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EIGENVALUES IN SPECTRAL GAPS OF DIFFERENTIAL OPERATORS

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Abstract. Spectral problems with band-gap spectral structure arise in numerous applications, including the study of crystalline structure and the determination of transmitted frequencies in photonic waveguides. Numerical discretization of these problems can result in spurious results, a phenomenon known as spectral pollution. We present a method for calculating eigenvalues in the gaps of self-adjoint operators which avoids spectral pollution. The method perturbs the problem into a dissipative problem in which the eigenvalues to be calculated are lifted out of the convex hull of the essential spectrum, away from the spectral pollution. The method is analysed here in the context of one-dimensional Schrödinger equations on the half line, but is applicable in a much wider variety of contexts, including PDEs, block operator matrices, multiplication operators, and others.

Keywords: eigenvalue, spectral pollution, self-adjoint, dissipative, Schrödinger, spectral gap, spectral band, essential spectrum, discretization, variational method.

1. Introduction

In the numerical calculation of the spectrum of a self-adjoint operator, one of the most difficult cases to treat arises when the spectrum has band-gap structure and one wishes to calculate eigenvalues in the spectral gaps above the infimum of the essential spectrum. The reason for this difficulty is that variational methods will generally result in spectral pollution (see, e.g., Rappaz , Sanchez Hubert, Sanchez Palencia and Vassiliev [15]): following discretization, the spectral gaps fill up with eigenvalues of the discrete problem which are so closely spaced that it is impossible to distinguish the spectral bands from the spectral gaps. A number of different strategies have been proposed to deal with this problem: see Mertins and Zimmermann [19], Davies and Plum [10] for variants of the classical variational methods, and Boulton and Levitin [7], Levitin and Shargorodsky [12] and the references therein for an approach based on quadratic relative spectrum. All of these methods work for general abstract self-adjoint operators in a Hilbert space. There is also a lot of work in the mathematical physics literature on choosing special bases which do not result in pollution for certain classes of operators: see, e.g., Lewin and Séré [12] and the references therein.

For differential operators on infinite domains or with singularities, spectral pollution caused by domain truncation is also well studied: see, e.g., [4], [18], [8]. Pollution can always be avoided by the choice of appropriate boundary conditions on the boundary

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of the truncated domain; in practice, however, devising such 'non-reflecting' boundary conditions can be just as difficult and problem-specific as devising non-polluting bases.

In [14], Marletta considered the calculation of eigenvalues for Schrödinger equations

$$-\Delta u + q(\mathbf{x})u = \lambda u,$$

in infinite domains in $\mathbb{R}^d$, with band-gap spectral structure. A different trick was proposed: exploiting the fact that for many such problems the eigenfunctions are rapidly decaying, the author proposed changing the problem by replacing the potential q, making the change

$$q(\mathbf{x}) \longrightarrow q(\mathbf{x}) + i\gamma s(\mathbf{x}), \tag{1}$$

where s is a compactly supported 'cutoff function' which takes the value 1 everywhere inside a ball of large radius. The parameter γ is a nonzero real. The fact that s is compactly supported means that the essential spectrum of the problem is unchanged. On the other hand, an eigenfunction belonging to an eigenvalue in a spectral gap, being exponentially decaying, will see the function s almost as if it took the value 1 everywhere, and so the corresponding eigenvalue λ will be perturbed according to

$$\lambda \longrightarrow \lambda_\gamma \sim \lambda + i\gamma. \tag{2}$$

In particular, $\lambda \approx \Re(\lambda_\gamma)$. Numerical results in [14] indicate that the quality of this approximation for many problems is surprisingly good, the error due to the perturbation being several orders of magnitude smaller than the error due to discretization, and that this does not require that γ be small. However no error bounds are presented in [14], which is concerned mainly with proving that spectral pollution remains close to the real axis for a wide class of potentials.

At this point, we make a brief historical digression. The use of complex function methods for apparently self-adjoint problems in computational science has a long history. In his PhD thesis in 1967, Tamás Vertse proposed a method for finding resonances which was independently discovered subsequently by several different authors and which is usually now called *dilation analyticity* or *complex scaling*: see, e.g., the 1971 paper of Aguilar and Combes [2], or the 1981 paper of Ritby et al. [16]. Numerical analysts discovered this technique somewhat later and call it the *perfectly matched layer* method, generally citing the 1994 paper of Berenger [5]. All of these techniques are designed to solve resonance or scattering problems by deforming them into eigenvalue problems for non-self-adjoint operators. Another well known technique is the *limiting absorption principle*, which also turns a scattering problem into a non-self-adjoint problem. The method which we analyse here has some flavour of both approaches but is actually quite different, and is designed for the problem of calculating eigenvalues when spectral pollution is an issue.

In the remainder of this paper we carry out an extensive analysis of this perturbation technique for an ODE problem on the half-line $[0, \infty)$. In particular we establish the following results for an eigenvalue λ_γ of the shifted problem:

1. We obtain rigorous error bounds on $|\lambda - \Re(\lambda_\gamma)|$ and $|\Im(\lambda_\gamma) - i\gamma|$ in the case in which q is a compact perturbation of a real periodic function. In particular, we show that if $s(x) = 0$ for $x \geq R$ and $s(x) = 1$ for $x \leq cR$, where $c \in (0, 1)$

is a fixed positive constant, then

$$|\lambda + i\gamma - \lambda_\gamma| \leq C_1 \exp(-c\, C_2 R), \tag{3}$$

for positive constants C_1 and C_2. We also obtain an a-posteriori error bound which replaces (3) in the case where q is any real-valued potential, locally L^1 at every point in $[0,\infty)$, for which the Schrödinger equation has exponentially decaying solutions for λ outside the essential spectrum.

2. We show that if the shifted problem is truncated to some interval $[0, X]$, $X > R$, so that λ_γ is perturbed to $\lambda_{\gamma,X,\mathrm{good}}$ then, regardless of the artificial boundary condition imposed at $x = X$, an error bound of the form

$$|\lambda_\gamma - \lambda_{\gamma,X,\mathrm{good}}| \leq C_3 \exp(-C_4(X - R)) \tag{4}$$

holds, where C_3 and C_4 are further positive constants.

3. If an eigenvalue $\lambda_{\gamma,X,\mathrm{bad}}$ of the truncated, shifted problem converges, as $X \to \infty$, to a point which is neither an eigenvalue λ_γ nor a point of essential spectrum — in other words, if $\lambda_{\gamma,X,\mathrm{bad}}$ is responsible for spectral pollution – then

$$|\Im(\lambda_{\gamma,X,\mathrm{bad}})| \leq C_5 \exp(-C_6(X - R)), \tag{5}$$

for further positive constants C_5 and C_6. In particular, combining (3,4,5), for all sufficiently large X,

$$|\Im(\lambda_{\gamma,X,\mathrm{good}})| \geq 3\gamma/4, \quad |\Im(\lambda_{\gamma,X,\mathrm{bad}})| \leq \gamma/4,$$

which allows one to avoid calculating polluting eigenvalues, simply by concentrating on eigenvalues whose imaginary part exceeds (say) $\gamma/2$.

