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Eigenvalues in spectral gaps of differential operators

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Abstract. Spectral problems with band-gap spectra arise in numerous applications, including the study of crystalline structures and the determination of transmitted frequencies in photonic waveguides. Numerical discretization of these problems can yield 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.

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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 [22]): 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 [26], Davies and Plum [13] for variants of the classical variational methods, and Boulton and Levitin [8], Levitin and Shargorodsky [17] and the references therein for an approach based on quadratic relative spectrum. All of these methods work for general

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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 [18] for some recent results and a review.

For differential operators on infinite domains or with singularities, spectral pollution caused by domain truncation is also well studied: see, e.g., [5], [25], and [11]. Pollution can always be avoided by the choice of appropriate boundary conditions on the boundary 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 [19], 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 [19] 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 [19], 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 non-self-adjoint methods and analytic function theory for apparently self-adjoint problems in computational science has a long history. In his Ph.D. thesis in 1967, the Hungarian computational chemist 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. [23]. Numerical analysts discovered this technique somewhat later and call it the *perfectly matched layer* method, generally citing the 1994 paper of Berenger [6]. 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.

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2. Summary of results

In this paper we carry out an extensive analysis of the dissipative perturbation technique for a Schrödinger problem on the half-line $[0, \infty)$. We establish the following results for an eigenvalue λ_γ of the problem with dissipative shift $i\gamma s(\cdot)$ which evolves from an eigenvalue λ for $\gamma = 0$.

(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

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

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 $[0, X]$, $X > R$, then whatever the boundary condition imposed at $x = X$, any eigenvalue $\lambda_{\gamma,X,\text{good}}$ of the truncated problem which converges to λ_γ as $X \to \infty$ satisfies

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

where C_3 and C_4 are positive constants depending on λ_γ.

(3) If an eigenvalue $\lambda_{\gamma,X,\text{bad}}$ 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 $\lambda_{\gamma,X,\text{bad}}$ is responsible for spectral pollution – then

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

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

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

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 $\lambda_{\gamma,X,\text{good}}$ and polluting eigenvalues $\lambda_{\gamma,X,\text{bad}}$, the truncated, shifted problems will also possess eigenvalues $\lambda_{\gamma,X,\text{ess}}$ which converge to the essential spectrum in such a way that for fixed $\gamma > 0$ and $X = R + Na$, where a is the period of the underlying background and $N \to \infty$, they satisfy

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

In fact all but finitely many points in any compact subset of the essential spectrum admit such approximations.

These results are not exhaustive.

Concerning the non-truncated problems, the "compact shift" trick (1) may generate further eigenvalues. We shall consider the behaviour of such eigenvalues as functions of γ. Taken together, the results in Proposition 1 and Theorem 12 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 $\gamma_{\text{crit}} > 0$ such that, as $\gamma \searrow \gamma_{\text{crit}}$, λ_γ converges to an interior point of a spectral band.

(4) As $\gamma \searrow 0$, λ_γ converges to a "pseudo-gap" in the essential spectrum of a self-adjoint operator described in Theorem 12. (By a pseudo-gap we mean a point in the essential spectrum at which the spectral measure has zero derivative.)

Numerical results will be presented to indicate that the second and third possibilities do appear to be realised 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.

All our analysis is one-dimensional with the exception of Theorem 10, which only uses exponential decay of eigenfunctions and some abstract operator theory. A result similar to Theorem 10 therefore holds for PDEs, and one of our numerical experiments in Section 6 is indeed a PDE.

3. 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

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

and

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

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 $\gamma \in \mathbb{R}$,

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

Proposition 1. *For any bounded, compactly supported s, the spectrum of $L_0 + i\gamma S$ converges to the spectrum of L_0 as $\gamma \to 0$.*

Proof. Since $\|S\| = \|s\|_{L^\infty(0,\infty)}$ and L_0 is self-adjoint,

$$\sup_{\lambda \in \sigma(L_0 + i\gamma S)} \operatorname{dist}(\lambda, \sigma(L_0)) \le \gamma \|S\| = \gamma \|s\|_{L^\infty(0,\infty)}$$

(see, e.g., the proof of Theorem V.4.10 in [16]). Thus every spectral point of $L_0 + i\gamma S$ must converge to a spectral point of L_0. Because s is compactly supported, $\sigma_{\text{ess}}(L_0) = \sigma_{\text{ess}}(L_0 + i\gamma S)$ by [15], Theorem IX.9.3, whatever definition of essential spectrum is used in the non-self-adjoint case. Thus it remains only to show that any isolated eigenvalue of L_0 can be approximated by an eigenvalue of $L_0 + i\gamma S$ as $\gamma \searrow 0$. Here we remark that the family $T(z) = L_0 + zS$ is holomorphic at $z = 0$ in the sense of Kato [16], Theorem VII.1.3, since $L_0 + iI$ is boundedly invertible and $(L_0 + iI + zS)^{-1}$ is holomorphic in z for small $|z|$. This means that each isolated eigenvalue of the family $T(z)$ has at worst an algebraic singularity at $z = 0$ [16], Theorem VII.1.8. In fact, because the Schrödinger equation has at most one square summable solution for any value of the spectral parameter, the isolated eigenvalues of L_0 are all simple, and hence each of the eigenvalues of $T(z)$ is holomorphic at $z = 0$: in other words, the eigenvalues of L_0 evolve holomorphically into eigenvalues of $L_0 + i\gamma S$ as functions of γ, for small $|\gamma|$. □

In order to describe the point spectrum of $L_0 + i\gamma S$ we use a technique called Glazman decomposition [3], § 130, which is equivalent to a two-sided shooting

[1] This is equivalent to assuming that the associated differential equation is in the so called limit-point case at infinity, see [12].

method. Fix $\lambda \in \mathbb{C}$; fix any non-zero constant h and consider the following two boundary value problems:

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

and

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

If these problems can be solved then we may define

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

The functions m_{left} and m_{right} are one-dimensional Dirichlet to Neumann maps. They are analytic functions; m_{left} is meromorphic with poles at the eigenvalues of the non-self-adjoint Sturm–Liouville problem on $[0, R]$ with the given boundary condition at 0 and homogeneous Dirichlet condition at R, see [9]; the function $-m_{\text{right}}$ is Nevanlinna [12], Chapter 9, eq. (3.14), if $\text{supp}(s) \subseteq [0, R]$.

