On the eigenvalues of spectral gaps of elliptic PDEs on waveguides

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Abstract. A method of calculating eigenvalues in the spectral gaps of self-adjoint elliptic partial differential equations on waveguides is presented. It is based on approximating the problem using domain truncation methods together with dissipative perturbation technique to the self-adjoint operator. The theoretical results essentially rely on the error estimate of Dirichlet-to-Neumann maps on the cross-section. The numerical examples show the efficiency of this approach.

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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. [24, 35]. There is therefore a keen interest in the study of spectral problems of band-gap structure of the differential operators on waveguides.

However it is well known that spectral approximation of selfadjoint problems with band-gap essential spectrum may lead to *spectral pollution*: the numerical approximation process may yield sequences of eigenvalues whose limit does not lie in the spectrum of the original problem. The term *spectral pollution* appears in 1981 in a paper of Rappaz [34] but the phenomenon had been noted before.

In the 1990s, several authors devised abstract methods which could be applied to any self-adjoint operator and which would avoid spectral pollution, at some cost. For example, Mertins and Zimmermann [39], Davies [12], and Davies and Plum [13] obtained enclosures to eigenvalues in spectral gaps which are based on combining min-max principles with a residual minimisation technique, which rejects approximate eigenvalues whose approximate eigenvectors do not come close to satisfying the appropriate eigenvalue equation. These methods rely on the spectral theorem for self-adjoint operators: they may not work well for non-selfadjoint operators, if the resolvent norm is large even very far from the spectrum [38]. Another abstract approach, which also relies on self-adjointness but which is generally more computationally efficient, is the method of second order relative spectra. Levitin and Shargorodsky [25] and Boulton and Levitin [8] applied this to perturbed periodic Schrödinger operators and computed upper and lower bounds of the discretised eigenvalues.

For special classes of operators, one may be able to devise classical projection methods which do not pollute. Lewin and Séré[26] described how this might be done for Schrödinger and Dirac operators of particular classes, though in practice the methods they describe are very difficult to realise unless one already has a very convenient decomposition of the operator (as in the Dirac case) or knows a great deal about the spectrum a priori. One special approach which requires little a-priori knowledge is the supercell method. This method turns a periodic PDE problem into a large-sized bounded domain problem with periodic boundary conditions. A Fourier method is then used for discretisation. The convergence of this method for two-dimensional problems, in particular, Maxwell's equation, was studied by Soussi [36]. Cancès et al. [10] proved that for a perturbed periodic Schrödinger operator the supercell method with Fourier bases is free from spectral pollution. The main disadvantage of this method is that the size of the supercell needs to be rather large in order to approximate an eigenfunction that is decaying slowly; thus the computation of the eigenvalues closes to the essential spectrum is costly.

In the present paper, which concerns waveguides, we concentrate on isolated eigenvalues of the elliptic differential expression $-\Delta + q$, in which q is any real, bounded potential having the property that when the expression $-\Delta + q$ is equipped with appropriate boundary conditions the resulting 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. The idea behind the dissipative barrier method is that if one has an eigenpair (λ, u) of a selfadjoint operator L, so that $Lu = \lambda u$, then without knowing too much about u one may nevertheless be able to choose a finite-rank, or relatively compact, operator s such that $su \approx u$. It follows that $(L + is)u \approx (\lambda + i)u$ and, setting aside possible concerns about pseudospectra, one may hope that the operator $L+is$ has an eigenvalue close to $\lambda + i$, which one may compute more easily by a variety of discretisation methods since it lies off the real axis and therefore is well separated from any spectral pollution. Of course it may also happen that $L + is$ has other eigenvalues which do not approximate those of L. A particularly illuminating analysis of dissipative barrier methods, both abstract and concrete, may be found in [41]; their combination with Galerkin methods is described in [42].

Dissipative barrier methods have their origins in computational chemistry, where they are often called *complex absorbing potential* methods. They have also been used to study quantum mechanical resonances, see [30, 31].

In this paper we suppose that a particular dissipative barrier has been fixed, and examine the process of approximating the resulting dissipative problem. 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 3.3 for the approximation of the Dirichlet-to-Neumann maps, Theorem 4.3 for absence of spectral pollution in the upper half plane, and Theorem 4.12 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. The name of Agmon [1] is often associated with such results, which have been proved in a variety of contexts, e.g. [4, 11, 14, 17]. For convenience we include the required result for our waveguide cases (Lemma 3.1), proved by a technique adapted from [20]. In [28], exponential decay was also used, but it was proved using Floquet theory and hence depended on periodicity in an essential way, which is avoided here. The results in [27], where the potentials are quite general but no convergence rates are given, could also be improved in a similar way. We have also included, for the reader's convenience, one result (Proposition 2.1) which describes how eigenvalues evolve when the dissipative barrier is 'switched on', though this is very similar to a theorem for ODEs in [3] and is not the main subject of the current work.

For the special case of periodic waveguides, our approach has both advantages and disadvantages compared to the methods of Joly et al. [21], Fliss [15], and Tausch and Butler [37]. While our analysis uses the Dirichlet-to-Neumann maps on cross-sections purely to prove theorems, and not for numerics, these papers exploit the additional periodicity assumption to construct approximations of the Dirichlet-to-Neumann maps. This approach avoids spectral pollution, but results in problems which are nonlinear in the spectral parameter. It is also more time-consuming to code. Another similar approach to the Dirichlet-to-Neumann maps was introduced by the first author in [44] in which matrix Schrödinger equations are considered. In [44], waveguides problems are discussed numerically, and the semi-discretisation is used to turn the waveguide problem to a family of matrix Schrödinger equations of arbitrarily high dimensions. Our own approach here can be implemented very quickly using off-the-shelf software for elliptic PDEs and large, sparse matrix eigenproblems. Of course our method also has its disadvantages, which we shall illustrate with numerical experiments in Section 5 below.

While our primary concern is with self-adjoint problems, there is also significant interest in non-selfadjoint waveguides, see e.g. [22, 32] which study the essential spectrum of the Laplacian operator equipped with complex

Robin boundary conditions, on waveguides, and derive 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 [23] and the many references therein.

The paper is organised as follows. In Section 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 3 establishes error bounds for truncated-domain approximations to the Dirichlet-to-Neumann maps. The main theorem is proved in Section 4. Finally, Section 5 represents some numerical examples to illustrate our results.

2. Preliminary and background theory

We consider the dissipative Schrödinger equation:

$$-\Delta u + (q + i\gamma s)u = \lambda u, \tag{2.1}$$

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. Homogeneous Dirichlet boundary conditions are imposed on the boundary of Ω. Fig. 1 illustrates the simplest model problem.

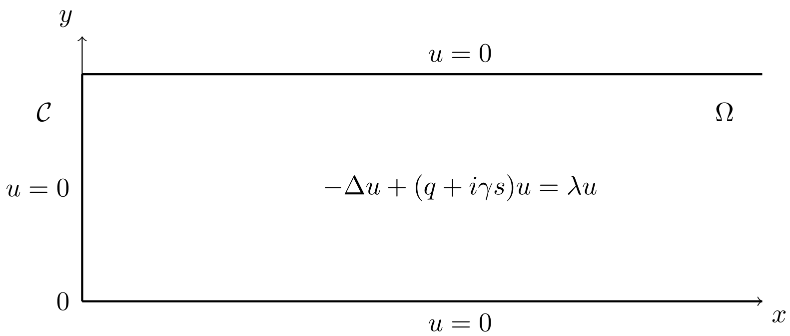

Figure 1. The domain of the semi infinite waveguide problem.

Associated with eqn. (2.1) and the Dirichlet boundary conditions is an operator L_0 on a domain $D(L_0) \subset L^2(\Omega)$; this operator will be described below. The parameter γ appearing in (2.1) 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

$$s(x, y) = \begin{cases} 1, & x < cR; \\ 0, & x \geq R. \end{cases} \tag{2.2}$$

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

$$L_0 u = (-\Delta + q)u, \tag{2.3}$$

with domain:

$$D(L_0) = \{\, u \in H^2_{loc}(\Omega) \cap H^1_0(\Omega) \mid (-\Delta + q)u \in L^2(\Omega)\}. \tag{2.4}$$

The following result describes the effect on an isolated, finite-multiplicity eigenvalue of introducing a dissipative barrier, and assumes exponential decay of the associated eigenfunctions (2.5), as discussed in Section 1.

Proposition 2.1. *Let λ be an isolated eigenvalue of L_0 with multiplicity ν, where $1 \le \nu \le n$, and normalised eigenvectors u_j, $j = 1, \dots, \nu$. For each sufficiently small $\gamma > 0$, let $\lambda_{\gamma,j}$, $j = 1, \dots, \nu$, be eigenvalues of the non-selfadjoint operator $L_0 + i\gamma s$ defined in* (2.3), (2.4) *with eigenvectors $u_{\gamma,j}$, $j = 1, \dots, \nu$, and suppose $\lambda_{\gamma,j} \to \lambda$ as $\gamma \to 0$. Then for each $1 \le j \le \nu$, the projection of $u_{\gamma,j}$ onto Span$\{u_1, \dots, u_\nu\}$ remains bounded away from zero, uniformly with respect to R and γ for sufficiently small γ.*
If, additionally, there exist functions $v_1, \dots, v_\nu \in L^2(\Omega)$, and a positive constant C_2, such that

$$u_j(x, \cdot) = v_j(x, \cdot)\exp(-C_2 x), \quad x \in [0, \infty), \quad j = 1, \dots, \nu, \tag{2.5}$$

then there exists $C_1 > 0$, independent of R, such that for all $R > 0$,

$$|\lambda + i\gamma - \lambda_{\gamma,j}| \le C_1 \gamma \exp(-cC_2 R), \tag{2.6}$$

where $c \in (0,1)$ is the constant appearing in assumption (2.2).

