Spectral approximation and eigenvalue bounds for differential operators

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Abstract

In this thesis, we study the spectrum of Schrödinger operators with complex potentials and Dirichlet Laplace operators on domains with rough boundaries. The focus is on spectral approximation results and a-priori bounds for the location and distribution of eigenvalues. Chapter 1 provides an overview of our main results and Chapters 2 - 5 are based on the papers [130, 129, 79, 121] respectively.

In Chapter 2, spectral inclusion and 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.

In Chapter 3, we consider Schrödinger operators of the form $H_R = -\mathrm{d}^2/\mathrm{d}x^2 + q + i\gamma\chi_{[0,R]}$ for large $R > 0$, where $q \in L^1(0,\infty)$ and $\gamma > 0$. Bounds for the maximum magnitude of an eigenvalue and for the number of eigenvalues are proved. These bounds complement existing general bounds applied to this operator, for sufficiently large R.

In Chapter 4, we prove upper and lower bounds for sums of eigenvalues of Lieb– Thirring type for non-self-adjoint Schrödinger operators on the half-line. The upper bounds are established for general classes of integrable potentials and are shown to be optimal in various senses by proving the lower bounds for specific potentials. We consider sums that correspond to both the critical and non-critical cases.

In Chapter 5, we prove a Mosco convergence theorem for H_0^1 spaces of bounded Euclidean domains satisfying a set of mild geometric hypotheses. For bounded domains, this notion implies norm-resolvent convergence for the Dirichlet Laplacian which in turn ensures spectral convergence. A key element of the proof is the development of a novel, explicit Poincaré-type inequality. These results allow us to construct a universal algorithm capable of computing the eigenvalues of the Dirichlet Laplacian on a wide class of rough domains. Many domains with fractal boundaries, such as the Koch snowflake and certain filled Julia sets, are included among this class. Conversely, we construct a counter example showing that there does not exist a universal algorithm of the same type capable of computing the eigenvalues of the Dirichlet Laplacian on an arbitrary bounded domain.

Contents

Chapter 1

Introduction

The spectral theory of differential operators plays a crucial role in the study of ordinary and partial differential equations, which are ubiquitous in the mathematical study of science and engineering. In this thesis, we approach this topic from two viewpoints. On one hand, we prove *spectral approximation* results, which rigorously justify algorithms for the numerical computation of spectra. On the other hand, we prove various bounds which give us a-priori information on the location and distribution of eigenvalues, without the need for any computation.

Spectral theory is a topic with a rich history, with the self-adjoint theory being particularly developed. Throughout much of this thesis, we work with *non-self-adjoint operators*, which present new challenges. We also address issues of a different nature, caused by the presence of *rough geometries*, for instance fractal boundaries.

This chapter is devoted to giving an overview of the results in the remaining chapters. The focus is on providing a clear exposition and we do not shy away from stating our results with less than full generality in order to improve the clarity of exposition. Note that the remaining chapters may be read independently of this chapter, and of each other.

Theorem 1.0. *In this chapter, the main results are underlined like this.*

Structure of chapter

Section 1.1: We present a detailed analysis of certain non-self-adjoint perturbations called dissipative barriers. Such perturbations have the curious property that they may induce eigenvalues accumulating to an approximate copy of the spectrum shifted in the complex plane, and have applications to numerical computation of spectra.
The main results are: Theorems 1.6, 1.8, 1.10, 1.11, 1.12.
Section 1.2: We present bounds describing the distribution of eigenvalues of Schrödinger operators with complex potentials on the half-line. These bounds generalise the clas-

sical Lieb-Thirring inequalities. In particular, our results illuminate the role of critical parameters in the case of non-self-adjoint operators.
The main results are: Theorems 1.13, 1.14, 1.15, 1.18, Corollaries 1.16, 1.17.
Section 1.3: Motivated by problems on the computational complexity of the eigenvalue problem, we present spectral approximation results for the Dirichlet Laplacian on rough domains. In particular, this involves establishing a new Poincaré-type inequality.
The main results are: Theorems 1.20, 1.22.