4. In addition to 'good' eigenvalues $\lambda_{\gamma,X,\mathrm{good}}$ and polluting eigenvalues $\lambda_{\gamma,X,\mathrm{bad}}$, the truncated, shifted problems will also possess eigenvalues $\lambda_{\gamma,X,\mathrm{ess}}$ which converge to the essential spectrum. We prove that for fixed $\gamma > 0$ and large X these satisfy

$$\Im(\lambda_{\gamma,X,\mathrm{ess}}) = O(X^{-1}). \tag{6}$$

These results are not exhaustive. The 'compact shift' trick (1) may generate further eigenvalues. In fact we shall consider the behaviour of such eigenvalues as functions of γ and show that the only possible behaviours are as follows:

1. λ_γ converges to an eigenvalue λ of the unperturbed problem as $\gamma \searrow 0$.
2. λ_γ converges to an endpoint of a spectral band as $\gamma \searrow 0$.
3. There exists $\gamma_{crit} > 0$ such that, as $\gamma \searrow \gamma_{crit}$, λ_γ converges to a point of a spectral band.

Numerical results will be presented to indicate that the second and third possibilities do appear to be realized in practice. It is worth observing that the critical constant γ_{crit} is strictly positive, something which is not true in the case of self-adjoint perturbations.

2. Problem statement and background theory

We consider on the half-line $[0,\infty)$ the Schrödinger equation

$$-u'' + (q(x) + i\gamma s(x))u = \lambda u, \tag{7}$$

with boundary condition

$$\cos(\alpha)u(0) - \sin(\alpha)u'(0) = 0. \tag{8}$$

defined by choosing some $\alpha \in [0, \pi)$. Here q is real-valued, locally L^1 and integrable near 0; the function s is positive, bounded and compactly supported.

We assume that the operator L_0 given by

$$D(L_0) = \{u \in L^2(0,\infty) \mid -u'' + qu \in L^2(0,\infty),\ \cos(\alpha)u(0) - \sin(\alpha)u'(0) = 0\} \tag{9}$$

$$L_0 u = -u'' + qu, \tag{10}$$

is self-adjoint[1]. It is known that the multiplication operator S given by

$$(Su)(x) = s(x)u(x), \quad u \in L^2(0,\infty) \tag{11}$$

is compact relative to L_0 and hence, for any $\gamma \in \mathbb{R}$,

$$\sigma_{ess}(L_0 + i\gamma S) = \sigma_{ess}(L_0) \subseteq \mathbb{R}$$

In order to describe the spectrum of $L_0 + i\gamma S$ we use a technique called Glazman decomposition [2, §130], which is equivalent to a two-sided shooting method. Fix $\lambda \in \mathbb{C}$; fix any non-zero constant h and consider the following two boundary value problems:

$$P_{\text{left}}: \quad \begin{cases} -v'' + (q + i\gamma s)v = \lambda v, \quad x \in (0, R); \\ \cos(\alpha)v(0) - \sin(\alpha)v'(0) = 0; \\ v(R) = h. \end{cases} \tag{12}$$

$$P_{\text{right}}: \quad \begin{cases} -w'' + (q + i\gamma s)w = \lambda w \quad x \in (R, \infty); \\ w(R) = h; \\ w \in L^2(R,\infty). \end{cases} \tag{13}$$

If these problems can be solved then we may define

$$m_{\text{left}}(\lambda) = v'(R)/v(R); \quad m_{\text{right}}(\lambda) = -w'(R)/w(R). \tag{14}$$

The functions m_{left} and m_{right} are one-dimensional Dirichlet to Neumann maps. They are analytic functions; m_{left} is meromorphic and m_{right} is Nevanlinna.

Suppose there exists $\mu \in \mathbb{C}$ such that for $\lambda = \mu$ we have

$$m_{\text{left}}(\mu) + m_{\text{right}}(\mu) = 0. \tag{15}$$

Then we can define a nontrivial function u by

$$u(x) = \begin{cases} v(x)/v(R), & x \le R, \\ w(x)/w(R), & x \ge R. \end{cases}$$

Now u solves the differential equation $-u'' + (q + i\gamma s)u = \mu u$ both on $(0, R)$ and on (R, ∞), is continuous at $x = R$ and, thanks to (15), has continuous first derivative at $x = R$. This implies that u is an eigenfunction with eigenvalue μ. The converse reasoning is equally straightforward, and we obtain the following result.

Lemma 1. *Suppose that $m_{\text{left}}(\lambda)$ and $m_{\text{right}}(\lambda)$ are well defined at $\lambda = \mu$. Then μ is an eigenvalue of $L_0 + i\gamma S$ if and only if μ is a zero of $m_{\text{left}} + m_{\text{right}}$.*

[1]This is equivalent to assuming that the associated differential equation is in the so called limit-point case at infinity, see [9].

In the remainder of this section we make the following assumptions:

(A1): q is real-valued, locally L^1, and there exists $R_0 \geq 0$ such that q is periodic with period $a > 0$ on $[R_0, \infty)$:

$$q(x+a) = q(x) \quad \forall x \geq R_0. \tag{16}$$

(A2): s is a cutoff function with support in $[0, R]$ for some $R \geq R_0$:

$$s(x) = \begin{cases} 1 & (x < cR); \\ 0 & (x \geq R). \end{cases} \tag{17}$$

Here $0 < c \leq 1$ is a fixed positive constant. For $x \in (cR, R)$ we simply assume that s is measurable and takes values in $[0, 1]$.

We now consider how to find m_{right} by using Floquet theory [11]. Since $q(x)$ is periodic for $x \geq R_0 \geq R$ and $s(x) = 0$ for $x \geq R$ it is known that for each $\lambda \in \mathbb{C}$ there exist solutions $\psi(x, \lambda)$ and $\phi(x, \lambda)$ of (7), and constants $\rho_1(\lambda)$, $\rho_2(\lambda)$ such that

$$\begin{pmatrix} \psi(x+a,\lambda) \\ \psi'(x+a,\lambda) \end{pmatrix} = \rho_1(\lambda) \begin{pmatrix} \psi(x,\lambda) \\ \psi'(x,\lambda) \end{pmatrix}, \quad \begin{pmatrix} \phi(x+a,\lambda) \\ \phi'(x+a,\lambda) \end{pmatrix} = \rho_2(\lambda) \begin{pmatrix} \phi(x,\lambda) \\ \phi'(x,\lambda) \end{pmatrix}, \quad x \geq R; \tag{18}$$

moreover we may write $\rho_1(\lambda) = \exp(ik(\lambda)a)$, $\rho_2(\lambda) = \exp(-ik(\lambda)a)$, where $\Im(k(\lambda)) > 0$ precisely when λ does not lie in $\sigma_{ess}(L_0)$. Thus for each $\lambda \notin \sigma_{ess}(L_0)$ the differential equation $-u'' + (q + i\gamma s)u = \lambda u$ has a unique (up to scalar multiples) solution $\psi(\cdot, \lambda) \in L^2(0, \infty)$. This solution decays exponentially while $\phi(\cdot, \lambda)$ grows exponentially.

Now consider the solution w of the boundary value problem P_{right} in (13). By direct verification, the solution exists if and only if $\psi(R; \lambda) \neq 0$ and is given by

$$w(x) = h\psi(x, \lambda)/\psi(R, \lambda).$$

Thus

$$m_{\text{right}}(\lambda) = -\psi'(R, \lambda)/\psi(R, \lambda), \tag{19}$$

and we deduce from Lemma 1 the following.