Suppose there exists $\mu \in \mathbb{C}$ such that

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

and define a nontrivial function u by

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

Then 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 of $L_0 + i\gamma S$ with eigenvalue μ. The converse reasoning is equally straightforward, and we obtain the following result.

Lemma 2. *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 $m_{\text{left}} + m_{\text{right}}$.*

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

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

$$q(x + a) = q(x) \quad \text{for all } x \ge R_0; \tag{16}$$

(**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 [14]. Since $q(x)$ is periodic for $x \geq R \geq R_0$ 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 $\varphi(x, \lambda)$ of (7), and constants $\rho_1(\lambda)$, $\rho_2(\lambda)$ such that for $x \geq R$,

$$\begin{aligned} \begin{pmatrix} \psi(x+a,\lambda) \\ \psi'(x+a,\lambda) \end{pmatrix} &= \rho_1(\lambda) \begin{pmatrix} \psi(x,\lambda) \\ \psi'(x,\lambda) \end{pmatrix}, \\ \begin{pmatrix} \varphi(x+a,\lambda) \\ \varphi'(x+a,\lambda) \end{pmatrix} &= \rho_2(\lambda) \begin{pmatrix} \varphi(x,\lambda) \\ \varphi'(x,\lambda) \end{pmatrix}; \end{aligned} \tag{18}$$

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 $\sigma_{\text{ess}}(L_0)$. Thus for each $\lambda \notin \sigma_{\text{ess}}(L_0)$ 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 $\varphi(\cdot, \lambda)$ 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 2 the following.

Corollary 3. *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*

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

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

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

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

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

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

The spectra of $L_{0,X}$ and $L_{0,X} + i\gamma S$ are now purely discrete. We can characterise the eigenvalues of $L_{0,X} + i\gamma S$ by replacing problem P_{right} in the Glazman decomposition (12), (13) by

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

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

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

where

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

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 2 and Corollary 3.

Lemma 4. *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

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

4. The effect of interval truncation: convergence rate estimates

Theorem 5. *Suppose that assumptions* (**A1**) *and* (**A2**) *hold; see* (16) *and* (17). *For* $\gamma > 0$ *let* λ_γ *be an eigenvalue of the non-self-adjoint Schrödinger operator* $L_0 + i\gamma S$ *defined in* (9)–(11). *Then any approximation* $\lambda_{\gamma,X,\text{good}}$ *to* λ_γ *obtained as an eigenvalue of the operator* $L_{0,X} + i\gamma S$ *defined in* (22) *and* (23), *satisfies*

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

where C_3 *and* C_4 *are positive constants which depend on* λ_γ.

Proof. Without loss of generality it is sufficient to check the cases $X = R + Na$ where $N \in \mathbb{N}$ is sufficiently large. The other cases follow by exploiting the latitude in the choice of the constants c and R in (22) and (23). For instance, if $X = R + Na + b$, with $0 < b < a$, then we can replace R by $R + b$ and use a smaller constant c in (23).

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

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

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 2 and 4. We know that

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

and we seek points $\lambda_{\gamma,X,\text{good}}$ which satisfy (30) together with the truncated-problem eigenvalue condition

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

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

$$C_X(\lambda) = \Big(\frac{\rho_1(\lambda)}{\rho_2(\lambda)}\Big)^N C_R(\lambda). \tag{33}$$

Observe that for some constants $c_- < 1$ and $c_+ > 1$, we have $|\rho_1(\lambda)| < c_- < 1$ and $|\rho_2(\lambda)| = |\rho_1(\lambda)|^{-1} > c_+ > 1$, uniformly with respect to λ in a neighbourhood of λ_γ, because λ_γ does not lie in a spectral band. It follows that $C_X(\lambda)$ is exponentially small in N, uniformly with respect to λ in a neighbourhood of λ_γ. Thus, in addition to (31), we have from (32) and (33) that

$$|(m_{\text{left}}(\lambda) + m_{\text{right}}(\lambda)) - (m_{\text{left}}(\lambda) + m_{\text{right},X}(\lambda))| \leq |C_R(\lambda)|\Big(\frac{c_-}{c_+}\Big)^N \tag{34}$$

uniformly with respect to λ in a neighbourhood of λ_γ. It follows by a standard zero-counting argument for analytic functions (Lemma 20 in the Appendix) that there exist points $\lambda_{\gamma,X,\text{good}}$ which satisfy (32) and are such that

$$|\lambda_\gamma - \lambda_{\gamma,X,\text{good}}| \leq O\Big(\frac{c_-}{c_+}\Big)^{N/\nu}, \tag{35}$$

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); moreover, any solutions of (32) which converge to λ_γ must satisfy (35).

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 6. *Suppose that assumptions* (**A1**) *and* (**A2**) *hold; see* (16) *and* (17). *For* $\gamma > 0$ *let* $\lambda_{\gamma,X,\text{bad}}$ *be an eigenvalue of the non-self-adjoint Schrödinger operator* $L_{0,X} + i\gamma S$ *defined in* (22) *and* (23) *which converges, as* $X \to +\infty$, *to a point which is not in the spectrum of* $L_0 + i\gamma S$. *Then for some positive constants* C_5 *and* C_6,

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

Proof. As in the proof of Theorem 5 it suffices to consider the case $X = R + Na$ where $N \in \mathbb{N}$. Let $\mu = \lim_{X\to\infty} \lambda_{\gamma,X,\text{bad}}$. We shall use the fact that $\lambda_{\gamma,X,\text{bad}}$ satisfies

$$m_{\text{left}}(\lambda_{\gamma,X,\text{bad}}) + m_{\text{right},X}(\lambda_{\gamma,X,\text{bad}}) = 0. \tag{36}$$

From (25), (26), and (27), and from (33) in the proof of Theorem 5, we deduce that

$$m_{\text{right},X}(\lambda) = m_{\text{right}}(\lambda)\left(\frac{1 - \left(\frac{\rho_1(\lambda)}{\rho_2(\lambda)}\right)^N C_R(\lambda)\frac{\varphi'(R,\lambda)}{\psi'(R,\lambda)}}{1 - \left(\frac{\rho_1(\lambda)}{\rho_2(\lambda)}\right)^N C_R(\lambda)\frac{\varphi(R,\lambda)}{\psi(R,\lambda)}}\right) \tag{37}$$

and we remark that off the real axis, the functions $\psi(R,\cdot)$, $\psi'(R,\cdot)$, $\varphi(R,\cdot)$ and $\varphi'(R,\cdot)$ have no 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 (37) 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 [12], Chapter 9). From this locally uniform convergence, together with the fact that $\lambda_{\gamma,X,\text{bad}} \to \mu$, we obtain, for large X,

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

and so $m_{\text{right},X}(\lambda_{\gamma,X,\text{bad}}) \to m_{\text{right}}(\mu)$ as $X \to \infty$. But from (36) this yields

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

From Lemma 2 this means that μ is an eigenvalue of $L_0 + i\gamma S$, a contradiction.

