rapid decay of eigenfunctions, but on rapid decay of the non-periodic part $R(\cdot)$ of the potential. By approximating $R(\cdot)$ with a compactly supported function $R_N(\cdot)$, with $\mathrm{supp}(R_N) \subseteq [0, Na]$ for some positive N, and identifying the boundary condition at $x = Na$ using Floquet theory, the problem turns into a finite-interval Schrödinger problem with λ-dependent boundary condition at the right endpoint $x = Na$.

For the scalar case this programme was carried out by Aceto et al. [2], but the fact that we are now dealing with a coupled system of differential equations introduces technical complications to almost every aspect. On the theoretical side, not only do we have to work with Cayley transforms and Atkinson Θ-matrices in order to avoid the usual effective-loss-of-rank problems associated with shooting for coupled systems [102], but we must also prove a monotonicity result (Proposition 6.2) which is completely new even for the scalar case, where it describes the λ-dependence of

the Prüfer θ-angles of the square-summable Floquet solutions in spectral gaps. This proposition is the key to establishing Theorem 6.12, which is a generalisation of one of the key results in [11] and [81]. Theorem 6.12 allows the characterisation of eigenvalues λ in a spectral gap in terms of eigenvalues of Atkinson Θ-matrices, whereas earlier results could only handle regular problems or eigenvalues below the essential spectrum.

On the numerical side, we have not used in this study either the piecewise constant coefficient approximation in [81] or its refinements in [74], nor indeed the BVM approach in [2]: instead we decided to use two approaches which are able to work directly with the differential equations satisfied by the (unitary) Atkinson Θ-matrices, specifically a 4th order Magnus integrator due to [34] and the projection integrator proposed in [44]. Both of these may seem odd choices: after all, coefficient approximation methods are good for dealing with highly oscillatory solutions, and solutions for λ above the infimum of the essential spectrum are oscillatory. However the Floquet theory automatically accounts for the oscillations and leaves us with a problem on a finite interval which typically has a very modest number of oscillations. The methods of [34] and [44] are also attractively easy to implement.

This chapter is organised as follows. Section 6.2 indicates the main results behind the theory of the proposed algorithm for matrix Schrödinger operators including the main theorem. Section 6.3 includes the numerical implementation of the proposed algorithm. Numerical examples, including ODE and PDE, are presented in Section 6.4. We conclude our study with some significant discussion in Section 6.5.

6.2   Theory of matrix Schrödinger operators

In this section, we highlight some concepts and main results from matrix differential equations which will be used throughout the rest of the chapter.

First of all, consider the unperturbed matrix Schrödinger equation:

$$- \underline{u}'' + Q_p \underline{u} = \lambda \underline{u}, \quad (0, \infty). \tag{148}$$

When λ lies outside the union of spectral bands, the solutions of this equation lying in $L^2(0, \infty)$ form a linear space of dimension precisely n. By following standard constructions as in Section 4.3, we may choose a basis of linearly independent Floquet solutions $\underline{u}_1(x, \lambda), \ldots, \underline{u}_n(x, \lambda)$ with

$$\underline{u}_j(x + a, \lambda) = \rho_j(\lambda) \underline{u}_j(x, \lambda), \quad j = 1, \ldots, n, \tag{149}$$

in which the $\rho_j(\lambda)$ are the Floquet multipliers and all satisfy $|\rho_j(\lambda)| < 1$ in spectral gaps. Introducing the $n \times n$ matrix $\Psi(x, \lambda)$ whose columns are $\underline{u}_1(x, \lambda), \ldots, \underline{u}_n(x, \lambda)$,

we can write (149) as

$$\Psi(x + a, \lambda) = \Psi(x, \lambda)\Lambda(\lambda) \tag{150}$$

in which $\Lambda(\lambda)$ is a Jordan matrix with diagonal entries $\rho_1(\lambda), \ldots, \rho_n(\lambda)$.

Definition 6.1. The *Atkinson Θ-matrix* associated with Ψ is the matrix

$$\Theta_F(x, \lambda) := (\Psi'(x, \lambda) + i\Psi(x, \lambda))(\Psi'(x, \lambda) - i\Psi(x, \lambda))^{-1}.$$

The following proposition collects some important properties of Θ_F.

Proposition 6.2. For λ in a fixed spectral gap, the following are true.

1. $\Theta_F(x, \lambda)$ is a well-defined unitary matrix.

2. $\Theta_F(x + a, \lambda) = \Theta_F(x, \lambda)$.

3. For each fixed x, the eigenvalues of $\Theta_F(x, \lambda)$ move strictly monotonically round the unit circle in $\mathbb{C}$, in a negative direction with increasing λ.

Remark 6.3. The third property stated above appears to be completely new even in the scalar case $n = 1$. In particular it is not available in standard texts such as [26] nor was it know to its authors. As we shall see, however, the essential ideas behind its proof have been available for more than fifty years.

Proof. (1) First we prove that Θ_F is well defined. The only way that this could fail would be if the matrix $\Psi'(x, \lambda) - i\Psi(x, \lambda)$ were rank deficient for some x and some λ. There would exist, for some x_0, $\mu \in \mathbb{R}$, a non-trivial vector $\underline{c} \in \ker(\Psi'(x_0, \mu) - i\Psi(x_0, \mu))$. The function $\underline{u}(\cdot) := \Psi(\cdot, \mu)\underline{c} \in L^2(x_0, \infty)$ would satisfy

$$-\underline{u}'' + Q_p\underline{u} = \mu\underline{u}, \quad x \in (x_0, \infty); \quad \underline{u}'(x_0) = i\underline{u}(x_0).$$

Left-multiplication by $\underline{u}^*(x, \mu)$ and integration by parts would then yield

$$i\|\underline{u}(x_0, \mu)\|^2 + \int_{x_0}^{\infty} \left\{ \|\underline{u}'(x, \mu)\|^2 + \underline{u}(x, \mu)^* Q_p(x)\underline{u}(x, \mu) \right\} dx = \mu\|\underline{u}(\cdot, \mu)\|_{L^2(x_0, \infty)}^2;$$

since μ is real and Q_p is Hermitian, taking imaginary parts would give a contradiction.

Now we prove that $\Theta_F(x, \lambda)$ is unitary. We assume first that 1 is not an eigenvalue of $\Theta_F(x, \lambda)$, which means that $\Psi(x, \lambda)$ is invertible. From Definition 6.1, proving that $\Theta_F(x, \lambda)$ is unitary is then the same as proving that $\Psi'(x, \lambda)\Psi(x, \lambda)^{-1}$ is Hermitian. For each fixed x, because $\Psi(\cdot, \lambda)$ captures the square summable solutions of the

matrix Schrödinger equation, of which there is precisely an n-dimensional space, $\Psi'(x, \lambda)\Psi(x, \lambda)^{-1}$ is the Dirichlet-to-Neumann map for the Schrödinger equation on $[x, \infty)$. Since this equation defines a self-adjoint operator when equipped with a homogeneous Dirichlet condition at x, it follows from abstract results on boundary triples [60] that its Dirichlet-to-Neumann map $\Psi'(x, \lambda)\Psi(x, \lambda)^{-1}$ is self-adjoint for real λ, and hence Hermitian. The case in which 1 is an eigenvalue of $\Theta_F(x, \lambda)$ can be dealt with similarly, by considering a Robin-to-Neumann map.

(2) By eqn. (150) it follows that $\Psi'(x + a, \lambda) = \Psi'(x, \lambda)\Lambda(\lambda)$ and hence

$$\Psi'(x + a, \lambda) \pm i\Psi(x + a, \lambda) = (\Psi'(x, \lambda) \pm i\Psi(x, \lambda))\Lambda(\lambda).$$

The result is then immediate from Definition 6.1.