Proof. The existence of $\lambda_{\gamma,j}$ with $|\lambda_{\gamma,j} - \lambda| \to 0$ as $\gamma \to 0$ is a consequence of results in [43] on analytic families. Let Γ be a contour which encloses the spectral point λ of L_0, and no other points of the spectrum of L_0. Let γ be small enough to ensure that $\lambda_{\gamma,j}$, $j = 1, \dots, \nu$ are the only spectral points of $L_0 + i\gamma s$ inside Γ. Clearly, $\|s\|_\infty = 1$ independently of R; since L_0 is a self-adjoint operator then $|\lambda - \lambda_{\gamma,j}| \le \gamma$ independently of R; thus the requirement 'γ small enough' can be satisfied independently of R. Suppose $u_{\gamma,j}$, $j = 1, \dots, \nu$ are eigenvectors of $L_0 + i\gamma s$, linearly independent with $\|u_{\gamma,j}\| = 1$. Following [43, VII,§3], let $P(\gamma)$ be the projection onto the eigenspace of $L_0 + i\gamma s$ spanned by the $u_{\gamma,j}$, $j = 1, \dots, \nu$, 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

$$\|P(\gamma) - P(0)\| \le O(\gamma). \tag{2.7}$$

Since

$$P(0)u_{\gamma,j} = u_{\gamma,j} + (P(0) - P(\gamma))u_{\gamma,j}, \tag{2.8}$$

taking the norm of (2.8) and using (2.7) 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:

$$\langle (L_0 + i\gamma s)u_{\gamma,j}, u_k\rangle = \lambda_{\gamma,j}\langle u_{\gamma,j}, u_k\rangle. \tag{2.9}$$

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

$$\langle (L_0 - i\gamma I)u_k, u_{\gamma,j}\rangle = (\lambda - i\gamma)\langle u_k, u_{\gamma,j}\rangle. \tag{2.10}$$

Because L_0 and s are self-adjoint and u_k and $u_{\gamma,j}$ are in the domain of L_0, then from (2.10) we have:

$$\langle (L_0 + i\gamma I)u_{\gamma,j}, u_k\rangle = (\lambda + i\gamma)\langle u_{\gamma,j}, u_k\rangle. \tag{2.11}$$

From (2.9) and (2.11), we obtain:

$$|\lambda + i\gamma - \lambda_{\gamma,j}|\ \langle u_{\gamma,j}, u_k\rangle = i\gamma\langle (1-s)u_{\gamma,j}, u_k\rangle = i\gamma\langle u_{\gamma,j}, (1-s)u_k\rangle.$$

Since $P(0)u_{\gamma,j}$ is bounded away from zero, 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 (2.5) and (A2) we deduce

$$\|(1-s)u_k\| \leq C_1 \exp(-cC_2 R),$$

for some positive constants C_1 and C_2. The result is proved. □

We now give an informal description of the Glazman decomposition method [2] 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, $(0,\infty)\times\partial\mathcal{C}$. Thus our main boundary value problem (2.1) with boundary conditions illustrated in Fig. 1 can be described as the following:

$$\left.\begin{aligned} -\Delta u + (q + i\gamma s)u = \lambda u, &\quad \text{on} \quad \Omega_{(0,\infty)}; \\ u = 0, &\quad \text{on} \quad \partial\Omega_{(0,\infty)}. \end{aligned}\right\} \tag{2.12}$$

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 $\mathcal{C}$ we consider the two boundary value problems P_{left} and P_{right} described as the following:

$$P_{left} : \begin{cases} -\Delta v + (q + i\gamma s)v = \lambda v, & \text{on} \ \ \Omega_{(0,R)}; \\ v = 0, & \text{on} \ \ \Sigma_{(0,R)}; \\ v(R,y) = f(y), & y \in \mathcal{C}. \end{cases} \tag{2.13}$$

$$P_{right} : \begin{cases} -\Delta w + qw = \lambda w, & \text{on} \ \ \Omega_{(R,\infty)}; \\ w = 0, & \text{on} \ \ \Sigma_{(R,\infty)}; \\ w(R,y) = f(y), & y \in \mathcal{C}. \end{cases} \tag{2.14}$$

Note that P_{left} is uniquely solvable provided λ lies outside the spectrum of $-\Delta_D + q + i\gamma s$ in $\Omega_{(0,R)}$, where $-\Delta_D$ denotes the Dirichlet Laplacian. This condition may be assumed to hold without loss of generality, if necessary by increasing R slightly to move the spectrum. Similarly P_{right} is solvable provided λ lies outside the spectrum of $-\Delta_D + q$ in $\Omega_{(R,\infty)}$ - in particular, for real-valued q, P_{right} is uniquely solvable for all non-real λ. 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 [27], and in [5], 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 (2.13)-(2.14) 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 $L^2(\mathcal{C})$ to $H^{-1}(\mathcal{C})$; 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 $L^2(\mathcal{C})$ into $H^{1/2}(\mathcal{C})$.

Lemma 2.2. *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 $L^2(\mathcal{C})$ into N_{left} and N_{right} respectively. Furthermore, the 'normal derivative' operators Γ_{left} and Γ_{right} on $\mathcal{C}$ from the left and right respectively, may be defined on the ranges Ran(S_{left}) and Ran(S_{right}), in such a way that

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

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

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

where $\Delta_{\mathcal{C}}$ is the Laplace (or Laplace-Beltrami) operator on $\mathcal{C}$ with Dirichlet boundary conditions. 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

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

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

$$(S_{right}f)(x,y) = \sum_{n=1}^{\infty} \langle f, \psi_n \rangle \psi_n(y) \exp(-\sqrt{\mu_n}(x-R)). \tag{2.15}$$

A direct calculation shows that $\|S_{right}\| = 1/(2\sqrt{\mu_1})$. 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 $H_0^1(\mathcal{C})$,

$$\begin{aligned} \left| \left\langle - \left. \frac{\partial (S_{right} f)}{\partial x} \right|_{x=R}, u \right\rangle \right| &= \left| \sum_{n=1}^{\infty} \langle f, \psi_n \rangle \sqrt{\mu_n} \overline{\langle u, \psi_n \rangle} \right| \\ &\leq \left(\sum_{n=1}^{\infty} |\langle f, \psi_n \rangle|^2 \right)^{1/2} \left(\sum_{n=1}^{\infty} \mu_n |\langle u, \psi_n \rangle|^2 \right)^{1/2} = \|f\|_{L^2(\mathcal{C}_R)} \|u\|_{H_0^1(\mathcal{C}_R)}. \end{aligned}$$

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

While Lemma 2.2 deals with harmonic extensions, for later use it will be convenient to use a compactly supported extension. The following lemma guarantees this.

Lemma 2.3. *For any $f \in L^2(\mathcal{C})$, 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, $\|F\|_{L^2(\Omega_{(R,\infty)})} \leq C\|f\|_{L^2(\mathcal{C})}$, in which the constant C depends only on the geometry of the domain $\Omega_{(R,\infty)}$.*

Proof. Let $\tilde{F} = S_{right} f$;

from Lemma 2.2, $\tilde{F}$ has all the properties required for F apart from compact support. We therefore introduce a smooth cut-off function χ satisfying

$$\chi(x,y) = \begin{cases} 1, & \text{on} \quad \Omega_{(R,R+\delta)}; \\ 0, & \text{on} \quad \Omega_{(R+1,\infty)}; \end{cases}$$

here $\delta \in (0,1)$ is fixed. Also, χ can be chosen with trivial dependence on y; formally $\chi(x,y) = \chi(x)$. Note that $\nabla \chi(x,y) = 0$ outside $(R+\delta, R+1) \times \mathcal{C}$. We set $F := \chi \tilde{F}$, and observe that $F|_{\mathcal{C}_R} = f$, and $F|_{\Sigma_{(R,\infty)}} = 0$. Because $\tilde{F}$ is harmonic,

$$\Delta F = \Delta(\chi \tilde{F}) = (\Delta \chi) \tilde{F} + 2 \nabla \chi \cdot \nabla \tilde{F}, \tag{2.16}$$

and

$$\|\Delta F\|_{L^2(\Omega_{(R,\infty)})} \leq \|\Delta \chi\|_{L^\infty(\Omega)} \|\tilde{F}\|_{L^2(\Omega_{(R,\infty)})} + 2\|\nabla \chi \cdot \nabla \tilde{F}\|_{L^2(\Omega_{(R,\infty)})} \tag{2.17}$$

To estimate the L^2-norm of ΔF we estimate the L^2-norm of each term in (2.17). 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

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

Using the explicit expression for $F=S_{right}f$ in (2.15) we have

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

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

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

from which we see that

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

and hence

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

Using this in conjunction with (2.17) and bearing in mind that $\|\Delta\chi\|_{L^\infty(\Omega)}$ is bounded, we see that ΔF admits a bound $\|\Delta F\|_{L^2(\Omega_{(R,\infty)})}\le C\|f\|_{L^2(\mathcal{C})}$, as required. □

Lemma 2.4. *If $\lambda\notin\mathrm{Sp}(-\Delta_D+q+i\gamma s)$ in $\Omega_{(0,R)}$ and $\lambda\notin\mathrm{Sp}(-\Delta_D+q)$ in $\Omega_{(R,\infty)}$, then the Dirichlet-to-Neumann maps $M_{left}(\lambda)$ and $M_{right}(\lambda)$, defined initially for smooth functions defined on $\mathcal{C}$, admit extensions as bounded linear maps from $L^2(\mathcal{C})$ to $H^{-1}(\mathcal{C})$.*

Proof. As in the proof of Lemma 2.2, we consider just the case of M_{right}; the case of M_{left} is similar. Given $f\in L^2(\mathcal{C})$ we seek the solution w of problem P_{right} in (2.14) 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 $\Omega_{(R,\infty)}$ and since $\lambda \notin \mathrm{Sp}(-\Delta_D + q)$ in $\Omega_{(R,\infty)}$ we have

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

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,

$$M_{right}(\lambda) = \Gamma_{right}S_{right} + \Gamma_{right}(-\Delta_D + q - \lambda)^{-1}(\lambda - q)S_{right}. \quad (2.18)$$

Because q is bounded, $(-\Delta_D + q - \lambda)^{-1}$ is a bounded map from $L^2(\Omega_{(R,\infty)})$ to $H^2(\Omega_{(R,\infty)}) \cap H_0^1(\Omega_{(R,\infty)})$. 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 $H^{1/2}(\mathcal{C})$, which is compactly embedded in $H^{-1}(\mathcal{C})$. The result now follows from Lemma 2.2. □

Remark 2.5. It follows from the proof of this result that the principal symbol of M_{right}, regarded as a pseudodifferential operator of order 1, coincides with the principal symbol of $\Gamma_{right}S_{right}$. In particular, the principal symbol is independent of λ as long as λ lies in the resolvent set of $-\Delta_D + q$. Similar results hold for M_{left} and for $\Gamma_{left}S_{left}$. Indeed, abstract versions of these results in the context of the theory of boundary triples are available e.g. in [9].

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

Lemma 2.6. *If μ satisfies the conditions on λ stated in Lemma* 2.4*, then μ is an eigenvalue of $L_0 + i\gamma s$ if and only if* $\ker\left\{M_{left}(\mu) + M_{right}(\mu)\right\} \neq \{0\}$.

Proof. If μ satisfies the conditions on λ in Lemma 2.4 then $M_{left}(\mu)$ and $M_{right}(\mu)$ are well-defined. Suppose that μ is an eigenvalue of $L_0 + i\gamma s$, with eigenfunction u. Moreover, for the problems P_{left} and P_{right} respectively, take $v = u$ on $\Omega_{(0,R)}$ and $w = u$ on $\Omega_{(R,\infty)}$. Hence

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

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

$$\ker\left\{M_{left}(\mu) + M_{right}(\mu)\right\} \neq \{0\}. \quad (2.19)$$

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

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

where $v \in L^2(\Omega_{(0,R)})$ and $w \in L^2(\Omega_{(R,\infty)})$ are the solutions of P_{left} and P_{right} in (2.13)-(2.14) respectively when $\lambda = \mu$. Then $u \in L^2(\Omega)$ 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 $\mathcal{C}_R$. It follows that u is a weak (i.e. H_0^1) solution of the boundary value problem (2.12) with $\lambda = \mu$, so that by standard elliptic bootstrapping arguments [18] we have $u \in H^2_{loc}(\Omega) \cap H_0^1(\Omega)$. This means that $u \in D(L_0)$ and so u is an eigenfunction of L_0 with eigenvalue μ. □

We now truncate our semi-infinite waveguide problem (2.1) 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 $u(X, y) = 0$, $y \in \mathcal{C}$. The truncated problem is given by:

$$\left.\begin{aligned} -\Delta u + (q + i\gamma s)u = \lambda u, \quad &\text{on} \quad \Omega_{(0,X)}; \\ u = 0, \quad &\text{on} \quad \partial\Omega_{(0,X)}. \end{aligned}\right\} \tag{2.20}$$

The operator L_0 is replaced by L_X:

$$L_X u = (-\Delta + q)u, \tag{2.21}$$

with domain:

$$D(L_X) = \{u \in H^2_{loc}(\Omega_{(0,X)}) \cap H_0^1(\Omega_{(0,X)}) \mid (-\Delta + q)u \in L^2(\Omega_{(0,X)})\}. \tag{2.22}$$

Remark 2.7. Other boundary conditions are possible apart from $u(X, y) = 0$, $y \in \mathcal{C}$; the study of non-reflecting boundary conditions is a very active area of research. 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 (2.14) as the following

$$P_{right,X} : \begin{cases} -\Delta w + qw = \lambda w, \quad \text{on} \ \Omega_{(R,X)}; \\ \ w = 0, \quad \text{on} \ \partial\Omega_{(R,X)} \setminus \mathcal{C}_R; \\ \ w(R, y) = f(y), \quad y \in \mathcal{C}. \end{cases} \tag{2.23}$$

Again if the boundary value problems (2.13)-(2.23) can be solved uniquely for f, then we may define a map $M_{right,X}(\lambda)$ informally as follows

$$M_{right,X}(\lambda) w|_{\mathcal{C}_R} = - \left.\frac{\partial w}{\partial \nu}\right|_{\mathcal{C}_R}. \tag{2.24}$$

Following the ideas in Lemma 2.2 it is straightforward to prove that $M_{right,X}(\lambda)$ is, like $M_{right}(\lambda)$, a bounded linear map from $L^2(\mathcal{C})$ to $H^{-1}(\mathcal{C})$, with the same λ-independent principal symbol as $\Gamma_{right} S_{right}$. The following result is proved in the same way as Lemma 2.6, replacing M_{right} by $M_{right,X}$.