Thus μ must be real and, by hypothesis, must lie in a spectral gap.

Case 2 (μ *is real and lies in a spectral gap*). Again μ lies off the essential spectrum so we still have

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

which is exponentially small. From (37) 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 $\psi(R, \lambda_{\gamma,X,\text{bad}})$, $\psi'(R, \lambda_{\gamma,X,\text{bad}})$ is exponentially small; equivalently, if and only if at least one of the following functions of λ,

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

is exponentially small when evaluated at $\lambda = \lambda_{\gamma,X,\text{bad}}$. 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 self-adjoint problems over one period $[R, R + a]$ would have eigenvalues with algebraic multiplicity exceeding 1, which is impossible). Thus $\lambda_{\gamma,X,\text{bad}}$ must be exponentially close to the real axis, which completes the proof. □

Finally we obtain an estimate which deals with rate of convergence of points approximating the essential spectrum. Note that for each $\lambda_{\text{ess}} \in \sigma_{\text{ess}}(L_0) = \sigma_{\text{ess}}(L_0 + i\gamma S)$ the existence of approximating points $\lambda_{\gamma,X,\text{ess}}$ in $\sigma(L_{0,X} + i\gamma S)$ is not difficult to establish in the self-adjoint case $\gamma = 0$, see, e.g., the results on spectral inclusion in [5]. The question here is to obtain both existence of such approximating points, and a rate of convergence, in the dissipative case $\gamma > 0$.

Theorem 7. *Assume that hypotheses* (**A1**) *and* (**A2**) *hold. Then for any point* λ_{ess} *of the essential spectrum which is neither a band end nor a zero of* $\psi'(R;\cdot)/\psi(R;\cdot) - m_{\text{left}}(\cdot)$, *there exists a constant* C *independent of* N *and an approximating sequence of eigenvalues* $\lambda_{\gamma,R+Na,\text{ess}}$ *such that* $\Im(\lambda_{\gamma,R+Na,\text{ess}}) \leq CN^{-1}$ *for all sufficiently large* N.

Proof. We first consider the result for a self-adjoint case. Let λ_{ess} be any interior point of a spectral band. Consider the self-adjoint problem on $[R, R+Na]$ for large N, equipped with Dirichlet boundary conditions at $x = R$ and at $x = R + Na$. Let λ_N be any eigenvalue of this problem; denote its eigenfunction by u_N. Up to normalization we must have

$$u_N(x) = \psi(x;\lambda_N) - \Big(\frac{\psi(R+Na;\lambda_N)}{\varphi(R+Na;\lambda_N)}\Big)\varphi(x,\lambda_N),$$

since this satisfies the differential equation together with the Dirichlet condition $u_N(R+Na) = 0$. This yields, in terms of the Floquet multipliers ρ_1 and ρ_2,

$$u_N(x) = \psi(x;\lambda_N) - \Big(\frac{\rho_1(\lambda_N)}{\rho_2(\lambda_N)}\Big)^N\Big(\frac{\psi(R;\lambda_N)}{\varphi(R;\lambda_N)}\Big)\varphi(x,\lambda_N). \tag{39}$$

Define a function of $(x;\lambda)$, following the notation of (25), by

$$\psi_{R+Na}(x;\lambda) = \psi(x;\lambda) - r(\lambda)^N\Big(\frac{\psi(R;\lambda)}{\varphi(R;\lambda)}\Big)\varphi(x,\lambda),$$

where $r(\lambda) = \rho_1(\lambda)/\rho_2(\lambda)$. The fact that $\psi_{R+Na}(R;\lambda_N) = u_N(R) = 0$ means that

$$1 - r(\lambda_N)^N = 0, \tag{40}$$

since $\psi(R;\lambda)$ is always non-zero for real λ. Using the representations $\rho_1(\lambda) = \exp(iak(\lambda))$, $\rho_2(\lambda) = \exp(-iak(\lambda))$, where $\Im(k(\lambda)) = 0$ on the spectral bands, we see that $r(\lambda) = \exp(2iak(\lambda))$ and so λ_N must be a root of one of the equations

$$k(\lambda) = \frac{\nu\pi}{Na}, \quad \nu = 0, \pm1, \pm2, \ldots. \tag{41}$$

We can now describe how to ensure that $\lambda_N - \lambda_{\text{ess}} = O(N^{-1})$.

Provided λ_{ess} is not an endpoint of a spectral band then $k'(\lambda_{\text{ess}}) > 0$, where dash denotes differentiation. This follows easily from results in Eastham [14]; see Lemma 21 in the appendix below. Now choose $\nu = \nu_N$ according to the formula

$$\nu_N = \lceil \pi^{-1} Nak(\lambda_{\text{ess}}) \rceil, \tag{42}$$

so that

$$k(\lambda_{\text{ess}}) - \frac{\nu_N\pi}{Na} = O(N^{-1}).$$

Hence (41) becomes $k(\lambda) = k(\lambda_{\text{ess}}) + O(N^{-1})$. Since $k'(\lambda_{\text{ess}}) > 0$ the Newton–Kantorovich [20] Theorem guarantees the existence, for all sufficiently large N, of a root λ_N such that

$$\lambda_N = \lambda_{\text{ess}} + O(N^{-1}).$$

Our next aim is to generalise this to the non-self-adjoint case over $[0, R+Na]$ with $\gamma \neq 0$. The condition which must be satisfied in this case is not $\psi_{R+Na}(R;\lambda) = 0$ but

$$\frac{\psi'_{R+Na}(R;\lambda)}{\psi_{R+Na}(R;\lambda)} = m_{\text{left}}(\lambda),$$

see (29). This rearranges to yield, instead of (40),

$$r(\lambda)^N = \frac{\psi'(R;\lambda)/\psi(R;\lambda) - m_{\text{left}}(\lambda)}{\varphi'(R;\lambda)/\varphi(R;\lambda) - m_{\text{left}}(\lambda)}. \tag{43}$$

