SPECTRAL INCLUSION AND POLLUTION FOR A CLASS OF DISSIPATIVE PERTURBATIONS

ALEXEI STEPANENKO

Cardiff University, School of Mathematics, Senghennydd Road, Cardiff, UK, CF24 4AG

ABSTRACT. Spectral inclusion and spectral pollution results are proved for sequences of linear operators of the form $T_0 + i\gamma s_n$ on a Hilbert space, where s_n is strongly convergent to the identity operator and $\gamma > 0$. We work in both an abstract setting and a more concrete Sturm-Liouville framework. The results provide rigorous justification for a method of computing eigenvalues in spectral gaps.

1. INTRODUCTION

In this paper, we study the eigenvalues of linear operators under a certain class of perturbations with an emphasis on Schrödinger operators of the form,

$$T_R = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q + i\gamma\chi_{[0,R]} \qquad \text{on } L^2(0,\infty), \tag{1.1}$$

where q is a possibly complex-valued function and χ is the characteristic function. Specifically, we are concerned with how the eigenvalues of T_R approximate the spectrum of the *limit operator* $T = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q + i\gamma$. As well as giving a precise account for the case of Schrödinger operators T_R with the *background potential* q either in L^1 or eventually real periodic, we give general results for abstract operators of this form, utilising the notion of limiting essential spectrum recently introduced by Bögli (2018) [3].

It is well known that the numerical approximation of the spectra of linear operators is often complicated by the possible presence of *spectral pollution* [2, 12, 23, 31]. The primary motivation for this paper is the justification of the *dissipative barrier method*, designed to circumvent such issues.

The perturbations we consider belong to a class of operators which are often referred to as *complex absorbing potentials* in the context of Schrödinger operators. These arise in the study of the damped wave equation [10, 11, 18], in the computation of resonances in quantum chemistry [32, 33, 37] and in the study of resonances in quantum chaos [29, 30].

1.1. **Spectral Inclusion and Pollution.** Suppose that we are interested in approximating the spectrum of a (linear) operator H on a Hilbert space $\mathcal{H}$ with domain $D(H)$. Let (H_n) be a sequence of operators on $\mathcal{H}$ whose spectra $\sigma(H_n)$ we hope will approximate the spectrum $\sigma(H)$ of H as $n \to \infty$. The *limiting spectrum* of (H_n) is defined by

$$\sigma((H_n)) = \{\lambda \in \mathbb{C} : \exists I \subset \mathbb{N} \text{ infinite}, \exists \lambda_n \in \sigma(H_n), n \in I \text{ with } \lambda_n \to \lambda\}. \quad (1.2)$$

(H_n) is said to be *spectrally inclusive* for H in some $\Omega \subset \mathbb{C}$ if

$$\sigma(H) \cap \Omega \subset \sigma((H_n)). \quad (1.3)$$

The set of *spectral pollution* for (H_n) with respect to H is defined by

$$\sigma_{\text{poll}}((H_n)) = \{\lambda \in \sigma((H_n)) : \lambda \notin \sigma(H)\}. \quad (1.4)$$

In order to reliably approximate the spectrum of H in $\Omega \subset \mathbb{C}$ using (H_n), we require that there is no spectral pollution in Ω, $\sigma_{\text{poll}}((H_n)) \cap \Omega = \emptyset$, and that (H_n) is spectrally inclusive for H in Ω. If this holds, we say that (H_n) is *spectrally exact* for H in Ω.

A typical scenario in which the set of spectral pollution may be non-empty is one in which the essential spectrum $\sigma_e(H)$ of H has a band-gap structure and the operators H_n have compact resolvents (i.e. H_n have purely discrete spectra). For this reason, spectral pollution often causes issues for the numerical computation of eigenvalues in spectral gaps. Various methods have been proposed to deal with such issues, we mention for instance [6, 12, 21, 24, 25, 36]. We focus on one such method, which involves perturbing the operator of interest such as to move the spectrum, in a predictable way, away from the set of spectral pollution caused by numerical discretisation [28].

1.2. **Dissipative Barrier Method.** Let us now describe this method. Let T_0 be a self-adjoint operator on a Hilbert space $\mathcal{H}$; suppose we are interested in numerically computing the spectrum of T_0. A dissipative barrier method for T_0 is defined by a bounded sequence of self-adjoint, T_0-compact operators (s_n) tending strongly to the identity operator on $\mathcal{H}$. If $\mathcal{H} = L^2(0, \infty)$, for instance, a typical choice for s_n would be $\chi_{[0,n]}$. Define the *perturbed operators* by

$$T_n = T_0 + i\gamma s_n \qquad (n \in \mathbb{N}) \quad (1.5)$$

where $\gamma > 0$. The *limit operator* T is defined by $T = T_0 + i\gamma$. The spectrum of T_0 is exactly encoded in the spectrum of T since $\sigma(T) = \sigma(T_0) + i\gamma$.

Under appropriate additional conditions on T_0 and s_n, it can be proved that there exist spectrally inclusive numerical methods for the computation of $\sigma(T_n)$ for fixed n [1, 5, 26, 27, 28, 35]. Furthermore, any spectral pollution for these numerical methods lies on $\mathbb{R}$, away from $\sigma(T)$ uniformly in n. The recently introduced notion of essential numerical range for unbounded operators can be used to prove general results of this form (see Theorems 4.5, 6.1 and 7.1 in [4]). Thanks to such numerical methods for $\sigma(T_n)$, if (T_n) can be shown to be spectrally exact for T in an open neighbourhood in $\mathbb{C}$ of a closed subset $i\gamma + I \subset i\gamma + \mathbb{R}$, then in principle one can reliably numerically compute the spectrum of T_0 in I.

1.3. **Analysis of Expanding Barriers.** The aim of this paper is to provide spectral inclusion and spectral pollution results for sequences of operators of the form (1.5).

In Section 2, we work in an abstract setting, utilising the limiting essential spectrum $\sigma_e((T_n))$ [3], which is a set enclosing the regions in $\mathbb{C}$ where spectral exactness for (T_n) with respect to T may fail. With additional assumptions on the operators s_n, for instance that they are projection operators, we prove new types of non-convex enclosures for $\sigma_e((T_n))$ and conclude for these cases that (T_n) is spectrally exact for T in an open neighbourhood of any eigenvalue of T. The paper [22] gives a similar spectral exactness conclusion for the case that (s_n) are projection operators. However, as well as including different classes of perturbations (s_n), both the statement and the proof of our results in Section 2 are far simpler than those of [22], owing to the use of the limiting essential spectrum.

The remainder of the paper is devoted to a more precise analysis for the case of Sturm-Liouville operators on the half-line. Our results in Sections 3 and 4 apply to operators for which the solutions of the corresponding Sturm-Liouville equation satisfy a certain decomposition. In particular, this decomposition is easily shown to be satisfied by Schrödinger operators T_R of the form (1.1) with the background potential q either in L^1 or real eventually periodic. In Section 3, we show that any eigenvalue of the limit operator $T \equiv T_0 + i\gamma \equiv -\mathrm{d}^2/\mathrm{d}x^2 + q + i\gamma$ for these cases is approximated by the spectrum of T_R with exponentially small error as $R \to \infty$. A similar result was proved in [28, Theorem 10], but only for γ sufficiently small. In Section 4 we show that the essential spectrum of T is approximated by the eigenvalues of T_R with an error of order $O(1/R)$[1]. The latter result is the first of its type to be reported.

We also characterise the set of spectral pollution for the two cases of perturbed Schrödinger operators T_R. Let $(R_n) \subset \mathbb{R}_+$ be any sequence such that $R_n \to \infty$. Since the dissipative barrier perturbations $i\gamma\chi_{[0,R_n]}$ are relatively compact, the essential spectrum $\sigma_e(T_0)$ is contained in the spectral pollution $\sigma_{\mathrm{poll}}((T_{R_n}))$ by Weyl's Theorem[2]. Note that this is in contrast to typical examples of spectral pollution, due to numerical discretisation, which are caused by spurious eigenvalues. It is shown in Section 3 that $\sigma_e(T_0)$ is the only possible source of spectral pollution for the case $q \in L^1$. We encourage the reader to inspect Figures 2 and 3 in Section 5, which illustrate the eigenvalues of T_R for this case. For q eventually real periodic, the set of spectral pollution outside $\sigma_e(T_0)$ is enclosed in the set of zeros of a certain analytic function constructed from solutions of (time-independent) Schrödinger equations. In fact, we prove that these zeros are contained inside the limiting essential spectrum $\sigma_e((T_{R_n}))$. Figure 4 in Section 5 shows how spectral pollution may occur in this second case.

1.4. **Summary of Results.** The definitions of the essential spectrum $\sigma_e(H)$ and the discrete spectrum $\sigma_d(H)$ for an operator H are given by equations (1.8) and (1.9) below.

Limiting Essential Spectrum and Spectral Pollution. In Section 2, we consider a self-adjoint operator T_0 on Hilbert space $\mathcal{H}$. It is assumed that the operators s_n ($n \in \mathbb{N}$) on $\mathcal{H}$ are self-adjoint, tend strongly to the identity operator as $n \to \infty$ and

---

[1]Although band-ends and embedded resonances may have a different rate of convergence.

[2]With the possible exception of a few isolated points if T_0 is non-self-adjoint.

are bounded independently of n. For $\gamma > 0$, we define the perturbed operators T_n ($n \in \mathbb{N}$) by (1.5) and the limit operator by $T = T_0 + i\gamma$.

The main tool in this section is the notion of *limiting essential spectrum* $\sigma_e((T_n))$ (see Definition 2.1). The results of [3] show that (Corollary 2.7)

$$(T_n) \text{ is spectrally exact for } T \text{ in } \mathbb{C} \backslash [\sigma_e((T_n)) \cup \sigma_e((T_n^*))^* \cup \sigma_e(T)].$$

The *limiting essential numerical range* $W_e((T_n))$ of (T_n) (see Definition 2.5), introduced by Bögli, Marletta and Tretter (2020), is a convex set which in our set-up satisfies (Propositions 2.6 and 2.9)

$$\sigma_e((T_n)) \cup \sigma_e((T_n^*))^* \subset W_e((T_n)) \subset [\text{conv}(\hat{\sigma}_e(T_0)) \backslash \{\pm \infty\}] \times i\gamma[s_-, s_+],$$

where $\hat{\sigma}_e(T_0)$ denotes the extended essential spectrum of T_0 (see Definition 2.8) and $s_\pm \in \mathbb{R}$ (defined by (2.5)) satisfy $s_- - \varepsilon \leqslant s_n \leqslant s_+ + \varepsilon$ for any $\varepsilon > 0$ and large enough n.

The main results of Section 2 are non-convex enclosures for $\sigma_e((T_n))$ complementing the enclosure provided by $W_e((T_n))$.

(A) (Theorem 2.11) If s_n is a projection operator for all n, that is $s_n^2 = s_n$, then $\sigma_e((T_n)) \cup \sigma_e((T_n^*))^* \subset \Gamma_a = \Gamma_a(\sigma_e(T_0), \gamma)$, where

$$\Gamma_a := \left\{ \lambda \in \mathbb{C} : \Im(\lambda) \in [0, \gamma], \ \text{dist}(\Re(\lambda), \sigma_e(T_0)) \leqslant \sqrt{\Im(\lambda)(\gamma - \Im(\lambda))} \right\}. \quad (1.6)$$

If for any sequence $(u_n) \subset D(T_0)$ bounded in $\mathcal{H}$ with $(T_0 u_n)$ bounded in $\mathcal{H}$ we have

$$\langle s_n u_n, T_0 u_n \rangle - \langle T_0 u_n, s_n u_n \rangle \to 0 \text{ as } n \to \infty$$

(Assumption 1) then $\sigma_e((T_n)) \cup \sigma_e((T_n^*))^* \subset \Gamma_b = \Gamma_b(\sigma_e(T_0), \gamma, s_\pm)$, where

$$\Gamma_b := \sigma_e(T_0) \times i\gamma[s_-, s_+].$$

In particular, if s_n are projection operators or if Assumption 1 is satisfied then

$$(T_n) \text{ is spectrally exact for } T \text{ in some open neighbourhood of any } \lambda \in \sigma_d(T).$$

We clarify that by open neighbourhood we mean open neighbourhood in $\mathbb{C}$. The enclosures Γ_a and Γ_b are illustrated in Figure 1. Assumption 1 is verified for a class of perturbations for Schrödinger operators on Euclidean domains in Example 2.13.

Second Order Operators on the Half-Line. In Section 3, we consider the case in which T_0 is a Sturm-Liouville operator on $L^2(0, \infty)$ and provide a more precise analysis compared to Section 2. The Sturm-Liouville operator T_0 is allowed to have complex coefficients and is endowed with a complex mixed boundary condition at 0.

We assume that for any $\lambda \in \mathbb{C} \backslash \sigma_e(T_0)$, the solution space of the equation $\tilde{T}_0 u = \lambda u$ (here, $\tilde{T}_0$ is the differential expression corresponding to T_0) is spanned by solutions $\psi_\pm(\cdot, \lambda)$ admitting the decomposition

$$\psi_\pm(x, \lambda) = e^{\pm ik(\lambda)x} \tilde{\psi}_\pm(x, \lambda).$$

Here, k and $\tilde{\psi}_\pm(x, \cdot)$ are analytic functions on $\mathbb{C} \backslash \sigma_e(T_0)$ with $\Im k > 0$ and with $\tilde{\psi}_\pm(\cdot, \lambda)$ bounded. A similar decomposition is required for $\psi'_\pm$ - see Assumption 2 for the precise statement.

The perturbed operators in Section 3 are defined by

$$T_R = T_0 + i\gamma\chi_{[0,R]} \qquad (R \in \mathbb{R}_+) \qquad (1.7)$$

where $\gamma \in \mathbb{C}\backslash\{0\}$. The limit operator is defined by $T = T_0 + i\gamma$. Under these assumptions, for any (R_n) with $R_n \to \infty$, we construct a set $S_{\mathfrak{p}}((R_n))$ (equation (3.20)) and prove the following:

(B) (Theorems 3.8 and 3.9) For any eigenvalue λ of T with $\lambda \notin S_{\mathfrak{p}}((R_n))$ and $\lambda \notin \sigma_e(T_0)$, there exists eigenvalues λ_n of T_{R_n} $(n \in \mathbb{N})$ such that

$$|\lambda - \lambda_n| = O(e^{-\beta R_n}) \text{ as } n \to \infty$$

for some $\beta > 0$ independent of n. Furthermore, the set of spectral pollution for (T_{R_n}) with respect to T satisfies

$$\sigma_{\mathrm{poll}}((T_{R_n})) \subset \sigma_e(T_0) \cup S_{\mathfrak{p}}((R_n)).$$

The proofs utilise Rouché's theorem applied to an analytic function (Lemma 3.4) whose zeros are the eigenvalues of T_R. (B) implies that

$$(T_{R_n}) \text{ is spectrally exact for } T \text{ in } \mathbb{C}\backslash(\sigma_e(T_0) \cup \sigma_e(T) \cup S_{\mathfrak{p}}((R_n))).$$

Assumption 2 is verified in two cases:

- (Examples 3.2 and 3.10) T_0 is a Schrödinger operator with an L^1 potential. In this case, $S_{\mathfrak{p}}((R_n)) = \emptyset$.
- (Examples 3.3 and 3.11) T_0 is a Schrödinger operator with an eventually real a-periodic potential, $\gamma > 0$ and $R_n - R_{n-1} = a$ for all n. In this case, $S_{\mathfrak{p}}((R_n))$ is expressed as the zeros of a certain analytic function (equation (3.29)). It is also proved that $S_{\mathfrak{p}}((R_n)) \subset \sigma_e((T_n))$.

Inclusion for the Essential Spectrum. In Section 4, we let T_0 be a Sturm-Liouville operator satisfying Assumption 2, as described above. In addition, we require that $\sigma_e(T_0) \subset \mathbb{R}$ and that k and $\tilde{\psi}_+(x,\cdot)$, hence $\psi_+(x,\cdot)$, admit analytic continuations into an open neighbourhood of any point in the interior of $\sigma_e(T_0)$. See Assumption 3 for the precise statement.