Corollary 2.8. *Suppose $X > R$. If μ does not lie in the spectrum of $-\Delta_D + q + i\gamma s$ in $\Omega_{(0,R)}$ and also does not lie in the spectrum of $-\Delta_D + q$ in $\Omega_{(R,X)}$, then μ is an eigenvalue of $L_X + i\gamma s$ if and only if* $\ker \left\{M_{left}(\mu) + M_{right,X}(\mu)\right\} \neq \{0\}$.

The following technical result will be useful in the sequel.

Lemma 2.9. *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 :*

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

Proof. Thanks to the simple geometry this can be proved by decomposing $u \in H_0^1 \cap H^2$ in a series of eigenfunctions of the cross-sectional Laplacian, tensor product with a Fourier sine transform in x. The calculations are similar to those in the proof of Lemma 2.2. □

3. Error bound of Dirichlet-to-Neumann maps

We start this section with an exponential decay result. While such results are well established in several contexts [4, 11, 14, 17, 20, 36], a proof is included for completeness. We assume that q is a bounded, real-valued potential.

Lemma 3.1. *Suppose v solves the boundary value problem:*

$$\left.\begin{aligned} (-\Delta + q - \lambda)v = -(-\Delta + q - \lambda)F, \quad &\textit{on} \quad \Omega_{(R,\infty)}; \\ v = 0, \quad &\textit{on} \quad \partial\Omega_{(R,\infty)}; \end{aligned}\right\} \tag{3.1}$$

where F is constructed as in Lemma 2.3 (in particular, $\mathrm{supp}(F) \subseteq \Omega_{(R,R+1)}$), and suppose $\mathrm{dist}(\lambda, \mathrm{Sp}((-\Delta_D + q)|_{\Omega_{(R,\infty)}})) > 0$. Then v admits a representation $v(x,\cdot) = \mathrm{e}^{-\alpha(x-R)}\tilde{v}(x,\cdot)$, where $\tilde{v} \in H^2_{loc}(\Omega_{(R,\infty)}) \cap H_0^1(\Omega_{(R,\infty)})$ and satisfies:

$$\|\tilde{v}\|_{H^2(\Omega_{(R,\infty)})} \leq C(\alpha, \lambda, \|q\|_{L^\infty(\Omega)})\|F\|_{L^2(\Omega_{(R,\infty)})},$$

in which $0 < \alpha < c\,\mathrm{dist}(\lambda, \mathrm{Sp}((-\Delta_D + q)|_{\Omega_{(R,\infty)}}))$, for some fixed $0 < c < 1$.

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

$$\begin{aligned} \mathrm{e}^{\alpha x}(-\Delta + q - \lambda)\mathrm{e}^{-\alpha x}\tilde{v} &= \mathrm{e}^{\alpha x}\Big(-\alpha^2 \mathrm{e}^{-\alpha x}\tilde{v} + 2\alpha \mathrm{e}^{-\alpha x}\frac{\partial \tilde{v}}{\partial x} + \mathrm{e}^{-\alpha x}(-\Delta + q - \lambda)\tilde{v}\Big) \\ &= (-\Delta + q - \lambda - \alpha^2)\tilde{v} + 2\alpha\frac{\partial \tilde{v}}{\partial x} \\ &= (T - \lambda - \alpha^2 + 2\alpha S)\tilde{v}, \end{aligned}$$

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:

$$\left.\begin{aligned} \mathrm{e}^{\alpha x}(-\Delta + q - \lambda)\mathrm{e}^{-\alpha x}\tilde{v} = \mathrm{e}^{\alpha(x-R)}F, \quad &\text{on} \quad \Omega_{(R,\infty)}; \\ \tilde{v} = 0, \quad &\text{on} \quad \partial\Omega_{(R,\infty)}. \end{aligned}\right\} \tag{3.2}$$

Recall that F is constructed as in Lemma 2.3; we deduce that $\mathrm{e}^{\alpha x}F$ is a compactly supported function with support contained in $\Omega_{(R,R+1)}$. Moreover, $\mathrm{e}^{\alpha(x-R)}F|_{\Sigma_{(R,\infty)}} = 0$, $\Delta(\mathrm{e}^{\alpha(x-R)}F) \in L^2(\Omega_{(R,\infty)})$, and $\mathrm{e}^{\alpha(x-R)}F \in$

$L^2(\Omega_{(R,\infty)})$ with a bound

$$\|\mathrm{e}^{\alpha(x-R)}F\|_{L^2(\Omega_{(R,\infty)})} \le \mathrm{e}^{\alpha}\|F\|_{L^2(\Omega_{(R,\infty)})}. \tag{3.3}$$

Solving (3.2) is equivalent to solving the operator equation

$$(T-\lambda-\alpha^2+2\alpha S)\tilde{v} = \mathrm{e}^{\alpha(x-R)}F. \tag{3.4}$$

Let $\Re(\lambda)\in(\eta,\zeta)$, where (η,ζ) is a spectral gap of the operator T. Thus our problem is uniquely solvable provided

$$\mathrm{dist}(\lambda,\mathrm{Sp}(T-\alpha^2)) = \min(|\lambda+\alpha^2-\eta|,|\zeta-\lambda-\alpha^2|)>0$$

and

$$2\alpha\|S(T-\lambda-\alpha^2)^{-1}\|_{L^2(\Omega_{(R,\infty)})\to H^1(\Omega_{(R,\infty)})}<1. \tag{3.5}$$

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

$$\|\omega\|_{L^2(\Omega_{(R,\infty)})} \le \|h\|_{L^2(\Omega_{(R,\infty)})}/\min(|\lambda+\alpha^2-\eta|,|\zeta-\lambda-\alpha^2|). \tag{3.6}$$

Moreover,

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

whence

$$\begin{aligned}\int_{\Omega_{(R,\infty)}}|\frac{\partial\omega}{\partial x}|^2 \le \int_{\Omega_{(R,\infty)}}|\nabla\omega|^2 \\ &\le \int_{\Omega_{(R,\infty)}}|(q-\lambda-\alpha^2)||\omega|^2+\epsilon\|\omega\|^2_{L^2(\Omega_{(R,\infty)})}+\frac{1}{4\epsilon}\|h\|^2_{L^2(\Omega_{(R,\infty)})} \\ &\le \big(|\lambda+\alpha^2|+\|q\|_{L^\infty(\Omega)}+\epsilon\big)\|\omega\|^2_{L^2(\Omega_{(R,\infty)})}+\frac{1}{4\epsilon}\|h\|^2_{L^2(\Omega_{(R,\infty)})} \\ &\le \left[\frac{|\lambda+\alpha^2|+\|q\|_{L^\infty(\Omega)}+\epsilon}{\min^2(|\lambda+\alpha^2-\eta|,|\zeta-\lambda-\alpha^2|)}+\frac{1}{4\epsilon}\right]\|h\|^2_{L^2(\Omega_{(R,\infty)})},\end{aligned}$$

in which the last inequality follows by (3.6). 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 (3.5) holds whenever α is small enough to ensure that

$$2\alpha\left[\frac{|\lambda+\alpha^2|+\|q\|_{L^\infty(\Omega)}+\epsilon}{\min^2(|\lambda+\alpha^2-\eta|,|\zeta-\lambda-\alpha^2|)}+\frac{1}{4\epsilon}\right]^{1/2}<1. \tag{3.7}$$

With all these calculations done, the solution $\tilde{v}$ of (3.4) exists and is unique. In addition, since

$$\int_{\Omega_{(R,\infty)}}|\nabla\tilde{v}|^2+\int_{\Omega_{(R,\infty)}}(q-\lambda-\alpha^2)|\tilde{v}|^2+2\alpha\int_{\Omega_{(R,\infty)}}\frac{\partial\tilde{v}}{\partial x}\overline{\tilde{v}} = \int_{\Omega_{(R,\infty)}}\mathrm{e}^{\alpha(x-R)}F\overline{\tilde{v}} \tag{3.8}$$

then taking the imaginary parts of (3.8) and using Young's inequality for $0<\delta<|\Im(\lambda)|$ yields

$$\|\tilde{v}\|^2_{L^2(\Omega_{(R,\infty)})} \leq \frac{1}{|\Im(\lambda)|-\delta}\Big[\frac{1}{4\delta}\|\mathrm{e}^{\alpha(x-R)}F\|^2_{L^2(\Omega_{(R,\infty)})}+\big(\delta+\frac{|\alpha|}{2\delta}\big)\|\tilde{v}\|^2_{H^1(\Omega_{(R,\infty)})}\Big]. \tag{3.9}$$

Moreover, (3.8) can be written as:

$$\int_{\Omega_{(R,\infty)}}|\nabla\tilde{v}|^2+\int_{\Omega_{(R,\infty)}}|\tilde{v}|^2=\int_{\Omega_{(R,\infty)}}\mathrm{e}^{\alpha(x-R)}F\overline{\tilde{v}}+\int_{\Omega_{(R,\infty)}}(\lambda-q+\alpha^2+1)|\tilde{v}|^2 \\ -2\alpha\int_{\Omega_{(R,\infty)}}\frac{\partial\tilde{v}}{\partial x}\overline{\tilde{v}}. \tag{3.10}$$

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 (3.10) with $\Re(\lambda-q+\alpha^2+1)\leq c$ we obtain:

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

Together with (3.3) and (3.9) 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:

$$\|\tilde{v}\|^2_{H^1_0(\Omega_{(R,\infty)})}\leq\tilde{C}\|F\|^2_{L^2(\Omega_{(R,\infty)})} \tag{3.11}$$

in which $\tilde{C}$ depends on λ,α, and $\|q\|_{L^\infty(\Omega_{(R,\infty)})}$. Furthermore, from (3.4) we have

$$-\Delta\tilde{v}=(\lambda-q+\alpha^2)\tilde{v}-2\alpha\frac{\partial\tilde{v}}{\partial x}+\mathrm{e}^{\alpha(x-R)}F.$$

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 (3.3)