When $\lambda = \lambda_{\text{ess}}$, the right hand side of (43) has modulus ≤ 1. To see this, we make two observations. Firstly, when λ is an interior point of the essential spectrum, some standard Floquet manipulations show that $\psi'(R;\lambda)/\psi(R;\lambda)$ is the complex conjugate of $\varphi'(R;\lambda)/\varphi(R;\lambda)$. Secondly, an integration-by-parts of the type in [12], p. 227, shows that $\Im(m_{\text{left}}(\lambda)) > 0$ for $\Im(\lambda) < \gamma$, that $\Im(\psi'(R;\lambda)/\psi(R;\lambda)) \geq 0$ for $\Im(\lambda) \geq 0$, and hence that $\Im(\varphi'(R;\lambda)/\varphi(R;\lambda)) \leq 0$ for $0 \leq \Im(\lambda) < \gamma$.

Thus provided $\psi'(R;\lambda_{\text{ess}})/\psi(R;\lambda_{\text{ess}}) - m_{\text{left}}(\lambda_{\text{ess}}) \neq 0$, (41) is replaced by

$$k(\lambda) = \frac{\nu\pi}{Na} + \frac{1}{2iNa}\log\Big(\frac{\psi'(R;\lambda)/\psi(R;\lambda) - m_{\text{left}}(\lambda)}{\varphi'(R;\lambda)/\varphi(R;\lambda) - m_{\text{left}}(\lambda)}\Big), \quad \nu = 0, \pm 1, \ldots,$$

in which the real part of the logarithm is negative. If we choose $\nu = \nu_N$ according to the previous criterion (42) then we get

$$k(\lambda) = k(\lambda_{\text{ess}}) + \frac{1}{2iNa}\log\Big(\frac{\psi'(R;\lambda)/\psi(R;\lambda) - m_{\text{left}}(\lambda)}{\varphi'(R;\lambda)/\varphi(R;\lambda) - m_{\text{left}}(\lambda)}\Big) + O(N^{-1}).$$

Since $k'(\lambda_{\text{ess}}) > 0$, this equation will have a root $\tilde{\lambda}_N$ for all sufficiently large N, by the Newton–Kantorovich Theorem [20], satisfying $\tilde{\lambda}_N = \lambda_{\text{ess}} + O(N^{-1})$, with $\Im(\tilde{\lambda}_N) > 0$. Denoting this root by $\lambda_{\gamma,R+Na,\text{ess}}$ yields the required result. □

Remark 8. The condition that $\psi'(R;\lambda_{\text{ess}})/\psi(R;\lambda_{\text{ess}}) - m_{\text{left}}(\lambda_{\text{ess}})$ be non-zero will be satisfied for almost every choice of γ, since m_{left} is an analytic non-constant function of γ.

Remark 9. A less satisfactory aspect of Theorem 7 is that since the quasi-momentum $k(\cdot)$ is generally not differentiable at the ends of the spectral bands, the theorem does not give any error estimate for the approximations to the endpoints of the spectral bands. However in the case $\gamma = 0$ a simpler approach using Weyl singular sequences establishes that every point of the essential spectrum can be approximated with error at worst $O(N^{-1/2})$, without exception: exploiting the fact that for $\lambda \in \sigma_{\text{ess}}(L_0)$, the function $|\psi(\cdot,\lambda)|$ (say) is a-periodic, one constructs functions u_N with support in $(R, R+Na)$ such that $-u_N'' + qu_N = \lambda u_N$ on $[R+a, R+(N-1)a]$ with the properties that

$$\int_{R+ja}^{R+(j+1)a} |u_N|^2 = 1, \quad j = 1, \ldots, N-2,$$

and, on $[R, R+a] \cup [R+(N-1)a, R+Na]$,

$$|-u_N'' + (q-\lambda)u_N| = O(1).$$

These have the properties that $Su_N = 0$ and

$$\frac{\|(L_0-\lambda)u_N\|}{\|u_N\|} = \frac{\|(L_0+i\gamma S-\lambda)u_N\|}{\|u_N\|} = O(N^{-1/2}).$$

The approximation property is then immediate for the self-adjoint operator L_0 but not for the non-self-adjoint operator $L_0 + i\gamma S$.

5. Eigenvalue evolution with respect to the coupling constant, for general potentials

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**). We already know from Proposition 1 that eigenvalues λ_γ must converge to spectral points of L_0 as $\gamma \searrow 0$: in other words, the perturbation $i\gamma S$ is not responsible for spectral pollution. We now consider in more detail the behaviour of eigenvalues λ_γ of $L_0 + i\gamma S$ whose real parts approximate eigenvalues of L_0, for small γ; we also consider the behaviour of those λ_γ which converge to points of the essential spectrum of L_0 with decreasing γ.