The perturbed operators T_R and the limit operator in Section 4 are defined by (1.7) and $T = T_0 + i\gamma$ respectively, as in Section 3. We construct a set $S_{\mathfrak{r}} \subset i\gamma + \mathbb{R}$ (equation (4.9)) and prove that:

(C) (Theorem 4.6) For any μ in the interior of $\sigma_e(T_0)$ with $\mu + i\gamma \notin S_{\mathfrak{r}}$, there exists eigenvalues λ_R of T_R $(R \in \mathbb{R}_+)$ such that

$$|\lambda_R - (\mu + i\gamma)| = O\left(\frac{1}{R}\right) \text{ as } R \to \infty.$$

The proof utilises Rouché's theorem applied to an analytic function (Lemma 4.3) whose zeros are the eigenvalues of T_R. In the case that

- (Examples 4.1 and 4.9) T_0 is a Schrödinger operator with an L^1 potential satisfying the Naimark condition or a dilation analyticity condition, or,
- (Examples 4.2 and 4.10) $\gamma > 0$ and T_0 is a Schrödinger operator with a real, eventually periodic potential, endowed with a real mixed boundary condition at 0,

it is proven that Assumption 3 is satisfied and that

$$\mu + i\gamma \in S_{\mathfrak{r}} \text{ if and only if } \mu \text{ is a resonance of } T_0 \text{ embedded in } \sigma_e(T_0).$$

See equation (4.23) for the precise definition of a resonance used here. For these cases, since resonances in the interior of $\sigma_e(T_0)$ are isolated, we can combine Theorem 4.6 with Theorem 3.9 and the characterisation of $S_\mathfrak{p}((R_n))$ to conclude that

(T_n) is spectrally exact for T in some open neighbourhood of any $\mu \in \mathrm{int}(\sigma_e(T))$.

Notation and Conventions. Let $\mathcal{H}$ be a separable Hilbert space with corresponding inner product $\langle \cdot, \cdot \rangle$ and norm $\|\cdot\|$. Let $B_n \xrightarrow{s} B$ as $n \to \infty$ denote strong convergence in $\mathcal{H}$ for bounded operators B_n and B on $\mathcal{H}$. Let $f_n \rightharpoonup f$ as $n \to \infty$ denote weak convergence in $\mathcal{H}$ for $f_n, f \in \mathcal{H}$. In this paper, we define the essential spectrum of an operator H on $\mathcal{H}$ by

$$\sigma_e(H) = \left\{ \lambda \in \mathbb{C} : \begin{array}{l} \exists (u_n) \subset D(H) \text{ with } \|u_n\| = 1, \\ u_n \rightharpoonup 0, \ \|(H - \lambda)u_n\| \to 0 \end{array} \right\} \tag{1.8}$$

which corresponds to σ_{e2} in [16]. The sequence (u_n) appearing in (1.8) is referred to as a singular sequence. The discrete spectrum is defined by

$$\sigma_d(H) = \sigma(H) \backslash \sigma_e(H). \tag{1.9}$$

The convention we take with regards to the square-root function is to make the branch-cut along the positive semi-axis, so that $\Im \sqrt{z} \geqslant 0$ for all $z \in \mathbb{C}$. We let $B_r(z)$ denote an open ball of radius $r > 0$ around a point $z \in \mathbb{C}$. In Sections 3 and 4, $\psi'(x, z) := \frac{\mathrm{d}}{\mathrm{d}x} \psi(x, z)$.

2. Limiting Essential Spectrum and Spectral Pollution

In this section, we study spectral exactness for sequences of abstract operators (T_n) of the form (1.5). In Section 2.1, we briefly review the notions of limiting essential spectrum and essential numerical range. We refer the reader to [3] and [4] for a more detailed exposition. In Section 2.2, we discuss the application of limiting essential spectrum and essential numerical range to (T_n). In Section 2.3, we prove enclosures for the limiting essential spectrum of (T_n).

2.1. **Limiting Essential Spectrum and Numerical Range.** Let $\mathcal{H}_n \subset \mathcal{H}$ ($n \in \mathbb{N}$) be closed subspaces and let $P_n : \mathcal{H} \to \mathcal{H}_n$ be the corresponding orthogonal projections. Assume that $P_n \xrightarrow{s} I$. Let H and H_n ($n \in \mathbb{N}$) be closed, densely-defined operators acting on $\mathcal{H}$ and $\mathcal{H}_n$ respectively.

Definition 2.1. The *limiting essential spectrum* of (H_n) is defined by

$$\sigma_e((H_n)) = \left\{ \lambda \in \mathbb{C} : \begin{array}{l} \exists I \subset \mathbb{N} \text{ infinite}, \exists u_n \in D(H_n), n \in I \text{ with} \\ \|u_n\| = 1, \ u_n \rightharpoonup 0, \ \|(H_n - \lambda)u_n\| \to 0 \end{array} \right\}. \tag{2.1}$$

Definition 2.2. (H_n) converges to H in the *generalised strong resolvent sense*, denoted by $H_n \xrightarrow{\text{gsr}} H$, if

$$\exists n_0 \in \mathbb{N} : \exists \lambda_0 \in \bigcap_{n \geqslant n_0} \rho(H_n) \cap \rho(H) : (H_n - \lambda_0)^{-1} P_n \xrightarrow{s} (H - \lambda_0)^{-1}.$$

In the case that $\mathcal{H}_n = \mathcal{H}$ for all n, generalised strong resolvent convergence is equivalent to strong resolvent convergence and denoted by $H_n \xrightarrow{\text{sr}} H$.

Theorem 2.3 ([3, Theorem 2.3]). *If $H_n \xrightarrow{\text{gsr}} H$ and $H_n^* \xrightarrow{\text{gsr}} H^*$ then*

$$\sigma_{\mathrm{poll}}((H_n)) \subset \sigma_e((H_n)) \cup \sigma_e((H_n^*))^* \tag{2.2}$$

and every isolated $\lambda \in \sigma(H)$ outside $\sigma_e((H_n)) \cup \sigma_e((H_n^*))^*$ is approximated by (H_n), that is,

$$\{\lambda \in \sigma(H) : \lambda \text{ isolated}, \lambda \notin \sigma_e((H_n)) \cup \sigma_e((H_n^*))^*\} \subset \sigma((H_n)).$$

Definition 2.4. The *essential numerical range* of H is defined by

$$W_e(H) = \{\lambda \in \mathbb{C} : \exists (u_n) \subset D(H) \text{ with } \|u_n\| = 1, \, u_n \rightharpoonup 0, \, \langle Hu_n, u_n \rangle \to \lambda\}.$$

Definition 2.5. The *limiting essential numerical range* of (H_n) is defined by

$$W_e((H_n)) = \left\{ \lambda \in \mathbb{C} : \begin{array}{l} \exists I \subset \mathbb{N} \text{ infinite, } \exists u_n \in D(H_n), n \in I \text{ with} \\ \|u_n\| = 1, \, u_n \rightharpoonup 0, \, \langle (H_n - \lambda)u_n, u_n \rangle \to 0 \end{array} \right\}. \tag{2.3}$$

Proposition 2.6 ([4, Proposition 5.6])**.** *The limiting essential numerical range of (H_n) is closed and convex with*

$$\mathrm{conv}(\sigma_e((H_n))) \subset W_e((H_n)).$$

Furthermore, if $D(H_n) \cap D(H_n^*)$ is a core of H_n^* for all n then

$$\mathrm{conv}(\sigma_e((H_n)) \cup \sigma_e((H_n^*))^*) \subset W_e((H_n)).$$

2.2. **Enclosures for the Limiting Essential Spectrum.** Throughout the remainder of the section, let T_0 and s_n ($n \in \mathbb{N}$) be self-adjoint operators on $\mathcal{H}$. Let $\gamma > 0$ and define the perturbed operators, as in the introduction, by

$$T_n = T_0 + i\gamma s_n. \qquad (n \in \mathbb{N}) \tag{2.4}$$

Assume that $s_n \xrightarrow{\text{s}} I$ and that $\|s_n\| \leqslant C$ for some $C > 0$ independent of n. Define the limit operator by $T = T_0 + i\gamma$ as in the introduction. T_n converges to T in the strong sense, and in fact, as we shall show in the following proof, in the strong resolvent sense.

Corollary 2.7. *(T_n) is spectrally exact for T in $\mathbb{C} \backslash [\sigma_e((T_n)) \cup \sigma_e((T_n^*))^* \cup \sigma_e(T)]$*

Proof. The fact that $T_n \xrightarrow{\text{sr}} T$ and $T_n^* = T_0 - i\gamma s_n \xrightarrow{\text{sr}} T_0 - i\gamma = T^*$ follows from an application of the resolvent identity, using $s_n \xrightarrow{\text{s}} I$, the self-adjointness of T_0 and the uniform boundedness of the sequence of operators (s_n). By Theorem 2.3, $\sigma_{\mathrm{poll}}((T_n)) \subset \sigma_e((T_n)) \cup \sigma_e((T_n^*))^*$ and

$$\{\lambda \in \sigma(T) : \lambda \text{ isolated}, \lambda \notin \sigma_e((T_n)) \cup \sigma_e((T_n^*))^*\} \subset \sigma((T_n)).$$

The corollary follows from the fact that every element of $\sigma_d(T) = \sigma_d(T_0) + i\gamma$ is isolated since T_0 is self-adjoint [16]. □

Since $D(T_n) = D(T_n^*) = D(T_0)$, Proposition 2.6 implies that the set $\sigma_e((T_n)) \cup \sigma_e((T_n^*))^*$ is contained in the limiting essential numerical range $W_e((T_n))$ and so (T_n) is spectrally exact for T in $\mathbb{C} \backslash [W_e((T_n)) \cup \sigma_e(T)]$. The limiting essential numerical range is typically easier to study than the limiting essential spectrum. For sequences of operators of the form (2.4), the limiting essential numerical range $W_e((T_n))$ is contained in a strip. To state this fact, we shall require the notion of extended essential spectrum.

Definition 2.8. The *extended essential spectrum* $\hat{\sigma}_e(H) \subset \sigma_e(H) \cup \{\pm \infty\}$ of a self-adjoint operator H on $\mathcal{H}$ is defined as the union of $\sigma_e(H)$ with $+\infty$ and/or $-\infty$ if H is unbounded from above and/or below respectively.
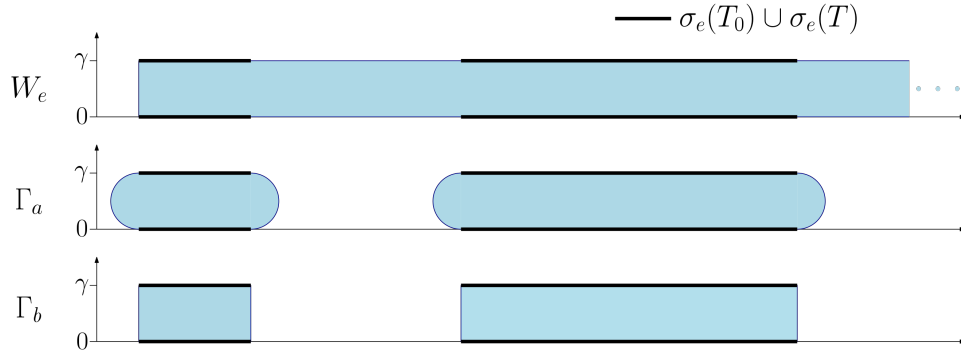
FIGURE 1. Illustration of various enclosures for the limiting essential spectrum: the limiting essential numerical range $W_e = W_e((T_n))$, the enclosure $\Gamma_a = \Gamma_a(\sigma_e(T_0), \gamma)$ of Theorem 2.11 (a) and the enclosure $\Gamma_b = \Gamma_b(\sigma_e(T_0), \gamma, s_\pm)$ of Theorem 2.11 (b). The illustration assumes that T_0 is unbounded only from above, $(s_-, s_+) = (0, 1)$ and that the plotted region shows the smallest two spectral bands.

Throughout the remainder of the section, let

$$s_- := \liminf_{n \to \infty} \inf_{u \in \mathcal{H}: \|u\|=1} \langle s_n u, u \rangle \quad \text{and} \quad s_+ := \limsup_{n \to \infty} \sup_{u \in \mathcal{H}: \|u\|=1} \langle s_n u, u \rangle. \quad (2.5)$$

Then, for any $\varepsilon > 0$ and sufficiently large n, $s_- - \varepsilon \leqslant s_n \leqslant s_+ + \varepsilon$.

Proposition 2.9. $W_e((T_n)) \subset [\text{conv}(\hat{\sigma}_e(T_0)) \backslash \{\pm\infty\}] \times i\gamma[s_-, s_+]$

Proof. Let $\lambda \in W_e((T_n))$. Then there exist $I \subset \mathbb{N}$ infinite and $(u_n)_{n \in I} \subset D(T_0)$ such that $\|u_n\| = 1$ for all $n \in I$, $u_n \rightharpoonup 0$ and $\langle (T_n - \lambda)u_n, u_n \rangle \to 0$. Taking the real part of the inner product, we have $\langle (T_0 - \Re(\lambda))u_n, u_n \rangle \to 0$ which implies that

$$\Re(\lambda) \in W_e(T_0) = \text{conv}(\hat{\sigma}_e(T_0)) \backslash \{\pm\infty\}$$

where we used [4, Theorem 3.8] in the equality. Finally, $\Im\langle (T_n - \lambda)u_n, u_n \rangle \to 0$ implies that $\Im(\lambda) = \gamma\langle s_n u_n, u_n \rangle + o(1) \in \gamma[s_-, s_+]$. □

2.3. **Main Abstract Results.** In the main result of this section, Theorem 2.11, we shall prove non-convex enclosures for the limiting essential spectrum $\sigma_e((T_n))$ that complement the enclosure provided by the limiting essential numerical range. We shall require additional assumptions on the perturbing operators (s_n). In part (a) of the theorem, we simply require that s_n are projection operators. An interesting feature of the enclosure of part (a) is that it is independent of the perturbing operators (s_n), depending only on $\sigma_e(T_0)$ and γ. The hypothesis for part (b) of the theorem, Assumption 1, is given below. An example of a class of perturbations for Schrödinger operators satisfying this assumption is provided in Example 2.13. The enclosures are illustrated in Figure 1.

Lemma 2.10. *Let H be a self-adjoint operator on $\mathcal{H}$. If for some $\eta \in \mathbb{R}$ and $\varepsilon > 0$ there exists a sequence $(u_n) \subset D(H)$ with $\|u_n\| = 1$ for all n, $u_n \rightharpoonup 0$ and $\|(H - \eta)u_n\| \to \varepsilon$ then*

$$\text{dist}(\eta, \sigma_e(H)) \leqslant \varepsilon.$$

Proof. For any $\delta > 0$ there exists $N_\delta \in \mathbb{N}$ such that $\|(H - \eta)u_n\| < (\varepsilon + \delta)\|u_n\|$ for all $n \geqslant N_\delta$. $(u_n)_{n \geqslant N_\delta}$ is a non-compact, bounded sequence so by [19, Chapter I, Theorem 10] the interval $(\eta - (\varepsilon + \delta), \eta + (\varepsilon + \delta))$ contains an infinite number of points in $\sigma(H)$. Taking the limit $\delta \to 0$ shows that the interval $[\eta - \varepsilon, \eta + \varepsilon]$ contains an infinite number of points in $\sigma(H)$. Finally, $[\eta - \varepsilon, \eta + \varepsilon]$ must contain a point of $\sigma_e(H)$ because any limit point of $\sigma_d(H)$ is in $\sigma_e(H)$. □

Assumption 1. *If $(u_n) \subset D(T_0)$ is bounded in $\mathcal{H}$ with $(T_0 u_n)$ bounded in $\mathcal{H}$ then*

$$\langle s_n u_n, T_0 u_n \rangle - \langle T_0 u_n, s_n u_n \rangle \to 0 \text{ as } n \to \infty.$$

Theorem 2.11. (a) *If s_n is a projection operator, that is $s_n^2 = s_n$, for all n then $\sigma_e((T_n)) \cup \sigma_e((T_n^*))^* \subset \Gamma_a = \Gamma_a(\sigma_e(T_0), \gamma)$ where Γ_a is defined by* (1.6).
(b) *If Assumption 1 holds then $\sigma_e((T_n)) \cup \sigma_e((T_n^*))^* \subset \Gamma_b = \Gamma_b(\sigma_e(T_0), \gamma, s_\pm)$ where*

$$\Gamma_b := \sigma_e(T_0) \times i\gamma[s_-, s_+]. \tag{2.6}$$

Proof. We will only prove that $\sigma_e((T_n)) \subset \Gamma_a$ or Γ_b - the proof that $\sigma_e((T_n^*))^* \subset \Gamma_a$ or Γ_b is similar since $T_n^* = T_0 - i\gamma s_n$.