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

Thus, from (3.11)

$$\|\Delta\tilde{v}\|_{L^2(\Omega_{(R,\infty)})}\leq C\|F\|_{L^2(\Omega_{(R,\infty)})}, \tag{3.12}$$

in which the constant C depends on λ,α, and $\|q\|_{L^\infty(\Omega_{(R,\infty)})}$. However, $v=\mathrm{e}^{-\alpha(x-R)}\tilde{v}$ is the solution of the original problem in (3.1) and using (3.11) we obtain a bound:

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

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

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

then

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

Inserting the estimates (3.11) and (3.12) in this inequality gives

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

again with C depending on λ, α, and $\|q\|_{L^\infty(\Omega_{(R,\infty)})}$. From Lemma 2.9 we conclude that $v \in H^2(\Omega_{(R,\infty)})$. □

Remark 3.2. The condition that appears in the proof, namely

$$\begin{aligned} \min(|\lambda+\alpha^2-\eta|, |\zeta-\lambda-\alpha^2|) &= \mathrm{dist}(\lambda+\alpha^2, \mathrm{Sp}(T)), \\ &\geq \mathrm{dist}(\lambda, \mathrm{Sp}(T)) - \alpha^2, \\ &\geq (1-c)^2\mathrm{dist}(\lambda, \mathrm{Sp}(T)). \end{aligned}$$

holds when $\alpha^2 < c\,\mathrm{dist}(\lambda, \mathrm{Sp}(T))$ for some $0 < c < 1$. However, Eq. (3.7) is satisfied if

$$2\alpha\left[\frac{|\lambda+\alpha^2| + ||q||_{L^\infty(\Omega)} + \epsilon}{(1-c)^4\mathrm{dist}^2(\lambda, \mathrm{Sp}(T))} + \frac{1}{4\epsilon}\right]^{1/2} < 1. \tag{3.13}$$

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

In the remainder of this section, we aim to prove that $M_{right,X}(\cdot)$ converges to $M_{right}(\cdot)$ at a certain rate. By applying Lemma 3.1 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 3.3. *Suppose $X > R$. Let $\lambda \in \mathbb{C} \setminus \mathbb{R}$ and suppose $\Re(\lambda) \in (\eta, \zeta)$, where (η, ζ) is a spectral gap of the Dirichlet operator $-\Delta + q$; $q \in L^\infty(\Omega)$, associated with the boundary value problem:*

$$\left.\begin{aligned} (-\Delta + q - \lambda)u = 0, \quad &on \quad \Omega_{(R,\infty)}; \\ u = 0, \quad &on \quad \partial\Omega_{(R,\infty)}. \end{aligned}\right\} \tag{3.14}$$

*Then there exist constants C and α_λ, as in Lemma (*3.1*), such that for all sufficiently large X*

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

Proof. Fix $f \in L^2(\mathcal{C})$. First, we prove the following inequality:

$$\|M_{right,X}(\lambda)f - M_{right}(\lambda)f\|_{H^{1/2}(\mathcal{C})} \leq c\|f\|_{L^2(\mathcal{C})}\exp(-\alpha_\lambda(X-R)). \tag{3.15}$$

By Lemma 2.3, there exists a function F with $\mathrm{supp}(F) \subset \Omega_{(R,X)}$ such that $F|_{\mathcal{C}_R} = f, F|_{\Sigma_{(R,\infty)}} = 0$, $F \in L^2(\Omega)$, $\Delta F \in L^2(\Omega)$, and

$$\|F\|_{L^2(\Omega)} \leq C\|f\|_{L^2(\mathcal{C})}. \tag{3.16}$$

Define $u := F + v$ and $u_X := F + v_X$ in which v and v_X are the solutions of the boundary value problems:

$$\left.\begin{aligned} (-\Delta+q-\lambda)v=-(-\Delta+q-\lambda)F=:G_\lambda, \quad \text{on} \quad \Omega_{(R,\infty)};\\ v=0, \quad \text{on} \quad \partial\Omega_{(R,\infty)}. \end{aligned}\right\} \tag{3.17}$$

$$\left.\begin{aligned} (-\Delta+q-\lambda)v_X=G_\lambda, \quad \text{on} \quad \Omega_{(R,X)};\\ v_X=0, \quad \text{on} \quad \partial\Omega_{(R,X)}. \end{aligned}\right\} \tag{3.18}$$

Then

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

and so we proceed to estimate $v-v_X$.

Observe that $G_\lambda := -(-\Delta+q-\lambda)F$ lies in L^2 since ΔF is in L^2, $q\in L^\infty(\Omega)$, and F in L^2. Moreover, G_λ inherits a compact support from F. We note that since $q\in L^\infty(\Omega)$, from Lemma 3.1 the solution v has the form $v=\mathrm{e}^{-\alpha_\lambda(x-R)}\tilde{v}$, where $\tilde{v}\in H^2_{loc}\cap H^1_0$ and α_λ satisfies $\alpha_\lambda<\operatorname{dist}(\lambda,\operatorname{Sp}(-\Delta_D+q)|_\Omega)$. We wish to obtain an estimate for $v-v_X$ in H^2 which, from Lemma 2.9, is equivalent to obtaining an estimate of $\|v-v_X\|_{L^2(\Omega_{(R,X)})}+\|\Delta(v-v_X)\|_{L^2(\Omega_{(R,X)})}$. To do so, let χ_X be a smooth cut-off function with

$$\operatorname{supp}(\chi_X)\subseteq\Omega_{(R,X)},\quad \operatorname{supp}(\nabla\chi_X)\subseteq\Omega_{(X-1,X)},\quad \|\nabla\chi_X\|_{L^\infty(\Omega)}\le 2, \tag{3.19}$$

and define $w_X:=\chi_X v-v_X$ which satisfies a BVP of the form

$$\left.\begin{aligned} (-\Delta+q-\lambda)w_X=g_X, \quad \text{on} \quad \Omega_{(R,X)};\\ w_X=0, \quad \text{on} \quad \partial\Omega_{(R,X)}. \end{aligned}\right\} \tag{3.20}$$

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

$$\begin{aligned} g_X:=(-\Delta+q-\lambda)w_X&=(-\Delta+q-\lambda)(\chi_X v-v_X)\\ &=(-\Delta+q-\lambda)(\chi_X v-v+v-v_X)\\ &=(-\Delta+q-\lambda)(\chi_X-1)v. \end{aligned}$$

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

$$g_X=-(\partial_x^2\chi_X)v-2(\partial_x\chi_X)(\partial_x v)+(\chi_X-1)(-\Delta v+(q-\lambda)v). \tag{3.21}$$

Note that by (3.19), the representation of $v=\mathrm{e}^{-\alpha_\lambda(x-R)}\tilde{v}$ and Lemma 3.1,

$$\begin{aligned} \|(\partial_x^2\chi_X)v\|^2{}_{L^2(\Omega_{(R,X)})}&=\int_{\Omega_{(R,X)}}(\partial_x^2\chi_X)^2v^2\\ &\le\|(\partial_x^2\chi_X)\|^2_{L^\infty(\Omega_{(X-1,X)})}\int_{\mathcal{C}}\int_{X-1}^{X}\exp(-2\alpha_\lambda(x-R))\tilde{v}^2\mathrm{d}x\mathrm{d}y,\\ &\le\|(\partial_x^2\chi_X)\|^2_{L^\infty(\Omega_{(X-1,X)})}\|\tilde{v}\|^2_{L^2(\Omega_{(R,X)})}\exp(-2\alpha_\lambda(X-R)),\\ &\le c_1\|F\|^2_{L^2(\Omega_{(R,X)})}\exp(-2\alpha_\lambda(X-R)), \end{aligned} \tag{3.22}$$

where c_1 is a constant depending on α_λ. Similarly, and since $\tilde{v}$ is in $H^2_{loc} \cap H^1_0$, then $\partial_x \tilde{v}$ is in $L^2(\Omega_{(R,X)})$, so we have:

$$\begin{aligned}
\|(\partial_x\chi_X)(\partial_x v)\|^2{}_{L^2(\Omega_{(R,X)})} &= \int_{\Omega_{(R,X)}} (\partial_x\chi_X)^2(\partial_x v)^2, \\
&\leq \|(\partial_x\chi_X)\|^2_{L^\infty(\Omega_{(X-1,X)})}\big[[\|\tilde{v}\|^2_{L^2(\Omega_{(R,X)})}\exp(-2\alpha_\lambda(X-R))] \\
&+ [\|\partial_x\tilde{v}\|^2_{L^2(\Omega_{(R,X)})}\exp(-2\alpha_\lambda(X-R))]\big], \\
&\leq c_2\|F\|^2_{L^2(\Omega_{(R,X)})}\exp(-2\alpha_\lambda(X-R)),
\end{aligned} \tag{3.23}$$

where c_2 is a constant depending on α_λ. To handle the last term of (3.21), observe that by (3.19) we know that

$$\begin{aligned}
\|(\chi_X-1)(-\Delta+q-\lambda)v\|^2_{L^2(\Omega_{(R,X)})} &= \int_{\Omega_{(R,X)}} (\chi_X-1)^2\big[(-\Delta+q-\lambda)v\big]^2, \\
&\leq \|(\chi_X-1)\|^2_{L^\infty(\Omega_{(R,X)})}\int_{\mathcal{C}}\int_{X-1}^{X}\big[(-\Delta+q-\lambda)v\big]^2\mathrm{d}x\mathrm{d}y, \\
&\leq \|(\chi_X-1)\|^2_{L^\infty(\Omega_{(R,X)})}\int_{\mathcal{C}}\int_{X-1}^{X}\exp(-2\alpha_\lambda(x-R)) \\
&\big[(-\Delta+q-\lambda)\tilde{v}+2\alpha_\lambda\partial_x\tilde{v}-\alpha_\lambda^2\tilde{v}\big]^2\mathrm{d}x\mathrm{d}y.
\end{aligned} \tag{3.24}$$

Since we have, from Lemma 3.1, a bound $\|\tilde{v}\|_{H^2} \leq C\|F\|_{L^2}$, and since $\mathrm{supp}(F) \subseteq \Omega_{(R,X)}$ for all sufficiently large X, we may combine (3.22), (3.23), and (3.24) in (3.21) to obtain the estimate:

$$\|g_X\|_{L^2(\Omega_{(R,X)})} \leq C\|F\|_{L^2(\Omega_{(R,X)})}\exp(-\alpha_\lambda(X-R)), \tag{3.25}$$

where C is a constant independent of F.