Theorem 10. *Suppose that assumption* (**A2**) *holds; see* (17). *Let λ be an isolated eigenvalue of L_0 with eigenfunction u. For each sufficiently small $\gamma > 0$, let λ_γ be an isolated eigenvalue of the non-self-adjoint Schrödinger operator $L_0 + i\gamma S$ defined in* (9)–(11) *with eigenfunction u_γ, and suppose $\lambda_\gamma \to \lambda$ as $\gamma \to 0$. Then the inner products $\langle u_\gamma, u\rangle$ remain bounded away from zero, uniformly with respect to R and γ, for all sufficiently small $\gamma > 0$.*

If, additionally, the following assumption

(**A1′**) $|u(x)| \le C\exp(-C_2 x)$ *for some positive constants C and C_2*

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

$$|\lambda + i\gamma - \lambda_\gamma| \le C_1\gamma\exp(-c\,C_2 R), \tag{44}$$

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

Proof. If γ is sufficiently small then we may surround λ by a contour Γ which is such that λ is the only spectral point of L_0 inside Γ and λ_γ is the only spectral point of $L_0 + i\gamma S$ inside Γ. Since $\|S\| = 1$ independently of R and as L_0 is self-adjoint, we have $|\lambda - \lambda_\gamma| \le \gamma$ independently of R so the contour Γ can be chosen independently

of R. The Riesz projection for $L_0 + i\gamma S$ associated with the λ_γ, u_γ is given by $P = \frac{1}{2\pi i}\int_\Gamma (\mu - (L_0 + i\gamma S))^{-1} d\mu$, which can be written as

$$P = \frac{1}{2\pi i}\int_\Gamma (\mu - L_0)^{-1} d\mu + \frac{\gamma}{2\pi}\int_\Gamma (\mu - L_0 - i\gamma S)^{-1}(S - I)(\mu - L_0 - i\gamma)^{-1} d\mu.$$

The second integral above is $O(\gamma)$ for small γ, uniformly in R since $\|S\| = 1$ independently of R. The first integral is just the projection for the unperturbed operator L_0. Thus $\langle u_\gamma, u\rangle = \langle u, u\rangle + O(\gamma)$, proving the first result.

Now we know that $(L_0 + i\gamma S)u_\gamma = \lambda_\gamma u_\gamma$ and that $(L_0 - i\gamma I)u = (\lambda - i\gamma)u$. Take the inner product of the first of these equations with u to obtain

$$\langle (L_0 + i\gamma S)u_\gamma, u\rangle = \lambda_\gamma \langle u_\gamma, u\rangle \tag{45}$$

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

$$\langle (L_0 - i\gamma I)u, u_\gamma\rangle = (\lambda - i\gamma)\langle u, u_\gamma\rangle; \tag{46}$$

use the fact that L_0 and S are self-adjoint and that u and u_γ both lie in the domain of L_0, which is contained in the domain of S, to rearrange (46) as

$$\langle (L_0 + i\gamma I)u_\gamma, u\rangle = (\lambda + i\gamma)\langle u_\gamma, u\rangle. \tag{47}$$

Now subtract (45) from (47) to obtain

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

The inner product $\langle u_\gamma, u\rangle$ on the left hand side is bounded away from zero for all sufficiently small γ, uniformly with respect to R. At the same time, using hypotheses (**A1′**) and (**A2**),

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

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

Remark 11. 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 $x \to +\infty$. The estimation of the exponential decay rate for an eigenfunction in terms of the distance of the corresponding eigenvalue from the essential spectrum is extensively studied in the literature: see, e.g., [21] and the references therein, in particular Agmon [1].

Let $L_{R,D}$ denote the self-adjoint operator on $[R, \infty)$ given by the expression $L_{R,D}u = -u'' + qu$ with Dirichlet boundary condition $u(R) = 0$ and suppose that its spectral measure ρ_{right} is absolutely continuous. Note that $\sigma_{\text{ess}}(L_{R,D}) = \sigma_{\text{ess}}(L_0)$ and denote by $\sigma_{\text{ess,inc}}(L_0) \subset \sigma_{\text{ess}}(L_0)$ the set of all points of the essential spectrum of L_0 at which ρ_{right} is strictly increasing.

Theorem 12. *Suppose that q is real-valued and locally L^1 and that the operator L_0 given by (9) and (10) is self-adjoint. Suppose further that the cutoff function s is a step function, taking the value 1 on $[0, R)$ and 0 on (R, ∞), as in (17) with $c = 1$. Let λ_γ be an eigenvalue of $L_0 + i\gamma S$ that converges non-tangentially to the real axis as $\gamma \searrow \gamma_{\text{crit}} \geq 0$, to a point $\mu \in \sigma_{\text{ess,inc}}(L_0)$. Then $\gamma_{\text{crit}} > 0$.*

Proof. Referring back to (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 (15),

$$m_{\text{left}}(\lambda_\gamma; \gamma) + m_{\text{right}}(\lambda_\gamma) = 0, \tag{48}$$

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. In (48) we observe that in view of the fact that s is a step-function satisfying the hypothesis (**A2**), we have $m_{\text{left}}(\lambda; \gamma) = m_{\text{left}}(\lambda - i\gamma; 0)$, so (48) becomes

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

It is known (see, e.g., [12], p. 228) that $\Im(-m_{\text{left}}(z; 0))$ is of the same sign as $\Im(z)$ and $\Im(-m_{\text{right}}(z))$ is of the same sign as $\Im(z)$. Taking imaginary parts in (49) immediately shows that $\Im(\lambda(\gamma) - i\gamma) < 0$ when $\Im(\lambda(\gamma)) > 0$, which can be proved more easily by numerical range estimates. We now let $\gamma \searrow \gamma_{\text{crit}}$ so that $\lambda(\gamma)$ approaches $\mu \in \mathbb{R}$. Because the limit is non-tangential, by hypothesis, the Titchmarsh–Kodaira formula gives

$$\lim_{\gamma \searrow \gamma_{\text{crit}}} \Im(-m_{\text{right}}(\lambda(\gamma))) = \pi \frac{d\rho_{\text{right}}}{d\lambda}(\mu) > 0,$$

where ρ_{right} is the spectral measure associated with $L_{R,D}$ and the strict inequality $\frac{d\rho_{\text{right}}}{d\lambda}(\mu) > 0$ holds by hypothesis. Thus, necessarily,

$$\lim_{\gamma \searrow \gamma_{\text{crit}}} \Im(-m_{\text{left}}(\lambda(\gamma) - i\gamma; 0)) < 0. \tag{50}$$

However the problem P_{left} has no essential spectrum, so m_{left} has no cut-line singularities on the real axis. Hence (50) gives

$$\Im(-m_{\text{left}}(\mu - i\gamma_{\text{crit}}; 0)) < 0,$$

which implies that $\gamma_{\text{crit}} > 0$ since $\Im m_{\text{left}}(z; 0) = 0$ for real z and $\Im(-m_{\text{left}}(z; 0)) > 0$ for $\Im(z) > 0$. This completes the proof. □

Remark 13. Borisov and Gadyl'shin [7] 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 $\gamma_{\text{crit}} > 0$ such that for $0 \leq \gamma < \gamma_{\text{crit}}$ there are no eigenvalues of $H_0 + \mathcal{L}_\gamma$ in $K \cap \sigma_{\text{ess}}(H_0)$. The present result, however, is stronger in one respect. It implies that if K contains no band ends then, for sufficiently small $\gamma > 0$, there are no eigenvalues either in $K \cap \mathbb{C}_+$ or in $K \cap \sigma_{\text{ess}}(L_0)$.