(3) Fix a spectral gap, so that Ψ and Ψ' are analytic functions of λ in that gap. The partial derivatives of $\Psi(x, \lambda)$ and $\Psi'(x, \lambda)$ with respect to λ are then well defined. Differentiating the formula in Definition 6.1 with respect to λ one may show that, see [10, Theorem 10.2.3]

$$\frac{\partial \Theta_F}{\partial \lambda}(x, \lambda) = i\Theta_F(x, \lambda)\Omega_F(x, \lambda), \tag{151}$$

in which, using λ subscripts to denote partial differentiation with respect to λ,

$$\Omega_F(x, \lambda) = 2\left((\Psi' - i\Psi)^{-1}\right)^* \left\{(\Psi')^*\Psi_\lambda - \Psi^*\Psi'_\lambda\right\}(\Psi' - i\Psi)^{-1}(x, \lambda).$$

The result will then follow immediately from (151) if we can show that Ω_F is negative definite, see [10, Theorem V.6.1]. By direct differentiation, using also the fact that Ψ satisfies the Schrödinger equation, Q is a Hermitian function and $\lambda \in \mathbb{R}$, it follows that

$$
\begin{aligned}
\frac{d}{dx}\left\{(\Psi')^*\Psi_\lambda - \Psi^*\Psi'_\lambda\right\}(x, \lambda) &= \left\{(\Psi'')^*\Psi_\lambda - \Psi^*\Psi''_\lambda\right\}(x, \lambda) \\
&= \left\{((Q - \lambda I)\Psi)^*\Psi_\lambda - \Psi^*((Q - \lambda I)\Psi_\lambda - \Psi)\right\}(x, \lambda) \\
&= \left\{\Psi^*(Q - \lambda I)^*\Psi_\lambda - \Psi^*(Q - \lambda I)\Psi_\lambda + \Psi^*\Psi\right\}(x, \lambda) \\
&= \left\{\Psi^*(Q - \lambda I)\Psi_\lambda - \Psi^*(Q - \lambda I)\Psi_\lambda + \Psi^*\Psi\right\}(x, \lambda) \\
&= \Psi^*\Psi(x, \lambda),
\end{aligned}
$$

see the proof of [10, Theorem 10.2.3] for details of a similar calculation. Since the Floquet solutions decay exponentially, along with their derivatives, an integration yields

$$\left\{(\Psi')^*\Psi_\lambda - \Psi^*\Psi'_\lambda\right\}(x, \lambda) = -\int_x^\infty \Psi^*\Psi(t, \lambda)dt,$$

which is strictly negative definite. This shows that

$$\Omega_F(x, \lambda) = -2\big((\Psi' - i\Psi)^{-1}\big)^*(x, \lambda) \left(\int_x^\infty \Psi^*\Psi(t, \lambda)dt\right) (\Psi' - i\Psi)^{-1}(x, \lambda)$$

is strictly negative definite, which completes our proof.

$\square$

From the Floquet matrix $\Psi(\cdot, \lambda)$ of square integrable solutions of (148) we can define a full rank matrix $\Psi_R(\cdot, \lambda)$ of square integrable solutions of (144).

Definition 6.4. By $\Psi_R(\cdot, \lambda)$ we denote the unique $n \times n$ matrix which satisfies the initial value problem

$$-\Psi_R''(x, \lambda) + (Q_p(x) + R(x))\Psi_R(x, \lambda) = \lambda\Psi_R(x, \lambda),$$

$$\Psi_R(X, \lambda) = \Psi(X, \lambda), \quad \Psi_R'(X, \lambda) = \Psi'(X, \lambda).$$

We define the Atkinson Θ-matrix associated with Ψ_R by

$$\Theta_R(x, \lambda) = (\Psi_R'(x, \lambda) + i\Psi_R(x, \lambda))(\Psi_R'(x, \lambda) - i\Psi_R(x, \lambda))^{-1}.$$

Note that by unique continuation, since $R(x) = 0$ for $x > X$, we have $\Psi(x, \lambda) = \Psi_R(x, \lambda)$ for $x \geq X$. This means, in turn, that

$$\Theta_R(x, \lambda) = \Theta_F(x, \lambda) \ \ \forall x \geq X. \tag{152}$$

In particular, this establishes that the eigenvalues of $\Theta_R(x, \lambda)$ move negatively round the unit circle, with increasing λ, for $x \geq X$. In fact this result is true for all x.

Proposition 6.5. For λ in a fixed spectral gap, the matrix $\Theta_R(x, \lambda)$ is well defined and unitary. Moreover its eigenvalues move negatively round the unit circle for all $x \geq 0$, for increasing λ.

Proof. The proofs of well-definedness and unitarity are essentially the same as for Proposition 6.2 part (1). The proof that the eigenvalues move negatively round the unit circle with increasing λ is essentially the same as for Proposition 6.2 part (3). In particular, the formula (151) still holds but with Θ_F replaced by Θ_R and Ψ replaced by Ψ_R in the formula for Ω_F. The resulting formula remains valid because the integral

$$\int_x^\infty \Psi_R^*\Psi_R(t, \lambda)dt$$

is still convergent and positive definite. $\square$

Suppose that Φ denotes an $n \times n$ matrix whose columns are linearly independent solutions of (144), and let

$$\Theta(x, \lambda) := (\Phi'(x, \lambda) + i\Phi(x, \lambda))(\Phi'(x, \lambda) - i\Phi(x, \lambda))^{-1}$$

be the associated Θ-matrix, if it exists. Differentiating with respect to x and using (144) to replace second derivatives $\Phi''(x, \lambda)$, one may show (see, e.g., [10, Theorem 10.2.2],[81]) that

$$\frac{d}{dx}\Theta(x, \lambda) = i\Theta(x, \lambda)\Omega(x, \lambda, \Theta), \tag{153}$$

in which $\Omega(x, \lambda, \bullet)$ is defined by the formula

$$\Omega(x, \lambda, \Theta) = \frac{1}{2}((\Theta^{-1} + I)(\Theta + I) - (\Theta^{-1} - I)(Q(x) - \lambda I)(\Theta - I)). \tag{154}$$

In particular, such a differential equation is satisfied by Θ_R and Θ_F. In addition, those matrices are unitary, meaning that the terms Θ^{-1} in the expression for Ω can be replaced by Θ^*.

Proposition 6.6. Suppose that $N \in \mathbb{N}$ is such that $Na \geq X$. Then $\Theta_R(x, \lambda)$ is the unique solution[9] of the initial value problem

$$\frac{d}{dx}\Theta_R(x, \lambda) = i\Theta_R(x, \lambda)\Omega(x, \lambda, \Theta_R), \quad \Theta_R(Na, \lambda) = \Theta_F(0, \lambda). \tag{155}$$

Proof. Using Proposition 6.2 part (2) inductively, it follows that $\Theta_F(Na, \lambda) = \Theta_F(0, \lambda)$. Also, by (152), since $Na \geq X$, we have $\Theta_R(Na, \lambda) = \Theta_F(Na, \lambda)$, and thus $\Theta_R(Na, \lambda) = \Theta_F(0, \lambda)$. This establishes the initial condition at $x = Na$ in (155). The differential equation is just (153). $\qquad\square$

Remark 6.7. For numerical purposes we shall be integrating the initial value problem in Proposition 6.6 backwards, from $x = Na$ back to $x = 0$. The value of $\Theta_F(0, \lambda)$ is obtained from the matrix $\Psi_F(0, \lambda)$, the initial condition satisfied by the Floquet solutions. This, in turn, can be found from the monodromy matrix for (148) over a single period $[0, a]$ and therefore requires only a finite numerical integration.