Notation and conventions

Let $\mathscr{H}$ be a separable Hilbert space with corresponding inner product $\langle\cdot,\cdot\rangle$ and norm $\|\cdot\|$. The domain and spectrum of a linear operator T on $\mathscr{H}$ is denoted by $D(T)$ and $\sigma(T)$ respectively

For bounded operators B_n, $n\in\mathbb{N}$, and B on $\mathscr{H}$, recall that strong convergence, denoted by $B_n \xrightarrow{s} B$ as $n\to\infty$, is said to hold if $B_n f \to Bf$ as $n\to\infty$ for every $f\in\mathscr{H}$. For $f_n\in\mathscr{H}$, $n\in\mathbb{N}$, and $f\in\mathscr{H}$, recall that weak convergence, denoted by $f_n \rightharpoonup f$ as $n\to\infty$, is said to hold if $\langle f_n, g\rangle \to \langle f, g\rangle$ as $n\to\infty$ for every $g\in\mathscr{H}$.

In this thesis, we define the essential spectrum of an operator T on $\mathscr{H}$ by

$$\sigma_e(T) = \left\{ \lambda\in\mathbb{C} : \begin{array}{c} \exists (u_n)\subset D(T) \text{ with } \|u_n\| = 1, \\ u_n \rightharpoonup 0,\ \|(T-\lambda)u_n\|\to 0 \end{array} \right\} \tag{1.1}$$

which corresponds to σ_{e2} in [61][1]. The sequence (u_n) appearing in (1.1) is referred to as a singular sequence. Furthermore, the set of isolated eigenvalues of finite algebraic multiplicity[2] is referred to as the discrete spectrum and is denoted by $\sigma_d(T)$. Note the geometric multiplicity of an eigenvalue (i.e. the dimension of the eigenspace) never exceeds the algebraic multiplicity.

We adopt the convention that $\mathbb{R}_+ = \mathbb{R}_{\geqslant 0} = \{x\in\mathbb{R} : x\geqslant 0\}$. $\mathbb{R}_{>0}$, $\mathbb{R}_{\leqslant 0}$, etc. are defined similarly. The convention we take with regards to the square-root function is to make the branch-cut along $\mathbb{R}_+$, so that $\operatorname{Im}\sqrt{z}\geqslant 0$ for all $z\in\mathbb{C}$. Finally, $B_X(0)$ denotes an open ball of radius X about the origin in $\mathbb{C}$ or $\mathbb{R}^2$.

[1] In fact, for non-self-adjoint operators there are at least five non-equivalent conventions for the definition of essential spectrum, which all coincide for self-adjoint operators [61, Theorem 1.6].

[2] The algebraic multiplicity of an eigenvalue is defined as the dimension of the image of the corresponding Riesz spectral projection [93, eqn. 2.47].

1.1 Dissipative barriers

In this section, we study a class of non-self-adjoint perturbations which we call *dissipative barriers*. In their most general form, the perturbed operators we consider take the form

$$T_n = T_0 + i\gamma s_n, \qquad n \in \mathbb{N}, \tag{1.2}$$

where T_0 is a unbounded operator on a Hilbert space $\mathscr{H}$, $\gamma > 0$ is regarded as a fixed parameter and s_n is a sequence of bounded, T_0-compact operators (see [61, Chapter III, Definition 7.3]) such that $s_n \to I$ strongly as $n \to \infty$ In addition, we pay particular attention to the model case of Schrödinger operators on $L^2(\mathbb{R}_+)$ perturbed by a "discontinuous" dissipative barriers,

$$H_R = H_0 + i\gamma\chi_{[0,R]} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q + i\gamma\chi_{[0,R]}, \qquad R > 0, \tag{1.3}$$

where q is a fixed multiplication operator referred to as a *background potential*, χ denotes the indicator function and $\gamma > 0$ is a fixed parameter.