To see this, recall that in (49) the functions m_{left} and m_{right} are analytic away from band ends. For $\gamma = 0$ there will be finitely many solutions of (49) in K, all on the real axis, and none in $K \cap \mathbb{C}_+$. For small $\gamma > 0$, say $0 < \gamma \leq \gamma_0$, there will still only be finitely many solutions of (49) in K, and hence only finitely many in $K \cap \mathbb{C}_+$, say $\lambda_1(\gamma), \ldots, \lambda_\nu(\gamma)$. Using Theorem 12, each of these solutions will have a corresponding strictly positive critical value of γ, say $\gamma_{\text{crit}}^{(1)}, \ldots, \gamma_{\text{crit}}^{(\nu)}$. Taking $\gamma_K \stackrel{\text{def}}{=} \min(\gamma_{\text{crit}}^{(1)}, \ldots, \gamma_{\text{crit}}^{(\nu)})$ we therefore find that for $0 < \gamma < \gamma_K$ there are no solutions of (49) in $K \cap \mathbb{C}_+$. There are also no eigenvalues in $K \cap \sigma_{\text{ess}}(L_0)$, since the differential equation does not have square summable solutions for $\lambda \in \sigma_{\text{ess}}(L_0)$.

This result depends on dissipativity. 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 $\gamma > 0$.

Remark 14. For the case of a trivial periodic background – $q \equiv 0$ – the proof of Theorem 12 becomes particularly straightforward. The solution of the differential equation which is in $L^2(0, \infty)$ is given by

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

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

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

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

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

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

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

$$\sqrt{\lambda - i\gamma} \approx \sqrt{\lambda}\Big(1 - \frac{i\gamma}{2\lambda}\Big),$$

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

show that (51) becomes

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

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

6. Examples and numerics

Example 15. For our first example we take

$$-u'' + \left(\frac{-40}{1+x^2} + \sin(x)\right)u = \lambda u, \quad u(0) = 0. \tag{52}$$

The first three spectral bands for this problem are

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

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 [24]). This makes it impossible to distinguish most of them from the band end.

We made the perturbation

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

and examined the resulting eigenvalues. For $\gamma = \frac{1}{4}$, Figure 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 $C_2 \approx 0.2006$.

With $R = 48$ fixed, Figure 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 (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 in [19], § 6.1, Table 1, and then vary R rather than X. The results in Figure 3 appear to show that (5) is tight, with $C_5 \approx 0.019$, $C_6 \approx 0.1376$.

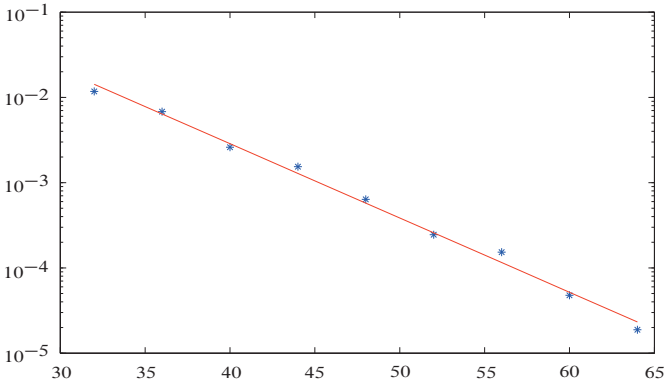

Figure 1. Logarithmic plot of $|\lambda + i\gamma - \lambda_\gamma|$ against R.

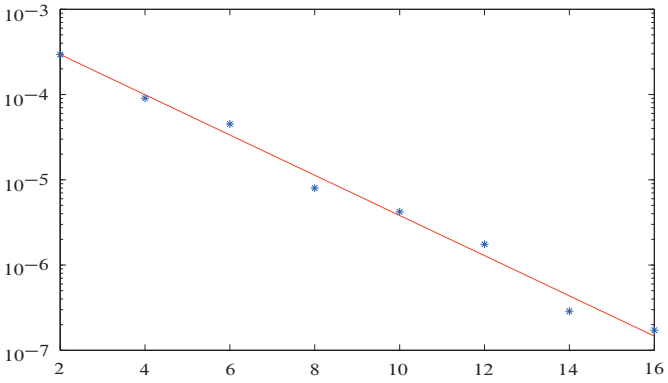

Figure 2. Logarithmic plot of $|\lambda_\gamma - \lambda_{\gamma,X,\text{good}}|$ against $X - R$.

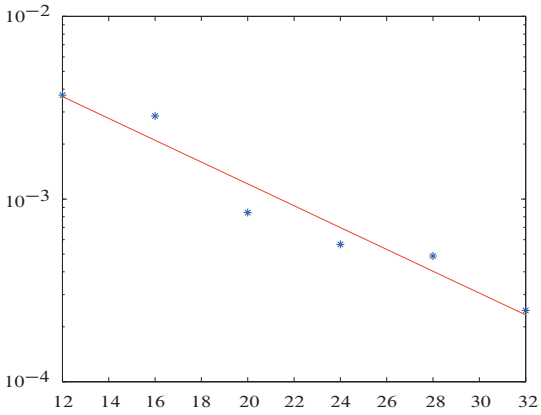

Figure 3. Logarithmic plot of $\Im(\lambda_{\gamma,X,\text{bad}})$ against $X - R$; $X = 64$ was fixed.

Finally, we attempted to verify whether or not the $O(N^{-1})$ error estimate in (6) for approximation of the essential spectrum is correct. This is a little more difficult again: if the eigenvalues $\lambda_{\gamma,X,\mathrm{ess}}$ 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 N, the eigenvalue $\lambda_{\gamma,R+Na,\mathrm{ess}}$ closest to μ, we were able to produce Figure 4, which gives very convincing numerical evidence that it is impossible to achieve better than $O(N^{-1})$ convergence.