Having estimated g_X we may now consider the BVP in (3.20). Taking inner products in the usual way gives

$$\int_{\Omega_{(R,X)}} (|\nabla w_X|^2 + (q-\lambda)|w_X|^2) = \int_{\Omega_{(R,X)}} g_X\overline{w_X}. \tag{3.26}$$

Taking imaginary parts of (3.26) and using the fact that q is real-valued, we obtain

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

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

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

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

$$\|w_X\|^2_{L^2(\Omega_{(R,X)})} \leq \frac{1}{4\delta[|\Im(\lambda)|-\delta]}\|g_X\|^2_{L^2(\Omega_{(R,X)})}; \tag{3.27}$$

upon using (3.25) we have the bound

$$\|w_X\|_{L^2(\Omega_{(R,X)})} \leq C\|F\|_{L^2(\Omega_{(R,X)})}\exp(-\alpha_\lambda(X-R)), \tag{3.28}$$

where C is a constant independent of F. Moreover, from the BVP in (3.20),

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

Since $q \in L^\infty(\Omega)$, and using (3.25), (3.28),

$$\begin{aligned}\|\Delta w_X\|_{L^2(\Omega_{(R,X)})} &\leq \|g_X\|_{L^2(\Omega_{(R,X)})} + \|\lambda - q\|_{L^\infty(\Omega_{(R,X)})}\|w_X\|_{L^2(\Omega_{(R,X)})}, \\ &\leq C\|F\|_{L^2(\Omega_{(R,X)})} \exp(-\alpha_\lambda(X - R)). \end{aligned} \tag{3.29}$$

Recalling that $w_X = \chi_X v - v_X = v - v_X$, from (3.28), (3.29) and Lemma 2.9 we conclude that

$$\|v - v_X\|_{H^2(\Omega_{(R,X)})} \leq c\|F\|_{L^2(\Omega)} \exp(-\alpha_\lambda(X - R));$$

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

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

but

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

Thus

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

and the inequality (3.15) follows immediately from the bound $\|F\|_{L^2(\Omega)} \leq C\|f\|_{L^2(\mathcal{C})}$ in Lemma 2.3, where C is a constant depends only on the domain of f and independent of f. The result follows upon taking sup over all $\|f\|_{L^2(\mathcal{C})} = 1$. □

4. Application to spectral problems

To state and prove our main result, we introduce some notation and technical lemmas.

Lemma 4.1. *Suppose $\Im(\lambda) > 0$ and suppose that*

$$\|M_{right,X}(\cdot) - M_{right}(\cdot)\|_{L^2(\mathcal{C})\to H^{1/2}(\mathcal{C})} \to 0 \text{ as } X \to \infty, \tag{4.1}$$

uniformly in a neighbourhood of $\lambda \in \mathbb{C}$ in which $M_{left}(\cdot)$ is well defined. 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

$$\begin{aligned} M_{left}(\cdot) + M_{right,X}(\cdot) &= \big(M_{left}(\cdot) + M_{right}(\cdot)\big) \\ &\quad \times \Big[I + \big(M_{left}(\cdot) + M_{right}(\cdot)\big)^{-1}\big(M_{right,X}(\cdot) - M_{right}(\cdot)\big)\Big]. \end{aligned}$$

The result follows immediately using this and the assumption (4.1), which implies that

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

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

$$\begin{aligned}M_{left}(\cdot)+M_{right}(\cdot)&=\big(M_{left}(\cdot)+M_{right,X}(\cdot)\big)\\&\quad\times\Big[I+\big(M_{left}(\cdot)+M_{right,X}(\cdot)\big)^{-1}\big(M_{right}(\cdot)-M_{right,X}(\cdot)\big)\Big].\end{aligned}$$

□

Theorem 4.2. *Suppose* $\lambda\in\mathrm{Sp}(L_0+i\gamma s)$, $\Im(\lambda)>0$. *Then* $\exists\,\lambda_X\in\mathrm{Sp}(L_X+i\gamma s)$ *such that* $\lambda_X\to\lambda$ *as* $X\to\infty$.

Proof. Since only the essential spectrum of $L_0+i\gamma s$ is real, λ must be an eigenvalue of $L_0+i\gamma s$. By Remark 2.5 we may assume without loss of generality that $M_{left}(\cdot)$ is well defined on a neighbourhood of λ. 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 a contour Γ (arbitrarily small) surrounding λ, see Fig. 2, such that $L_X+i\gamma s$ has no eigenvalues in a neighbourhood enclosed by Γ.

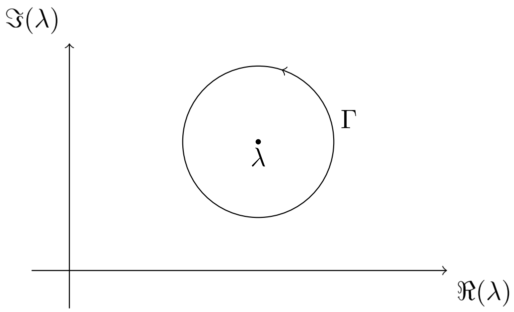

FIGURE 2. A contour Γ surrounding the eigenvalue λ.

This means that $M_{left}(\cdot)+M_{right,X}(\cdot)$ is invertible in a neighbourhood of Γ. From the Cauchy Theorem:

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

However from Theorem 3.3 and Lemma 4.1, this means that

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

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, $\ker\big\{M_{left}(\lambda)+M_{right}(\lambda)\big\}=\{0\}$, so λ is not in $\mathrm{Sp}(L_0+i\gamma s)$ by Lemma 2.6. □

Theorem 4.3. *Suppose* $\lambda_X \in \mathrm{Sp}(L_X + i\gamma s)$; $\lambda_X \to \lambda$, *with* $\Im(\lambda) > 0$. *Then* $\lambda \in \mathrm{Sp}(L_0 + i\gamma s)$.

Proof. Assume for a contradiction that $\lambda \notin \mathrm{Sp}(L_0 + i\gamma s)$. Hence λ is in the resolvent of $L_0 + i\gamma s$, which is open, so 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 4.1. Following Theorem 3.3, 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 4.1, the operator $M_{left}(\cdot) + M_{right,X}(\cdot)$ is invertible in a neighbourhood of λ for all sufficiently large X. From Lemma 2.6, $\ker\left\{M_{left}(\cdot) + M_{right,X}(\cdot)\right\} = \{0\}$ in a neighbourhood of λ. Hence, there are no eigenvalues of $L_X + i\gamma s$ in a neighbourhood of λ. This contradicts the assumption that $\lambda_X \in \mathrm{Sp}(L_X + i\gamma s)$ converges to λ. □

Lemma 4.4. *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* $L^2(\mathcal{C})$ *into* $H^{1/2}(\mathcal{C})$. *Similarly, if* $M_{right}(\lambda)$ *and* $M_{right}(\lambda^\dagger)$ *are well defined then* $M_{right}(\lambda) - M_{right}(\lambda^\dagger)$ *maps* $L^2(\mathcal{C})$ *into* $H^{1/2}(\mathcal{C})$.

Proof. We present the proof for M_{right}; the proof for M_{left} is similar. Using (2.18) in the proof of Lemma 2.4, 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 $L^2(\mathcal{C})$, the operator S_{right} maps into $L^2(\Omega_{(R,\infty)})$. In turn, the resolvent $(-\Delta_D + q - \lambda^\dagger)^{-1}$ maps $L^2(\Omega_{(R,\infty)})$ into $H_0^1(\Omega_{(R,\infty)}) \cap H^2(\Omega_{(R,\infty)})$. Applying the normal derivative operator Γ_{right} loses $3/2$ orders of smoothness, taking the final image into $H^{1/2}(\mathcal{C})$. □

Lemma 4.5. *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* $H^{-1}(\mathcal{C})$ *to* $L^2(\mathcal{C})$.

Proof. Let $M_{left}(\lambda, 0)$ and $M_{right}(\lambda, 0)$ be the Dirichlet-to-Neumann maps defined from the problems (2.13) and (2.14), respecetively, when $q \equiv 0$ and $s \equiv 0$. An explicit calculation using separation of variables, following the method in the proof of Lemma 2.2, 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 $H^{-1}(\mathcal{C})$ to $L^2(\mathcal{C})$. This completes the proof when the coefficients q and s are trivial.

By using the Hilbert resolvent identity in a manner analogous to the proof of Lemma 4.4, we have 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 $\tilde{N}_{q,s}(\lambda)$ map from $L^2(\mathcal{C}) \to H^{1/2}(\mathcal{C})$; for instance, one may use eqn. (2.18) of Lemma 2.4 to see that

$$\begin{aligned} N_q(\lambda) &= M_{right}(\lambda) - M_{right}(\lambda,0) \\ &= \Gamma_{right}(-\Delta_D + q - \lambda)^{-1}(-\lambda q(-\Delta_D - \lambda)^{-1} - q)S_{right}, \end{aligned}$$

together with a similar expression for $\tilde{N}_{q,s}(\lambda)$; the fact that $N_q(\lambda)$ maps $L^2(\mathcal{C})$ to $H^{1/2}(\mathcal{C})$ then follows from the fact that $\Gamma_{right}(-\Delta_D + q - \lambda)^{-1}$ maps from $L^2(\Omega_{(R,\infty)})$ to $H^{1/2}(\mathcal{C})$, see the proof of Lemma 2.4.

We have therefore established $M_{left}(\lambda) + M_{right}(\lambda)$ is a compact perturbation of $M_{left}(\lambda,0) + M_{right}(\lambda,0)$. Since all the M-operators are analytic functions [9], the Analytic Fredholm Theorem lifts the result from the case $q \equiv 0$, $s \equiv 0$ to the general case.

For $M_{left}(\lambda) + M_{right,X}(\lambda)$ the proof is essentially the same, starting from the formula

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

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

□

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

$$\begin{aligned} K(\lambda) =& \big(M_{left}(\lambda^\dagger) + M_{right}(\lambda^\dagger)\big)^{-1} \\ &\times \big(M_{left}(\lambda) - M_{left}(\lambda^\dagger) + M_{right}(\lambda) - M_{right}(\lambda^\dagger)\big), \end{aligned} \tag{4.2}$$

so that

$$\big(M_{left}(\lambda^\dagger) + M_{right}(\lambda^\dagger)\big)^{-1}\big(M_{left}(\lambda) + M_{right}(\lambda)\big) = I + K(\lambda). \tag{4.3}$$

Similarly, if

$$\begin{aligned} K_X(\lambda) =& \left(M_{left}(\lambda^\dagger) + M_{right,X}(\lambda^\dagger) \right)^{-1} \\ &\times \left(M_{left}(\lambda) - M_{left}(\lambda^\dagger) + M_{right,X}(\lambda) - M_{right,X}(\lambda^\dagger) \right) \end{aligned} \tag{4.4}$$

then

$$\begin{aligned} K(\lambda) - K_X(\lambda) =& (I - (I + Q^{-1}(\lambda^\dagger)E_X(\lambda^\dagger))^{-1})Q^{-1}(\lambda^\dagger)R(\lambda) \\ &- (I + Q^{-1}(\lambda^\dagger)E_X(\lambda^\dagger))^{-1}Q^{-1}(\lambda^\dagger)\tilde{E}_X(\lambda), \end{aligned} \tag{4.5}$$

in which

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

We observe the following results.

Lemma 4.6. *If $M_{left}(\lambda)$ is well-defined then λ is an eigenvalue of $L_0 + i\gamma s$ if and only if $I + K(\lambda)$ has a nontrivial kernel.*

Proof. Assume that λ is an eigenvalue of $L_0 + i\gamma s$ then from Lemma 2.6 $\ker\left\{M_{left}(\lambda) + M_{right}(\lambda)\right\} \neq \{0\}$. Following the formula of $I + K(\lambda)$ in (4.3) we derive the desired result; the converse reasoning is analogous. □

Definition 4.7. For $0 < p < \infty$, the Schatten p-class, $\mathfrak{S}_p$, is the class of all compact operators T in a Hilbert space such that

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

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

$\mathfrak{S}_1$ is called the trace class and $\mathfrak{S}_2$ is the Hilbert-Schmidt class. See e.g., Gohberg et al. [19] for basic properties of Schatten classes.