Having introduced the $n \times n$ matrix Ψ_R of L^2 solutions of (144) and its associated Atkinson Θ-matrix, it remains only to define an $n \times n$ full rank matrix of solutions of (144) satisfying the boundary condition at $x = 0$.

---

[9]See Remark 6.11.

Definition 6.8. We define Ψ_L to be the solution of the initial value problem

$$-\Psi_L''(x, \lambda) + (Q_p(x) + R(x))\Psi_L(x, \lambda) = \lambda \Psi_L(x, \lambda),$$

$$\Psi_L(0, \lambda) = B^*, \quad \Psi_L'(0, \lambda) = A^*. \tag{156}$$

The corresponding Θ-matrix is

$$\Theta_L(x, \lambda) := (\Psi_L'(x, \lambda) + i\Psi_L(x, \lambda))(\Psi_L'(x, \lambda) - i\Psi_L(x, \lambda))^{-1}.$$

The following result is proved in [81].

Proposition 6.9. For each $x \geq 0$, and every $\lambda \in \mathbb{R}$, the matrix $\Theta_L(x, \lambda)$ is unitary. Moreover for $x > 0$ its eigenvalues move positively round the unit circle with increasing λ.

Proposition 6.10. $\Theta_L(x, \lambda)$ is the unique solution[10] of the initial value problem

$$\frac{d}{dx}\Theta_L(x, \lambda) = i\Theta_L(x, \lambda)\Omega(x, \lambda, \Theta_L), \quad \Theta_L(0, \lambda) = (A^* + iB^*)(A^* - iB^*)^{-1}, \tag{157}$$

in which $\Omega(x, \lambda, \bullet)$ is given by (154).

Proof. Since Ψ_L and Ψ_R satisfy the same Schrödinger equation, their Θ-matrices satisfy the same first order differential equation. It remains only to check the initial condition. This follows immediately from the initial condition $\Psi_L(0, \lambda) = B^*$, $\Psi_L'(0, \lambda) = A^*$. □

Remark 6.11. The uniqueness of the solutions of the initial value problems (155) and (157) is taken for granted in Atkinson, see [10, Chapter 10]. To show that the initial value problem

$$\frac{d}{dx}\Theta(x, \lambda) = i\Theta(x, \lambda)\Omega(x, \lambda, \Theta), \quad \Theta(0, \lambda) = \Theta_0;$$

$\Omega(x, \lambda, \Theta)$ is given by (154), has a unique solution, we need to show that $F(x, \Theta) = i\Theta(x, \lambda)\Omega(x, \lambda, \Theta)$ is locally Lipschitz. Note that

$$F(x, \Theta_1) - F(x, \Theta_2) = (\Theta_1 - \Theta_2)\Omega(x, \Theta_1) + \Theta_2(\Omega(x, \Theta_1) - \Omega(x, \Theta_2))$$

Hence,

$$\|F(x, \Theta_1) - F(x, \Theta_2)\| \leq \|\Theta_1 - \Theta_2\|\|\Omega(x, \Theta_1)\| + \|\Theta_2\|\|\Omega(x, \Theta_1) - \Omega(x, \Theta_2)\|,$$

---

[10]See Remark 6.11.

and it suffices to show that Ω is locally Lipschitz. We know that from (154)

$$2\Omega(x, \Theta) = (\Theta + I)^*(\Theta + I) - (\Theta - I)^*(Q - \lambda I)(\Theta - I).$$

Hence,

$$2\Omega(x, \Theta) = \Theta^*(\lambda I - Q + I)\Theta + \Theta^* M_1 + M_2\Theta + M_3;$$

where M_1, M_2, and M_3 are matrices and depend on x. We need to show that the map:

$$\Theta \mapsto \Theta^* M_4(x)\Theta$$

is locally Lipschitz when $\|M_4(x)\|$ is locally bounded. Hence,

$$\Theta_1^* M_4 \Theta_1 - \Theta_2^* M_4 \Theta_2 = (\Theta_1 - \Theta_2)^* M_4 \Theta_1 + \Theta_2^* M_4(\Theta_1 - \Theta_2)$$

and so

$$\|\Theta_1^* M_4 \Theta_1 - \Theta_2^* M_4 \Theta_2\| \leq \|\Theta_1 - \Theta_2\|\|M_4\|\big(\|\Theta_1\| + \|\Theta_2\|\big).$$

Theorem 6.12. *Fix $c \in [0, \infty)$ and fix a spectral gap $\mathcal{J}$ of the essential spectrum associated with the Schrödinger equation (144)-(145). Then the following are true.*

1. *A real value $\lambda \in \mathcal{J}$ is an eigenvalue for the original problem (144) if and only if 1 is an eigenvalue of the matrix $\Theta_R^*(c, \lambda)\Theta_L(c, \lambda)$.*

2. *The multiplicity of λ as an eigenvalue of the original problem (144) is equal to the multiplicity of 1 is an eigenvalue of the matrix $\Theta_R^*(c, \lambda)\Theta_L(c, \lambda)$.*

3. *The eigenvalues of $\Theta_R^*(c, \lambda)\Theta_L(c, \lambda)$ move positively round the unit circle as λ increases in $\mathcal{J}$.*

Proof. **Parts (1) and (2)**

Suppose that λ is an eigenvalue of the problem (144)-(145), and let $\underline{u}$ be a corresponding eigenfunction. Because $\underline{u}$ satisfies the boundary condition at $x = 0$, there exists a vector $\underline{c}_L$ such that $\underline{u}(x) = \Psi_L(x, \lambda)\underline{c}_L$. Because $\underline{u} \in L^2(0, \infty)$ there exists a vector $\underline{c}_R$ such that $\underline{u}(x) = \Psi_R(x, \lambda)\underline{c}_R$. Thus we have

$$\Psi_L(x, \lambda)\underline{c}_L = \Psi_R(x, \lambda)\underline{c}_R, \quad \Psi_L'(x, \lambda)\underline{c}_L = \Psi_R'(x, \lambda)\underline{c}_R$$

for all $x \geq 0$, and in particular for $x = c$. These imply that

$$(\Psi_L'(c, \lambda) + i\Psi_L(c, \lambda))\underline{c}_L = (\Psi_R'(c, \lambda) + i\Psi_R(c, \lambda))\underline{c}_R,$$

which we may write as

$$\Theta_L(c,\lambda)(\Psi'_L(c,\lambda) - i\Psi(c,\lambda))\underline{c}_L = \Theta_R(c,\lambda)(\Psi'_R(c,\lambda) - i\Psi(c,\lambda))\underline{c}_R.$$

However since also $(\Psi'_L(c,\lambda) - i\Psi_L(c,\lambda))\underline{c}_L = (\Psi'_R(c,\lambda) - i\Psi_R(c,\lambda))\underline{c}_R$, this implies

$$\Theta_L(c,\lambda)\underline{v} = \Theta_R(c,\lambda)\underline{v}, \tag{158}$$

in which $\underline{v} = (\Psi'_L(c,\lambda) - i\Psi_L(c,\lambda))\underline{c}_L = (\Psi'_R(c,\lambda) - i\Psi_R(c,\lambda))\underline{c}_R$. We know that $\underline{v} \neq 0$, e.g. since $\Psi'_L(c,\lambda) - i\Psi_L(c,\lambda)$ is invertible. As Θ_R is unitary, from (158) we obtain that 1 is an eigenvalue of $\Theta^*_R(c,\lambda)\Theta_L(c,\lambda)$ with eigenvector $\underline{v}$. If λ has multiplicity $\nu \geq 1$ as an eigenvalue of (144)-(145) then there are ν linearly independent choices of $\underline{c}_L$, giving ν linearly independent choices of $\underline{v}$, and proving hence that 1 is an eigenvalue of $\Theta^*_R(c,\lambda)\Theta_L(c,\lambda)$ of multiplicity at least ν.