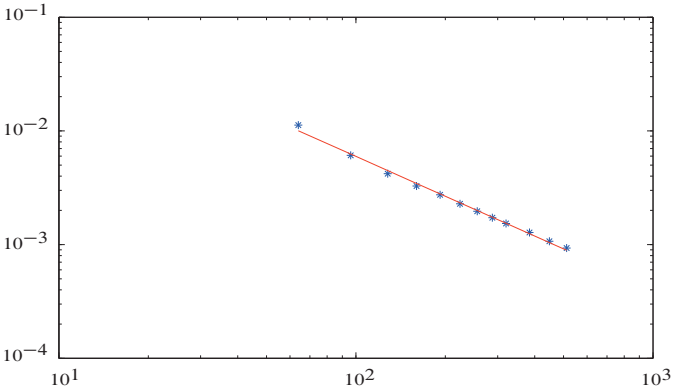

Figure 4. Plot of $\Im(\lambda_{\gamma,R+Na,\mathrm{ess}})$ against $R + Na$.

Example 16. Continuing with (52), we examined the behaviour of eigenvalues as functions of γ under the perturbation

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

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 of the spectral band, some of which may correspond to spectral concentrations [10]. 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 $\gamma_{\mathrm{crit}} \approx 0.025$ 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.

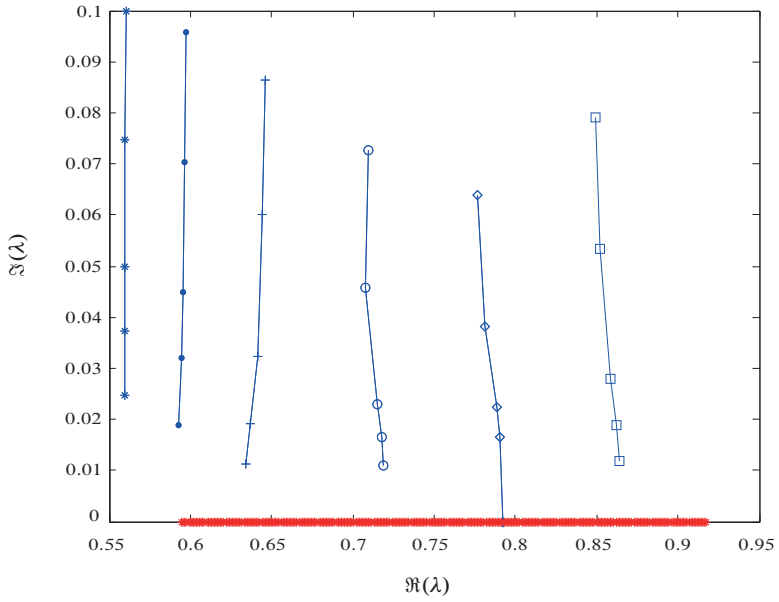

Figure 5. One gap eigenvalue and five points of essential spectrum giving rise to six eigenvalues for a dissipative perturbation of the original self-adjoint operator.

Example 17. As mentioned in Remark 14, 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

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

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

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

Example 18. This example falls slightly outside the scope of the ODE theory of this paper; however the methods used to prove Theorem 10 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 truncated to the rectangle $[-60, 60]^2$, equipped with Dirichlet boundary conditions and solved using MATLAB PDETool with a user-adapted mesh. Figure 6 shows an eigenvalue lifted into the upper half plane by the dissipative perturbation.

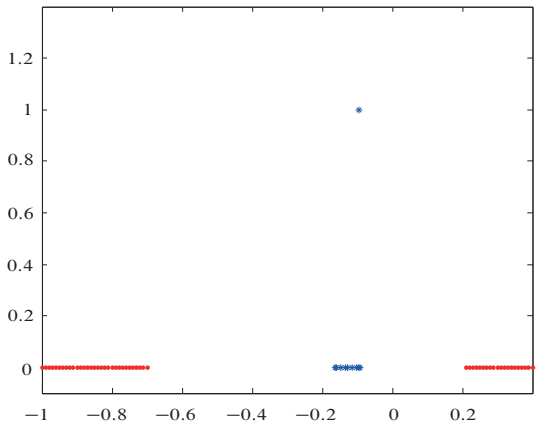

Figure 6. Computed spectrum of perturbed periodic Schrödinger equation. The genuine eigenvalue has been shifted into the upper half plane. Spectral pollution stays close to the real axis, as one would guess by Theorem 6.

The eigenvalue calculated was

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

Boulton and Levitin [8] obtained $\lambda \in [-0.09697 - \varepsilon, -0.09697 + \varepsilon]$ with $\varepsilon = 3.39 \times 10^{-4}$. The real part of our computed λ_γ agrees with the result in [8] so well that we suspect that both results are 30 times more accurate than the error bound in [8]. The error in the imaginary part (10^{-9}) is also very small. 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.