Corollary 1. *Suppose that $m_{\text{left}}(\lambda)$ is well defined and that $\psi(R, \lambda)$ is nonzero. Then λ is an eigenvalue of $L_0 + i\gamma S$ if and only if*

$$m_{\text{left}}(\lambda) - \psi'(R, \lambda)/\psi(R, \lambda) = 0. \tag{20}$$

Now suppose that we truncate our problem over $[0, \infty)$ to a problem on $[0, X]$ for some $X > R$. At $x = X$ we impose, for some $\beta \in \mathbb{R}$, a selfadjoint artificial boundary condition

$$\cos(\beta)u(X) - \sin(\beta)u'(X) = 0. \tag{21}$$

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

$$\begin{aligned} D(L_{0,X}) = \{u \in L^2(0, X) \mid & -u'' + qu \in L^2(0, X), \\ & \cos(\alpha)u(0) - \sin(\alpha)u'(0) = 0 = \cos(\beta)u(X) - \sin(\beta)u'(X)\}, \end{aligned} \tag{22}$$

$$L_{0,X}u = -u'' + qu. \tag{23}$$

The spectra of $L_{0,X}$ and $L_{0,X}+i\gamma S$ are now purely discrete. We can characterize the eigenvalues of $L_{0,X}+i\gamma S$ by replacing problem P_{right} in the Glazman decomposition (13,14) by

$$P_{\text{right,X}}: \quad \begin{cases} -w''+(q+i\gamma s)w=\lambda w \quad x\in(R,X); \\ w(R)=h; \\ \cos(\beta)w(X)-\sin(\beta)w'(X)=0. \end{cases} \tag{24}$$

Let ψ and ϕ be the functions determined (up to scalar multiples) by (18) and let

$$\psi_X(x,\lambda)=\psi(x,\lambda)-C_X(\lambda)\phi(x,\lambda), \tag{25}$$

where

$$C_X(\lambda)=\frac{\cos(\beta)\psi(X,\lambda)-\sin(\beta)\psi'(X,\lambda)}{\cos(\beta)\phi(X,\lambda)-\sin(\beta)\phi'(X,\lambda)}. \tag{26}$$

Then a direct calculation shows that the solution of (24), if it exists, is given by

$$w(x)=h\psi_X(x,\lambda)/\psi_X(R,\lambda).$$

Defining

$$m_{\text{right},X}(\lambda)=-w'(R)/w(R)=-\psi_X'(R,\lambda)/\psi_X(R,\lambda), \tag{27}$$

we obtain the following analogue of Lemma 1 and Corollary 1.

Lemma 2. *Suppose that $m_{\text{left}}(\lambda)$ is well defined and that $m_{\text{right},X}(\lambda)$ is well defined. Then λ is an eigenvalue of $L_{0,X}+i\gamma S$ if and only if*

$$m_{\text{left}}(\lambda)+m_{\text{right},X}(\lambda)=0; \tag{28}$$

equivalently, if and only if

$$m_{\text{left}}(\lambda)-\psi_X'(R,\lambda)/\psi_X(R,\lambda)=0. \tag{29}$$

3. The effect of interval truncation: convergence rate estimates

Theorem 1. *Suppose that assumptions (A1) and (A2) hold — see (16,17). For $\gamma>0$ let λ_γ be an eigenvalue of the non-selfadjoint Schrödinger operator $L_0+i\gamma S$ defined in (9,10,11) and let $\lambda_{\gamma,X,\text{good}}$ be the approximation to this eigenvalue obtained as an eigenvalue of the operator $L_{0,X}+i\gamma S$ defined in (22,23). Then*

$$|\lambda_\gamma-\lambda_{\gamma,X,\text{good}}|\le C_3\exp(-C_4(X-R)) \tag{30}$$

holds, where C_3 and C_4 are positive constants.

Proof. Without loss of generality it is sufficient to check the cases $X=R+Na$ where $N\in\mathbb{N}$ is sufficiently large; the other cases follow by interpolation, with possible adjustment of the constants C_3 and C_4.

First we observe that λ_γ has strictly positive imaginary part for $\gamma>0$; in fact if u_γ is the corresponding normalized eigenfunction then a standard integration by parts yields

$$\Im(\lambda_\gamma)=\gamma\int_0^R s(x)|u_\gamma(x)|^2dx>0.$$

Next we observe that as a consequence, neither $\psi(R,\cdot)$ nor $\psi_X(R,\cdot)$ can be zero in a neighbourhood of $\lambda=\lambda_\gamma$. If we had $\psi(R,\lambda_\gamma)=0$ then from the Floquet equation (18) we would also have $\psi(R+a,\lambda_\gamma)=0$. Since the cutoff function s is zero on

$[R, R+a]$, this would mean that the strictly complex number λ_γ was an eigenvalue of a self-adjoint Dirichlet problem over $[R, R+a]$, which is impossible. If we had $\psi_X(R, \lambda_\gamma) = 0$ a similar argument would immediately apply since ψ_X satisfies the self-adjoint boundary condition (21). Since $\psi(R, \cdot)$ and $\psi_X(R, \cdot)$ are both nonzero in a neighbourhood of λ_γ it follows that $m_{\text{right}}(\cdot)$ and $m_{\text{right},X}(\cdot)$ are well defined in a neighbourhood of λ_γ.

If $m_{\text{left}}(\lambda_\gamma)$ is well defined, then we can use Lemmata 1 and 2. We know that

$$m_{\text{left}}(\lambda_\gamma) + m_{\text{right}}(\lambda_\gamma) = 0, \tag{31}$$

$$m_{\text{left}}(\lambda_{\gamma,X,\text{good}}) + m_{\text{right},X}(\lambda_{\gamma,X,\text{good}}) = 0; \tag{32}$$

using (25) and the definitions of m_{right} and $m_{\text{right},X}$ it follows that for each fixed λ,

$$m_{\text{right}}(\lambda) - m_{\text{right},X}(\lambda) = O(C_X(\lambda)).$$

Now we exploit the Floquet equation (18) together with the fact that $X = R + Na$ to deduce that

$$C_X(\lambda) = \left(\frac{\rho_1(\lambda)}{\rho_2(\lambda)}\right)^N C_R(\lambda); \tag{33}$$

since $|\rho_1| < 1$ and $|\rho_2| = |\rho_1|^{-1} > 1$, this is exponentially small in N. Thus, in addition to (31), we have from (32) and (33) that

$$m_{\text{left}}(\lambda_{\gamma,X,\text{good}}) + m_{\text{right}}(\lambda_{\gamma,X,\text{good}}) = O\left(\left(\frac{\rho_1(\lambda_{\gamma,X,\text{good}})}{\rho_2(\lambda_{\gamma,X,\text{good}})}\right)^N\right). \tag{34}$$

It follows by a standard extension of the implicit function theorem that

$$|\lambda_\gamma - \lambda_{\gamma,X,\text{good}}| = O\left(\frac{\rho_1(\lambda_\gamma)}{\rho_2(\lambda_\gamma)}\right)^{N/\nu},$$

where ν is the algebraic multiplicity of λ_γ (i.e. the order of the zero of $m_{\text{left}}(\cdot)+m_{\text{right}}(\cdot)$ at λ_γ).