Now suppose that 1 is an eigenvalue of $\Theta^*_R(c,\lambda)\Theta_L(c,\lambda)$ with some eigenvector $\underline{w}$; then $\Theta_L(c,\lambda)\underline{w} = \Theta_R(c,\lambda)\underline{w}$, which means

$$(\Psi'_L(c,\lambda) + i\Psi_L(c,\lambda))(\Psi'_L(c,\lambda) - i\Psi_L(c,\lambda))^{-1}\underline{w}$$
$$= (\Psi'_R(c,\lambda) + i\Psi_R(c,\lambda))(\Psi'_R(c,\lambda) - i\Psi_R(c,\lambda))^{-1}\underline{w}. \tag{159}$$

If we define

$$\underline{c}_L := (\Psi'_L(c,\lambda) - i\Psi_L(c,\lambda))^{-1}\underline{w},$$

and

$$\underline{c}_R := (\Psi'_L(c,\lambda) - i\Psi_L(c,\lambda))^{-1}\underline{w},$$

then we have

$$(\Psi'_L(c,\lambda) - i\Psi_L(c,\lambda))\underline{c}_L = (\Psi'_R(c,\lambda) - i\Psi_R(c,\lambda))\underline{c}_R = \underline{w},$$

but also from (159)

$$(\Psi'_L(c,\lambda) + i\Psi_L(c,\lambda))\underline{c}_L = (\Psi'_R(c,\lambda) + i\Psi_R(c,\lambda))\underline{c}_R.$$

It follows that

$$\Psi_L(c,\lambda)\underline{c}_L = \Psi_R(c,\lambda)\underline{c}_R, \quad \Psi'_L(c,\lambda)\underline{c}_L = \Psi'_R(c,\lambda)\underline{c}_R.$$

If we define a function $\underline{u}$ by

$$\underline{u}(x) = \begin{cases} \Psi_L(x,\lambda)\underline{c}_L, & x \in [0,c), \\ \Psi_R(x,\lambda)\underline{c}_R, & x \in [c,\infty), \end{cases}$$

then $\underline{u}$ lies in $L^2(0, \infty)$, satisfies the boundary condition (145) and the differential equation (144), and is therefore an eigenfunction of the Schrödinger problem with eigenvalue λ. If 1 has multiplicity $\nu \geq 1$ as an eigenvalue of $\Theta_R^*(c, \lambda)\Theta_L(c, \lambda)$ then there are ν linearly independent choices of $\underline{w}$, giving ν linearly independent $\underline{c}_L$ and corresponding $\underline{c}_R$. These define ν linearly independent eigenfunctions $\underline{u}$ and prove that λ is a Schrödinger eigenvalue with multiplicity at least ν.

Part (3) Following the derivation of equation (151), see also [10, Theorem V.6.1], we know that

$$\frac{\partial \Theta_R}{\partial \lambda}(x, \lambda) = -i\Theta_R(x, \lambda)\Omega_R(x, \lambda)$$

and

$$\frac{\partial \Theta_L}{\partial \lambda}(x, \lambda) = i\Theta_L(x, \lambda)\Omega_L(x, \lambda),$$

in which Ω_R and Ω_L are positive definite. The partial derivative of $\Theta_R^*\Theta_L(x, \lambda)$ with respect to λ is given by:

$$
\begin{aligned}
\frac{\partial \Theta_R^*\Theta_L}{\partial \lambda}(x, \lambda) &= \left(\frac{\partial \Theta_R}{\partial \lambda}(x, \lambda)\right)^* \Theta_L(x, \lambda) + \Theta_R^*(x, \lambda)\frac{\partial \Theta_L}{\partial \lambda}(x, \lambda) \\
&= \left(-i\Theta_R\Omega_R(x, \lambda)\right)^*\Theta_L(x, \lambda) + \Theta_R^*(x, \lambda)\left(i\Theta_L\Omega_L(x, \lambda)\right) \\
&= i(\Omega_R(x, \lambda))^*\Theta_R^*\Theta_L(x, \lambda) + i\Theta_R^*\Theta_L(x, \lambda)\Omega_L(x, \lambda) \\
&= i\Theta_R^*\Theta_L(x, \lambda)\left(\Omega_L(x, \lambda) + \left(\Theta_R^*\Theta_L(x, \lambda)\right)^*\Omega_R^*(x, \lambda)\left(\Theta_R^*\Theta_L(x, \lambda)\right)\right) \\
&= i\Theta_R^*\Theta_L(x, \lambda)\Omega_{LR}(x, \lambda),
\end{aligned}
$$

where $\Omega_{LR}(x, \lambda) = \Omega_L(x, \lambda) + \left(\Theta_R^*\Theta_L(x, \lambda)\right)^*\Omega_R(x, \lambda)\left(\Theta_R^*\Theta_L(x, \lambda)\right) > 0$. Thus Ω_{LR} is strictly positive definite, and the results follows from [10, Theorem V.6.1]. $\qquad\square$

Remark 6.13. Theorem 6.12 gives a characterisation of the eigenvalues of the problem (144)-(145) which we shall use as the basis of a shooting procedure in Section 6.3 below.

We shall shortly introduce (eqn. (164) below) a miss-distance function which plays an important role in locating eigenvalues of our problem. First we require a replacement for the Prüfer angles of the one-dimensional case.

Let the eigenvalues of $\Theta_L(x, \lambda)$ be $\exp(i\phi_j^L(x))$, $j = 1, \ldots, n$, and let the eigenvalues of $\Theta_R(x, \lambda)$ be $\exp(i\phi_j^R(x))$, $j = 1, \ldots, n$. The so-called *phase angles* $\phi_j^L(x, \lambda)$ and $\phi_j^R(x, \lambda)$ should be chosen to be continuous functions of x and λ. Since the initial

condition $\Theta_L(0, \lambda) = (A^* + iB^*)(A^* - iB^*)^{-1}$ is independent of λ, continuity may be ensured, and the phase angles determined uniquely up to ordering, by insisting that

$$0 \leq \phi_j^L(0, \lambda) < 2\pi.$$

However the initial condition for Θ_R, viz. $\Theta_R(Na, \lambda) = \Theta_F(Na, \lambda) = \Theta_F(0, \lambda)$, is λ-dependent. In order to ensure that the $\phi_j^R(x, \lambda)$ are continuous with respect to λ we must ensure that we have a canonical way to choose the phase angles of the eigenvalues of $\Theta_F(0, \lambda)$ as continuous functions of λ. This requires an additional hypothesis.

Proposition 6.14. If the pure-periodic problem has pure a.c. spectrum [99, Chapter VII], then 1 cannot be an eigenvalue of the unitary matrix $\Theta_F(0, \lambda)$. Consequently, the phase angles of $\Theta_F(0, \lambda)$ may be chosen as continuous functions of λ with values in $(0, 2\pi)$, in each spectral gap.