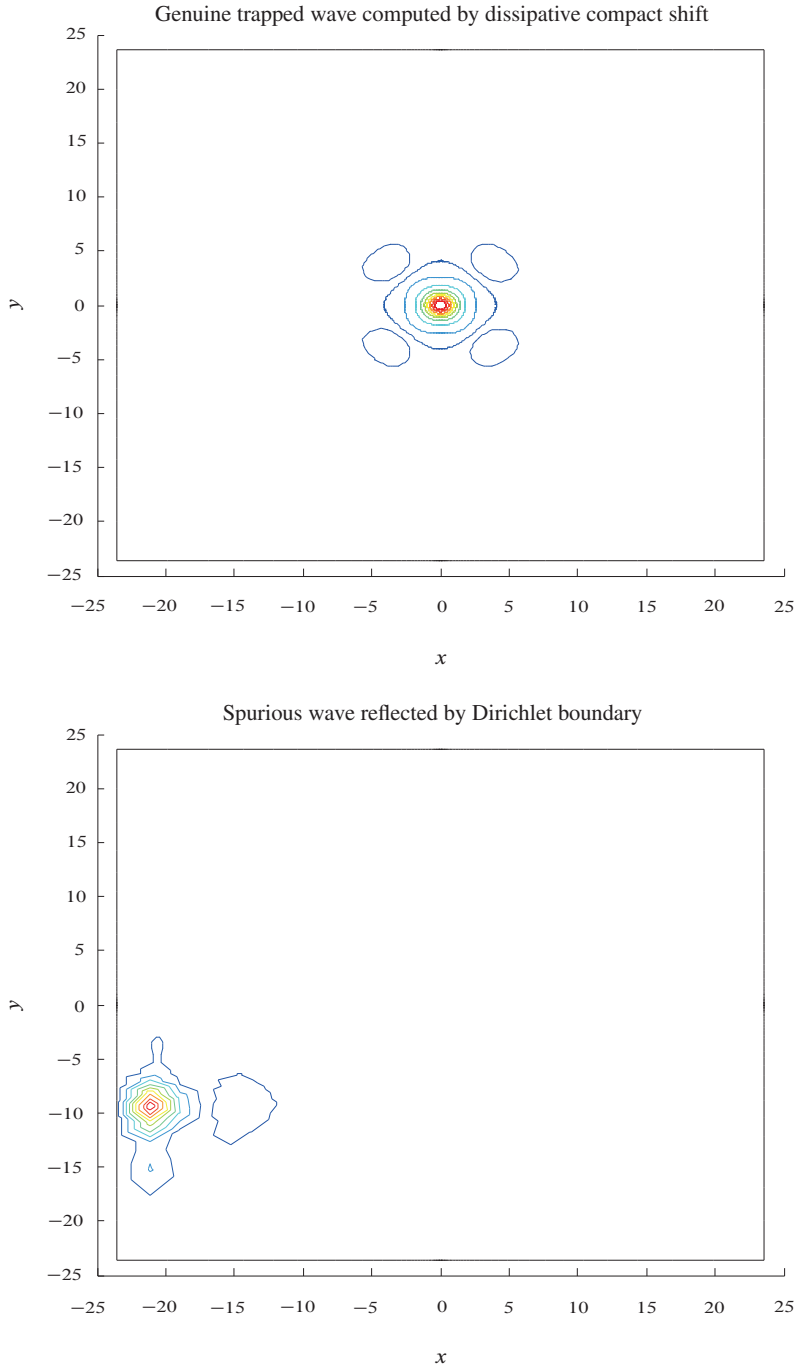

Figure 7. Genuine and polluting eigenfunction: it is clear which is which.

Example 19. We consider for $\delta \geq 0$, $x \in [0, \infty)$ the problem

$$-u'' + x^2 \exp(-\delta x^2)u = \lambda u, \quad u(0) = 0. \tag{53}$$

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 [4].

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.

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.

Pole of m_{left} (Dirichlet eigenvalues)	Zero of m_{left} (Neumann eigenvalues)	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	$17.5519026 + 0.1959618i$

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; requires very few additional lines of programming; and appears to be much more computationally efficient than the pessimistic remarks at the end of the introduction in [19] suggest.

8. Appendix

Lemma 20. *Let f be an analytic function having a zero of order $\nu \geq 1$ at a point z_0 and let (f_ε) be a family of analytic functions parametrised by a (small) parameter ε such that for some constants $C, r > 0$, and all sufficiently small $|\varepsilon|$,*

$$|f(z) - f_\varepsilon(z)| \leq C|\varepsilon| \tag{54}$$

for all $|z - z_0| \leq r$. Then there exists a constant K such that for all sufficiently small $|\varepsilon|$, the function f_ε has ν zeros in the disc with centre z_0 and radius $K|\varepsilon|^{1/\nu}$. Moreover there are no other zeros of f_ε which converge to z_0 as ε tends to zero.

Proof. By making an affine change of variables if necessary, we may assume without loss of generality that $z_0 = 0$. On a circle $|z| = \rho$ of sufficiently small radius $\rho > 0$, inside which f has only the isolated zero of multiplicity ν at the origin, there will exist positive constants m_1, m_2 such that

$$m_1\rho^\nu \leq |f(z)| \leq m_2\rho^\nu. \tag{55}$$

Provided ε is sufficiently small to ensure that $m_1\rho^\nu > C|\varepsilon|$, then (55) and (54) will yield

$$|f(z) - f_\varepsilon(z)| < |f(z)|, \quad |z| = \rho,$$

so by Rouché's theorem f and f_ε have the same number of zeros in the disc $|z| < \rho$. Taking $\rho = 2(C|\varepsilon|/m_1)^{1/\nu}$ gives the required existence result with $K = 2(C/m_1)^{1/\nu}$; taking $\rho = \rho(\varepsilon)$ to be greater than the greatest absolute value of any zero of f_ε which converges to 0 as ε tends to zero, we also deduce that there can be no others beyond those already counted. □

Lemma 21. *In terms of the Hill discriminant $D(\lambda)$ the quasi-momentum $k(\lambda)$ satisfies, at the interior points of any spectral band,*

$$ak'(\lambda) = \frac{\pm D'(\lambda)}{\sqrt{4 - (D(\lambda))^2}}, \tag{56}$$

in which the sign is chosen so that $k'(\lambda) > 0$. Consequently, $k'(\lambda)$ is non-zero at all interior points of spectral bands, and if $\lambda = \mu$ is such a point then

$$ak(\mu + i\varepsilon) \sim ak(\mu) + i\varepsilon k'(\mu) \tag{57}$$

in which $k'(\mu) > 0$.

Proof. The quasi-momentum k is related to the Hill discriminant by the equation

$$\exp(2iak(\lambda)) - D(\lambda)\exp(iak(\lambda)) + 1 = 0;$$

see [14], p. 2. This means that $D(\lambda) = 2\cos(ak(\lambda))$. Differentiating with respect to λ gives (56). The fact that $D'(\lambda)$ does not vanish at interior points of spectral bands is part of the proof of [14], Theorem 2.3.1. Equation (57) is immediate by Taylor expansion. The sign of k' is determined to ensure $\Re(iak(\mu + i\varepsilon)) < 0$ for $\varepsilon > 0$, so that our solution $\psi(\cdot, \mu + i\varepsilon)$ lies in $L^2(0, \infty)$ for $\varepsilon > 0$; this means we require $k'(\lambda) > 0$ for real λ in a spectral band. □

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