This proves the result for the case when $m_{\text{left}}(\lambda_\gamma)$ is well defined. When m_{left} has a pole at λ, then λ cannot be an eigenvalue of $L_0 + i\gamma S$ because m_{right} and $m_{\text{right},X}$ cannot have poles off the real axis: as already shown, $\psi(R, \lambda)$ and $\psi_X(R, \lambda)$ cannot have zeros off the real axis. □

Theorem 2. *Suppose that assumptions (A1) and (A2) hold — see (16,17). For $\gamma > 0$ let $\lambda_{\gamma,X,\text{bad}}$ be an eigenvalue of the non-selfadjoint Schrödinger operator $L_{0,X} + i\gamma S$ defined in (22,23) which converges, as $X \to +\infty$, to a point which is not in the spectrum of $L_0 + i\gamma S$. If $X = R + Na$, where $N \in \mathbb{N}$, then for some positive constants C_5 and C_6,*

$$\Im(\lambda_{\gamma,X,\text{bad}}) \le C_5 \exp(-C_6 X).$$

Proof. Let $\mu = \lim_{X\to\infty} \lambda_{\gamma,X,\text{bad}}$. We shall use the fact that $\lambda_{\gamma,X,\text{bad}}$ satisfies

$$m_{\text{left}}(\lambda_{\gamma,X,\text{bad}}) + m_{\text{right},X}(\lambda_{\gamma,X,\text{bad}}) = 0. \tag{35}$$

From (25,26,27), and from eqn. (33) in the proof of Theorem 1, we deduce that

$$m_{\text{right},X}(\lambda) = m_{\text{right}}(\lambda) \left(\frac{1 - \left(\frac{\rho_1(\lambda)}{\rho_2(\lambda)}\right)^N C_R(\lambda) f(\lambda)}{1 - \left(\frac{\rho_1(\lambda)}{\rho_2(\lambda)}\right)^N C_R(\lambda) g(\lambda)} \right) \tag{36}$$

where

$$f(\lambda) = \frac{\phi(R,\lambda)}{\psi(R,\lambda)}, \quad g(\lambda) = \frac{\phi'(R,\lambda)}{\psi'(R,\lambda)}. \tag{37}$$

Both of these functions are analytic off the real axis as it is only on the real axis that $\psi(R,\cdot)$ and $\phi(R,\cdot)$ can have zeros.

The Floquet multipliers ρ_1 and ρ_2 are also continuous functions of λ with $|\rho_1(\lambda)| < 1$ and $|\rho_2(\lambda)| = |\rho_1(\lambda)|^{-1} > 1$ for λ outside the essential spectrum. There are two cases to consider.

Case 1, $\Im(\mu) \neq 0$: Then μ lies off the essential spectrum, and so from (36) we can deduce that $m_{\text{right},X}(\cdot)$ converges locally uniformly to $m_{\text{right}}(\cdot)$ as $X \to \infty$ (this fact also follows even for more general problems from the classical Titchmarsh-Weyl nesting circle analysis; see, e.g., Coddington and Levinson [9, Chapter 9]). From this locally uniform convergence, together with the fact that $\lambda_{\gamma,X,\text{bad}} \to \mu$, we obtain, for large X,

$$m_{\text{right},X}(\lambda_{\gamma,X,\text{bad}}) \sim m_{\text{right}}(\mu) + O\left(\frac{\rho_1(\mu)}{\rho_2(\mu)}\right)^N,$$

and so $m_{\text{right},X}(\lambda_{\gamma,X,\text{bad}}) \to m_{\text{right}}(\mu)$ as $X \to \infty$. But from (35) this yields

$$m_{\text{left}}(\mu) + m_{\text{right}}(\mu) = 0.$$

From Lemma 1 this means that μ is an eigenvalue of $L_0 + i\gamma S$, a contradiction. Thus μ must be real; but recall that by assumption we also know that μ must not lie in one of the spectral bands.

Case 2, μ is real but does not lie in a spectral band: Again μ lies off the essential spectrum so we still have

$$\left(\frac{\rho_1(\lambda_{\gamma,X,\text{bad}})}{\rho_2(\lambda_{\gamma,X,\text{bad}})}\right)^N \sim \left(\frac{\rho_1(\mu)}{\rho_2(\mu)}\right)^N,$$

which is exponentially small. From eqns. (36,37) we have

$$m_{\text{right},X}(\lambda) = m_{\text{right}}(\lambda) \left(\frac{\psi(R,\lambda) - \left(\frac{\rho_1(\lambda)}{\rho_2(\lambda)}\right)^N C_R(\lambda)\phi(R,\lambda)}{\psi'(R,\lambda) - \left(\frac{\rho_1(\lambda)}{\rho_2(\lambda)}\right)^N C_R(\lambda)\phi'(R,\lambda)} \right) \frac{\psi'(R,\lambda)}{\psi(R,\lambda)}$$

and so the only way that we can fail to have $m_{\text{right},X}(\lambda_{\gamma,X,\text{bad}}) \to m_{\text{right}}(\mu)$ as $X \to \infty$ is if either $C_R(\lambda_{\gamma,X,\text{bad}})$ is exponentially large or if one of $\psi(R,\lambda)$, $\psi'(R,\lambda_{\gamma,X,\text{bad}})$ is exponentially small; equivalently, if and only if at least one of the following functions of λ,

$$\psi(R,\lambda), \quad \psi'(R,\lambda), \quad \cos(\beta)\phi(R,\lambda) - \sin(\beta)\phi'(R,\lambda) \tag{38}$$

is exponentially small when evaluated at $\lambda = \lambda_{\gamma,X,\mathrm{bad}}$. But the functions of λ defined in (38) have no zeroes off the real axis and have non-zero derivatives with respect to λ on the real axis (otherwise certain selfadoint problems over one period $[R, R+a]$ would have eigenvalues with algebraic multiplicity exceeding 1, which is impossible). Thus $\lambda_{\gamma,X,\mathrm{bad}}$ must be exponentially close to the real axis, which completes the proof. □

Finally we obtain an estimate on $\Im(\lambda_{\gamma,X,\mathrm{ess}})$ which deals with rate of convergence of points approximating the essential spectrum.

Theorem 3. *Under the hypotheses (A1) and (A2), there exists a constant C independent of X such that $\Im(\lambda_{\gamma,X,\mathrm{ess}}) \le CX^{-1}$ for all sufficiently large X.*

Proof. Let u be the eigenfunction of $L_{0,X} + iS$ whose eigenvalue is $\lambda_{\gamma,X,\mathrm{ess}}$. A simple calculation yields

$$\Im(\lambda_{\gamma,X,\mathrm{ess}}) = \frac{\int_0^R s|u|^2}{\int_0^R |u|^2 + \int_R^X |u|^2} = \frac{\int_0^R |u|^2 - \int_{R-r}^R (1-s)|u|^2}{\int_0^R |u|^2 + \int_R^X |u|^2}. \tag{39}$$

In order to obtain an upper bound on $\Im(\lambda_{\gamma,X,\mathrm{ess}})$ we need to consider the worst case scenario in which $\int_R^X |u|^2$ is as small as possible. This will occur when u is a multiple of the exponentially decaying solution $\psi(\cdot,\cdot)$ introduced in (18). For simplicity we restrict our attention to the case $X = R + Na$, in which case

$$\int_R^X |u|^2 = (1 + |\rho_1|^2 + \cdots + |\rho_1|^{2(N-1)}) \int_R^{R+a} |u|^2. \tag{40}$$

Here ρ_1 denotes the Floquet multiplier $\rho_1(\lambda_{\gamma,X,\mathrm{ess}})$ with $|\rho_1| < 1$. Combining (39,40) we obtain

$$\Im(\lambda_{\gamma,X,\mathrm{ess}}) \le \frac{1-\tilde{Q}}{1 + Q(1 + |\rho_1|^2 + \cdots + |\rho_1|^{2N-2})} = \frac{(1-\tilde{Q})(1-|\rho_1|^2)}{(1-|\rho_1|^2) + Q(1-|\rho_1|^{2N})}, \tag{41}$$

in which

$$Q = \frac{\int_R^{R+a} |u|^2}{\int_0^R |u|^2},$$

$$\tilde{Q} = \frac{\int_{R-r}^R (1-s)|u|^2}{\int_0^R |u|^2} < 1.$$

Suppose now that there exist positive exponents p and ν such that

$$|\rho_1|^2 \sim 1 - \alpha \Im(\lambda_{\gamma,X,\mathrm{ess}})^\nu \quad \text{and} \quad \Im(\lambda_{\gamma,X,\mathrm{ess}}) = O(1/N^p).$$

(In fact it is known that $\nu = 1$ except near endpoints of spectral bands, where $\nu = 1/2$.) Then for some constant c,

$$|\rho_1|^2 \le 1 - \frac{c}{N^{p\nu}}.$$

The cases $0 < p\nu < 1$, $p\nu = 1$ and $p\nu > 1$ must be considered separately.