Proof. Suppose that 1 is an eigenvalue of

$$\Theta_F(0, \lambda) = (\Psi'(0, \lambda) + i\Psi(0, \lambda))(\Psi'(0, \lambda) - i\Psi(0, \lambda))^{-1}.$$

Then $\Psi(0, \lambda)$ has eigenvalue 0. Hence there exists a constant $\underline{c} \neq \underline{0}$ such that $\underline{u}(\cdot) := \Psi(\cdot, \lambda)\underline{c} \in L^2(0, \infty)$ and solves

$$-\underline{u}'' + Q_p\underline{u} = \lambda\underline{u}, \quad \underline{u}(0) = \underline{0}.$$

This means that λ is an eigenvalue of the pure-periodic problem. We assumed that the spectrum of the periodic problem is pure a.c., so this cannot happen. $\quad\square$

We are now able to introduce two continuous functions of x and λ.

Remark 6.15. The sum of the functions $\phi_j^L(x, \lambda)$ is given by

$$\arg\det(\Theta_L(x, \lambda)) = \sum_{j=1}^{n} \phi_j^L(x, \lambda).$$

Similarly, the sum of the $\phi_j^R(x, \lambda)$ is given by

$$\arg\det(\Theta_R(x, \lambda)) = \sum_{j=1}^{n} \phi_j^R(x, \lambda).$$

Working from (153), standard calculations show, see, e.g., [10, Equation 10.2.26], that both $\arg\det(\Theta_L)$ and $\arg\det(\Theta_R)$ satisfy the differential equation:

$$\frac{d}{dx}\arg\det(\Theta(x)) = \mathrm{trace}(\Omega(x)),$$

where Ω is defined in (154). The following two propositions therefore hold.

Proposition 6.16. The function $\arg\det(\Theta_L(x))$ is the unique solution[11] of the initial value problem:

$$\left.\begin{aligned}
\frac{d}{dx}\arg\det(\Theta_L(x)) &= \mathrm{trace}(\Omega(x)), \\
\arg\det(\Theta_L(0)) &= \arg\det((A^* + iB^*)(A^* - iB^*)^{-1})
\end{aligned}\right\} \tag{160}$$

in which $\Omega(x)$ is given in (154).

Proposition 6.17. The function $\arg\det(\Theta_R(x))$ is the unique solution[12] of the initial value problem:

$$\left.\begin{aligned}
\frac{d}{dx}\arg\det(\Theta_R(x)) &= \mathrm{trace}(\Omega(x)), \\
\arg\det(\Theta_R(Na)) &= \arg\det(\Theta_F(0)),
\end{aligned}\right\} \tag{161}$$

in which $\Omega(x)$ is given in (154).

Remark 6.18. The uniqueness of the solution of the initial value problem

$$\frac{d}{dx}\arg\det(\Theta(x)) = \mathrm{trace}(\Omega(x)), \quad \arg\det(\Theta(0)) = \arg\det(\Theta_0) \tag{162}$$

follows from the fact that once Θ is uniquely determined then so is Ω and hence so is the trace of Ω. Hence the right hand side of the differential equation (162) is completely determined. The solution of the initial value problem (162) is then just given by The Fundamental Theorem of Calculus, see [40, Section 2.9]:

$$\arg\det(\Theta(x)) = \arg\det(\Theta(x_0)) + \int_{x_0}^{x} \mathrm{trace}(\Omega(s))ds.$$

---

[11]See Remark 6.18.

[12]See Remark 6.18.

Choose $c \in [0, X]$ and let the eigenvalues of the unitary matrix $\Theta_R^*(c)\Theta_L(c)$ be $\exp(i\omega_j)$, $j = 1, \dots, n$, where

$$0 \leq \omega_j < 2\pi. \tag{163}$$

(From this normalisation, the angles ω_j are not generally continuous functions of λ : they will have jump discontinuities whenever an eigenvalue $\exp(i\omega_j)$ passes through the point 1 on the unit circle).

Now we define an integer-valued function $M(\lambda)$ as follows.

Definition 6.19. The miss-distance function associated with $\Theta_R^*(c)\Theta_L(c)$ is given by

$$M(\lambda) = \frac{1}{2\pi}\left\{ \arg \det(\Theta_L(c)) - \arg \det(\Theta_R(c)) - \sum_{j=1}^{n} \omega_j \right\}. \tag{164}$$

The following theorem indicates important properties of $M(\lambda)$.

Theorem 6.20. *Suppose that the pure periodic problem has pure a.c. spectrum [99, Chapter VII]. Fix $c \in [0, \infty)$. For each spectral gap $\mathcal{J}$ of the essential spectrum associated with the Schrödinger equation (144)-(145), let $\Theta_R^*(c)\Theta_L(c)$ be the unitary matrix in Theorem 6.12. Then the following are true.*

1. *$M(\lambda)$ is an integer-valued function.*

2. *$M(\lambda)$ is a monotonically increasing function inside the spectral gap $\mathcal{J}$ whose points of increase are the eigenvalues of the equation (144)-(145).*

Proof. **Part (1)** See [81, Proposition 1].
Part (2) $M(\lambda)$ is an increasing function as λ increases inside $\mathcal{J}$. This follows directly from Theorem 6.12 since eigenvalues of the unitary matrix $\Theta_R^*(c)\Theta_L(c)$ move positively round the unit circle as λ increases in $\mathcal{J}$. Moreover, since $\arg \det(\Theta_L)$ and $\arg \det(\Theta_R)$ are continuous functions of λ, the latter being so by Proposition 6.14, it follows that $M(\lambda)$ can change if one, or more, of ω_j passes through a multiple of 2π and jumps because of the conditions (163). This happens only when 1 is an eigenvalue of $\Theta_R^*(c)\Theta_L(c)$. Thus from Theorem 6.12 the corresponding λ is an eigenvalue of the original problem (144)-(145). □

Remark 6.21. The purpose of using $M(\lambda)$ here is to locate the eigenvalues of the problem (144)-(145) reliably. Every eigenvalue is reflected in a discontinuity of $M(\lambda)$ and vice-versa; even if $M(\lambda)$ is only evaluated on a widely spaced set of values of λ, the monotonicity ensures that no discontinuities can 'hide' from the algorithm. See Figure 6.3 below.

6.3   Numerical implementation

In view of Theorem 6.12 we shall find eigenvalues by calculating the unitary matrix $\Theta_R^*(c,\lambda)\Theta_L(c,\lambda)$ together with $\arg\det(\Theta_L(c,\lambda))$ and $\arg\det(\Theta_R(c,\lambda))$, computing $M(\lambda)$ and finding its discontinuities. To do this we must solve the initial value problems (157)-(160) and (155)-(161). We describe the necessary ingredients below.

Ingredient 1: the matrix $\Theta_F(0,\lambda)$

We must find the Floquet solutions for the unperturbed equation

$$-\underline{u}'' + Q_p\underline{u} = \lambda\underline{u}, \quad x \in (0,a). \tag{165}$$

We rewrite this problem as a first order system

$$\begin{pmatrix} \underline{u} \\ \underline{u}' \end{pmatrix}' = \begin{pmatrix} 0 & I \\ Q_p(x) - \lambda I & 0 \end{pmatrix}\begin{pmatrix} \underline{u} \\ \underline{u}' \end{pmatrix}, \quad x \in (0,a),$$

and consider the $2n \times 2n$ matrix-valued solutions of the associated initial value problem

$$Y' = \begin{pmatrix} 0 & I \\ Q_p(x) - \lambda I & 0 \end{pmatrix} Y, \; x \in (0,a); \quad Y(0) = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}.$$

The *monodromy matrix* is the matrix

$$A(\lambda) = Y(a,\lambda), \tag{166}$$

and its eigenvalues are the *Floquet multipliers*. In a spectral gap (i.e. outside the essential spectrum), precisely n of the $2n$ Floquet multipliers have absolute value strictly less than 1; the other n have absolute value strictly greater than 1. Denoting by $V(\lambda)$ the n by $2n$ matrix whose columns are the eigen and associated vectors of $A(\lambda)$ corresponding to the Floquet multipliers of modulus less than 1, then the matrix Ψ of $L^2(0,\infty)$ solutions appearing in (150) is given by

$$\begin{pmatrix} \Psi(x,\lambda) \\ \Psi'(x,\lambda) \end{pmatrix} = Y(x,\lambda)V(\lambda),$$

and in particular

$$\begin{pmatrix} \Psi(0,\lambda) \\ \Psi'(0,\lambda) \end{pmatrix} = V(\lambda).$$

We immediately compute $\Theta_F(0,\lambda) = (\Psi'(0,\lambda) + i\Psi(0,\lambda))(\Psi'(0,\lambda) - i\Psi(0,\lambda))^{-1}$.