Let $\lambda \in \sigma_e((T_n))$. Then there exist $I \subset \mathbb{N}$ infinite and $(u_n)_{n \in I} \subset D(T_0)$ with $\|u_n\| = 1$ for all $n \in I$, $u_n \rightharpoonup 0$ and $\|(T_n - \lambda)u_n\| = o(1)$. By Cauchy-Schwarz, we have $\langle (T_n - \lambda)u_n, u_n \rangle = o(1)$, whose real and imaginary parts imply that

$$\langle T_0 u_n, u_n \rangle = \Re(\lambda) + o(1) \quad \text{and} \quad \gamma\langle s_n u_n, u_n \rangle = \Im(\lambda) + o(1). \tag{2.7}$$

Since both $(T_n u_n)$ and $(s_n u_n)$ are bounded in $\mathcal{H}$, $(T_0 u_n)$ must be bounded in $\mathcal{H}$. Hence by Cauchy-Schwarz we have $\langle (T_n - \lambda)u_n, T_0 u_n \rangle = o(1)$ whose real part implies that

$$\|T_0 u_n\|^2 - \Re(\lambda)\langle T_0 u_n, u_n \rangle - \gamma\Im\langle s_n u_n, T_0 u_n \rangle = o(1). \tag{2.8}$$

The first equation in (2.7) gives

$$\|(T_0 - \Re(\lambda))u_n\|^2 = \|T_0 u_n\|^2 - \Re(\lambda)\langle T_0 u_n, u_n \rangle + o(1),$$

which, combined with (2.8), yields,

$$\|(T_0 - \Re(\lambda))u_n\|^2 = \gamma\Im\langle s_n u_n, T_0 u_n \rangle + o(1). \tag{2.9}$$

(a) In this case, $\sigma(s_n) = \{0, 1\}$ so $0 \leqslant s_n \leqslant 1$ for all n, and so by the second equation in (2.7),

$$\forall n \in I : \langle s_n u_n, u_n \rangle \in [0, 1] \quad \Rightarrow \quad \Im(\lambda) \in [0, \gamma]. \tag{2.10}$$

Focusing now on $\Re(\lambda)$, Cauchy-Schwarz gives us $\langle (T_n - \lambda)u_n, s_n u_n \rangle = o(1)$, whose imaginary part combined with the hypothesis $s_n^2 = s_n$ and the second equation in (2.7) gives,

$$\Im\langle s_n u_n, T_0 u_n \rangle = \gamma\|s_n u_n\|^2 - \Im(\lambda)\langle s_n u_n, u_n \rangle + o(1)$$

$$= (\gamma - \Im(\lambda))\frac{\Im(\lambda)}{\gamma} + o(1). \tag{2.11}$$

Combining (2.9) and (2.11), we have

$$\|(T_0 - \Re(\lambda))u_n\| = \sqrt{(\gamma - \Im(\lambda))\Im(\lambda)} + o(1) \tag{2.12}$$

which by Lemma 2.10 implies that

$$\mathrm{dist}(\Re(\lambda), \sigma_e(T_0)) \leqslant \sqrt{(\gamma - \Im(\lambda))\Im(\lambda)}.$$

(b) In this case, by the definitions of $s_\pm$ in (2.5), a similar reasoning as in (2.10) yields $\Im(\lambda) \in \gamma[s_-, s_+]$. Assumption 1 implies that

$$\Im\langle s_n u_n, T_0 u_n \rangle = o(1) \quad \Rightarrow \quad \|(T_0 - \Re(\lambda))u_n\| = o(1)$$

so (u_n) is a singular sequence proving that $\Re(\lambda) \in \sigma_e(T_0)$.

$\square$

Remark 2.12. It is interesting to note that Lemma 2.10 is not required in case (b) of Theorem 2.11. This is because Assumption 1 ensures that the following holds:

$$(u_n) \subset D(T_n) = D(T_0), \|u_n\| = 1, u_n \rightharpoonup 0, \|(T_n - \lambda)u_n\| \to 0$$
$$\Rightarrow (u_n) \subset D(T_0), \|u_n\| = 1, u_n \rightharpoonup 0, \|(T_0 - \Re(\lambda))u_n\| \to 0,$$

that is, if (u_n) is a singular-type sequence for a point λ in the limiting essential spectrum then (u_n) is also a singular sequence for $\Re(\lambda) \in \sigma_e(T_0)$.

Example 2.13. Suppose that $q \in L^1_{\mathrm{loc}}(\Omega)$ is real-valued and bounded from below. Suppose that $T_0 = -\Delta + q$ on $L^2(\Omega)$ is endowed with Dirichlet boundary conditions (see, for example, [16, Chapter VII, Theorem 1.4]). Then, T_0 is self-adjoint.

Let $\varphi \in W^{1,\infty}(0, \infty)$ be real-valued and such that $\varphi(0) = 1$. Let $(R_n) \subset \mathbb{R}_+$ be any sequence such that $R_n \to \infty$. For any $n \in \mathbb{N}$, define multiplication operator s_n on $L^2(\Omega)$ by

$$(s_n u)(x) = \varphi\left(\frac{\langle x \rangle}{R_n}\right)u(x) \qquad (u \in L^2(\Omega), \ x \in \Omega) \tag{2.13}$$

where $\langle x \rangle := (1 + |x|^2)^{\frac{1}{2}}$.

Then s_n is uniformly bounded, $s_n \xrightarrow{\mathrm{s}} I$ and Assumption 1 is satisfied.

Proof. Define $\varphi_n : \Omega \to \mathbb{R}$ by

$$\varphi_n(x) = \varphi\left(\frac{\langle x \rangle}{R_n}\right). \qquad (x \in \Omega)$$

Step 1 (Uniform boundedness). The uniform boundedness of the sequence of operators (s_n) follows from the fact that, for all $u \in L^2(\Omega)$ and all $n \in \mathbb{N}$,

$$\operatorname*{ess\,inf}_{t \in (0,\infty)} \varphi(t)\|u\|^2 \leqslant \langle s_n u, u \rangle \leqslant \operatorname*{ess\,sup}_{t \in (0,\infty)} \varphi(t)\|u\|^2.$$

Step 2 ($s_n \xrightarrow{\mathrm{s}} I$). Let $u \in L^2(\Omega)$ and let $(X_n) \subset \mathbb{R}_+$ be any sequence such that $X_n \to \infty$ and $X_n = o(R_n)$. For any $n \in \mathbb{N}$,

$$\|(s_n - I)u\| \leqslant \|\varphi(\langle \cdot \rangle / R_n) - 1\|_{L^\infty(\Omega \cap B_{X_n}(0))}\|u\| + (\|s_n\| + 1)\|u\|_{L^2(\Omega \backslash B_{X_n}(0))}. \tag{2.14}$$

By Morrey's inequality, φ is continuous, so, since $\varphi(0) = 1$, the first term on the right hand side of (2.14) tends to zero as $n \to \infty$. The second term tends to zero because $u \in L^2(\Omega)$ and $(\|s_n\|)$ is bounded.

Step 3 (Assumption 1). Let $(u_n) \subset D(T_0)$ be any sequence which is bounded in $\mathcal{H}$ such that $(T_0 u_n)$ is bounded in $\mathcal{H}$. Then,

$$\langle s_n u_n, T_0 u_n \rangle - \langle T_0 u_n, s_n u_n \rangle = -\int_\Omega \varphi_n u_n \Delta(\overline{u}_n) + \int_\Omega \varphi_n \overline{u}_n \Delta(u_n)$$
$$= \int_\Omega u_n \nabla(\varphi_n) \cdot \nabla(\overline{u}_n) - \int_\Omega \overline{u}_n \nabla(\varphi_n) \cdot \nabla(u_n).$$

The second equality above holds by integration by parts and the product rule since T_0 is endowed with Dirichlet boundary conditions. Hence we have,

$$|\langle s_n u_n, T_0 u_n \rangle - \langle T_0 u_n, s_n u_n \rangle| \leqslant 2\|\nabla \varphi_n\|_{L^\infty(\Omega)}\|\nabla u_n\|\|u_n\|. \qquad (2.15)$$

By the chain rule and the fact that $\varphi \in W^{1,\infty}(0,\infty)$, $\|\nabla \varphi_n\|_{L^\infty(\Omega)} \to 0$ as $n \to \infty$. (u_n) is bounded in $\mathcal{H}$ by hypothesis. (∇u_n) can be seen to be bounded in $\mathcal{H}$ by applying integration by parts to $\langle T_0 u_n, u_n \rangle$, using the hypotheses that $(\|T_0 u_n\|)$ is bounded and that q is bounded below. The right hand side of (2.15) tends to zero as $n \to \infty$ hence Assumption 1 is satisfied. $\qquad \square$

3. Second Order Operators on the Half-Line

Consider the differential expression

$$\tilde{T}_0 u = \frac{1}{r}(-(pu')' + qu) \quad \text{on} \quad [0,\infty)$$

where p, q and r are functions on $[0,\infty)$ satisfying the minimal hypotheses: p and q are complex in general, $r > 0$, $p \neq 0$ and $q, 1/p, r \in L^1_{\text{loc}}[0,\infty)$. These assumptions on p, q and r ensure that for any $\lambda, u_1, u_2 \in \mathbb{C}$ there exists a unique solution u to the initial value problem

$$\tilde{T}_0 u = \lambda u \quad \text{on} \quad [0,\infty), \, u(0) = u_1, \, pu'(0) = u_2$$

such that $u, pu' \in AC_{\text{loc}}[0,\infty)$. The solution space of $\tilde{T}_0 u = \lambda u$ on $[0,\infty)$ is therefore a two-dimensional complex vector space.

Consider a Sturm-Liouville operator T_0 on the weighted Lebesgue space $L^2_r(0,\infty)$, endowed with a complex mixed boundary condition at 0,

$$BC[u] := \cos(\eta)u(0) - \sin(\eta)pu'(0) = 0 \qquad (3.1)$$

for some $\eta \in \mathbb{C}$. T_0 is defined by

$$T_0 u = \tilde{T}_0 u$$
$$D(T_0) = \{u \in L^2_r(0,\infty) : u, pu' \in AC_{\text{loc}}[0,\infty), \tilde{T}_0 u \in L^2_r(0,\infty), BC[u] = 0\}. \qquad (3.2)$$

Fix $\gamma \in \mathbb{C}\backslash\{0\}$. Define the perturbed operators by

$$T_R u = T_0 u + i\gamma\chi_{[0,R]}u, \, D(T_R) = D(T_0) \qquad (R \in \mathbb{R}_+) \qquad (3.3)$$

and define the limit operator by $T = T_0 + i\gamma$.

Next, we introduce the main hypotheses of this section, which we will later assume holds throughout the section. The assumption ensures that for any $\lambda \in \mathbb{C}\backslash\sigma_e(T_0)$, one solution of $\tilde{T}_0 u = \lambda u$ is exponentially decaying and the other is exponentially growing.

Assumption 2. There exists $k : \mathbb{C}\backslash\sigma_e(T_0) \to \mathbb{C}$, $\tilde{\psi}_\pm : [0,\infty) \times \mathbb{C}\backslash\sigma_e(T_0) \to \mathbb{C}$ and $\tilde{\psi}_\pm^d : [0,\infty) \times \mathbb{C}\backslash\sigma_e(T_0) \to \mathbb{C}$ such that:

(i) k is analytic and satisfies $\Im k > 0$.
(ii) $\tilde{\psi}_\pm(x,\cdot)$ and $\tilde{\psi}_\pm^d(x,\cdot)$ are analytic for all x and satisfy

$$\|\tilde{\psi}_\pm(\cdot,z)\|_{L^\infty(0,\infty)} < \infty, \quad \|\tilde{\psi}_\pm^d(\cdot,z)\|_{L^\infty(0,\infty)} < \infty \qquad (3.4)$$

for all z.

(iii) The solution space of $\tilde{T}_0 u = zu$ is spanned by $\psi_\pm(\cdot, z)$, where,

$$\psi_\pm(x, z) := e^{\pm ik(z)x} \tilde{\psi}_\pm(x, z)$$
$$\psi'_\pm(x, z) := e^{\pm ik(z)x} \tilde{\psi}^d_\pm(x, z).$$
(3.5)

Remark 3.1 (See [8]). The conditions of Assumption 2 do not exclude a situation in which $\sigma(T_0) = \sigma_e(T_0) = \mathbb{C}$. A sufficient condition to ensure that this does not occur is that

$$\overline{\text{co}} \left\{ \frac{q(x)}{r(x)} + yp(x) : x, y \in [0, \infty) \right\} \neq \mathbb{C},$$

where $\overline{\text{co}}$ denotes the closed convex hull, and that $\tilde{T}_0$ is in Sims case I.

Example 3.2 (Schrödinger operators with L^1 potentials). Consider the case $p = r = 1$ with $q \in L^1(0, \infty)$. Then,

$$\sigma_e(T_0) = [0, \infty).$$

By the Levinson asymptotic theorem [15, Theorem 1.3.1], for any $z \in \mathbb{C} \backslash \{0\}$, the solution space of $\tilde{T}_0 u = zu$ is spanned by $\psi_\pm(\cdot, z)$, where

$$\psi_\pm(x, z) = e^{\pm i\sqrt{z}x} (1 + E_\pm(x, z))$$
(3.6)

$$\psi'_\pm(x, z) = \pm i\sqrt{z} e^{\pm i\sqrt{z}x} (1 + E^d_\pm(x, z))$$
(3.7)

and

$$|E_\pm(x, z)|, |E^d_\pm(x, z)| \to 0 \text{ as } x \to \infty.$$

(i) $k(z) := \sqrt{z}$ is analytic and satisfies $\Im k > 0$ on $\mathbb{C} \backslash \sigma_e(T_0) = \mathbb{C} \backslash [0, \infty)$.

(ii) $\tilde{\psi}_\pm(x, z) := 1 + E_\pm(x, z)$ and $\tilde{\psi}^d_\pm(x, z) := \pm i\sqrt{z}(1 + E^d_\pm(x, z))$ are bounded in x for any fixed $z \in \mathbb{C} \backslash \{0\}$. For any x, $\psi_\pm(x, \cdot)$ and $\psi^d_\pm(x, \cdot)$ are analytic on $\mathbb{C} \backslash [0, \infty)$ so $\tilde{\psi}_\pm(x, \cdot)$ and $\tilde{\psi}^d_\pm(x, \cdot)$ are analytic on $\mathbb{C} \backslash [0, \infty)$.

Consequently, Assumption 2 is satisfied in this case.

Example 3.3 (Eventually periodic Schrödinger operators). Consider the case $p = r = 1$ with q eventually real periodic, that is, there exists $a > 0$ and $X \geqslant 0$ such that $q|_{[X, \infty)}$ is real-valued and a-periodic. Below, we briefly review some Floquet theory and show that the conditions of Assumption 2 are met in this case. See, for example, [14] for a detailed exposition of Floquet theory.

For any $z \in \mathbb{C}$, let $\phi_1(\cdot, z)$ and $\phi_2(\cdot, z)$ be the solutions of the Schrödinger equation $-\phi'' + q\phi = z\phi$ on $[0, \infty)$, subject to the boundary conditions

$$\phi_1(X, z) = 1, \ \phi'_1(X, z) = 0 \text{ and } \phi_2(X, z) = 0, \ \phi'_2(X, z) = 1.$$
(3.8)

The *discriminant* is defined by

$$D(z) = \phi_1(X + a, z) + \phi'_2(X + a, z).$$
(3.9)

The essential spectrum of T_0 is

$$\sigma_e(T_0) = \{z \in \mathbb{R} : |D(z)| \leqslant 2\}.$$
(3.10)

The *Floquet multipliers* $\rho_\pm$ are defined by

$$\rho_\pm(z) = \frac{1}{2}\left(D(z) \pm i\sqrt{4 - D(z)^2}\right).$$
(3.11)

Note that $\rho_\pm$ have branch cuts along $\sigma_e(T_0)$, $|\rho_+(z)| < 1$ for all $z \in \mathbb{C}\backslash\sigma_e(T_0)$ and $\rho_+(z)\rho_-(z) = 1$. Define k by

$$k(z) = -\frac{i}{a}\ln(\rho_+(z)). \tag{3.12}$$

In this setting, k is referred to as the *Floquet exponent*. k is analytic and satisfies $\Im k > 0$ on $\mathbb{C}\backslash\sigma_e(T_0)$ hence satisfies Assumption (i).

Define the *Floquet solutions* $\psi_\pm$ by

$$\psi_\pm(x, z) = -\phi_2(X + a, z)\phi_1(x, z) + (\phi_1(X + a, z) - \rho_\pm(z))\phi_2(x, z) \tag{3.13}$$

for any $x \in [0, \infty)$ and $z \in \mathbb{C}$. $\psi_\pm(\cdot, z)$ span the solution space of $\tilde{T}_0 u = zu$ and satisfy

$$\psi_\pm(x_0 + na, z) = e^{\pm ik(z)na}\psi_\pm(x_0, z)$$
$$\psi'_\pm(x_0 + na, z) = e^{\pm ik(z)na}\psi'_\pm(x_0, z) \tag{3.14}$$

for any $x_0 \in [X, X + a)$ and $n \in \mathbb{N}$. For any x, the Floquet solutions $\psi_\pm(x, \cdot)$ and $\psi'_\pm(x, \cdot)$ are analytic on $\mathbb{C}\backslash\sigma_e(T_0)$. Define the *band-ends* B_{ends} by

$$B_{\text{ends}} = \{\lambda \in \mathbb{C} : |D(\lambda)| = 2\}. \tag{3.15}$$

For any $z_0 \in \sigma_e(T_0)\backslash B_{\text{ends}}$, $\rho_\pm$ and k can be analytically continued into an open neighbourhood of z_0 in $\mathbb{C}$, hence for any $x \in [0, \infty)$, $\psi_\pm(x, \cdot)$ and $\psi'_\pm(x, \cdot)$ can be analytically continued into an open neighbourhood of z_0.