In the case $0 < p\nu < 1$, we have $|\rho_1|^{2N} \sim \exp(-cN^{1-p\nu})$ which tends to zero faster than any inverse power of N. From (41) we find that the terms $1 - |\rho_1|^2 = O(1/N^{p\nu})$ are the dominant terms in both numerator and denominator, giving $\Im(\lambda_{\gamma,X,\mathrm{ess}}) \sim$

$1 - \tilde{Q} > 0$. This is impossible as $\lambda_{\gamma,X,\mathrm{ess}}$ is meant to approximate the essential spectrum, which lies on the real axis.

In the case $p\nu = 1$ we have $|\rho_1|^{2N} \sim \exp(-c)$, which is a nonzero constant. Thus from (41), $\Im(\lambda_{\gamma,X,\mathrm{ess}}) = O(1 - |\rho_1|^2) = O(1/N^{p\nu}) = O(1/N)$, as required.

Finally, in the case $p\nu > 1$, we have $|\rho_1|^{2N} \sim 1$ and from (41) we again get $\Im(\lambda_{\gamma,X,\mathrm{ess}}) = O(1 - |\rho_1|^2) = O(1/N^{p\nu}) \leq O(1/N)$. □

4. When the potential is not perturbed-periodic

In this section we consider problems on half-lines without truncation and examine the evolution of spectral points as functions of the 'coupling constant' γ. We maintain the assumption (A2) on the cutoff function s but drop the assumption of eventual periodicity in (A1). First we consider the behaviour of eigenvalues λ_γ of $L + i\gamma S$ whose real parts approximate eigenvalues of L, for small γ; then we consider the behaviour of those λ_γ which do not converge to eigenvalues of L with decreasing γ.

Theorem 4. *Suppose that assumption (A2) holds — see (17). For $\gamma > 0$ let λ_γ be an eigenvalue of the non-selfadjoint Schrödinger operator $L_0 + i\gamma S$ defined in (9,10,11) with eigenfunction u_γ; suppose that $\lambda_\gamma \to \lambda$, $\|u_\gamma - u\| \to 0$ uniformly with respect to R, as $\gamma \searrow 0$. Suppose also that the following assumption holds:*

(A1'): *$|u(x)| \leq C \exp(-C_2 x)$ for some positive constants C and C_2.*

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

$$|\lambda + i\gamma - \lambda_\gamma| \leq C_1 \exp(-c\, C_2 R), \tag{42}$$

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

Proof. We know that $(L + i\gamma S)u_\gamma = \lambda_\gamma u_\gamma$ and that $(L - i\gamma I)u = (\lambda - i\gamma)u$. Take the inner product of the first of these equations with u to obtain

$$\langle (L + i\gamma S)u_\gamma, u\rangle = \lambda_\gamma \langle u_\gamma, u\rangle \tag{43}$$

and take the inner product of the second equation with u_γ to obtain

$$\langle (L - i\gamma I)u, u_\gamma\rangle = (\lambda - i\gamma)\langle u, u_\gamma\rangle; \tag{44}$$

use the fact that L and S are self-adjoint and that u and u_γ both lie in the domain of L, which is contained in the domain of S, to rearrange (44) as

$$\langle (L + i\gamma I)u_\gamma, u\rangle = (\lambda + i\gamma)\langle u_\gamma, u\rangle. \tag{45}$$

Now subtract (43) from (45) to obtain

$$[(\lambda + i\gamma) - \lambda_\gamma]\, \langle u_\gamma, u\rangle = i\gamma \langle (I - S)u_\gamma, u\rangle = i\gamma \langle u_\gamma, (I - S)u\rangle.$$

Because u_γ tends to u as γ tends to zero, the inner product on the left hand side is bounded away from zero. At the same time, using hypotheses (A1') and (A2),

$$\|(I - S)u\| \leq C \exp(-c\, C_2 R)$$

for some positive constants C and C_2. This proves the result. □

Remark 1. *There are many potentials for which eigenfunctions u exhibit exponential or super-exponential decay: potentials satisfying (A1), for instance, as well as potentials for which $q(x) \to +\infty$ as $x \to +\infty$. Suitable results can be found in any good textbook on asymptotics of solutions of differential equations.*

Theorem 5. *Suppose that q is real valued and locally L^1; that the cutoff function s is a step function taking the value 1 on $[0, R)$ and 0 on (R, ∞), as in (17) with $c = 1$; and that the operator L_0 given by (9,10) is self-adoint and that its essential spectrum is purely absolutely continuous. Let λ_γ be an eigenvalue of $L_0 + i\gamma S$ which converges, as $\gamma \searrow \gamma_{crit} \geq 0$, to a point μ of the essential spectrum of L_0. Then $\gamma_{crit} > 0$.*

Remark 2. *Borisov and Gadyl'shin* [6] *consider an abstract perturbation $H_0 + \mathcal{L}_\gamma$ of a periodic Schrödinger operator H_0, in which $\mathcal{L}_\gamma$ is bounded but not necessarily self-adjoint. They prove that, given a compact set K intersecting the essential spectrum of H_0, there exists a constant $\gamma_{crit} > 0$ such that for $0 \leq \gamma < \gamma_{crit}$ there are no eigenvalues of $H_0 + \mathcal{L}_\gamma$ in $K \cap \sigma_{ess}(H_0)$. The present result is stronger and implies that there are no eigenvalues in K. This depends heavily on the fact that our operator $\mathcal{L}_\gamma = i\gamma S$ is dissipative. In the case where iS is replaced by just S, the result is false, in general, as eigenvalues may immediately emerge from the top of spectral bands as soon as $\gamma > 0$.*

Proof. Referring back to eqn. (13), denote by $\psi(x, \lambda)$ the solution of P_{right} for the particular choice $h = 1$. The solvability of P_{right} is guaranteed for any non-real λ since the underlying operator is self-adjoint and hence has a resolvent which is well defined for non-real λ. The existence of $m_{\text{right}}(\lambda) = -\psi'(R, \lambda)$ is thus guaranteed for $\Im(\lambda) \neq 0$, and we have, as in eqn. (15),

$$m_{\text{left}}(\lambda_\gamma; \gamma) + m_{\text{right}}(\lambda_\gamma) = 0, \tag{46}$$

where we make the dependence of m_{left} on γ explicit in the notation. It will also be convenient to denote λ_γ by $\lambda(\gamma)$ throughout the rest of this proof. Note that $\lambda(\gamma)$ is differentiable with respect to γ as long as $\gamma > \gamma_{crit}$ (to keep $\lambda(\gamma)$ off the real axis) and, by a standard calculation,

$$\lambda'(\gamma) = \frac{\int_0^R \psi(x, \lambda(\gamma))^2 dx}{\int_0^R \psi(x, \lambda(\gamma))^2 dx + \int_R^\infty \psi(x, \lambda(\gamma))^2 dx}. \tag{47}$$