It is well known that reliable computation of Floquet multipliers is not straightforward if the problem is stiff - for instance, if λ is large and negative. Dieci et al.

[44] propose a multiple shooting algorithm, resulting in a generalized eigenproblem, to circumvent this difficulty. In our experiments (Section 6.4 below) it was never necessary to use a full-blown multiple-shooting technique: it was always sufficient to apply the repeated bisection over the interval $[0, a]$.

Ingredient 2: a numerical method for the differential equations (155)-(157)

Both (155) and (157) require the integration of an $n \times n$ matrix differential equation of the form

$$\Theta' = i\Theta \left(\frac{1}{2}(\Theta^* + I)(\Theta + I) - \frac{1}{2}(\Theta^* - I)(Q - \lambda I)(\Theta - I) \right), \qquad (167)$$

either integrating forward from a condition at $x = 0$ (for Θ_L) or integrating backwards from a condition $\Theta_R(Na, \lambda) = \Theta_F(0, \lambda)$ (for Θ_R). The key difficulty is to preserve the unitarity of Θ, see Section 6.2, without which a catastrophic exponential accumulation of error is not unusual. It is well known (see, e.g., Casas and Iserles [34]) that among Runge-Kutta methods, only special classes of implicit formulae preserve quadratic invariants. Iserles therefore developed special *Magnus integrators* which work on the associated Lie algebra - roughly speaking, they represent Θ in the form $\Theta = \exp(i\Sigma)$, in which Σ is Hermitian, and integrate the differential equation for Σ. (Early numerical methods based on this idea were also used by Alex Dragt in the 1970s, in codes which he wrote for nonlinear dynamics in particle accelerators.) These methods require reliable algorithms for computation of matrix exponentials, see [87].

For our numerics, we compared a Magnus-type integrator from [34] with the projection method proposed in [44]. This second approach involves taking any one-step method and performing a QR factorisation after each step, to map the non-unitary numerical approximation to the unitary Θ-matrix back onto the unitary group. In fact we modified this slightly, making an a-priori division of the interval of integration into equal sub-intervals and performing projections only at the ends of the subintervals. Integration over the sub-intervals was performed with MATLAB's **ode45**. We never needed more than ten sub-intervals for this purpose, because one of the advantages of good non-reflecting boundary conditions is that the range of integration never had to be too long.

Because $\arg \det(\Theta_L)$ and $\arg \det(\Theta_R)$ appear in Theorem 6.20, we also need to integrate the differential equation for $\arg \det(\Theta)$ which is an immediate consequence of the differential equation (167):

$$\arg \det(\Theta)' = \text{trace} \left(\frac{1}{2}(\Theta^* + I)(\Theta + I) - \frac{1}{2}(\Theta^* - I)(Q - \lambda I)(\Theta - I) \right). \qquad (168)$$

115

This can be included in either approach (Magnus or projected RK45) with a single additional line. In the Magnus method, for instance, the step from x_n to x_{n+1} is given by a formula

$$\Theta_{n+1} = \Theta_n \exp(i(x_{n+1} - x_n)\Sigma_n),$$

in which Σ_n is Hermitian. This gives

$$\arg\det(\Theta_{n+1}) = \arg\det(\Theta_n) + (x_{n+1} - x_n)\mathrm{trace}(\Sigma_n).$$

6.4   Numerical examples

In this section we test the algorithm on two different problems. In the first example, we consider a matrix-valued Schrödinger problem of small dimension $n = 3$ for which we know the essential spectrum already. In the second example, we look at an elliptic PDE on a semi-infinite waveguide. Using semi-discretisation by a spectral method, this problem generates a family of matrix Schrödinger equations of arbitrarily high dimension, for which we do not know the essential spectrum.

All our computations were performed using Matlab. In particular for the projected Runge-Kutta method we used Matlab's `ode45`; for the Magnus method we implemented the algorithm given in [34], which we equipped with an automatic step size control.

Example 6.22. Consider the matrix Schrödinger equation:

$$-\underline{u}'' + \left(-(2\pi - \min(x, 2\pi))^2 I_3 + Q_p(x) \right)\underline{u} = \lambda\underline{u}, \quad \underline{u}(0) = \underline{0}, \qquad (169)$$

such that

$$Q_p(x) = \begin{pmatrix} \frac{\sin(x)+\cos(x)+40}{6} & \frac{\sin(x)-\cos(x)}{2\sqrt{3}} & -\frac{\sin(x)+\cos(x)-20}{3\sqrt{2}} \\ \frac{\sin(x)-\cos(x)}{2\sqrt{3}} & \frac{\sin(x)+\cos(x)}{2} & \frac{\cos(x)-\sin(x)}{\sqrt{2}\sqrt{3}} \\ -\frac{\sin(x)+\cos(x)-20}{3\sqrt{2}} & \frac{\cos(x)-\sin(x)}{\sqrt{2}\sqrt{3}} & \frac{\sin(x)+\cos(x)+10}{3} \end{pmatrix}.$$

The first two spectral gaps in the essential spectrum of this problem are given by, see e.g., Example 4.15 in Section 4.6:

$$(-\infty, -0.3785), (-0.3404, 0.5959).$$

We started by comparing our algorithm using the integer-valued miss distance $M(\lambda)$ with a contour integral method [19] which can handle a wide range of λ-nonlinear generalized matrix eigenvalue problems: to be precise, we discretised the

problem using the standard three-point finite difference scheme with a fixed step size, with λ-dependent coefficients in the last row of the matrix giving the discrete version of our non-reflecting boundary conditions. Table 6.1 shows approximations of five different isolated eigenvalues of the problem using the proposed algorithm and the $\lambda-$nonlinear eigenvalue algorithm. Approximations are obtained with interval truncation $[0, 6\pi]$. For the computation of $M(\lambda)$ we used $c = 2\pi$, though of course the positions of the discontinuities in $M(\lambda)$ do not depend on the choice of c. In addition, the tolerance is set to 10^{-6} for the shooting methods and the step size for the finite difference scheme was $h = \frac{6\pi}{1000}$.

Surprisingly, given the ad-hoc nature of the step size control algorithm which we wrote for the Magnus integrator, the approximations using the two shooting methods are identical for the decimal places given. The three-point finite difference scheme is much less accurate and, because of the contour integral approach to eigenvalue location, more expensive by a factor of at least 20. While the accuracy could be improved by using a higher order finite difference or by Richardson extrapolation, the computational cost reflects the fact that the contour integral method is really adapted to problems in which eigenvalues lie in the complex plane, and cannot compete with methods which exploit self-adjointness to reduce the dimension of the search region from 2 to 1.