Finally, Assumption 2 can be satisfied by setting

$$\tilde{\psi}_\pm(x, z) = \begin{cases} e^{\mp ik(z)x}\psi_\pm(x, z) & \text{if } x \in [0, X) \\ e^{\mp ik(z)x_0(x)}\psi_\pm(x_0(x), z) & \text{if } x \in [X, \infty) \end{cases} \tag{3.16}$$

and

$$\tilde{\psi}^d_\pm(x, z) = \begin{cases} e^{\mp ik(z)x}\psi'_\pm(x, z) & \text{if } x \in [0, X) \\ e^{\mp ik(z)x_0(x)}\psi'_\pm(x_0(x), z) & \text{if } x \in [X, \infty) \end{cases} \tag{3.17}$$

where $x_0(x) := X + (x - X)\bmod a$.

Throughout the remainder of the section, let

$$S := \sigma_e(T_0) \cup (i\gamma + \sigma_e(T_0)) \tag{3.18}$$

and suppose that the conditions of Assumption 2 are satisfied. Also, let $(R_n) \subset \mathbb{R}_+$ be any sequence such that $R_n \to \infty$ as $n \to \infty$. Recall that BC denotes the boundary condition functional defined by equation (3.1).

Lemma 3.4. *$\lambda \in \mathbb{C}\backslash S$ is an eigenvalue of T_R if and only if*

$$f_R(\lambda) := \alpha_+(R, \lambda)e^{ik(\lambda - i\gamma)R} + \alpha_-(R, \lambda)e^{-ik(\lambda - i\gamma)R} = 0$$

where

$$\alpha_+(R, \lambda) := BC[\psi_-(\cdot, \lambda - i\gamma)]\Big(\tilde{\psi}_+(R, \lambda - i\gamma)\tilde{\psi}^d_+(R, \lambda) - \tilde{\psi}^d_+(R, \lambda - i\gamma)\tilde{\psi}_+(R, \lambda)\Big)$$

and

$$\alpha_-(R, \lambda) := BC[\psi_+(\cdot, \lambda - i\gamma)]\Big(\tilde{\psi}_+(R, \lambda)\tilde{\psi}^d_-(R, \lambda - i\gamma) - \tilde{\psi}^d_+(R, \lambda)\tilde{\psi}_-(R, \lambda - i\gamma)\Big).$$

Furthermore, f_R is analytic on $\mathbb{C}\backslash S$.

Proof. Let $\lambda \in \mathbb{C}\backslash S$ and $R > 0$. λ is an eigenvalue of T_R if and only if there exists a solution to the problem

$$(\tilde{T}_0 + i\gamma\chi_{[0,R]})u = \lambda u, \ BC[u] = 0, \ u \in L_r^2(0,\infty) \tag{3.19}$$

on $[0,\infty)$. Any solution to (3.19) on $[0,R]$ must be of the form $C_1 u_1(\cdot,\lambda)$, where u_1 is defined by

$$u_1(x,\lambda) = BC[\psi_-(\cdot,\lambda-i\gamma)]\psi_+(x,\lambda-i\gamma) - BC[\psi_+(\cdot,\lambda-i\gamma)]\psi_-(x,\lambda-i\gamma)$$

and $C_1 \in \mathbb{C}$ is independent of x. Any solution to (3.19) on $[R,\infty)$ must be of the form $C_2\psi_+(x,\lambda)$, where $C_2 \in \mathbb{C}$ is independent of x. Hence λ is an eigenvalue if and only if there exists $C_1, C_2 \in \mathbb{C}\backslash\{0\}$ independent of x such that the function

$$x \mapsto \begin{cases} C_1 u_1(x,\lambda) & \text{if } x \in [0,R) \\ C_2\psi_+(x,\lambda) & \text{if } x \in [R,\infty) \end{cases}$$

is absolutely continuous. This holds if and only if

$$u_1(R,\lambda)\psi_+'(R,\lambda) - u_1'(R,\lambda)\psi_+(R,\lambda) = 0$$

which holds if and only if the following quantity is zero

$$(BC[\psi_-(\cdot,\lambda-i\gamma)]\psi_+(R,\lambda-i\gamma) - BC[\psi_+(\cdot,\lambda-i\gamma)]\psi_-(R,\lambda-i\gamma))\tilde{\psi}_+^d(R,\lambda)$$
$$- \big(BC[\psi_-(\cdot,\lambda-i\gamma)]\psi_+'(R,\lambda-i\gamma) - BC[\psi_+(\cdot,\lambda-i\gamma)]\psi_-'(R,\lambda-i\gamma)\big)\tilde{\psi}_+(R,\lambda)$$

which in turn is equivalent to $f_R(\lambda) = 0$. The analyticity claim follows from Assumptions 2 (i) and (ii). $\square$

In the regions of the complex plane for which $\alpha_-(R,\cdot)$ becomes small for large R, we are unable to prove the spectral pollution and spectral inclusion results of Theorems 3.8 and 3.9. We now define a subset of the complex plane capturing such regions.

Definition 3.5. Define subset $S_\mathfrak{p}((R_n))$ of $\mathbb{C}$ by

$$S_\mathfrak{p}((R_n)) = \left\{ z \in \mathbb{C}\backslash S : \liminf_{n\to\infty} |\Lambda(R_n,z)| = 0 \right\} \tag{3.20}$$

where the function $\Lambda : [0,\infty) \times \mathbb{C}\backslash S \to \mathbb{C}$ is defined by

$$\Lambda(R,\lambda) = \tilde{\psi}_+(R,\lambda)\tilde{\psi}_-^d(R,\lambda-i\gamma) - \tilde{\psi}_+^d(R,\lambda)\tilde{\psi}_-(R,\lambda-i\gamma). \tag{3.21}$$

Note that with the above definition of Λ, we have

$$\alpha_-(R,\lambda) = BC[\psi_+(\cdot,\lambda-i\gamma)]\Lambda(R,\lambda)$$

and that the zeros of $\lambda \mapsto BC[\psi_+(\cdot,\lambda-i\gamma)]$ are exactly the eigenvalues of the limit operator $T = T_0 + i\gamma$.

The set $S \cup S_\mathfrak{p}((R_n))$ plays a similar role in this section as the limiting essential spectrum did in Section 2. We shall show in Theorems 3.8 and 3.9 that there is no spectral pollution for (T_{R_n}) with respect to T outside of $S \cup S_\mathfrak{p}((R_n))$ and that eigenvalues of T lying outside of $S \cup S_\mathfrak{p}((R_n))$ are approximated (with exponentially small error) by the eigenvalues of T_{R_n}.

Proposition 3.6. $S \cup S_\mathfrak{p}((R_n))$ *is a closed subset of* $\mathbb{C}$.

Proof. By Assumption 2 (ii), $\Lambda(R_n, \cdot)$ is analytic for all n and $\Lambda(\cdot, z)$ is bounded for all z. Let λ be a limit point of $S \cup S_{\mathfrak{p}}((R_n))$. The desired lemma holds if and only if λ lies in either S or in $S_{\mathfrak{p}}((R_n))$. If λ is a limit point of S then $\lambda \in S$ since S is closed. In the only other case, λ is a limit point of $S_{\mathfrak{p}}((R_n))$ so there exists $(\lambda_k) \subset S_{\mathfrak{p}}((R_n))$ such that $\lambda_k \to \lambda$ as $k \to \infty$. Since $\liminf_{n \to \infty} |\Lambda(R_n, \lambda_k)| = 0$ for all k, there exists a subsequence (R_{n_k}) such that $|\Lambda(R_{n_k}, \lambda_k)| \to 0$ as $k \to \infty$. Let $\varepsilon > 0$ be small enough so that $\overline{B_\varepsilon(\lambda)} \subset \mathbb{C}\backslash S$. Since the magnitude of $\Lambda(R, z)$ is bounded above uniformly for all $R > 0$ and all $z \in \overline{B_\varepsilon(\lambda)}$, by Cauchy's formula,

$$\Lambda(R_{n_k}, \lambda) - \Lambda(R_{n_k}, \lambda_k) = \frac{1}{2\pi i} \oint_{\partial B_\varepsilon(\lambda)} \frac{\lambda_k - \lambda}{(z - \lambda)(z - \lambda_k)} \Lambda(R_{n_k}, z) \, dz \to 0 \quad (3.22)$$

as $k \to \infty$. Finally,

$$|\Lambda(R_{n_k}, \lambda)| \leqslant |\Lambda(R_{n_k}, \lambda_k)| + |\Lambda(R_{n_k}, \lambda) - \Lambda(R_{n_k}, \lambda_k)| \to 0 \text{ as } k \to \infty$$

so $\lambda \in S_{\mathfrak{p}}((R_n))$, completing the proof. □

Corollary 3.7. *For any $\lambda \in \mathbb{C}\backslash(S \cup S_{\mathfrak{p}}((R_n)))$ there exists a bounded, open neighbourhood U of λ with $\overline{U} \subset \mathbb{C}\backslash S$ and $|\Lambda(R_n, z)| \geqslant C$ for all $z \in U$ and $n \geqslant N_0$, where $C, N_0 > 0$ are some constants independent of n and z.*

Proof. Let $\lambda \in \mathbb{C}\backslash(S \cup S_{\mathfrak{p}}((R_n)))$. $\mathbb{C}\backslash(S \cup S_{\mathfrak{p}}((R_n)))$ is an open subset of $\mathbb{C}$ so there exists a bounded open neighbourhood U of λ such that $\overline{U} \subset \mathbb{C}\backslash(S \cup S_{\mathfrak{p}}((R_n)))$. Suppose that the desired result does not hold with this choice for U. Then there exists a subsequence (R_{n_k}) and a sequence $(z_k) \subset U$ such that $|\Lambda(R_{n_k}, z_k)| \to 0$ as $k \to \infty$. Since $\overline{U}$ is compact, there exists $z \in \mathbb{C}\backslash(S \cup S_{\mathfrak{p}}((R_n)))$ such that $z_k \to z$. By the arguments in (a), $\liminf_{n \to \infty} |\Lambda(R_n, z)| = 0$, which is the desired contradiction. □

Next, we prove the main results of this section, regarding spectral inclusion and pollution for the operators T_R defined by equation (3.3) such that T_0 satisfies Assumption 2. Recall, also, that S is defined by equation (3.18), $S_{\mathfrak{p}}((R_n))$ is defined by (3.20) and $(R_n) \subset \mathbb{R}_+$ is an arbitrary sequence such that $R_n \to \infty$.

Theorem 3.8. *Let μ be an eigenvalue of T_0 and assume that $\mu + i\gamma \notin S \cup S_{\mathfrak{p}}((R_n))$. Then there exists eigenvalues λ_n of T_{R_n} ($n \in \mathbb{N}$) and constants $C_0 = C_0(T_0, \gamma, \mu) > 0$ and $\beta = \beta(T_0, \gamma, \mu) > 0$ such that*

$$|\lambda_n - (\mu + i\gamma)| \leqslant C_0 e^{-\beta R_n} \quad (3.23)$$

for all large enough n.

Proof. Let $C, C_1, C_2, C_3, N_0 > 0$ denote constants independent of λ and n, where C may change from line to line.

Since μ is an eigenvalue of T_0, $\mu + i\gamma$ is a zero of the analytic function

$$\lambda \mapsto \tilde{f}(\lambda) := BC[\psi_+(\cdot, \lambda - i\gamma)].$$

Since it is assumed that $\mu + i\gamma \notin S \cup S_{\mathfrak{p}}((R_n))$, Corollary 3.7 guarantees the existence of an open neighbourhood U of $\mu + i\gamma$ such that $\overline{U} \subset \mathbb{C}\backslash S$ and $|\Lambda(R_n, \lambda)| \geqslant C$ ($\lambda \in U$, $n \geqslant N_0$) for some sufficiently large $N_0 \in \mathbb{N}$. For $n \geqslant N_0$, $\lambda \in U$ is an eigenvalue of T_{R_n} if and only if

$$\tilde{f}_n(\lambda) := e^{ik(\lambda - i\gamma)R_n} \frac{f_{R_n}(\lambda)}{\Lambda(R_n, \lambda)} = 0.$$

Since $\overline{U} \in \mathbb{C}\backslash S$, Assumption 2 guarantees that $|\alpha_+(R_n, \lambda)| \leqslant C$ $(\lambda \in U, n \in \mathbb{N})$ and $\Im k(\lambda - i\gamma) \geqslant C$ $(\lambda \in U)$. Combined with the bound below for Λ, this implies that

$$|\tilde{f}_n(\lambda) - \tilde{f}(\lambda)| = \left| e^{2ik(\lambda - i\gamma)R_n} \frac{\alpha_+(R_n, \lambda)}{\Lambda(R_n, \lambda)} \right| \leqslant C_1 e^{-C_2 R_n} \qquad (\lambda \in U, n \geqslant N_0) \quad (3.24)$$

for some $C_1, C_2 > 0$. Since $\tilde{f}$ is analytic at $\mu + i\gamma$, there exists $\varepsilon > 0$ such that

$$|\tilde{f}(\lambda)| \geqslant C_3 |\lambda - (\mu + i\gamma)|^\nu \qquad (\lambda \in B_\varepsilon(\mu + i\gamma)) \qquad (3.25)$$

for some $C_3 > 0$. Here, ν is the algebraic multiplicity of the eigenvalue μ of T_0, that is, the multiplicity of the zero μ of the analytic function $z \mapsto BC[\psi_+(\cdot, z)]$. Let $C_0 = (2C_1/C_3)^{1/\nu}$ and $\beta = C_2/\nu$. Make $N_0 \in \mathbb{N}$ large enough such that $C_0 e^{-\beta R_n} < \varepsilon$ $(n \geqslant N_0)$. Combining (3.24) and (3.25), for all $n \geqslant N_0$ and all $\lambda \in \mathbb{C}$ with

$$|\lambda - (\mu + i\gamma)| = C_0 e^{-\beta R_n}$$

we have

$$|\tilde{f}_n(\lambda) - \tilde{f}(\lambda)| \leqslant \frac{1}{2} |\tilde{f}(\lambda)| < |\tilde{f}(\lambda)|.$$

By Rouché's theorem, for all $n \geqslant N_0$ there exists a zero $\lambda_n \in U$ of $\tilde{f}_n$ satisfying inequality (3.23). $\qquad \square$

The next result concerns spectral pollution - the set of spectral pollution is defined by equation (1.4).

Theorem 3.9. *The set of spectral pollution of the sequence of operators (T_{R_n}) with respect to the limit operator $T = T_0 + i\gamma$ satisfies*

$$\sigma_{\mathrm{poll}}((T_{R_n})) \subset \sigma_e(T_0) \cup S_{\mathfrak{p}}((R_n)).$$

Proof. Let $C > 0$ denote an arbitrary constant independent of λ and n.

Let $\mu \in \mathbb{C}\backslash(S \cup S_{\mathfrak{p}}((R_n)))$ and assume that μ is not an eigenvalue of T. Then μ is an arbitrary element of $\rho(T)\backslash(\sigma_e(T_0) \cup S_{\mathfrak{p}}((R_n)))$. We aim to show that $\mu \notin \sigma_{\mathrm{poll}}((T_{R_n}))$, for which it suffices to show that there exists a neighbourhood U of μ such that f_{R_n} has no zeros in U for large enough n.