Lemma 4.8. *If $p > 2\dim(\mathcal{C})$ then $K(\lambda)$ and $K_X(\lambda)$ lie in the Schatten p-class $\mathfrak{S}_p$.*

Proof. We obtain, from (4.2), (4.4) and Lemmas 4.4 and 4.5, the following diagrams, in which J_1 and J_2 are imbeddings:

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

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

In fact, since the cross-section $\mathcal{C}$ is bounded then the Sobolev imbedding J_1 belongs to Schatten class $\mathfrak{S}_p$ for $p > 2\dim(\mathcal{C})$ (see [29]). 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 $\|AB\|_p \le \|A\|\|B\|_p$,

$$\begin{aligned}
&\|K(\lambda)\|_p = \|Q^{-1}(\lambda^\dagger)R(\lambda)\|_p = \|Q^{-1}(\lambda^\dagger)J_2J_1R(\lambda)\|_p\\
&\le \|Q^{-1}(\lambda^\dagger)J_2\|_{L^2(\mathcal{C})\to L^2(\mathcal{C})}\|J_1R(\lambda)\|_p\\
&\le C\|Q^{-1}(\lambda^\dagger)J_2\|_{L^2(\mathcal{C})\to L^2(\mathcal{C})}\|R(\lambda)\|_{L^2(\mathcal{C})\to H^{1/2}(\mathcal{C})},
\end{aligned}$$

the last inequality holding for $p > 2\dim(\mathcal{C})$; similar reasoning applies to $K_X(\lambda)$. $\square$

Lemma 4.9. *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, see [9], in the natural norm for maps from $L^2(\mathcal{C})$ to $H^{1/2}(\mathcal{C})$. Note that $K(\lambda)$ is analytic in the $\mathfrak{S}_p$-norm for λ in the domain of analyticity of $M_{left}(\lambda) + M_{right}(\lambda)$, see Lemma 2.4; $K_X(\lambda)$ is analytic in the $\mathfrak{S}_p$-norm for λ in the domain of analyticity of $M_{left}(\lambda) + M_{right,X}(\lambda)$, see Corollary 2.8. 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 [40]. A brief summary is included in the Appendix.

Lemma 4.10. *If $M_{left}(\lambda)$ is well-defined then λ is an eigenvalue of $L_0 + i\gamma s$ if and only if $\det_p(I + K(\lambda)) = 0$.*

Proof. If λ is an eigenvalue of $L_0 + i\gamma s$ then from Lemma 4.6 $I + K(\lambda)$ has nontrivial kernel. The proof follows directly from [19] since $K(\lambda) \in \mathfrak{S}_p$. The converse reasoning is similar. $\square$

Proposition 4.11. *Suppose $X > R$. If $p > 2\dim(\mathcal{C})$ then*

$$\|K(\lambda) - K_X(\lambda)\|_p \leq c \exp(-\alpha_\lambda (X - R)); \tag{4.6}$$

c is a constant depending on α_λ which is chosen as in Lemma 3.1. Moreover,

$$|\det_p(I + K(\lambda)) - \det_p(I + K_X(\lambda))| \leq C \exp(-\alpha_\lambda (X - R)); \tag{4.7}$$

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 (4.5), we start by considering $Q^{-1}(\lambda^\dagger) E_X(\lambda^\dagger)$:

$$Q^{-1}(\lambda^\dagger) E_X(\lambda^\dagger) : L^2(\mathcal{C}) \xrightarrow{E_X(\lambda^\dagger)} H^{1/2}(\mathcal{C}) \overset{J_1}{\hookrightarrow} L^2(\mathcal{C}) \overset{J_2}{\hookrightarrow} H^{-1}(\mathcal{C}) \xrightarrow{Q^{-1}(\lambda^\dagger)} L^2(\mathcal{C}).$$

Here we apply the chain of inequalities

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

provided p is such that the imbedding J_1 is Schatten class, i.e, $p > 2\dim(\mathcal{C})$. Hence

$$\|Q^{-1}(\lambda^\dagger) E_X(\lambda^\dagger)\|_p \leq C_1 \|E_X(\lambda^\dagger)\|_{L^2(\mathcal{C}) \to H^{1/2}(\mathcal{C})}, \tag{4.8}$$

where C_1 is independent of X. Inserting this estimate into the first term of (4.5) and using $\|AB\|_p \le \|A\|_p\|B\|$, for $A \in \mathfrak{S}_p$ and a bounded B, we have:

$$\begin{aligned}
&\|I - (I + Q^{-1}(\lambda^\dagger)E_X(\lambda^\dagger))^{-1}Q^{-1}(\lambda^\dagger)R(\lambda)\|_p \\
&\quad = \|(Q^{-1}(\lambda^\dagger)E_X(\lambda^\dagger))\sum_{n=0}^{\infty}(Q^{-1}(\lambda^\dagger)E_X(\lambda^\dagger))^n Q^{-1}(\lambda^\dagger)R(\lambda)\|_p \\
&\quad \le \|Q^{-1}(\lambda^\dagger)E_X(\lambda^\dagger)\|_p \|\sum_{n=1}^{\infty}(Q^{-1}(\lambda^\dagger)E_X(\lambda^\dagger))^n\| \|Q^{-1}(\lambda^\dagger)R(\lambda)\|_{L^2(\mathcal{C})\to L^2(\mathcal{C})}
\end{aligned}$$

provided $p > 2\dim(\mathcal{C})$. Hence, using (4.8):

$$\begin{aligned}
&\|I - (I + Q^{-1}(\lambda^\dagger)E_X(\lambda^\dagger))^{-1}Q^{-1}(\lambda^\dagger)R(\lambda)\|_p \\
&\quad \le \|Q^{-1}(\lambda^\dagger)E_X(\lambda^\dagger)\|_p \frac{1}{1 - \|Q^{-1}(\lambda^\dagger)E_X(\lambda^\dagger)\|} \|Q^{-1}(\lambda^\dagger)R(\lambda)\|_{L^2(\mathcal{C})\to L^2(\mathcal{C})} \\
&\quad \le C\|E_X(\lambda^\dagger)\|_{L^2(\mathcal{C})\to H^{1/2}(\mathcal{C})}; \qquad (4.9)
\end{aligned}$$

where C is a constant independent of X. For the second term of the right hand side of (4.5) the same ideas can be applied to the term $Q^{-1}(\lambda^\dagger)\tilde{E}_X(\lambda)$ to obtain the $\mathfrak{S}_p$-norm:

$$\|Q^{-1}(\lambda^\dagger)\tilde{E}_X(\lambda)\|_p \le C_2\|\tilde{E}_X(\lambda)\|_{L^2(\mathcal{C})\to H^{1/2}(\mathcal{C})};$$

again C_2 is independent of X. Therefore, the estimate of the second term of (4.5) becomes

$$\|(I + Q^{-1}(\lambda^\dagger)\tilde{E}_X(\lambda))^{-1}Q^{-1}(\lambda^\dagger)\tilde{E}_X(\lambda)\|_p \le \tilde{C}\|\tilde{E}_X(\lambda)\|_p. \qquad (4.10)$$

Inserting the Inequalities (4.9) and (4.10) in (4.5) we derive the following estimate:

$$\|K(\lambda) - K_X(\lambda)\|_p \le C\|E_X(\lambda)\|_{L^2(\mathcal{C})\to H^{1/2}(\mathcal{C})} + \tilde{C}\|\tilde{E}_X(\lambda)\|_{L^2(\mathcal{C})\to H^{1/2}(\mathcal{C})}.$$

Employing Theorem 3.3 on $E_X(\lambda^\dagger)$ and $\tilde{E}_X(\lambda)$ on the corresponding domain $\Omega_{(R,\infty)}$ leads to the desired estimate (4.6), locally uniformly with respect to λ, where c is a constant depending on α_λ.
Now in order to obtain (4.7), we use Theorem 2.2 of [19, p.194], to obtain

$$|\det_p(I + K(\lambda)) - \det_p(I + K_X(\lambda))| \le C\|K(\lambda) - K_X(\lambda)\|_p, \qquad (4.11)$$

where C is a constant independent of X. Hence (4.7) is obtained by inserting (4.6) into (4.11). □

We can now put the previous lemmas together to derive the following key result.

Theorem 4.12. *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 (2.3,2.4). 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 (2.21,2.22) which satisfies*

$$|\lambda_\gamma - \lambda_{\gamma,X}| \le C_3\exp(-C_4(X - R)), \qquad (4.12)$$

where C_3 and C_4 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 2.6:

$$\ker\left\{M_{left}(\lambda_\gamma) + M_{right}(\lambda_\gamma)\right\} \neq \{0\}.$$

Consequently, the existence of the approximating eigenvalues $\lambda_{\gamma,X}$ follows immediately from Theorem 4.2. Next, in order to obtain the estimate (4.12), observe that since λ_γ 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 (4.2) and (4.3) make sense. Furthermore, the corresponding truncated problem generates $K_X(\lambda)$ which is given by (4.4). Moreover, from Lemma 4.8 $K(\lambda)$ and $K_X(\lambda)$ lie in Schatten class $\mathfrak{S}_p$ with $p > 2\dim(\mathcal{C})$. We then follow Prop. 4.11 and obtain the estimate

$$|\det_p(I + K(\lambda)) - \det_p(I + K_X(\lambda))| \leq C \exp(-\alpha_{\lambda_\gamma}(X - R));$$

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 6.1 in the Appendix 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., [28, 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. □

5. Numerical Examples

In this section we present several examples of elliptic PDEs on waveguides and study approximations of isolated eigenvalues. Computations were performed using piecewise linear finite elements with the help of MATLAB's PDETool package. Fig. 3 shows our algorithm schematically.

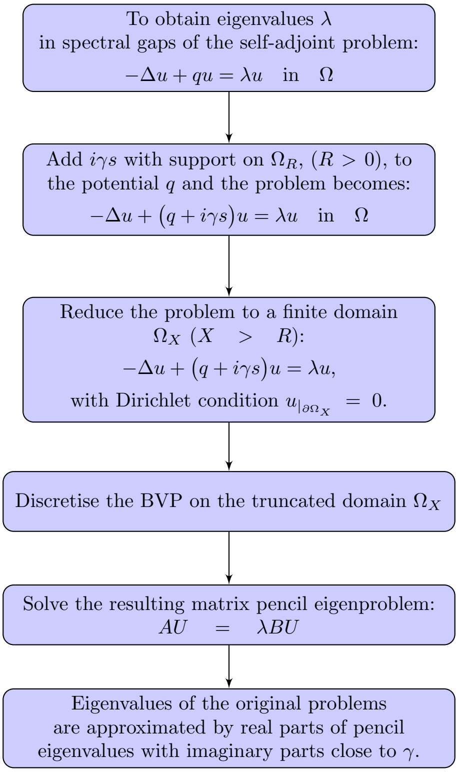

FIGURE 3. Dissipative barrier technique with domain truncation for eigenvalues in spectral gaps of Schrödinger problems.

For the discretisation step, we used MATLAB PDETool, which uses piecewise linear basis functions defined on a triangular mesh. The default mesh used is everywhere fine, which results in excessively large matrices in the pencil problem $AU = \lambda BU$, and run-times of many hours on a normal laptop computer. In order to circumvent this difficulty, we exploit the fact that due to exponential decay, the eigenfunctions which we wish to calculate should be concentrated towards the left-hand end of the waveguide, and the mesh refined there accordingly. To this end we used a simple mesh adaptation $(x, y) \mapsto (\mathcal{M}(x), y)$, in which

$$\mathcal{M}(x) = \min(x, X^*)\exp\left(\frac{\min(x, X^*)}{3}\right) + \max(x - X^*, 0)\left(1 + \frac{X^*}{3}\right)\exp\left(\frac{X^*}{3}\right). \tag{5.1}$$

The parameter $X^* > 0$ was chosen heuristically and depended also on the value of X, the length of the truncated waveguide. The effects of this mapping may be seen in Fig. 4, for the case $X = \mathcal{M}(7) \approx 50$ and $X^* = 14/3$. Of course much finer meshes were used for the computations. In fact, the mesh can appear to be degenerating when X is large, but this does not happen since, in principle, one takes the limit of small mesh-size ($h \to 0$) before the limit of large X.