λ_k	Magnus integrator	Projected RK45	$\lambda-$nonlinear algorithm
λ_1	0.4792	0.4792	0.47
CPU	11 secs[1]	3 secs	221 secs
λ_2	-1.5373	-1.5373	-1.5
CPU	11 secs	3 secs	225 secs
λ_3	-4.31273	-4.31273	-4.31
CPU	8 secs	3 secs	224 secs
λ_4	-7.8236	-7.8236	-7.82
CPU	7 secs	3 secs	230 secs
λ_5	-12.3525	-12.3525	-12.35
CPU	6 secs	3 secs	230 secs

[1] secs=seconds

Table 6.1: Approximation of some eigenvalues of (169) comparing shooting method (Magnus/projected RK45) vs. finite difference scheme with contour integral method.

The test in Table 6.1 shows no difference in accuracy between the two shooting methods, so we performed a second test of accuracy vs. cost, fixing our attention on one particular eigenvalue, namely $\lambda_1 \approx 0.4792$ in the spectral gap $(-0.3404, 0.5959)$.

In order to do this we first computed our best guess of the 'true' eigenvalue, using both integrators with a tolerance of 10^{-9}, and used this to assess the error at slacker tolerances. The results are in Table 6.2 with a logarithmic plot of error vs. cost in Figure 6.1. It can be seen that the projected RK45 method consistently out-performs the Magnus integrator. This is not surprising, given the difference in orders (5 for RK45, 4 for the Magnus method).

Magnus	CPU[1]	Projected RK45	CPU[1]	Tol
0.4792653809	3	0.4794997559	1	10^{-4}
0.4792129822	6	0.4790531311	2	10^{-5}
0.4792103462	11	0.4792057991	3	10^{-6}
0.4792096562	19	0.4792102885	5	10^{-7}
0.4792096138	35	0.4792096526	9	10^{-8}
0.4792096136	60	0.4792096202	15	10^{-9}

[1] in seconds

Table 6.2: Comparison between approximations and time consuming for an isolated eigenvalue in the gap $(-0.3404, 0.5959)$ using Magnus and the projected RK45 with different values of tolerance.
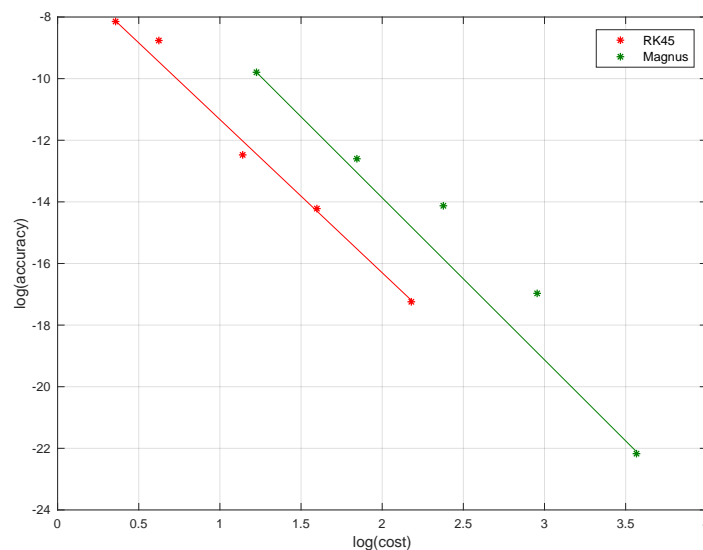

Figure 6.1: Logarithmic plot of cost against accuracy of approximations given in Table 6.2.

We repeated this test for an eigenvalue below the essential spectrum, $\lambda_5 \approx -12.3525$, for which the problem would be more stiff. However the results in Table 6.3 and Figure 6.2 still show that projected RK45 is winning. In Section 6.5 below we discuss this slightly unfair comparison further, and indicate how the performance of the Magnus method could be improved.

Magnus	CPU[1]	Projected RK45	CPU[1]	Tol
-12.352502441	2	-12.354650879	1	10^{-4}
-12.352507820	4	-12.352698517	2	10^{-5}
-12.352514172	6	-12.352522373	3	10^{-6}
-12.352514637	11	-12.352514899	4	10^{-7}
-12.352514461	18	-12.352514461	6	10^{-8}
-12.352514416	29	-12.352514360	11	10^{-9}

[1] in seconds

Table 6.3: Comparison between approximations and time consuming for one of an eigenvalue below the essential spectrum using Magnus and the projected RK45 with different values of tolerance.
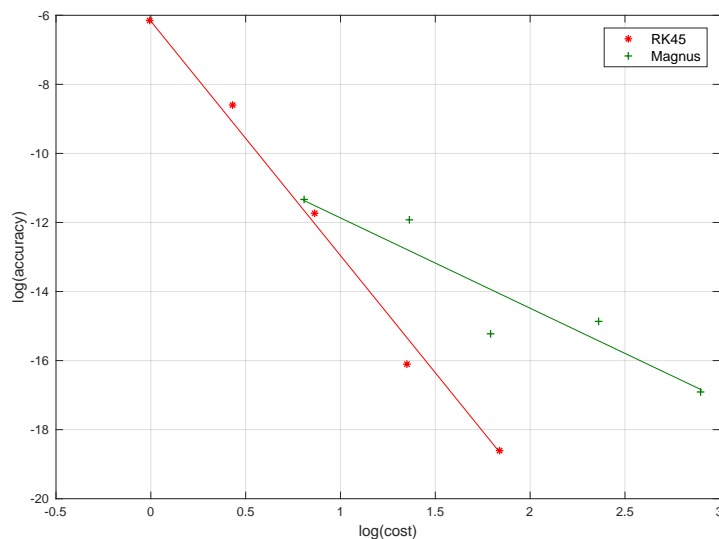

Figure 6.2: Logarithmic plot of cost against accuracy of approximations given in Table 6.3.

Example 6.23. In Example 5.27, Section 5.5, we considered a PDE problem on
a waveguide, which we here transform into a matrix Schrödinger equation using a
semi-discretisation method. We would like to know if this approach can beat the
'dissipative barrier plus finite element' approach of our previous chapter. The PDE
is

$$-\Delta u + \left(\cos(x) - 25\exp(-x)(1 - \epsilon(\pi - y)^2) \right) u = \lambda u, \tag{170}$$

in a waveguide $[0, \infty) \times [0, 2\pi]$, with Dirichlet boundary conditions. By separation
of variables eqn. (170) turns into a family of ODEs:

$$-u_n''(x) + \frac{n^2}{4}u_n(x) + \sum_{m=1}^{\infty} \left(\int_0^{2\pi} \phi_n(y)Q(x,y)\phi_m(y)dy \right) u_n(x) = \lambda u_n(x); \tag{171}$$

$Q(x,y) = \cos(x) - 25\exp(-x)(1 - \epsilon(\pi - y)^2)$ and $\phi_n(y) = \frac{1}{\sqrt{\pi}}\sin(\frac{ny}{2})$; $n, m = 1, 2, \ldots$.
The sum in (171) must be truncated to yield a suitable matrix problem. We shall
consider various choices of truncation in the numerics below.