Since $\mu \notin S_{\mathfrak{p}}((R_n))$ and $BC[\psi_+(\cdot, \mu - i\gamma)] \neq 0$,

$$|\alpha_-(R_n, \mu)| = |BC[\psi_+(\cdot, \mu - i\gamma)]\Lambda(R_n, \mu)| \geqslant C \qquad (3.26)$$

for large enough n. Let $\varepsilon > 0$ be small enough so that $\overline{B_\varepsilon(\mu)} \subset \mathbb{C}\backslash S$. Then by Assumption 2 we have

$$|\alpha_\pm(R_n, \lambda)| \leqslant C \text{ and } \Im k(\lambda - i\gamma) \geqslant C \qquad (\lambda \in B_\varepsilon(\mu), n \in \mathbb{N}) \qquad (3.27)$$

Using Cauchy's integral formula as in (3.22), and making $\varepsilon > 0$ small enough, we have

$$|\alpha_\pm(R_n, \lambda) - \alpha_\pm(R_n, \mu)| \leqslant C|\lambda - \mu| \qquad (\lambda \in B_\varepsilon(\mu), n \in \mathbb{N}). \qquad (3.28)$$

Define approximation $f_n^{(\mu)}$ to f_{R_n} by

$$f_n^{(\mu)}(\lambda) := \alpha_+(R_n, \mu)e^{ik(\lambda - i\gamma)R_n} + \alpha_-(R_n, \mu)e^{-ik(\lambda - i\gamma)R_n}.$$

By (3.28) we have

$$|f_{R_n}(\lambda) - f_n^{(\mu)}(\lambda)| \leqslant C|\lambda - \mu|e^{\Im k(\lambda - i\gamma)R_n} \qquad (\lambda \in B_\varepsilon(\mu), n \in \mathbb{N}).$$

Using (3.26) and (3.27) we have

$$|e^{ik(\lambda-i\gamma)R_n} f_n^{(\mu)}(\lambda)| \geqslant \left||\alpha_-(R_n,\mu)| - |\alpha_+(R_n,\mu)|e^{-2\Im k(\lambda-i\gamma)R_n}\right|$$
$$\geqslant \frac{|\alpha_-(R_n,\mu)|}{2} \geqslant C \qquad (\lambda \in B_\varepsilon(\mu))$$

for large enough n. Finally, making $\varepsilon > 0$ small enough if necessary, we have

$$|f_{R_n}(\lambda) - f_n^{(\mu)}(\lambda)| < |f_n^{(\mu)}(\lambda)| \qquad (\lambda \in B_\varepsilon(\mu))$$

for large enough n. f_{R_n} therefore has no zeros in $U := B_\varepsilon(\mu)$ for large enough n, completing the proof.

□

In the case of Schrödinger operators on $L^2(0,\infty)$ with L^1 potentials, described in Example 3.2, $S_\mathfrak{p}((R_n))$ can be easily computed to be the empty set.

Example 3.10 (Schrödinger operators with L^1 potentials, continued). Consider again the case $p = r = 1$ with $q \in L^1(0,\infty)$. Then, using expression (3.21) for Λ and the expressions for $\tilde{\psi}_\pm$, $\tilde{\psi}_\pm^d$ in Example 3.2 (ii), Λ satisfies

$$\Lambda(R,\lambda) \to -i\left(\sqrt{\lambda-i\gamma} + \sqrt{\lambda}\right) \text{ as } R \to \infty$$

for any $\lambda \in \mathbb{C}\backslash S$. Since $\sqrt{\lambda-i\gamma} \neq -\sqrt{\lambda}$ for all $\lambda \in \mathbb{C}$ we have

$$S_\mathfrak{p}((R_n)) = \emptyset$$

for any $(R_n) \subset \mathbb{R}_+$ with $R_n \to \infty$ as $n \to \infty$.

For Schrödinger operators with eventually real periodic potentials, described in Example 3.3, the computation of $S_\mathfrak{p}((R_n))$ is more involved.

Example 3.11 (Eventually periodic Schrödinger operators, continued). Consider again the case $p = r = 1$ with $q|_{[X,\infty)}$ real-valued and a-periodic for some $X \geqslant 0$ and $a > 0$. Assume that $\gamma > 0$ and let $R_n = x_0 + na$ $(n \in \mathbb{N})$ for any fixed $x_0 \in [X, X + a)$.

Using the expressions (3.16) and (3.17) for $\tilde{\psi}_\pm$ and $\tilde{\psi}_\pm^d$ as well as the definition of $S_\mathfrak{p}((R_n))$ in equation (3.20), we infer that $\lambda \in S_\mathfrak{p}((R_n))$ if and only if

$$\psi_+(x_0,\lambda)\psi_-'(x_0,\lambda-i\gamma) - \psi_+'(x_0,\lambda)\psi_-(x_0,\lambda-i\gamma) = 0. \tag{3.29}$$

$\psi_\pm(x_0,\cdot)$ and $\psi_\pm'(x_0,\cdot)$ are analytic on $\mathbb{C}\backslash\sigma_e(T_0)$ and can be analytically continued into an open neighbourhood in $\mathbb{C}$ of any point in $\sigma_e(T_0)\backslash B_{\text{ends}}$ (recall that B_{ends} denotes the set of band-ends for the essential spectrum of T_0). Consequently, $S_\mathfrak{p}((R_n))$ consists of isolated points in the complex plane that can only accumulate to the band-ends of either T_0 or T, that is, to the set $B_{\text{ends}} \cup (i\gamma + B_{\text{ends}})$.

Recall that $\sigma_e((T_{R_n}))$ denotes the limiting essential spectrum of the sequence of operators (T_{R_n}). $S_\mathfrak{p}((R_n))$ satisfies the inclusion

$$S_\mathfrak{p}((R_n)) \subset \sigma_e((T_{R_n})). \tag{3.30}$$

Proof of inclusion (3.30). Throughout the proof, $C > 0$ denotes an arbitrary constant independent of n.

By $\|\cdot\|_{L^2}$ and $\|\cdot\|_{L^\infty}$, we mean $\|\cdot\|_{L^2(0,\infty)}$ and $\|\cdot\|_{L^\infty(0,\infty)}$ respectively.

Let $\lambda \in S_\mathfrak{p}((R_n))$. Then, using the property (3.14) of the Floquet solutions, (3.29) implies that,

$$\psi_+(R_n,\lambda)\psi_-'(R_n,\lambda-i\gamma) - \psi_+'(R_n,\lambda)\psi_-(R_n,\lambda-i\gamma) = 0 \tag{3.31}$$

for all n. (3.31) ensures that there exists $C_{1,n}, C_{2,n} \in \mathbb{C} \backslash \{0\}$ independent of x such that

$$u_n(x) := \begin{cases} C_{1,n}\psi_-(x, \lambda - i\gamma) & \text{if } x \in [0, R_n) \\ C_{2,n}\psi_+(x, \lambda) & \text{if } x \in [R_n, \infty) \end{cases} \qquad (3.32)$$

is absolutely continuous and solves the Schrödinger equation $\tilde{T}_{R_n}u = \lambda u$, where $\tilde{T}_{R_n}$ denotes the differential expression on $[0, \infty)$ corresponding to T_{R_n}. Define

$$v_n = \frac{\tilde{\chi}_n u_n}{\|\tilde{\chi}_n u_n\|_{L^2}}.$$

where $\tilde{\chi}_n(x) := \tilde{\chi}(x/R_n)$ and $\tilde{\chi} : [0, \infty) \to [0, 1]$ is any smooth function such that $\tilde{\chi} = 0$ on $[0, \frac{1}{4}]$ and $\tilde{\chi} = 1$ on $[\frac{1}{2}, \infty)$. Then $v_n \in D(T_0) = D(T_{R_n})$, $\|v_n\|_{L^2} = 1$ and, since $\langle v_n, \varphi \rangle_{L^2} = 0$ for any $\varphi \in C_c^\infty[0, \infty)$ and any large enough n, $v_n \rightharpoonup 0$ in $L^2(0, \infty)$.

By unique continuation,

$$\|\psi'_-(\cdot, \lambda - i\gamma)\|_{L^2(I)} \leqslant C\|\psi_-(\cdot, \lambda - i\gamma)\|_{L^2(I)}$$

for $I = [0, X]$, $[X, X + a]$ or $[X, x_0]$ so, using the property (3.14) of the Floquet solutions

$$\|\psi'_-(\cdot, \lambda - i\gamma)\|^2_{L^2(0,R_n)} \leqslant C\|\psi_-(\cdot, \lambda - i\gamma)\|^2_{L^2(0,R_n)} \qquad (3.33)$$

for all n. Also, noting that $\|\psi_-(\cdot, \lambda - i\gamma)\|_{L^2(0,x)}$ is exponentially growing in x, we deduce that,

$$\|u_n\|_{L^2} \leqslant C\|u_n\|_{L^2(\frac{1}{2}R_n, \infty)} \leqslant C\|\tilde{\chi}_n u_n\|_{L^2}. \qquad (3.34)$$

for all large enough n.

By the product rule,

$$\|(T_{R_n} - \lambda)v_n\|_{L^2} \leqslant \frac{1}{\|\tilde{\chi}_n u_n\|_{L^2}}\left[\|\tilde{\chi}_n(\tilde{T}_{R_n} - \lambda)u_n\|_{L^2} + 2\|\tilde{\chi}'_n u'_n\|_{L^2} + \|\tilde{\chi}''_n u_n\|_{L^2}\right].$$

The first term in the square brackets above vanishes and $\tilde{\chi}_n^{(k)}$ are supported in $[0, R_n]$ with $\|\tilde{\chi}_n^{(k)}\|_{L^\infty} \leqslant C/R_n^k$ so

$$\|(T_{R_n} - \lambda)v_n\|_{L^2} \leqslant C\frac{\|u_n\|_{L^2}}{\|\tilde{\chi}_n u_n\|_{L^2}}\left[\frac{1}{R_n}\frac{\|\psi'_-(\cdot, \lambda - i\gamma)\|_{L^2(0,R_n)}}{\|\psi_-(\cdot, \lambda - i\gamma)\|_{L^2(0,R_n)}} + \frac{1}{R_n^2}\right] \to 0 \text{ as } n \to \infty.$$

Here, we used estimates (3.33) and (3.34). Consequently, by the definition of limiting essential spectrum (see Definition 2.1), we have $\lambda \in \sigma_e((T_{R_n}))$.

$\square$

4. INCLUSION FOR THE ESSENTIAL SPECTRUM

Consider the Sturm-Liouville operator T_0 introduced in Section 3. Suppose that the conditions of Assumption 2 are met. As before, fix $\gamma \in \mathbb{C} \backslash \{0\}$, define the perturbed operators by

$$T_R u = T_0 u + i\gamma\chi_{[0,R]}u, \ D(T_R) = D(T_0) \qquad (R \in \mathbb{R}_+)$$

and define the limit operator by $T = T_0 + i\gamma$.

In this section, we prove that the essential spectrum of the limit operator T is approximated by the eigenvalues of T_R as $R \to \infty$. To achieve this, we require an additional assumption which ensures that the solution ψ_+ of $\tilde{T}_0 u = \lambda u$ introduced in Assumption 2 can be analytically continued, with respect to the spectral parameter λ, into an open neighbourhood in $\mathbb{C}$ of any point in the interior of $\sigma_e(T_0)$. The

interior of the essential spectrum is denoted by $\mathrm{int}(\sigma_e(T_0))$ and defined with respect to the subspace topology.

Assumption 3. T_0 is such that $\sigma_e(T_0) \subset \mathbb{R}$. For any $\mu \in \mathrm{int}(\sigma_e(T_0))$, there exists an open neighbourhood V_μ of μ such that:

(i) k admits analytic continuations κ_u (κ_l) from the half-planes $\mathbb{C}_+$ $(\mathbb{C}_-)$ respectively into V_μ, with

$$\Im\kappa_u(z),\ -\Im\kappa_l(z) \begin{cases} > 0 & \text{if } z \in \mathbb{C}_+ \cap V_\mu \\ = 0 & \text{if } z \in \mathbb{R} \cap V_\mu \\ < 0 & \text{if } z \in \mathbb{C}_- \cap V_\mu \end{cases}. \tag{4.1}$$

(ii) For any $R > 0$, $\tilde{\psi}_+(R,\cdot)$ admits analytic continuations $\tilde{\varphi}_u(R,\cdot)$ $(\tilde{\varphi}_l(R,\cdot))$ from $\mathbb{C}_+$ $(\mathbb{C}_-)$ respectively into V_μ and $\tilde{\psi}_+^d(R,\cdot)$ admits analytic continuations $\tilde{\varphi}_u^d(R,\cdot)$ $(\tilde{\varphi}_l^d(R,\cdot))$ from $\mathbb{C}_+$ $(\mathbb{C}_-)$ respectively into V_μ. $\tilde{\varphi}_j$ and $\tilde{\varphi}_j^d$ satisfy

$$\|\tilde{\varphi}_j(\cdot,z)\|_{L^\infty(0,\infty)},\ \|\tilde{\varphi}_j^d(\cdot,z)\|_{L^\infty(0,\infty)} < \infty \qquad (j = u \text{ or } l) \tag{4.2}$$

for all $z \in V_\mu$.

(iii) For each $z \in V_\mu$, the functions $\varphi_u(\cdot,z)$ and $\varphi_l(\cdot,z)$, defined by

$$\varphi_j(x,z) := e^{i\kappa_j(z)x}\tilde{\varphi}_j(x,z), \qquad (j = u \text{ or } l), \tag{4.3}$$

solve the equation $\tilde{T}_0\varphi = z\varphi$ and satisfy

$$\varphi_j'(x,z) = e^{i\kappa_j(z)x}\tilde{\varphi}_j^d(x,z). \qquad (j = u \text{ or } l) \tag{4.4}$$

In the following two examples, by analytic continuations we mean analytic continuations from $\mathbb{C}_+$ and $\mathbb{C}_-$ into V_μ.

Example 4.1 (Schrödinger operators with L^1 potentials, continued). Consider again the case $p = r = 1$ with $q \in L^1(0,\infty)$, introduced in Example 3.2. Recall that $k(\lambda) = \sqrt{\lambda}$ so Assumption 3 (i) is satisfied in this case. Recall that

$$\tilde{\psi}_\pm(x,z) = 1 + E_\pm(x,z) \text{ and } \tilde{\psi}_\pm^d(x,z) = \pm i\sqrt{z}(1 + E_\pm^d(x,z)).$$

In order to show that Assumption 3 (ii) and (iii) hold in this case it suffices to show that for any $\mu \in \mathrm{int}(\sigma_e(T_0))$ and any $x \in [0,\infty)$, $E_+(x,\cdot)$ and $E_+^d(x,\cdot)$ admit analytic continuations $E(x,\cdot)$ and $E^d(x,\cdot)$ (respectively) into an open neighbourhood V_μ of μ independent of x, such that the function $\varphi(\cdot,z)$ defined by

$$\varphi(x,z) := e^{i\sqrt{z}x}(1 + E(x,z)) \tag{4.5}$$

satisfies

$$\varphi'(x,z) = i\sqrt{z}e^{i\sqrt{z}x}(1 + E^d(x,z)), \tag{4.6}$$

solves the Schrödinger equation $-\varphi'' + q\varphi = z\varphi$ and satisfies

$$|E_\pm(x,z)|, |E_\pm^d(x,z)| \to 0 \text{ as } x \to \infty$$

for any fixed $z \in V_\mu$. Note that $\sqrt{\cdot}$ is understood to have been analytically continued into V_μ in (4.5) and (4.6). Additional conditions on the potential q are required to ensure that this holds. Two such conditions are:

(a) (Naimark condition [34, Lemma 1]) There exists $a > 0$ such that

$$\int_0^\infty e^{ax}|q(x)|\,\mathrm{d}x < \infty. \tag{4.7}$$

(b) (Dilation analyticity [7]) q is real-valued and can be analytically continued into some open, convex region $U \subset \mathbb{C}$ containing a sector $\{z \in \mathbb{C} : \arg(z) \in [-\theta, \theta]\}$ for some $\theta \in (0, \frac{\pi}{2}]$. Furthermore, there exists $C_0 > 0$ and $\beta > 1$ independent of z such that

$$|q(z)| \leqslant C_0 |z|^{-\beta} \tag{4.8}$$

for all $z \in U$.

Example 4.2 (Eventually periodic Schrödinger operators, continued). Consider again the case $p = r = 1$ with q eventually real periodic, introduced in Example 3.3. As mentioned in Example 3.3, for any $\mu \in \text{int}(\sigma_e(T_0)) = \sigma_e(T_0) \backslash B_{\text{ends}}$ and any $x \in [0, \infty)$, the functions k, $\psi_+(x, \cdot)$ and $\psi'_+(x, \cdot)$ admit analytic continuations into an open neighbourhood V_μ of μ.

(i) By the expression (3.11) for ρ_+, the analytic continuations $\tilde{\rho}_+$ for ρ_+, from $\mathbb{C}_\pm$ into V_μ, satisfies

$$|\tilde{\rho}_+| \begin{cases} < 1 & \text{if } z \in \mathbb{C}_\pm \cap V_\mu \\ = 1 & \text{if } z \in \mathbb{R} \cap V_\mu \\ > 1 & \text{if } z \in \mathbb{C}_\mp \cap V_\mu \end{cases} .$$

Hence, the analytic continuations of k satisfy equation (4.1).
(ii) The analytic continuations of $\tilde{\psi}_+(x, \cdot)$ and $\tilde{\psi}^d_+(x, \cdot)$ satisfy the L^∞ estimates (4.2) by their definitions (3.16) and (3.17).
(iii) The analytic continuations with respect to z of $\psi_+(\cdot, z)$ solve the Schrödinger equation $-\psi'' + q\psi = z\psi$ since by (3.13) they are linear combinations of the solutions $\phi_1(\cdot, z)$ and $\phi_2(\cdot, z)$. Expressions (4.3) and (4.4) for the analytic continuations of ψ_+ and ψ'_+ hold by the definition of (the analytic continuations of) $\tilde{\psi}_+$ and $\tilde{\psi}^d_+$ respectively.