Remark 5.1. Typically the size of the matrices A and B appearing in Fig. 3 were at most 10000×10000 and the experiments used 3 refinements of PDETool's initial mesh.

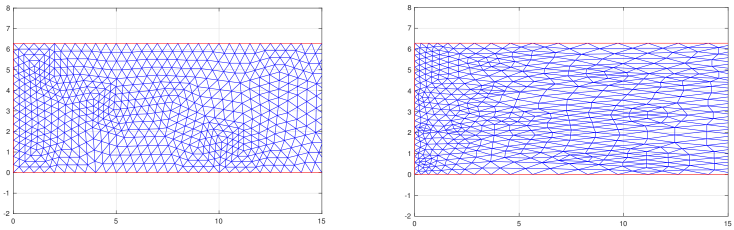

FIGURE 4. Mesh before (left) and after (right) mapping.

5.1. General discussion of the dissipative barrier scheme

We consider the following PDE problem:

$$-\Delta u + \cos(x)u - 25\exp(-x)u = \lambda u, \tag{5.2}$$

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

$$-u_n'' + \left(\cos(x) + \frac{n^2}{4} - 25\exp(-x)\right)u_n = \lambda u_n; \quad n = 1, 2, \cdots, \quad \text{on} \quad [0,\infty). \tag{5.3}$$

The spectral bands of the Mathieu equation are reported to high accuracy in [8]. Shifting these bands by $n^2/4$ for $n = 1, 2, \ldots$, we obtain the spectral bands of (5.2). The first two spectral bands are approximately given in Table 1.

m	I_m
1	[-0.12849,-0.09767]
2	[0.62151,0.65233]

TABLE 1. Spectral bands for (5.2)

In order to obtain approximations of eigenvalues in the gaps of (5.2), we first introduce a dissipative barrier to obtain

$$-\Delta u + \cos(x)u - 25\exp(-x)u + i\gamma s(x)u = \lambda u, \tag{5.4}$$

where $s(x) = \frac{1}{2}(1-\tanh(x-20))$ and the defined R in **A2** is approximately 25. 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 as described in Fig. 3.

Table 2 shows approximating eigenvalues for the self-adjoint problem (5.2) and non-self-adjoint problem (5.4). The computations were performed using three MATLAB PDETool mesh refinements, followed by the mesh mapping (5.1). The results in Table 2 show spectral pollution in the self-adjoint case (no dissipative barrier; $\gamma = 0$), which does not appear near the eigenvalues in the dissipative case ($\gamma = 1$). More discussion of the influence of the choice of γ and s will be given later. Now, by taking the real parts of the three computed eigenvalues for the dissipative problem we obtain approximations to three eigenvalues for the original problem (5.2), lying in the gap implied in Table 1. The second eigenvalue, which is the closest to the origin, appears to be calculated less accurately than the other two.

Self-adjoint ($\gamma = 0$)	Non-self-adjoint ($\gamma = 1$)
-0.084962803557113	-0.084961545990299 + 0.999988974782084i
0.065250381213409	
0.075056449171371	
0.075920453707749	
0.082342277041306	
0.094868041295541	
0.395135728508211	0.395135728509314 + 0.999999999980165i

TABLE 2. True and spurious eigenvalues with range of real part between $[-0.08, 0.6]$ for (5.4).

Table 2 only shows the results using a fixed mesh. Since eigenvalue error is approximately quadratic in the typical mesh-size, which is halved every time a mesh refinement is performed, one expects that after each mesh refinement the discretisation error is approximately divided by four. Richardson extrapolation can therefore be used to estimate the discretisation error and enhance accuracy. Applying this technique to one of the isolated eigenvalues in Table 2, with three further mesh refinements, yields the results in Table 3. Comparing the final result 0.36418887 in Table 3 with the two estimates 0.395135728508211 (self-adjoint) and 0.395135728509314 (non-self-adjoint) in Table 2, one sees that the error in the real parts of the eigenvalues due to the introduction of the dissipative barrier, which is of order 10^{-12}, is much smaller than the error due to the use of finite elements. It seems most unlikely that the estimate 0.36418887 is accurate to all of its eight quoted decimal places.

refinement	eigenvalues		
3	0.39513573		
4	0.37196251	0.36423810	
5	0.36613459	0.36419195	0.36418887

TABLE 3. Richardson extrapolation of order 2, 4, and 6 for an eigenvalue in a gap.

Now, we discuss the influence of the choice of γ and s. Let

$$s(x) = \frac{1}{2}(1 - \tanh(5(x - (R - 1)))). \tag{5.5}$$

The following table shows approximate eigenvalues for the self-adjoint problem of (5.2) and the non-self-adjoint problem (5.4) when $R = 21$ and the mesh refinement here is 3.

Self-adjoint $\gamma = 0$	Non-self-adjoint $\gamma = 1$
-0.003424652193865	-0.003033208595515 + 0.999647134982003i
0.065250381213409	
0.075056449171371	
0.075920453707749	
0.082342277041306	
0.094868041295541	
0.395135728508211	0.395135728507996 + 0.999999999996618i

TABLE 4. True and spurious eigenvalues with range of real part between $[-0.08, 0.6]$ for (5.4) when $R = 21$ in (5.5)

Again, the results in Table 4 show spectral pollution in the self-adjoint case which does not appear near the eigenvalues in the dissipative case, i.e., when $\gamma = 1$. On the other hand, these true eigenvalues do not appear when $R = 2$. It can be seen that in Table 5 the results no longer have imaginary parts close to 1.

Non-self-adjoint $\gamma = 1$
-0.003424852843047 + 0.000001234534508i
0.394655527181139 + 0.065229989814277i

TABLE 5. True eigenvalues for (5.4) when $R = 21$ do not appear when $R = 2$

Comparing the results of Tables 4 and 5, we can see that $R = 2$ gives far too short a barrier to lift genuine eigenvalues close to the line $\Im(\lambda) = \gamma$; by contrast $R = 21$ is sufficient, while also being small enough to ensure $X - R$ is large enough to kill off the various error terms of order $\exp(-c(X - R))$ from our analysis.

We now keep the same length of the waveguide, $X \approx 50$, and vary R to see the effect on the eigenvalues. Fig. 5 shows transition of genuine eigenvalue 0.39513573 and spurious eigenvalue 0.07505645, which appear in Table 4, for different values of R. It can be seen that, the imaginary part of the genuine eigenvalue starts from 0 when $R = 1$ and grows rapidly until it reaches 1 when $R = 10$. The imaginary part of the spurious eigenvalue does not reach the value of γ until the very end of the waveguide i.e., $R = X$.

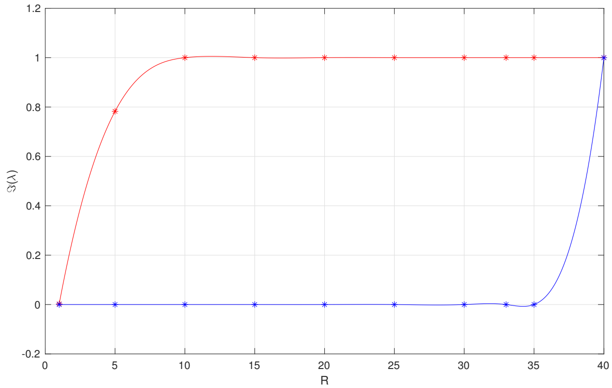

FIGURE 5. Imaginary parts of genuine eigenvalue (red) vs spurious eigenvalue (blue) with different values of R

Fig. 6 and Fig. 7 show contour plots of eigenfunctions of the eigenvalues 0.39513573 and 0.07505645 respectively. In particular, in Fig. 6, we can see the line of symmetry across the middle of the figure which is close to π on the y-axis, and the genuine eigenfunction appears on the left hand side of the waveguide. Fig. 7 shows the spurious eigenfunction which appears at the right hand side of the waveguide. We note that even though the mesh is quite stretched at the right hand end, it is remarkable that the scheme can properly manage to capture the eigenfunctions of that end of the waveguide.

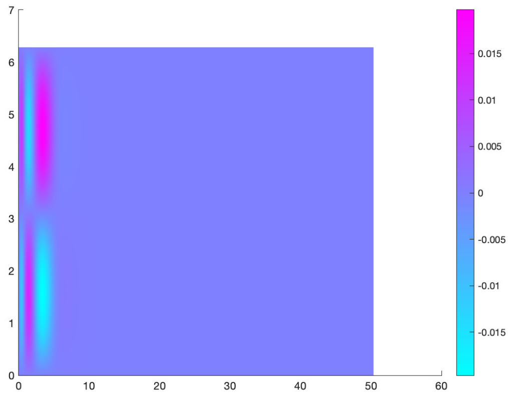

FIGURE 6. Contour plot of genuine eigenfunction

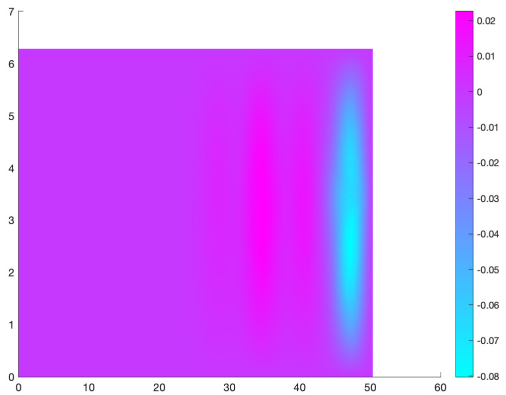

FIGURE 7. Contour plot of spurious eigenfunction

Finally, we indicate Table 6 to show the effect of changing γ on the eigenvalues. In the first column, when $\gamma = 0.1$, we can see three genuine eigenvalues, -0.00342463, 0.08238489, 0.09314387 and 0.39513573, whose imaginary part is close to 0.1. Similarly, in the second column, when $\gamma = 5$, four genuine eigenvalues have imaginary parts close to γ : -0.00342352, 0.08246694, 0.2771197 and 0.39513573. As before, all other eigenvalues whose imaginary part is away from γ are part of the spectral pollution. In this table, $X \approx 50$ and the mesh refinement is 3. Here we choose $R = 30$ in order to get all the potential eigenvalues.

$\gamma = 0.1$	$\gamma = 5$
-0.003424626734283 + 0.09999985i	-0.003423518167252 + 4.99999974i
0.065250640518402 + 0.00000007i	0.065250679159489 + 0.00000004i
0.075108913318926 + 0.00000379i	0.075118320886019 + 0.00000642i
0.077907611578600 + 0.00043861i	0.078972277513691 + 0.00136792i
0.082384889001159 + 0.09992834i	0.082466936544064 + 4.99998793i
0.093143871536771 + 0.08991193i	-
-	0.277119701218018 + 4.83463623i
0.395135728508214 + 0.09999999i	0.395135728508222 + 4.99999999i

TABLE 6. True and spurious eigenvalues on the spectral gap $[-0.08, 0.6]$ for eqn. (5.4) with different values of γ.