Now consider what happens as $\gamma \searrow \gamma_{crit}$. We know that μ is an interior point of the essential spectrum and that the operator has purely a.c. essential spectrum, so $\psi(x, \mu)$ cannot lie in L^2. Thus

$$\lim_{\gamma \searrow \gamma_{crit}} \Re \left(\int_R^\infty \psi(x, \lambda(\gamma))^2 dx \right) = +\infty,$$

and hence from (47) we deduce that

$$\lim_{\gamma \searrow \gamma_{crit}} \lambda'(\gamma) = 0. \tag{48}$$

Now we return to (46) and observe that in view of the fact that s is a step-function satisfying the hypothesis (A2), we have $m_{\text{left}}(\lambda; \gamma) = m_{\text{left}}(\lambda - i\gamma; 0)$. Substituting

into (46) and differentiating with respect to γ now yields

$$m'_{\text{left}}(\lambda(\gamma) - i\gamma; 0)(\lambda'(\gamma) - i) + m'_{\text{right}}(\lambda(\gamma))\lambda'(\gamma) = 0. \tag{49}$$

Now since the essential spectrum is assumed purely a.c., m_{right} remains bounded as the essential spectrum on the real axis is approached from above. Thus we obtain, in view of (48),

$$m'_{\text{left}}(\mu - i\gamma_{crit}; 0) = 0. \tag{50}$$

However the Titchmarsh-Weyl functions for Sturm-Liouville problems cannot have zero derivatives with respect to λ on the real axis: if they did, it would contradict the well known fact that they are Nevanlinna functions. Thus (50) implies that $\gamma_{crit} > 0$. □

Remark 3. *For the case of a trivial periodic backround — $q \equiv 0$ — the proof of Theorem 5 becomes particularly straightforward. The solution of the differential equation which is in $L^2(0,\infty)$ is given by*

$$\psi(x) = \begin{cases} \cos(\sqrt{\lambda - i\gamma}(x - R)) + i\sqrt{\frac{\lambda}{\lambda - i\gamma}}\sin(\sqrt{\lambda - i\gamma}(x - R)), & x < R, \\ \exp(i\sqrt{\lambda}(x - R)), & x > R. \end{cases}$$

Here $\sqrt{\lambda}$ is chosen to have positive imaginary part when $\Im(\lambda) > 0$. Imposing the boundary condition $\psi(0) = 0$ yields, for λ, the transcendental equation

$$i\sqrt{\lambda}\frac{\tan(\sqrt{\lambda - i\gamma}R)}{\sqrt{\lambda - i\gamma}} = 1. \tag{51}$$

If we suppose that λ_γ is a family of solutions of this equation with $\Im(\lambda_\gamma) \to 0$ as $\gamma \to \gamma_{crit}$, then we can deduce that $\gamma_{crit} > 0$: otherwise, with $\lambda_\gamma \to \mu \geq 0$, and $\gamma \to \gamma_{crit} = 0$, we would obtain

$$i\tan(R\sqrt{\mu}) = 1,$$

which is impossible for $\mu \geq 0$.

It should also be mentioned that there is a uniform $\gamma_{crit} > 0$ for this problem: there exists $\gamma_{crit} > 0$ such that for $0 \leq \gamma < \gamma_{crit}$ the problem has no eigenvalues at all. Some simple asymptotic expansions for large λ and small γ, namely

$$\sqrt{\lambda - i\gamma} \approx \sqrt{\lambda}\left(1 - \frac{i\gamma}{2\lambda}\right), \quad \tan(\sqrt{\lambda - i\gamma}R) \approx \frac{\tan(R\sqrt{\lambda}) + i\tanh\left(\frac{R\gamma}{2\sqrt{\lambda}}\right)}{1 - i\tan(R\sqrt{\lambda})\tanh\left(\frac{R\gamma}{2\sqrt{\lambda}}\right)},$$

show that (51) becomes

$$\tan(R\sqrt{\lambda}) + i\tanh\left(\frac{R\gamma}{2\sqrt{\lambda}}\right) \approx -i - \left(1 + i\frac{\gamma}{2\lambda}\right)\tan(R\sqrt{\lambda})\tanh\left(\frac{R\gamma}{2\sqrt{\lambda}}\right).$$

Comparing real and imaginary parts shows that this equation has no solutions for large λ.

5. Spectral concentrations

In view of Theorem 5 it is useful to understand which points μ in $\sigma_{ess}(L)$ will be first to give rise to eigenvalues when γ is 'turned on'. Eqn. (50) tells us that we should seek those values of μ for which there exists a zero of $m'_{\text{left}}(\lambda, 0)$ on the line $\Re(\lambda) = \mu$ as close as possible to the real axis, since it is the distance to the real axis which is precisely γ_{crit}.

Consider the case in which m_{left} has a pole and a zero at two close points on the real axis; we shall call these points $\mu - \epsilon/2$ and $\mu + \epsilon/2$. The point $\mu - \epsilon/2$ will be the zero of m_{left}, and is an eigenvalue of the self-adjoint problem

$$-v'' + qv = \lambda v, \quad x \in (0, R),$$
$$\cos(\alpha)v(0) - \sin(\alpha)v'(0) = 0 = v'(R);$$

the point $\mu + \epsilon/2$ is a pole of m_{left} and is an eigenvalue for the case of a Dirichlet boundary condition $v(R) = 0$. We can write

$$m_{\text{left}}(\lambda) = \left(\frac{\lambda - \mu + \epsilon/2}{\lambda - \mu - \epsilon/2}\right) M(\lambda), \tag{52}$$

where M is non-zero at $\lambda = \mu - \epsilon/2$ and is analytic at $\lambda = \mu + \epsilon/2$. In fact M will be the m_{left} for the case when q is replaced by some different L^2-function: $q \mapsto Q$. This follows from standard results in the theory of inverse Sturm-Liouville problems, and means in particular that just as m_{left} has the Nevanlinna property $\Im(m_{\text{left}}(\zeta + i\nu)) > 0$ for $\Im(\nu) > 0$, so M will satisfy

$$\Im(M(\zeta + i\nu)) > 0 \text{ for } \Im\nu > 0. \tag{53}$$

Now M will have a Taylor expansion about $\lambda = \mu + \epsilon/2$:

$$M(\lambda) = a + b(\lambda - \mu - \epsilon/2) + c(\lambda - \mu - \epsilon/2)^2 + \cdots,$$

and in particular

$$M(\mu + \epsilon + i\nu) = a + ib\nu - c\nu^2 + \cdots. \tag{54}$$

The Nevanlinna property of M means that $b > 0$.

But from (52) we also have the expansion

$$m_{\text{left}}(\mu + \epsilon/2 + i\nu) = \left(1 + \frac{\epsilon}{i\nu}\right)(a + ib\nu - c\nu^2 + \cdots) = -i\frac{a\epsilon}{\nu} + a + b\epsilon + O(\nu);$$

using the Nevanlinna property of m_{left} it follows, considering small $\nu > 0$, that $a\epsilon < 0$. Now an elementary calculation shows that in a neighbourhood of $\lambda = \mu + \epsilon/2$,

$$m'_{\text{left}}(\lambda) = -\frac{a\epsilon}{(\lambda - \mu - \epsilon/2)^2} + b + 2\epsilon c + O(\lambda - \mu - \epsilon/2).$$

It follows that m'_{left} will have a zero at a point in $\mathbb{C}^+$ given approximately by

$$\lambda \sim \mu + \epsilon/2 + i\sqrt{\frac{-a\epsilon}{b - \epsilon c}}; \tag{55}$$

note that the fact that $b > 0$ and $a\epsilon < 0$ is important here.

In view of eqn. (50), formula (55) gives an approximation to the value of γ_{crit} at which an eigenvalue of the problem with the dissipative perturbation $q \mapsto q + i\gamma s$,

for $s = \chi_{[0,R]}$, can be expected to emerge from the essential spectrum into the upper half plane.