Throughout the remainder of the section, let $\mu \in \text{int}(\sigma_e(T_0))$ and suppose that the conditions of Assumption 3 are satisfied. Also, assume without loss of generality that $(i\gamma + V_\mu) \cap \mathbb{R} = \emptyset$.

Lemma 4.3. $\lambda \in i\gamma + V_\mu$ is an eigenvalue of T_R if and only if

$$g_R(\lambda) := \beta_u(R, \lambda) e^{i\kappa_u(\lambda - i\gamma)R} + \beta_l(R, \lambda) e^{i\kappa_l(\lambda - i\gamma)R} = 0$$

where

$$\beta_u(R, \lambda) := BC[\varphi_l(\cdot, \lambda - i\gamma)]\Big(\tilde{\varphi}_u(R, \lambda - i\gamma)\tilde{\psi}^d_+(R, \lambda) - \tilde{\varphi}^d_u(R, \lambda - i\gamma)\tilde{\psi}_+(R, \lambda)\Big)$$

and

$$\beta_l(R, \lambda) := BC[\varphi_u(\cdot, \lambda - i\gamma)]\Big(\tilde{\psi}_+(R, \lambda)\tilde{\varphi}^d_l(R, \lambda - i\gamma) - \tilde{\psi}^d_+(R, \lambda)\tilde{\varphi}_l(R, \lambda - i\gamma)\Big).$$

Furthermore, g_R is analytic on $i\gamma + V_\mu$.

Proof. The proof is similar to the proof of Lemma 3.4.
Let $\lambda \in i\gamma + V_\mu$. Any solution of the boundary value problem

$$(\tilde{T}_0 + i\gamma\chi_{[0,R]})u = \lambda u \text{ on } [0, R], \ BC[u] = 0$$

must lie in $\text{span}_\mathbb{C}\{u_1(\cdot, \lambda)\}$, where u_1 is defined by

$$u_1(x, \lambda) = BC[\varphi_l(\cdot, \lambda - i\gamma)]\varphi_u(x, \lambda - i\gamma) - BC[\varphi_u(\cdot, \lambda - i\gamma)]\varphi_l(x, \lambda - i\gamma).$$

Since $(i\gamma + V_\mu) \cap \mathbb{R} = \emptyset$, any L_r^2 solution of $(\tilde{T}_0 + i\gamma\chi_{[0,R]})u = \lambda u$ on $[R, \infty)$ must lie in $\mathrm{span}_{\mathbb{C}}\{\psi_+(\cdot, \lambda)\}$. λ is an eigenvalue if and only if

$$u_1(R, \lambda)\psi_+'(R, \lambda) - u_1'(R, \lambda)\psi_+(R, \lambda) = 0$$

which holds if and only if $g_R(\lambda) = 0$.   □

We proceed on to the proof of inclusion for the essential spectrum of T, which consists in proving that there exists eigenvalues of T_R accumulating to $\mu + i\gamma$ as $R \to \infty$. We can only achieve this with the additional assumption that $\mu + i\gamma$ does not lie in a region of the complex plane in which either $\beta_u(R, \cdot)$ or $\beta_l(R, \cdot)$ become small as $R \to \infty$. We now define a subset of the complex plane capturing such regions.

Definition 4.4. Define a subset $S_{\mathfrak{r}} \subset \mathbb{C}$ by

$$S_{\mathfrak{r}} = \left\{\lambda \in i\gamma + V_\mu \cap \mathbb{R} : \liminf_{R \to \infty} |\beta_j(R, \lambda)| = 0, \, j = u \text{ or } l\right\}. \tag{4.9}$$

The strategy of the proof is to first introduce an approximation $g_R^\infty(\lambda)$ to $g_R(\lambda)$ which is valid for λ near $\mu + i\gamma$. It is then shown that there exists zeros λ_R^∞ of g_R^∞ converging to $\mu + i\gamma$ as $R \to \infty$. A family of simple closed contours ℓ_R surrounding λ_R^∞ are constructed such that $\mathrm{dist}(\ell_R, \mu + i\gamma) \to 0$ as $R \to \infty$. We estimate $|g_R^\infty|$ from below and $|g_R - g_R^\infty|$ from above on ℓ_R to conclude, using Rouché's Theorem, that there exists a zero λ_R of g_R inside ℓ_R for all large enough R. Such (λ_R) would be eigenvalues of T_R and would converge to $\mu + i\gamma$ as $R \to \infty$, giving the result.

Lemma 4.5. The function $\kappa_u - \kappa_l$ has an analytic inverse $(\kappa_u - \kappa_l)^{-1} : B_\delta(w_0) \to \mathbb{C}$ for some small enough $\delta > 0$, where $w_0 := (\kappa_u - \kappa_l)(\mu)$,

Proof. Let $h = \kappa_u - \kappa_l - w_0$. Let $\varepsilon > 0$ be small enough so that $|h| > 0$ on $\partial B_\varepsilon(\mu)$. Assumption 3 (i) implies that any $z \in \partial B_\varepsilon(\mu)$ satisfies

$$\arg\left(\frac{h}{|h|}(z)\right) = \arg(h(z)) \in \begin{cases} (0, \pi) & \text{if } z \in \mathbb{C}_+ \cap V_\mu \\ \{0, \pi\} & \text{if } z \in \mathbb{R} \cap V_\mu \\ (\pi, 2\pi) & \text{if } z \in \mathbb{C}_- \cap V_\mu \end{cases}. \tag{4.10}$$

Note that arg is set so that $\arg(z) = 0$ if $z \in \mathbb{R}_+$. The topological degree (i.e. the winding number) of the map $h/|h| : \partial B_\varepsilon(0) \to \partial B_1(0)$ is equal to the number of zeros for h in $B_\varepsilon(0)$, counted with multiplicity [20, pg. 110]. (4.10) implies that the topological degree of $h/|h|$ can only be 1, hence μ is a simple zero of $\kappa_u - \kappa_l$. The lemma now follows from the inverse function theorem.

□

Theorem 4.6. Assume that $\mu \in \mathrm{int}(\sigma_e(T_0))$ is such that $\mu + i\gamma \notin S_{\mathfrak{r}}$. There exists eigenvalues λ_R of T_R $(R \in \mathbb{R}_+)$ and a constant $C_0 = C_0(T_0, \gamma, \mu) > 0$ such that

$$|\lambda_R - (\mu + i\gamma)| \leqslant \frac{C_0}{R}$$

for all large enough R.

Proof. Let $C > 0$ be an arbitrary constant independent of R and θ.
Define approximation g_R^∞ to g_R by

$$g_R^\infty(\lambda) = \beta_{u,R}e^{i\kappa_u(\lambda - i\gamma)R} - \beta_{l,R}e^{i\kappa_l(\lambda - i\gamma)R}$$

where $\beta_{u,R} := \beta_u(R, \mu + i\gamma)$ and $\beta_{l,R} := -\beta_l(R, \mu + i\gamma)$. By the definition of $S_{\mathfrak{r}}$, the L^∞ estimates (3.4) of Assumption 2 (ii) and the L^∞ estimates (4.2) of Assumption 3 (ii), there exists $C_1, C_2 > 0$ independent of R such that $\beta_{u,R}$ and $\beta_{l,R}$ satisfy

$$C_1 \leqslant |\beta_{j,R}| \leqslant C_2 \qquad (j = u \text{ or } l) \tag{4.11}$$

for all large enough R. $g_R^\infty(\lambda) = 0$ holds if and only if

$$(\kappa_u - \kappa_l)(\lambda - i\gamma) = -\frac{i}{R}\left(\ln\left(\frac{\beta_{l,R}}{\beta_{u,R}}\right) + 2\pi i n\right) =: \tilde{\kappa}(n) \tag{4.12}$$

for some $n \in \mathbb{Z}$.

Let $w_0 := (\kappa_u - \kappa_l)(\mu)$ and $n(R) := \lfloor Rw_0/(2\pi) \rfloor$. Note that $n(R)$ is well-defined since $\mu \in \mathbb{R}$ and $\Im w_0 = 0$ by Assumption 3. Using (4.11),

$$|\tilde{\kappa}(n(R)) - w_0| \leqslant \frac{1}{R}\left|\ln\left(\frac{\beta_{l,R}}{\beta_{u,R}}\right)\right| + \left|\frac{2\pi n(R)}{R} - w_0\right| \leqslant \frac{C}{R} \tag{4.13}$$

for large enough R. By Lemma 4.5, there exists an analytic inverse $(\kappa_u - \kappa_l)^{-1} : B_{2\delta}(w_0) \to \mathbb{C}$ for some small enough $\delta > 0$. Let $R_0 > 0$ be large enough such that $\tilde{\kappa}(n(R))$ lies in $B_\delta(w_0)$ for all $R \geqslant R_0$. Define

$$\lambda_R^\infty = (\kappa_u - \kappa_l)^{-1}(\tilde{\kappa}(n(R))) + i\gamma \qquad (R \geqslant R_0). \tag{4.14}$$

Then $g_R^\infty(\lambda_R^\infty) = 0$ and, by the analyticity of $(\kappa_u - \kappa_l)^{-1}$ as well as (4.13),

$$|\lambda_R^\infty - (\mu + i\gamma)| \leqslant C|\tilde{\kappa}(n(R)) - w_0| \leqslant \frac{C}{R} \tag{4.15}$$

for large enough R. For $R \geqslant R_0$, define family $\ell_R = \{\ell_R(\theta) : \theta \in [0, 2\pi)\}$ of simple closed contours around λ_R^∞ by

$$\ell_R(\theta) = (\kappa_u - \kappa_l)^{-1}\left(\tilde{\kappa}(n(R)) + \frac{\delta}{R}e^{i\theta}\right) + i\gamma. \tag{4.16}$$

By the analyticity of $(\kappa_u - \kappa_l)^{-1}$ and estimate (4.15), we have that

$$|\ell_R(\theta) - (\mu + i\gamma)| \leqslant |\ell_R(\theta) - \lambda_R^\infty| + |\lambda_R^\infty - (\mu + i\gamma)| \leqslant \frac{C}{R} \tag{4.17}$$

for large enough R.

By a direct computation, we have

$$e^{i\kappa_u(\ell_R(\theta) - i\gamma)R} = \frac{\beta_{l,R}}{\beta_{u,R}}e^{i\delta e^{i\theta}}e^{i\kappa_l(\ell_R(\theta) - i\gamma)R}. \tag{4.18}$$

By Assumption 3 (ii), $\beta_u(R, \cdot)$ and $\beta_l(R, \cdot)$ are analytic and bounded in R uniformly in a small enough neighbourhood of $\mu + i\gamma$, so, using the Cauchy integral formula as in (3.22) and using (4.17),

$$|\beta_j(R, \ell_R(\theta)) - \beta_j(R, \mu + i\gamma)| \leqslant C|\ell_R(\theta) - (\mu + i\gamma)| \leqslant \frac{C}{R} \qquad (j = u \text{ or } l) \tag{4.19}$$

for large enough R. Using (4.11), (4.18) and (4.19),

$$|g_R(\ell_R(\theta)) - g_R^\infty(\ell_R(\theta))|$$
$$\leqslant \left(|\beta_u(R, \ell_R(\theta)) - \beta_{u,R}|\left|\frac{\beta_{l,R}}{\beta_{u,R}}e^{i\delta e^{i\theta}}\right| + |\beta_l(R, \ell_R(\theta)) + \beta_{l,R}|\right)e^{-\Im\kappa_l(\ell_R(\theta) - i\gamma)R}$$
$$\leqslant \frac{C}{R}e^{-\Im\kappa_l(\ell_R(\theta) - i\gamma)R}$$

for large enough R. Similarly,

$$|g_R^\infty(\ell_R(\theta))| = |\beta_{l,R}|\left|e^{i\delta e^{i\theta}} - 1\right|e^{-\Im\kappa_l(\ell_R(\theta)-i\gamma)R} \geqslant Ce^{-\Im\kappa_l(\ell_R(\theta)-i\gamma)R}.$$

For each large enough R, Rouché's condition

$$|g_R(\ell_R(\theta)) - g_R^\infty(\ell_R(\theta))| < |g_R^\infty(\ell_R(\theta))|$$

is satisfied so there exists a zero λ_R of g_R in the interior of ℓ_R such that

$$|\lambda_R - (\mu + i\gamma)| \leqslant |\lambda_R - \lambda_R^\infty| + |\lambda_R^\infty - (\mu + i\gamma)| \leqslant \frac{C_0}{R}$$

for some $C_0 > 0$ independent of R. $\qquad\square$

We finish this section with a characterisation of the set $S_{\mathfrak{r}}$ in the case that T_0 is a Schrödinger operator with an L^1 or an eventually real periodic potential.

Definition 4.7. Define function $\Lambda_u : [0,\infty) \times (i\gamma + V_\mu) \to \mathbb{C}$ by

$$\Lambda_u(R,\lambda) = \tilde{\varphi}_u(R,\lambda - i\gamma)\tilde{\psi}_+^d(R,\lambda) - \tilde{\varphi}_u^d(R,\lambda - i\gamma)\tilde{\psi}_+(R,\lambda) \tag{4.20}$$

and define function $\Lambda_l : [0,\infty) \times (i\gamma + V_\mu) \to \mathbb{C}$ by

$$\Lambda_l(R,\lambda) = \tilde{\psi}_+(R,\lambda)\tilde{\varphi}_l^d(R,\lambda - i\gamma) - \tilde{\psi}_+^d(R,\lambda)\tilde{\varphi}_l(R,\lambda - i\gamma). \tag{4.21}$$

By the definition of β_u and β_l in Theorem 4.3,

$$\beta_u(R,\lambda) = BC[\varphi_l(\cdot,\lambda - i\gamma)]\Lambda_u(R,\lambda) \text{ and } \beta_l(R,\lambda) = BC[\varphi_u(\cdot,\lambda - i\gamma)]\Lambda_l(R,\lambda)$$

hence we have the following characterisation of $S_{\mathfrak{r}}$:

Corollary 4.8. $S_{\mathfrak{r}}$ *can be decomposed as*

$$S_{\mathfrak{r}} = (i\gamma + S_{\mathfrak{r},0}) \cup S_{\mathfrak{r},u} \cup S_{\mathfrak{r},l} \tag{4.22}$$

where

$$S_{\mathfrak{r},0} := \{z \in V_\mu \cap \mathbb{R} : BC[\varphi_u(\cdot,z)] = 0 \text{ or } BC[\varphi_l(\cdot,z)] = 0\} \tag{4.23}$$

and

$$S_{\mathfrak{r},j} := \left\{\lambda \in i\gamma + V_\mu \cap \mathbb{R} : \liminf_{R\to\infty} |\Lambda_j(R,\lambda)| = 0\right\} \qquad (j = u \text{ or } l). \tag{4.24}$$

The elements of $S_{\mathfrak{r},0}$ are precisely the resonances of T_0 in $V_\mu \cap \mathbb{R}$, by definition.

Example 4.9 (Schrödinger operators with L^1 potentials, continued)**.** Consider again the case $p = r = 1$ with $q \in L^1(0,\infty)$ satisfying the necessary conditions ensuring that Assumption 3 holds, as discussed in Example 4.1. In this case, since the functions $E_\pm(R,\lambda)$ and $E_\pm^d(R,\lambda)$ tend to zero as $R \to \infty$ for any λ, Λ_u and Λ_l satisfy

$$|\Lambda_j(R,\lambda)| \to \left|\sqrt{\lambda - i\gamma} - \sqrt{\lambda}\right| \text{ as } R \to \infty \qquad (j = u \text{ or } l)$$

for all $\lambda \in i\gamma + V_\mu$, where the square-root is understood to have been analytically continued from $\mathbb{C}_+$ ($\mathbb{C}_-$) into V_μ in the case $j = u$ ($j = l$) respectively. Since $\sqrt{\lambda - i\gamma} \neq \sqrt{\lambda}$ for all $\lambda \in i\gamma + V_\mu$, regardless of which branch-cut for the square-root is chosen, we have

$$S_{\mathfrak{r},u} = S_{\mathfrak{r},l} = \emptyset.$$

Consequently,

$$S_{\mathfrak{r}} = i\gamma + S_{\mathfrak{r},0},$$

that is, $\mu + i\gamma \in S_{\mathfrak{r}}$ if and only if μ is a resonance of T_0

Example 4.10 (Eventually periodic Schrödinger operators, continued)**.** Consider the case $p = r = 1$ with q real-valued and $q|_{[X,\infty)}$ a-periodic for some $X \geqslant 0$ and $a > 0$. Assume that $\eta \in [0, \pi)$, so that T_0 is equipped with a real mixed boundary condition at 0. Note that T_0 is self-adjoint in this case. q is eventually real periodic so by Example 4.2, Assumption 3 is satisfied. The sets $S_{\mathfrak{r},u}$ and $S_{\mathfrak{r},l}$ satisfy

$$S_{\mathfrak{r},u} = S_{\mathfrak{r},l} = \emptyset. \tag{4.25}$$

Consequently,

$$S_{\mathfrak{r}} = i\gamma + S_{\mathfrak{r},0},$$

that is, $\mu + i\gamma \in S_{\mathfrak{r}}$ if and only if μ is a resonance of T_0

Proof of (4.25). We will only prove (4.25) for $j = u$, the proof for $j = l$ is similar.