The case $\epsilon = 0$ As a warm-up we checked the case $\epsilon = 0$, for which the prob-
lem (170) has a gap $(-0.08, 0.61)$ in the essential spectrum. In this case the matrix
potential becomes diagonal. Table 6.4 shows approximations of an isolated eigen-
value in this spectral gap using the shooting algorithm and the dissipative barrier
scheme, when the matrix (171) is truncated to $d = 5$, on a finite interval $[0, 6\pi]$. The
numerical integrations were performed using the projected RK45 method at different
tolerances, and the matching point for shooting was chosen to be $c = 2\pi$. On the
other hand, for the dissipative barrier technique, the PDE (170) was solved via the
finite element method implemented in the PDEtool solver. The waveguide is trun-
cated to $[0, 7] \times [0, 2\pi]$ and result is obtained after three mesh refinements, 3, 4 and
5, followed by Richardson's extrapolation, see Example 5.27 in Section 5.5 for more
details. Looking closely to results of Table 6.4, approximations of both methods are
agreed to six decimal places starting from 10^{-6}. The shooting method is marginally
cheaper, attaining better accuracy and a lower run time for tolerance 10^{-7}.

Shooting algorithm			Dissipative barrier	
Tol	eigenvalue	CPU[1]	eigenvalue	CPU[1]
10^{-5}	**0.36418**0151	3		
10^{-6}	**0.364188**400	6		
10^{-7}	**0.364188**628	10	**0.36418**887	13
10^{-8}	**0.364188**623	18		
10^{-9}	**0.364188**617	32		

[1] in seconds

Table 6.4: Approximations of an isolated eigenvalue of problem (170) when $\epsilon = 0$ using the proposed algorithm and the dissipative barrier technique.

The case $\epsilon > 0$ The essential spectrum of the PDE (170) when $\epsilon > 0$ is not known, but this does not prevent us from using our shooting method or the dissipative barrier technique. One of the eigenvalues obtained from solving the PDE using the dissipative barrier method and domain truncation, as described before, is $\lambda \approx 0.45599$. Therefore, we test the proposed algorithm on the interval $[0, 6\pi]$ with the projected RK45 and $c = 2\pi$ when the size the system (171) using $d = 5, 10, 15$. Figure 6.3 shows the integer-valued miss-distance $M(\lambda)$ for these values of d; only the cases $d = 10$ and $d = 15$ have discontinuities close to 0.45599. The value $d = 5$ is simply too small to yield good agreement between the PDE and the matrix Schrödinger equation.
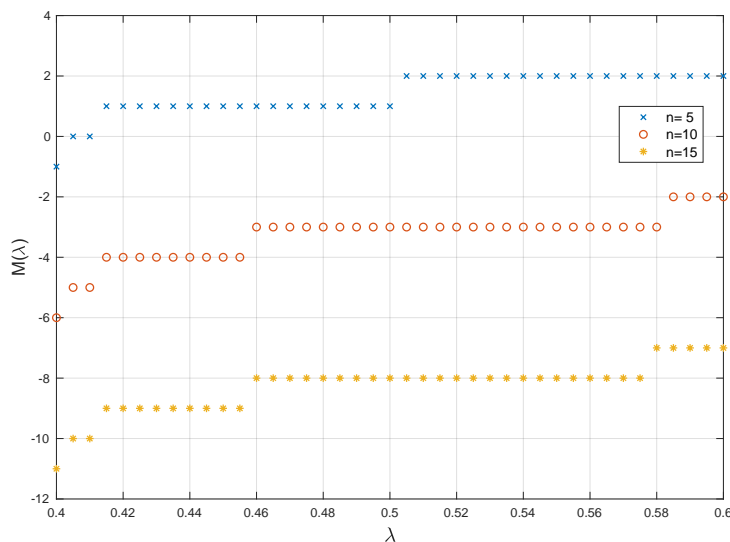

Figure 6.3: Plot of $M(\lambda)$ for the problem (171) when $\epsilon = 0.8$.

Table 6.5 and Table 6.6 show approximations of the underlying eigenvalue when the size of the system is 10 and 15 respectively. For each calculation we present the numerical value, the tolerance, and the CPU time for the computations. The difference between the shooting eigenvalues and the dissipative barrier eigenvalue is approximately 10^{-6} for $d = 10$ and 10^{-7} for $d = 15$, independently of the tolerance used for the shooting. From this it appears that

- the dominant source of error is semi-discretisation, i.e. the value of d;

- the dissipative barrier finite element method is remarkably accurate;

- the shooting method can win on CPU time - but only if we know which tolerance to use, which is not clear a priori.

Shooting algorithm, $d = 10$			Dissipative barrier	
Tol	eigenvalue	CPU[1]	eigenvalue	CPU[1]
10^{-5}	0.455989960936	4		
10^{-6}	0.455989997559	7		
10^{-7}	0.455989999695	13	0.45599186	13
10^{-8}	0.455989999962	23		
10^{-9}	0.455989999998	43		

[1] in seconds

Table 6.5: Approximations of an isolated eigenvalue of (170) when $\epsilon = 0.8$, comparing projected RK45 shooting with dissipative barrier plus finite elements. Here $d = 10$.

Shooting algorithm, $d = 15$			Dissipative barrier	
Tol	eigenvalue	CPU[1]	eigenvalue	CPU[1]
10^{-5}	0.455990968750	5		
10^{-6}	0.455990996094	9		
10^{-7}	0.455990999756	18	0.45599186	13
10^{-8}	0.455990999969	33		
10^{-9}	0.455990999996	60		

[1] in seconds

Table 6.6: Approximations of an isolated eigenvalue of (170) when $\epsilon = 0.8$, comparing projected RK45 shooting with dissipative barrier plus finite elements. Here $d = 15$.

6.5   Some remarks on the Magnus implementation

The Magnus method gives a mathematically elegant approach to the integration of the matrix differential equation (167), which does not require additional user interventions such as projections onto the unitary group. We have also seen that it is more expensive. Part of the reason is the difference in orders between the methods compared. However a much more significant contributor is that the matrix exponential is expensive to compute. The Matlab function `expm` uses precisely the scaling and squaring method to compute the matrix exponential which is based on the approximation:

$$e^A = (e^{2^{-s}A})^{2^s} \approx r_m(2^{-s}A)^{2^s},$$

where r_m is the $[m/m]$ Padé approximate to e^x and m and s are nonnegative integers chosen particularly to minimise machine computational cost, see [4, 87]. The implementation aims to deliver, whenever possible, results which are of comparable accuracy to those available from scalar-valued intrinsic functions. This is much more than we need for numerical solution of an initial value problem, even at the tightest feasible tolerance. The cost of the Magnus approach could, we believe, be substantially reduced by implementing lower-order approximations to `expm` which nevertheless preserve the property that $\exp(iH)$ is unitary when H is Hermitian.

6.6   Conclusion

We have shown that the integer-valued function $M(\lambda)$, which counts eigenvalues below the essential spectrum, is also well-defined and monotone increasing in each gap of the essential spectrum. Although, in general, it no longer counts eigenvalues in the gaps, its monotonicity in each gap means that all eigenvalues can be clearly identified. None is missed and it would be possible, with a careful implementation, to compute several eigenvalues at a time - though we did not do this here.

Of the matrix-based approaches (finite differences/elements) the only one which is guaranteed not to 'miss' an eigenvalue is the contour integral method, which is significantly more expensive in CPU time.

Combining finite difference/element methods with a dissipative barrier technique lifts eigenvalues away from the spectral gaps and hence out of the essential numerical range of the underlying operator. Arnoldi-type methods must then be used, as the problem becomes non-self-adjoint. These generally perform well, but there is the potential for the subspace iterations to fail to converge, with eigenvalues being missed. Our shooting method with $M(\lambda)$ avoids this problem.

Finally, projected RK45 is not as elegant a solution as the Magnus method for

unitary integration. To the already existing nineteen dubious ways to compute a matrix exponential [87] it would therefore be nice to add a twentieth, which performs the task with lower accuracy but greater speed, while preserving the property that the exponential of an anti-Hermitian matrix is unitary.

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