6. Examples and numerics

Example 1. *For our first example we take*

$$-u'' + \left(\frac{-40}{1+x^2} + \sin(x)\right) u = \lambda u, \quad u(0) = 0. \tag{56}$$

The first three spectral bands for this problem are

$$[-0.378489, -0.347669],\ [0.594800, 0.918058],\ [1.293166, 2.285157].$$

There are infinitely many eigenvalues in the gaps between the spectral bands, accumulating at the lower ends of the bands, and their spacing is exponentially small (see Schmidt [17]*). This makes it impossible to distinguish most of them from the band end.*

We made the perturbation

$$q(x) \mapsto q(x) + i\gamma\chi_{[0,R]}(x)$$

and examined the resulting eigenvalues. For $\gamma = \frac{1}{4}$*, Fig. 1 shows a plot of* $|\lambda + i\gamma - \lambda_\gamma|$ *against* R *for one of the eigenvalues in the spectral gap* $(-0.347669, 0.594800)$*, with the vertical axis on a logarithmic scale. This appears to indicate that our formula (3) is a tight estimate, with* $C_1 \approx 8.72$ *and* $C_2 \approx 0.2006$*.*

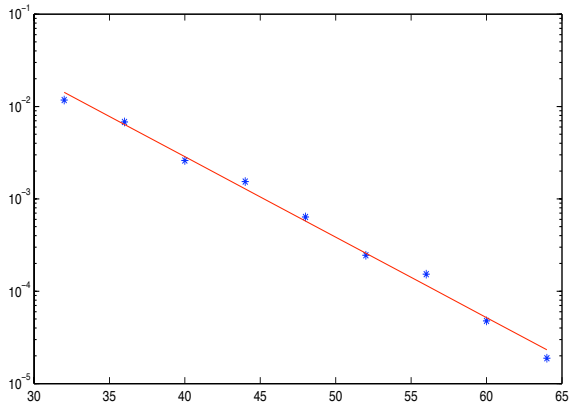

FIGURE 1. Logarithmic plot of $|\lambda + i\gamma - \lambda_\gamma|$ against R.

With $R = 48$ *fixed, Fig. 2 shows the effect of truncating the problem to a fixed interval* $[0, X]$*,* $X > R$*. The horizontal axis is* $X - R$*. This plot indicates that our estimate (4) is tight, with* $C_3 \approx 0.00087$ *and* $C_4 \approx 0.5431$*.*

Examining the behaviour of spurious eigenvalues predicted by eqn. (5) is rather more difficult because, for second order ODEs with one regular and one singular endpoint, there is at most one spurious eigenvalue in each spectral gap. The approach taken was to fix X *at a value which gives a spurious eigenvalue following the approach*

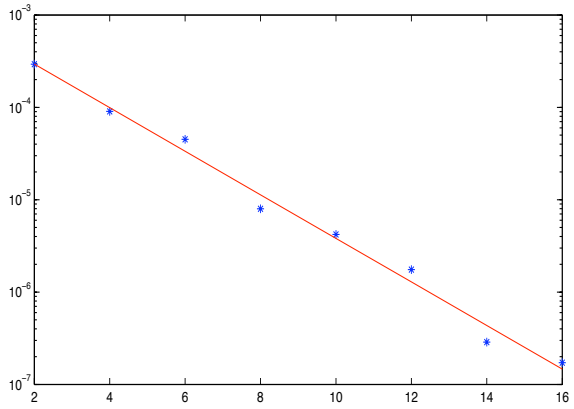

FIGURE 2. Logarithmic plot of $|\lambda_\gamma - \lambda_{\gamma,X,\mathrm{good}}|$ against $X - R$.

in [14, §6.1, Table 1]*, and then vary R rather than X. The results in Fig. 3 appear to show that (5) is tight, with $C_5 \approx 0.019$, $C_6 \approx 0.1376$.*

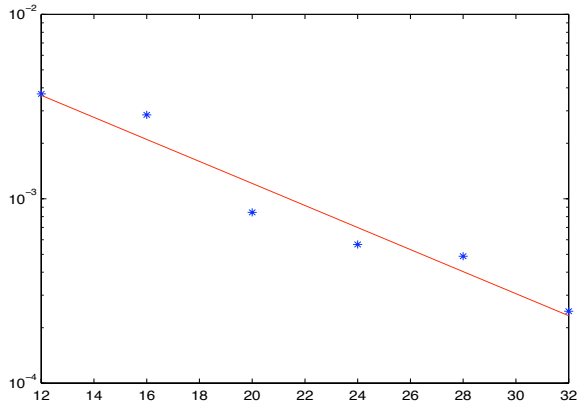

FIGURE 3. Logarithmic plot of $\Im(\lambda_{\gamma,X,\mathrm{bad}})$ against $X - R$; $X = 64$ was fixed.

Finally, we attempted to verify whether or not the $O(X^{-1})$ error estimate in eqn. (6) for approximation of the essential spectrum is correct. This is a little more difficult again: if the eigenvalues are indexed so as to behave as continuous functions of X, then all but finitely many eigenvalues will converge to the bottom of the essential spectrum. However by fixing a value μ in the middle of a spectral band and always choosing, for each X, the eigenvalue $\lambda_{\gamma,X,\mathrm{ess}}$ closest to μ, we were able to produce Fig. 4, which gives very convincing numerical evidence that it is impossible to achieve better than $O(X^{-1})$ convergence.

Example 2. *Continuing with eqn. (56), we examined the behaviour of eigenvalues as functions of γ under the perturation*

$$q(x) \mapsto q(x) + i\gamma\chi_{[0,50]}(x).$$

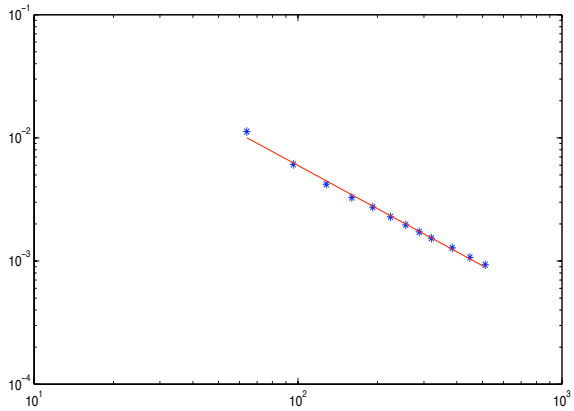

FIGURE 4. Plot of $\Im(\lambda_{\gamma,X,\mathrm{ess}})$ against X

Figure 5 shows the trajectories of six eigenvalues for $\gamma \in [0.025, 0.1]$. *The essential spectrum is marked by dense asterisks along a part of the real axis. The leftmost eigenvalue (real part approximately 0.56) emerges from an eigenvalue in a spectral gap for* $\gamma = 0$. *The second eigenvalue, real part approximately 0.59, appears to emerge from the lower endpoint of a spectral band; recall, however, that there are infinitely many eigenvalues in the gap, accumulating at the lower end of the band, with exponentially small spacing. The remaining eigenvalues all appear to arise from interior points*

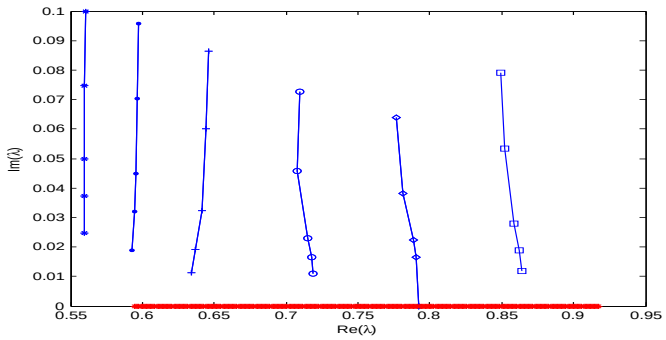

FIGURE 5. One gap eigenvalue and five points of essential spectrum giving rise to six eigenvalues for a dissipative perturbation of the original selfadjoint operator.