Assume for contradiction that $S_{\mathfrak{r},u}$ is non-empty and let $\lambda \in S_{\mathfrak{r},u}$. By unique continuation, expressions analogous to (3.16) and (3.17) hold for $\tilde{\varphi}_u$ and $\tilde{\varphi}_u^d$. By these expressions, there exists a sequence $(x_{0,n}) \subset [X, X + a)$ such that $\Lambda_u(x_{0,n}, \lambda) \to 0$ as $n \to \infty$. Let x_0 be any accumulation point of $(x_{0,n})$. Then, since $\Lambda_u(\cdot, \lambda)$ is absolutely continuous, it holds that $\Lambda_u(x_0, \lambda) = 0$, so,

$$\varphi_u(x_0, \lambda - i\gamma)\psi'_+(x_0, \lambda) - \varphi'_u(x_0, \lambda - i\gamma)\psi_+(x_0, \lambda) = 0. \tag{4.26}$$

Noting that the solutions $\phi_1(\cdot, \lambda - i\gamma)$ and $\phi_2(\cdot, \lambda - i\gamma)$ defined by (3.8) are real since $\lambda - i\gamma \in \mathbb{R}$ and that the analytic continuations $\rho_u(\rho_l)$ for ρ_+ from $\mathbb{C}_+(\mathbb{C}_-)$ respectively satisfy $\overline{\rho_u(\lambda - i\gamma)} = \rho_l(\lambda - i\gamma)$, the expression analogous to (3.13) for the Floquet solution φ_u implies that

$$\overline{\varphi_u}(x, z) = -\phi_2(X + a, z)\phi_1(x, z) + (\phi_1(X + a, z) - \overline{\rho_u(z)})\phi_2(x, z) = \varphi_l(x, z)$$

where $z := \lambda - i\gamma$. Consequently we have,

$$\varphi_l(x_0, \lambda - i\gamma)\overline{\psi'_+}(x_0, \lambda) - \varphi'_l(x_0, \lambda - i\gamma)\overline{\psi_+}(x_0, \lambda) = 0. \tag{4.27}$$

By (4.26) and (4.27), there exists $C_{1,u}, C_{2,u}, C_{1,l}, C_{2,l} \in \mathbb{C}\backslash\{0\}$ independent of x such that the functions

$$u_u(x, \lambda) := \begin{cases} C_{1,u}\varphi_u(x, \lambda - i\gamma) & \text{if } x \in [0, x_0) \\ C_{2,u}\psi_+(x, \lambda) & \text{if } x \in [x_0, \infty) \end{cases}$$

and

$$u_l(x, \lambda) := \begin{cases} C_{1,l}\varphi_l(x, \lambda - i\gamma) & \text{if } x \in [0, x_0) \\ C_{2,l}\overline{\psi_+}(x, \lambda) & \text{if } x \in [x_0, \infty) \end{cases}$$

are absolutely continuous and solve the Schrödinger equation $\tilde{T}_{x_0}u = \lambda u$. Note that $\overline{\psi_+}$ solves the Schrödinger equation $\tilde{T}_{x_0}u = \lambda u$ on $[x_0, \infty)$ because q is real-valued. By orthogonality, there exists $(a_u, a_l) \in \mathbb{C}^2\backslash\{(0,0)\}$ such that

$$BC[a_u u_u(\cdot, \lambda) + a_l u_l(\cdot, \lambda)] = a_u C_{1,u} BC[\varphi_u(\cdot, \lambda - i\gamma)] + a_l C_{1,l} BC[\varphi_l(\cdot, \lambda - i\gamma)] = 0$$

This implies that λ is an eigenvalue of T_{x_0} with corresponding eigenfunction $u := a_u u_u + a_l u_l$. By a standard integration by parts,

$$\Im(\lambda) = \gamma \frac{\int_0^{x_0} |u|^2}{\int_0^\infty |u|^2} < \gamma$$

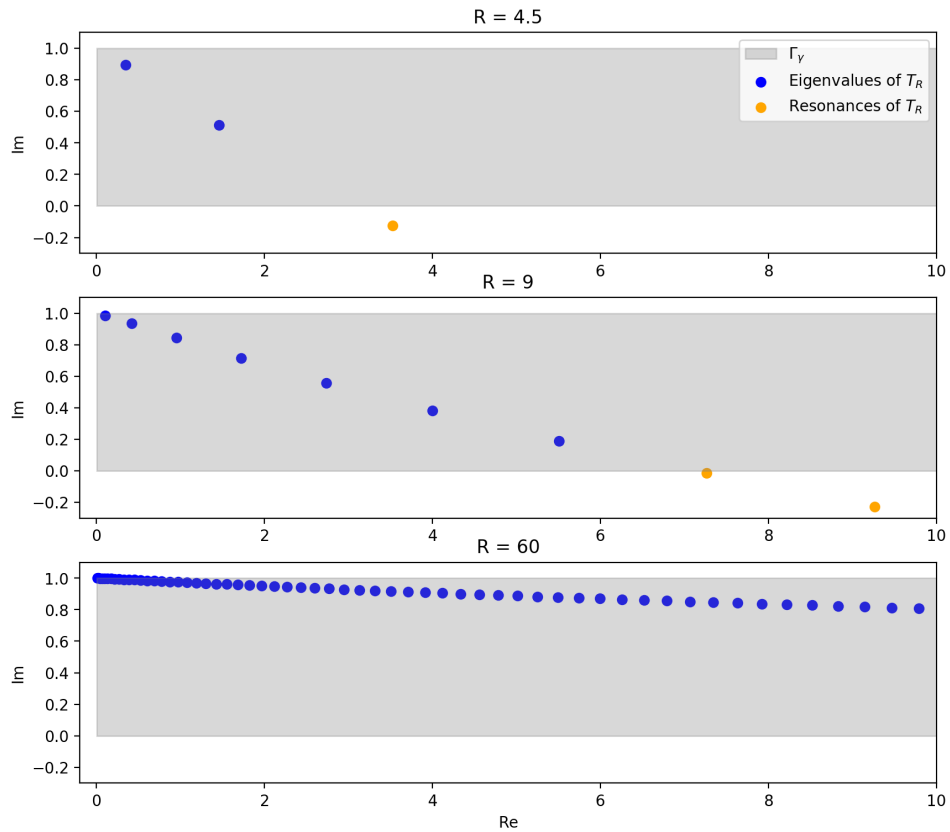which is the desired contradiction. $\square$

FIGURE 2. Plot of the eigenvalues and resonances of the operator T_R defined by (5.1).

5. NUMERICAL EXAMPLES

In this section, we illustrate the results from Sections 3 and 4 with numerical examples.

Example 5.1. Consider perturbed operators of the form

$$T_R = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + i\chi_{[0,R]}(x) \qquad (R \in \mathbb{R}_+) \tag{5.1}$$

endowed with Dirichlet boundary conditions at 0. This corresponds to the case $p = r = 1$, $q = 0$, $\eta = 0$ and $\gamma = 1$ in Sections 3 and 4.

By an explicit computation, $\lambda \in \mathbb{C}\backslash[0,\infty)$ is an eigenvalue of T_R if and only if

$$f_R(\lambda) = i\sqrt{\lambda}\sin(\sqrt{\lambda - i}R) - \sqrt{\lambda - i}\cos(\sqrt{\lambda - i}R) = 0. \tag{5.2}$$

Note that our convention is that the branch cut of the square-root is along $[0,\infty)$. By suitably analytically continuing the square root function in (5.2), any λ in the lower right quadrant of the complex plane is a resonance of T_R if and only if $f_R(\lambda) = 0$.
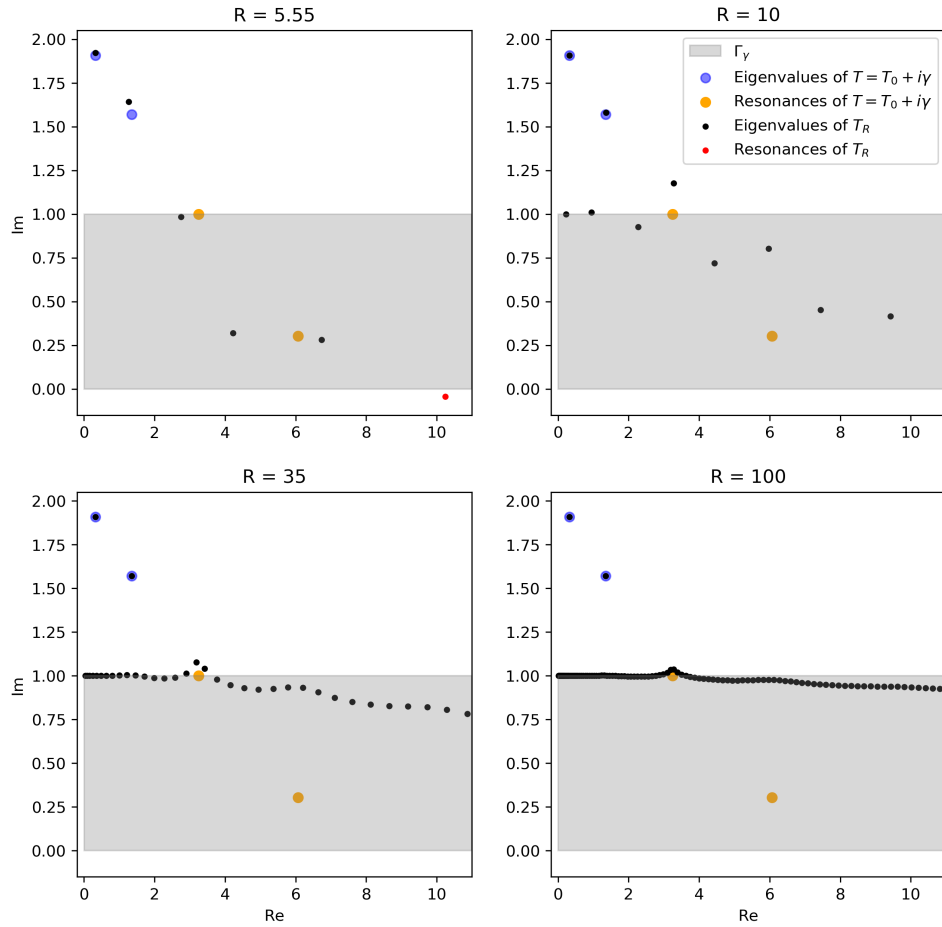
FIGURE 3. Plot of eigenvalues and resonances of the operators T_R and $T = T_0 + i\gamma$ defined by (5.3), with $R_0 = 4.7$.

To numerically compute the zeros of f_R, hence the eigenvalues and resonances of T_R, in a fixed bounded region, we use a Python implementation of an algorithm utilising the argument principle [13]. The results are illustrated in Figure 2.

For small enough $R > 0$, T_R has no eigenvalues [17]. As R increased, we observe resonances in the lower half plane emerging out of $\sigma_e(T_R) = [0, \infty)$, to become eigenvalues in the numerical range

$$\Gamma_\gamma := \sigma_e(T_0) \times i[0, \gamma] = [0, \infty) \times i[0, \gamma]$$

of T_0 accumulating to $\sigma_e(T) = i\gamma + [0, \infty)$, as expected by Theorem 4.6.

Example 5.2. Consider perturbed operator of the form

$$T_R = T_0 + i\chi_{[0,R]}(x) = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + i\chi_{[0,R_0]}(x) + i\chi_{[0,R]}(x) \qquad (R \in \mathbb{R}_+) \qquad (5.3)$$

endowed with Dirichlet boundary conditions at 0. This corresponds to the case $p = r = 1$, $\eta = 0$, $q = i\chi_{[0,R_0]}$ for some $R_0 > 0$ and $\gamma = 1$ in Sections 3 and 4.

By an explicit computation, $\lambda \in \mathbb{C} \backslash [0, \infty)$ is an eigenvalue of T_R if and only if

$$f_R(\lambda) = i\sqrt{\lambda - i}\left[e^{-2i\sqrt{\lambda - i}(R - R_0)} - \frac{\sqrt{\lambda - i} - \sqrt{\lambda}}{\sqrt{\lambda - i} + \sqrt{\lambda}}\right]\sin(\sqrt{\lambda - 2i}R_0)$$

$$- \sqrt{\lambda - 2i}\left[e^{-2i\sqrt{\lambda - i}(R - R_0)} + \frac{\sqrt{\lambda - i} - \sqrt{\lambda}}{\sqrt{\lambda - i} + \sqrt{\lambda}}\right]\cos(\sqrt{\lambda - 2i}R_0) = 0 \quad (5.4)$$

As before, by suitably analytically continuing the square root function in (5.4), any λ in the lower right quadrant of the complex plane is a resonance of T_R if and only if $f_R(\lambda) = 0$.

A numerical computation of the zeros of f_R, hence the eigenvalues and resonances of T_R is shown in Figure 3. We observe that there are eigenvalues of T_R converging rapidly to the eigenvalues of T and that eigenvalues of T_R accumulate to $\sigma_e(T) = i\gamma + [0, \infty)$, as expected by Theorems 3.8 and 4.6.

Recall that Example 4.10 guarantees that the rate of convergence of eigenvalues of T_R to $\mu \in \text{int}(\sigma_e(T)) = i\gamma + (0, \infty)$ is $O(1/R)$, unless μ is a resonance of T. The limit operator T for our choice of parameters has a resonance embedded in $\sigma_e(T)$. We seem to observe a distinction between the way the eigenvalues of T_R accumulate to the resonance compared to other points in the interior of $\sigma_e(T)$. It seems reasonable to conjecture that the rate of convergence to embedded resonances is indeed slower that $O(1/R)$.

Example 5.3. Consider perturbed operators of the form

$$T_R = T_0 + \frac{i}{4}\chi_{[0,R]}(x) = -\frac{d^2}{dx^2} + \sin(x) + \frac{i}{4}\chi_{[0,R]}(x) \qquad (R \in \mathbb{R}_+) \qquad (5.5)$$

endowed with a Dirichlet boundary condition at 0. This corresponds to the case $p = r = 1$, $\eta = 0$, $q(x) = \sin(x)$ and $\gamma = \frac{1}{4}$ in Section 3 and 4. The essential spectrum of T_0 has a band gap structure - the first spectral band, which we denote by B, is approximately $[-0.3785, -0.3477]$ [28, Example 15].

To numerically compute the eigenvalues of T_R, we first perform a domain truncation onto an interval $[0, X]$, imposing a Dirichlet boundary condition at X. Applying a finite difference method with step-size h, we obtain a finite matrix $T_{R,X,h}$. For fixed R, the eigenvalues of $T_{R,X,h}$ accumulate to every point in $\sigma(T_R)$ as $X \to \infty$ and $h \to 0$. Moreover, any point of accumulation that does not lie in $\sigma(T_R)$ must lie on the real-line (see [9] and [28]).

For a fixed small value of h, a fixed large value of $X - R$, the eigenvalues of $T_{R,X,h}$ for increasing R are plotted in Figure 4. We first observe an accumulation of eigenvalues of $T_{R,X,h}$ to the interval B in $\mathbb{R}$. These eigenvalues of $T_{R,X,h}$ are due to the domain truncation method approximating $\sigma_e(T_R)$ and should not be interpreted as approximations of the eigenvalues of T_R. All other points in the plots are approximations of the eigenvalues of T_R.