5.2. The effect of the perturbation term on the eigenvalues

We consider the following PDE problem:

$$-\Delta u + \left(\cos(x) - 25\exp(-x)(1 - \epsilon(\pi - y)^2) + \frac{i\gamma}{2}(1 - \tanh(x - 20)) \right) u = \lambda u, \tag{5.6}$$

in a waveguide $[0, \infty) \times [0, 2\pi]$, with Dirichlet boundary conditions. Clearly, Example 5.1 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 is the same as in Example 5.1. 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 for the underlying self-adjoint problem ($\gamma = 0$) eigenvalues in the gaps merge into the essential spectrum as ϵ becomes large enough, i.e., larger than $\frac{1}{\pi^2}$. This is reflected in the behaviour of the real parts of the eigenvalues of the dissipative problem ($\gamma = 1$): Fig. 8 shows the behaviour of the real parts of 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.

5.3. The effect of the potential on the eigenvalues

Consider the PDE

$$-\Delta u + \left(\cos(x + \epsilon y) - 25\exp(-x) + \frac{i\gamma}{2}(1 - \tanh(x - 20)) \right) u = \lambda u, \tag{5.7}$$

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. Fig. 9 shows the computed eigenvalues with real parts in $[-1, 1]$, for three values of ϵ. It illustrates some of the difficulties encountered when interpreting numerical results from the dissipative barrier method. Considering the points near the real axis, between -0.05 and 0.7, one may be tempted to speculate that the bands of essential spectrum do depend on ϵ: the computed eigenvalue

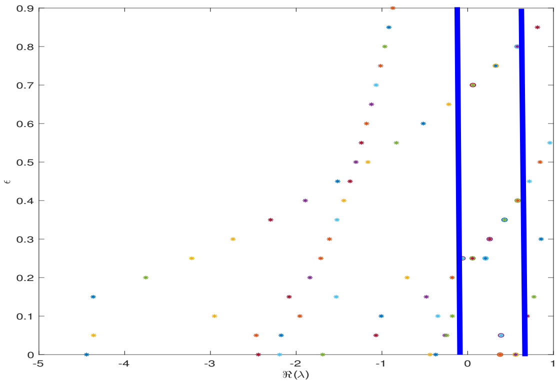

FIGURE 8. Eigenvalues of the PDE (5.6) with $|\Im(\lambda) - 1| < 0.01$ for different values of ϵ between 0 and 0.9. Isolated eigenvalues of the problem with real part in $[-0.08, 0.59]$, are marked as asterisks surrounded by circles. The blue shaded lines indicate the spectral bands, which are ϵ-independent.

clusters close to 0 move to the right, and clusters close to 0.6 move to the left, with increasing ϵ. In fact, these results should be treated with scepticism as we have not proved any approximation results for points of the essential spectrum. The eigenvalues with imaginary part very close to 1 are likely to give good approximations to the eigenvalues of the underlying self-adjoint problem; other eigenvalues should be treated with scepticism, being artefacts of the dissipative barrier or of the domain truncation. Fig. 10 zooms in on eigenvalues with imaginary parts close to 1, for values of ϵ between 0 and 1. Unlike in (5.6), the potential no longer has a real part which is increasing with ϵ, so the non-monotone behaviour of the eigenvalues in Fig. 10 is not surprising.

5.4. Optics with complex index of refraction

We consider the following PDE problem:

$$-\Delta u - 25\exp(-x)u = \lambda(2 + \sin(x) - is(x))u, \tag{5.8}$$

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. By separation of variables the PDE can be reduced to a Schrödinger equation with an infinite matrix-valued potential, suggesting that in addition to a finite

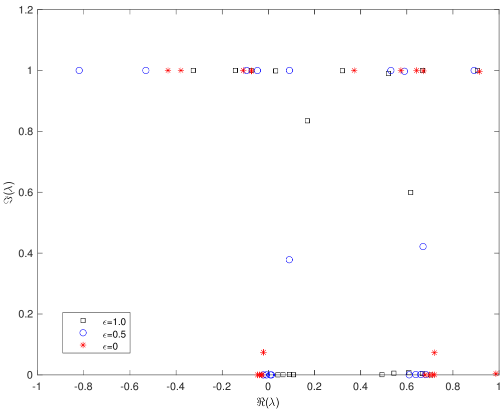

FIGURE 9. Computed eigenvalues of (5.7) with $\Re(\lambda) \in [-1, 1]$, for $\gamma = 1$ and different values of ϵ.

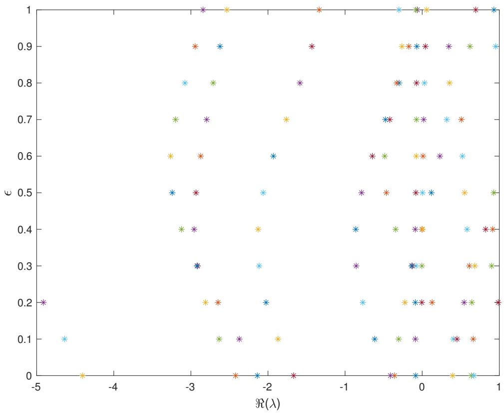

FIGURE 10. Eigenvalues of the PDE (5.7) with $\Re(\lambda) \in [-5, 1]$ and $|\Im(\lambda) - 1| < 0.02$, for different values of ϵ.

element approach one also perform numerics on the system

$$-\underline{u}'' + (D - 25\exp(-x)I)\underline{u} = \lambda((2 + \sin(x))I - is(x)I)\underline{u}, ; \quad x \in (0, \infty), \quad (5.9)$$
$$\underline{u}(0) = \mathbf{0},$$

where $D(j, j) = j^2, j = 1, \cdots, n$. Fig. 11 (left part) indicates the spectral bands of this ODE system with $n = 5$, as discussed by the authors in [3] and computed using the Numerov discretisation [33]. For comparison, Fig. 11 (right part) shows approximating eigenvalues produced by a finite element approach with the same MATLAB settings as in Example 5.1. Despite the fact that an infinity of differential equations has been replaced by just five, there are some surprising qualitative similarities. In order to understand

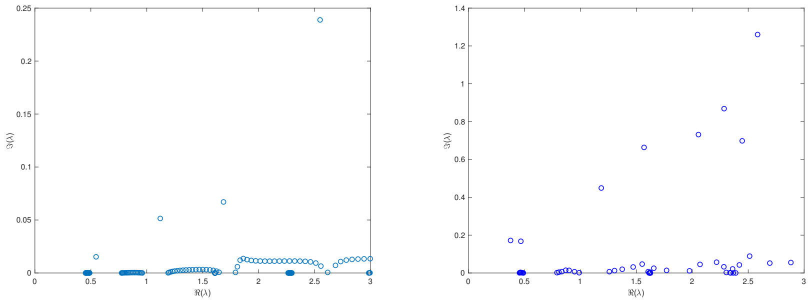

FIGURE 11. (Left) Eigenvalues of the ODE (5.9) with $\Re(\lambda) \in [0, 3]$, using $\pi/20$ mesh intervals. (Right) Eigenvalues of the PDE (5.8) using 5 PDETool mesh refinements.

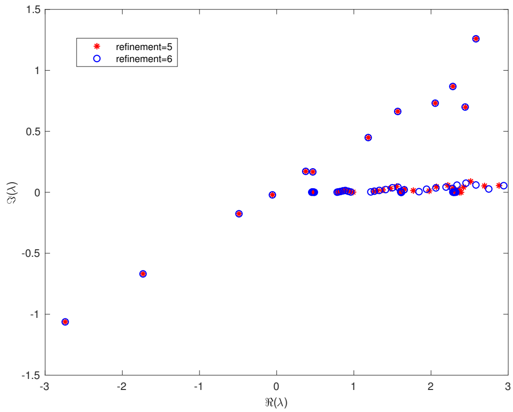

FIGURE 12. Eigenvalues of the PDE (5.8) with refinements 5 and 6 and real part of λ in the interval $[-3, 3]$.

the difficulty of obtaining accurate results for (5.8), we performed two very high-accuracy finite element calculations which are shown in Fig. 12. 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 5.2 below, the error is clearly not very small.

Remark 5.2. 1. The essential spectrum of the PDE pencil (5.8) 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 $\mathrm{Sp}_{ess}(A, B) \subseteq \mathrm{Sp}_{ess}(A, B_0) \subseteq \mathbb{R}$.

2. For each eigenvalue λ of the pencil (5.8):
   (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 6.2 in the Appendix the essential numerical range of the pencil satisfies that $W_e(A,B) \subseteq \mathbb{R}$.

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

$$\det_2(I + A) = \det(I + A)\exp(-\mathrm{trace}(A)).$$

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

$$\det_p(I + A) := \Pi_{j=1}^{\infty}(1 + r_p(\alpha_j)), \quad A \in \mathfrak{S}_p. \tag{6.1}$$

In every case, $\det_p(I + A)$ is non-zero if and only if $I + A$ is invertible.

Lemma 6.1. *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:

$$F(\lambda) = \sum_{n=0}^{\infty} (\lambda - \lambda_0)^n G_n, \quad \sum_{n=0}^{\infty} |\lambda - \lambda_0|^n \|G_n\|_p < \infty \quad \text{for } |\lambda - \lambda_0| < \rho,$$

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:

$$\|F(\lambda) - \sum_{n=0}^{N} (\lambda - \lambda_0)^n G_n\|_p < \epsilon \quad \text{for all } |\lambda - \lambda_0| \le \frac{1}{2}\rho.$$

2. For each $n \in \{0, \cdots, N\}$ choose a finite rank operator $G_{n,\epsilon}$ such that:

$$\|G_n - G_{n,\epsilon}\|_p \le \frac{\epsilon \cdot 2^{-n}}{\max(1, (\frac{1}{2}\rho)^n)}$$

and define a finite-rank analytic operator-valued function F_ϵ by

$$F_\epsilon = \sum_{n=0}^{N} (\lambda - \lambda_0)^n G_{n,\epsilon}, \quad |\lambda - \lambda_0| \le \frac{1}{2}\rho.$$

Then

$$\|F(\lambda) - F_\epsilon(\lambda)\|_p < \epsilon + \sum_{n=0}^{\infty} \epsilon \cdot 2^{-n} = 3\epsilon, \quad \text{for all } |\lambda - \lambda_0| \le \frac{1}{2}\rho.$$

Following [19, Theorem 2.2, p.194], we have, for $|\lambda - \lambda_0| \le \rho/2$,

$$|\det_p(I + F_\epsilon(\lambda)) - \det_p(I + F(\lambda))| \le C\|F_\epsilon(\lambda) - F(\lambda)\|_p < 3C\epsilon,$$

where C is a positive constant. Since F_ϵ is finite rank, it is not difficult to show that $\det_p(I + F_\epsilon(\lambda)) = \det(I + F_\epsilon(\lambda)) \exp(-\mathrm{trace}(F_\epsilon(\lambda)) + \cdots)$ is analytic. As the locally uniform limit of an analytic function is analytic (Hurwitz), then $\det_p(I + F(\lambda))$ is analytic in λ. □

Lemma 6.2. *Consider the PDE problem* $-\Delta u + qu = \lambda(w - is)u$ *on a semi infinite waveguide* Ω *in which* q *is bounded and* s *tends to zero in the precise sense that* $s(x, y) \to 0$ *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* $W_e(A, B)$ *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 [6, Theorem 2.26] that $W_e(A, B) = W_e(A, B + is) = W_e(A, w)$. Since w is real-valued and A is selfadjoint, $W_e(A, w) \subseteq \mathbb{R}$. □

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Declaration

Conflict of interest

The authors declare that they have no conflict of interest.

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