of the spectral band, some of which may correspond to spectral concentrations. The slowest to emerge is the one giving rise to the eigenvalue with real part approximately 0.78. At the level of resolution shown in this graph it looks as if $\gamma_{crit} \approx 0.025$ *for this eigenvalue, because with* $\gamma = 0.025$ *we see that the other eigenvalues have already lifted off, while this particular one appears still to be stuck on the real axis. However since* $\Im(\lambda)$ *does not change sign as* γ *passes through* γ_{crit} *it is actually almost impossible to determine* γ_{crit} *accurately by numerical means.*

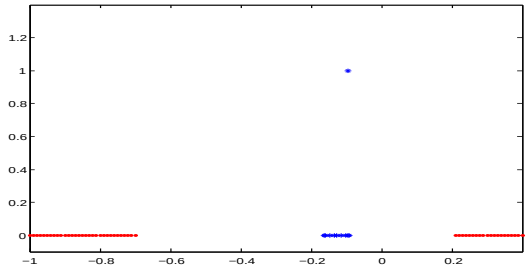

FIGURE 6. Computed spectrum of perturbed periodic Schrödinger equation. The genuine eigenvalue has been shifted into the upper half plane. Spectral pollution stays close to the real axis, as one would guess by Theorem 2.

Example 3. *As mentioned in Remark 3, in the case of a zero periodic background we can find the critical value(s) of γ at which eigenvalues emerge from the essential spectrum of the free Laplacian under perturbation,*

$$-\frac{d^2u}{dx^2} + i\gamma\chi_{[0,R]}(x)u = \lambda u, \quad u(0) = 0,$$

by solving, for real $\lambda \geq 0$ and $\gamma > 0$, the transcendental equation

$$\Phi(\lambda, \gamma) = iR\sqrt{\lambda}\frac{\tan(\sqrt{\lambda - i\gamma}R)}{\sqrt{\lambda - i\gamma}R} - 1 = 0.$$

We solved this equation numerically with $R = 50$ by minimizing $|\Phi|$, obtaining

$$\gamma_{crit} \approx 0.0379727, \quad \lambda \approx 0.3003689.$$

Example 4. *This example falls slightly outside the scope of the ODE theory of this paper; however the methods used to prove Theorem 4 are not specific to ordinary differential equations, and apply equally to partial differential equations with exponentially decaying eigenfunctions.*

Our problem is to compute an eigenvalue of the Schrödinger equation

$$-\Delta u + q(\mathbf{x})u = \lambda u, \quad \mathbf{x} \in \mathbb{R}^2,$$

in which q describes a perturbed periodic medium:

$$q(x, y) = \cos(x) + \cos(y) - 5\exp(-x^2 - y^2).$$

This problem has band-gap spectral structure, and we treated it with the perturbation

$$q(x, y) \mapsto q(x, y) + \frac{i}{4}(1 - \tanh(|x| - 30))(1 - \tanh(|y| - 30)).$$

The resulting problem was solved on the rectangle $[-60, 60]^2$ using Dirichlet boundary conditions, solved using MATLAB PDETool with a user-adapted mesh. Figure 6 shows an eigenvalue lifted into the upper half plane by the dissipative perturbation. The eigenvalue calculated was

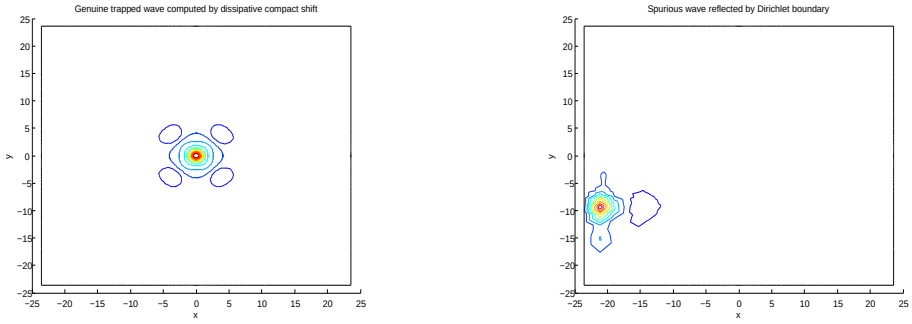

FIGURE 7. Genuine and polluting eigenfunction: it is clear which is which.

$$\lambda_\gamma = -0.09698 + (1 - 10^{-9})i;$$

Boulton and Levitin [7] *obtained the enclosure* $\lambda \in [-0.09697 - \epsilon, -0.09697 + \epsilon]$ *with* $\epsilon = 3.39 \times 10^{-4}$*; the real part of our computed* λ_γ *therefore agrees with the result in* [7] *with accuracy 30 times smaller than the error bound in* [7]*. Note the spectral pollution on the real axis below* λ_γ*, caused by domain truncation. In fact this pollution will fill the whole spectral gap if the domain is large enough. One can also see in Figure 7 the qualitative difference between the contour plot of a genuine eigenfunction and a polluting eigenfunction.*

Example 5. *We consider for* $\delta \geq 0$*,* $x \in [0, \infty)$ *the problem*

$$-u'' + x^2 \exp(-\delta x^2)u = \lambda u, \quad u(0) = 0. \tag{57}$$

For $\delta = 0$ *this is the harmonic oscillator problem and its eigenvalues are well known to be the integers* $4k - 1$*,* $k \in \mathbb{N}$*. For* $\delta > 0$*, however small, the problem has no eigenvalues at all, and the spectrum is purely absolutely continuous. The problem with small* $\delta > 0$ *exhibits* spectral concentrations *near the integers* $4k - 1$*: - see Aslanyan and Davies* [3].

Table 1 shows numerical results for the case $\delta = 10^{-2}$*. Taking* $R = 5$ *for this problem results in an* $m_{\text{left}}(\lambda)$ *which has some very close (pole,zero) pairs – the Dirichlet and Neumann eigenvalues in the first two columns of the table. The eigenvalues of the dissipative problem which emerge upon adding a perturbation* $i\gamma\chi_{[0,5]}(x)$ *do indeed emerge with real parts in the intervals between the corresponding Neumann and Dirichlet eigenvalues.*

7. CONCLUSIONS

The technique of relatively compact dissipative perturbation appears to be a computationally attractive tool for avoiding spectral pollution. Eigenvalues of interest are moved into a part of the complex plane where they are well isolated from spurious points, giving numerical methods which are much quicker and more efficient. There is no evidence of problems with pseudospectra, even though the resulting problems are non-normal. The approach can easily be implemented as an add-on to legacy codes and requires very few additional lines of programming.

Pole of m_{left} (Dirichlet eigenvalue)	*Zero of m_{left} (Neumann eigenvalue)*	*Dissipative, $\gamma = 0.2$*
2.9621125	*2.9621124*	*2.9621125 + 0.2000000i*
6.8083144	*6.8082846*	*6.8083001 + 0.1999999i*
10.5272610	*10.5247488*	*10.5260768 + 0.1999939i*
14.1401140	*14.0178056*	*14.1095773 + 0.1997539i*
17.8348945	*17.2277815*	*17.5519026+0.1959618i*

TABLE 1. Dirichlet and Neumann eigenvalues for problem on $[0, 5]$ compared with eigenvalues in upper half plane for dissipatively perturbed problem on $[0, \infty)$. Note that the un-perturbed problem on $[0, \infty)$ has no eigenvalues.

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