In Figure 4, we observe that as R increases, eigenvalues of T_R emerge out of the spectral band B and tend to the shifted spectral band $i\gamma + B$, which is a subset of $\sigma_e(T)$. For large R, we observe an accumulation of eigenvalues to $i\gamma + B$. The eigenvalues of T_R accumulating to $i\gamma + B$ seem to be contained in $B \times i(0, \gamma)$. If this is indeed the case then by Bolzano-Weierstrass we expect that there is spectral pollution in $B \times i(0, \gamma)$
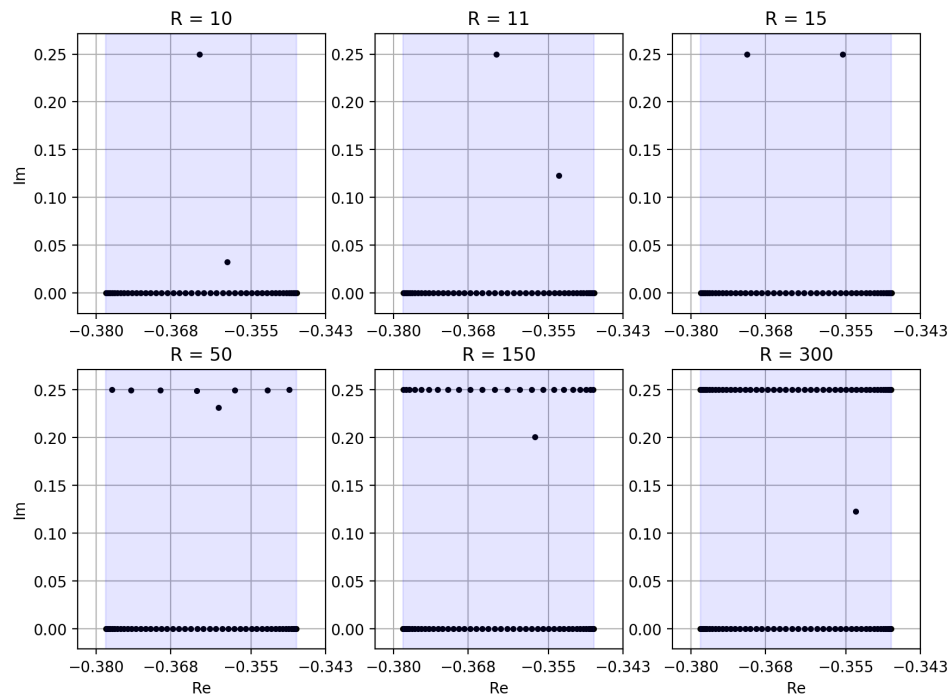
FIGURE 4.   Plot of eigenvalues of the domain truncation and finite difference approximation $T_{R,X,h}$ of the operator T_R defined by (5.5). $h = 0.05$ and $X - R = 300$ are fixed. The region $B \times i\mathbb{R}$ is shaded in light blue.

Data Availability. Data available on request from the author.

REFERENCES

[1] Salma Aljawi and Marco Marletta. On the eigenvalues of spectral gaps of matrix-valued Schrödinger operators. *Numerical Algorithms*, 2020.
[2] Daniele Boffi, Franco Brezzi, and Lucia Gastaldi. On the problem of spurious eigenvalues in the approximation of linear elliptic problems in mixed form. *Mathematics of computation*, 69(229):121–140, 2000.
[3] Sabine Bögli. Local convergence of spectra and pseudospectra. *Journal of Spectral Theory*, 8(3):1051–1098, 2018.
[4] Sabine Bögli, Marco Marletta, and Christiane Tretter. The essential numerical range for unbounded linear operators. *Journal of Functional Analysis*, 279(1):108509, 2020.
[5] Sabine Bögli, Petr Siegl, and Christiane Tretter. Approximations of spectra of Schrödinger operators with complex potentials on $\mathbb{R}$d. *Communications in Partial Differential Equations*, 42(7):1001–1041, 2017.

[6] Lyonell Boulton and Michael Levitin. On approximation of the eigenvalues of perturbed periodic Schrodinger operators. *Journal of Physics A: Mathematical and Theoretical*, 40(31):9319–9329, 2007.

[7] B Malcolm Brown and Michael SP Eastham. Analytic continuation and resonance-free regions for Sturm–Liouville potentials with power decay. *Journal of computational and applied mathematics*, 148(1):49–63, 2002.

[8] B Malcolm Brown, DKR McCormack, W Desmond Evans, and Michael Plum. On the spectrum of second-order differential operators with complex coefficients. *Proceedings of the Royal Society of London. Series A: Mathematical, Physical and Engineering Sciences*, 455(1984):1235–1257, 1999.

[9] Françoise Chatelin. *Spectral Approximation of Linear Operators*, volume 65. SIAM, 1983.

[10] Hans Christianson. Applications of cutoff resolvent estimates to the wave equation. *Mathematical Research Letters*, 16(4):577–590, 2009.

[11] Hans Christianson, Emmanuel Schenck, András Vasy, and Jared Wunsch. From resolvent estimates to damped waves. *Journal d'Analyse Mathématique*, 122(1):143–162, 2014.

[12] Edward B Davies and Michael Plum. Spectral pollution. *IMA journal of numerical analysis*, 24(3):417–438, 2004.

[13] Michael Dellnitz, Oliver Schütze, and Qinghua Zheng. Locating all the zeros of an analytic function in one complex variable. *Journal of Computational and Applied mathematics*, 138(2):325–333, 2002.

[14] Michael Stephen Patrick Eastham. *The Spectral Theory of Periodic Differential Equations*. Scottish Academic Press, 1973.

[15] Michael Stephen Patrick Eastham. *The Asymptotic Solution of Linear Differential Systems: Application of the Levinson Theorem*, volume 4. Oxford University Press, 1989.

[16] David E Edmunds and W Desmond Evans. *Spectral Theory and Differential Operators*. Oxford University Press, 2018.

[17] Rupert L Frank, Ari Laptev, and Oleg Safronov. On the number of eigenvalues of Schrödinger operators with complex potentials. *Journal of the London Mathematical Society*, 94(2):377–390, 2016.

[18] Pedro Freitas, Petr Siegl, and Christiane Tretter. The damped wave equation with unbounded damping. *Journal of Differential Equations*, 264(12):7023–7054, 2018.

[19] Izrail' Markovich Glazman. *Direct Methods of Qualitative Spectral Analysis of Singular Differential Operators*, volume 2146. Israel Program for Scientific Translations, 1965.

[20] Victor Guillemin and Alan Pollack. *Differential Topology*, volume 370. American Mathematical Soc., 2010.

[21] Anders C Hansen. On the approximation of spectra of linear operators on Hilbert spaces. *Journal of Functional Analysis*, 254(8):2092–2126, 2008.

[22] James Hinchcliffe and Michael Strauss. Spectral enclosure and superconvergence for eigenvalues in gaps. *Integral Equations and Operator Theory*, 84(1):1–32, 2016.

[23] Werner Kutzelnigg. Basis set expansion of the Dirac operator without variational collapse. *International Journal of Quantum Chemistry*, 25(1):107–129, 1984.

[24] Michael Levitin and Eugene Shargorodsky. Spectral pollution and second-order relative spectra for self-adjoint operators. *IMA journal of numerical analysis*, 24(3):393–416, 2004.

[25] Mathieu Lewin and Éric Séré. Spectral pollution and how to avoid it. *Proceedings of the London Mathematical Society*, 100(3):864–900, 2010.

[26] Marco Marletta. Neumann-Dirichlet maps and analysis of spectral pollution for non-self-adjoint elliptic PDEs with real essential spectrum. *IMA journal of numerical analysis*, 30(4):917–939, 2010.

[27] Marco Marletta and Sergey Naboko. The finite section method for dissipative operators. *Mathematika*, 60(2):415–443, 2014.

[28] Marco Marletta and Rob Scheichl. Eigenvalues in spectral gaps of differential operators. *Journal of Spectral Theory*, 2(3):293–320, 2012.

[29] Stéphane Nonnenmacher and Maciej Zworski. Quantum decay rates in chaotic scattering. *Acta Mathematica*, 203(2):149–233, 2009.

[30] Stéphane Nonnenmacher and Maciej Zworski. Decay of correlations for normally hyperbolic trapping. *Inventiones mathematicae*, 200(2):345–438, 2015.
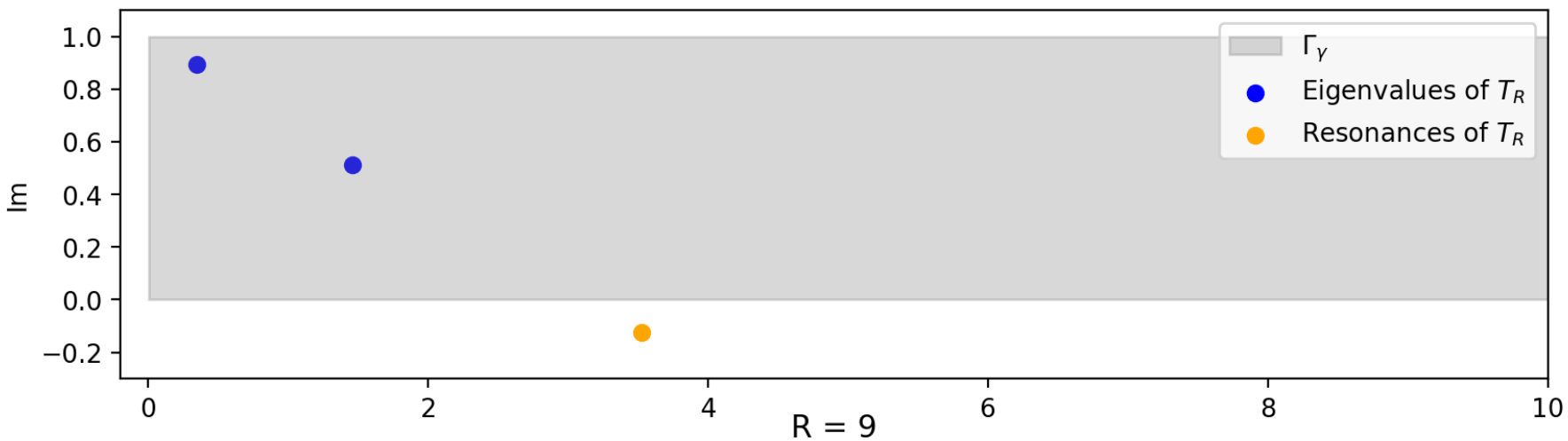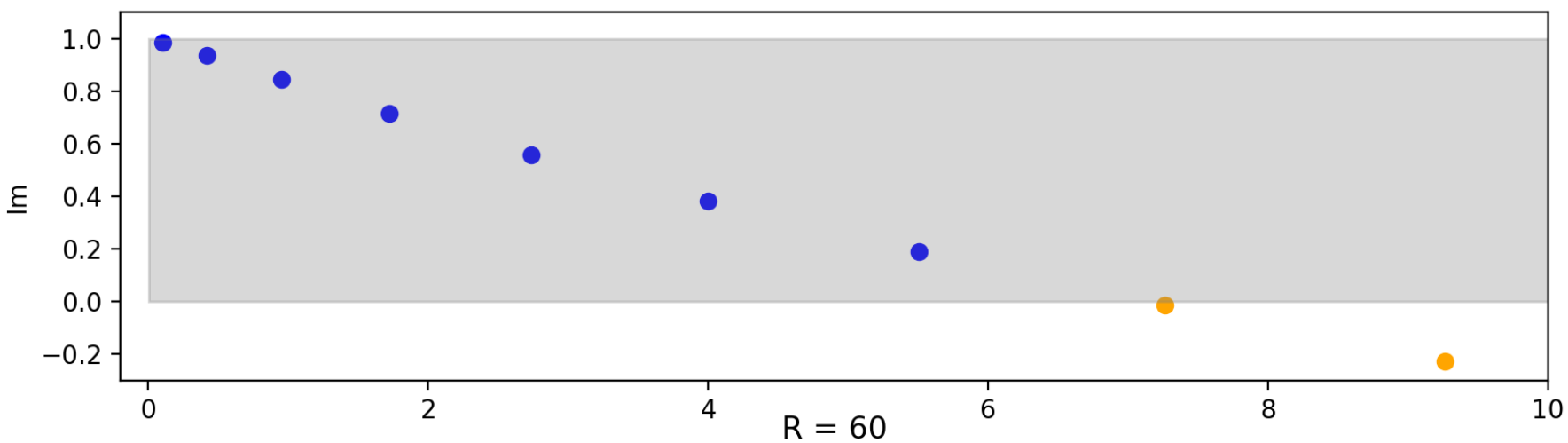
[31] Jacques Rappaz, J Sanchez Hubert, Evariste Sanchez-Palencia, and Dmitri Vassiliev. On spectral pollution in the finite element approximation of thin elastic "membrane" shells. *Numerische Mathematik*, 75(4):473–500, 1997.

[32] UV Riss and HD Meyer. Calculation of resonance energies and widths using the complex absorbing potential method. *Journal of Physics B: Atomic, Molecular and Optical Physics*, 26(23):4503–4535, 1993.

[33] Plamen Stefanov. Approximating resonances with the complex absorbing potential method. *Communications in Partial Differential Equations*, 30(12):1843–1862, 2005.

[34] S A Stepin. Complex potentials: Bound states, quantum dynamics and wave operators. In *Semigroups of Operators-Theory and Applications*, pages 287–297. Springer, 2015.

[35] Michael Strauss. The Galerkin method for perturbed self-adjoint operators and applications. *Journal of Spectral Theory*, 4(1):113–151, 2014.

[36] S Zimmermann and U Mertins. Variational bounds to eigenvalues of self-adjoint eigenvalue problems with arbitrary spectrum. *Zeitschrift für Analysis und ihre Anwendungen*, 14(2):327–345, 1995.

[37] Maciej Zworski. Scattering Resonances as Viscosity Limits. In *Algebraic and Analytic Microlocal Analysis*, Springer Proceedings in Mathematics & Statistics, pages 635–654, 2018.
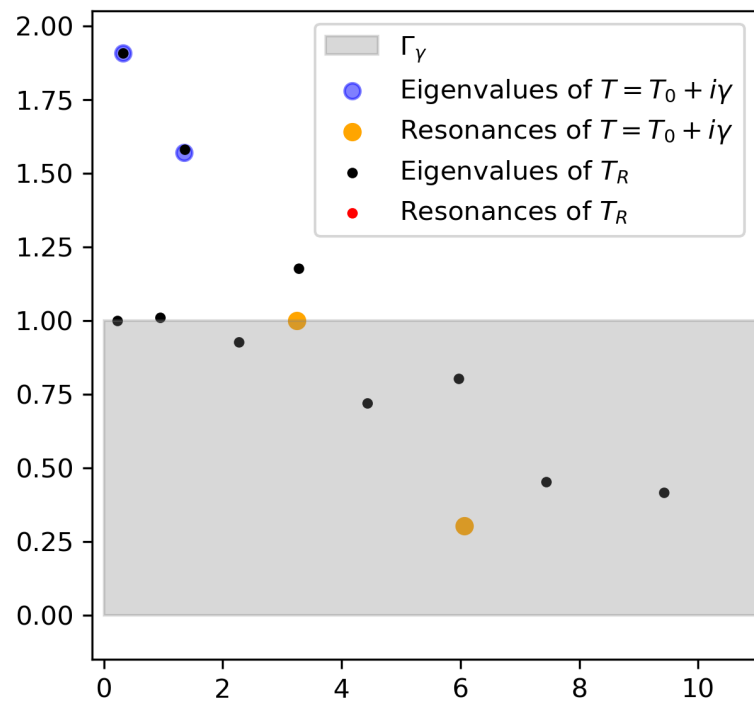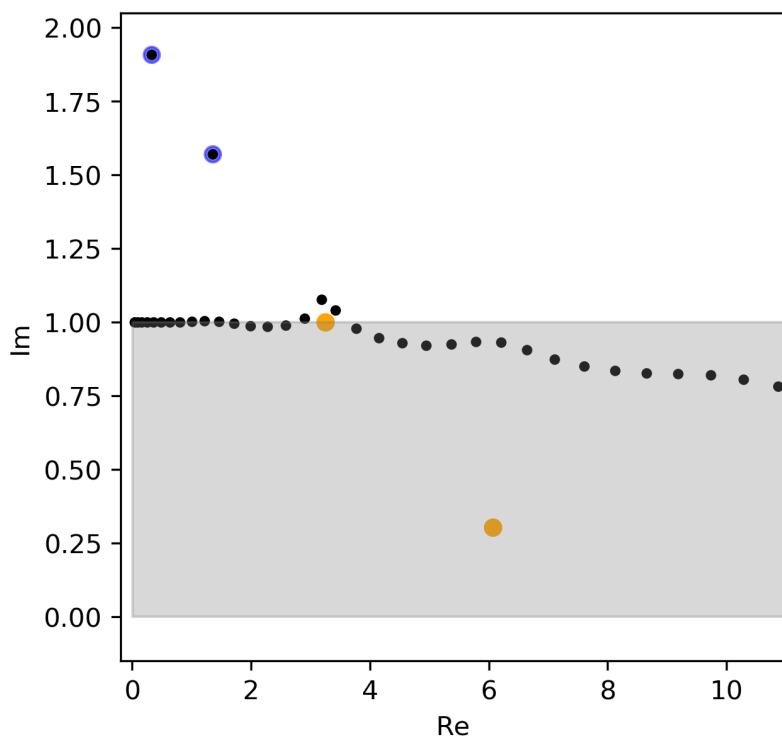
$$\boxed{\phantom{\rule{4cm}{0.4cm}}}\ \sigma_e(T_0) \cup \sigma_e(T)$$

W_e

γ

0

Γ_a

γ

0

Γ_b

γ

0