Our results shall require additional assumptions, which shall be stated as we go along. For instance, the abstract result Theorem 1.8 holds for the case that T_0 is self-adjoint. For Schrödinger operators H_0, we also deal with non-self-adjoint operators H_0 (i.e. complex potentials q). In this case, we shall require other assumptions on q such as integrability or reality and periodicity outside a compact interval, which allows for the application of technical tools such that Levinson's asymptotic theorem or Floquet theory (resp.).

A key property of dissipative barrier perturbations is that they leave the essential spectrum invariant. Assume that T_0 and H_0 are closed [61, pg. 95]. By the relative compactness of the dissipative barrier perturbations $i\gamma s_n$ and $i\gamma\chi_{[0,R]}$, Weyl's theorem guarantees that

$$\sigma_e(T_n) = \sigma_e(T_0) \qquad \text{and} \qquad \sigma_e(H_R) = \sigma_e(H_0), \tag{1.4}$$

respectively (see [61, Chapter IX, Theorem 2.1]).

One of our key results on dissipative barriers states that, under suitable hypotheses on q, for any point in the spectrum $\mu \in \sigma(H_0)$, $\mu + i\gamma$ is approximated by eigenvalues $\lambda_R(\mu) \in \sigma_d(H_R)$, in the sense that

$$\lambda_R(\mu) \to \mu + i\gamma \qquad \text{as} \qquad R \to \infty.$$

In other words, for large R, the dissipative barrier $i\gamma\chi_{[0,R]}$ generates an approximate "copy" of the spectrum shifted by $i\gamma$ in the complex plane. The importance of such results lies in the fact that, by numerically computing this "copy" of the spectrum, one may avoid problems of spurious eigenvalues (that is, spectral pollution due to numerical discretisation) that are often encountered when trying to numerically compute $\sigma(H_0)$ directly. This is explained further in Sections 1.1.1 and 1.1.2.

The rich behaviour of the eigenvalues of H_R for large R also makes it an interesting example in the wider context of Schrödinger operators with complex potentials. The operators H_R are studied from this perspective in Chapter 3 and Section 4.3; these results are summarised below in Section 1.1.4. In particular, the special case $q \equiv 0$ is an important counter-example in the theory of Lieb–Thirring-type inequalities for non-self-adjoint Schrödinger operators and can be used as a building block in the construction of more sophisticated counter-examples (see Section 4.4).

1.1.1 Motivation: spectral pollution

Consider a sequence of operators T_n, $n \in \mathbb{N}$, intended to approximate a given *limit operator* T. A point $\mu \in \sigma(T)$ is approximated by the spectra of T_n if there exists $\lambda_n(\mu) \in \sigma(T_n)$, n large enough, such that

$$\lambda_n(\mu) \to \mu \qquad \text{as} \qquad n \to \infty.$$

Even if every point in $\sigma(T)$ is approximated by the spectra of T_n, we cannot conclude that $\sigma(T_n)$ is a good approximation for $\sigma(T)$ as $n \to \infty$; one must also ensure that there is no spectral pollution. The formal definition of spectral pollution is as follows.

Definition 1.1. $\mu \in \mathbb{C}$ belongs to the the set of *spectral pollution* of $(T_n)_{n\in\mathbb{N}}$ with respect to T if it lies in the resolvent set $\rho(T) = \mathbb{C}\backslash\sigma(T)$ and there exists a subsequence $(T_{n_k})_{k\in\mathbb{N}} \subset (T_n)_{n\in\mathbb{N}}$ along with spectral points $\lambda_{n_k}(\mu) \in \sigma(T_{n_k})$, $k \in \mathbb{N}$, such that

$$\lambda_{n_k}(\mu) \to \mu \qquad \text{as} \qquad k \to \infty.$$

Spectral pollution is known to cause serious issues for the numerical computations of spectra, particularly when the operator in question has essential spectrum with band gap structure (see [84, Figure 8] for instance). Let us look at a basic example of this phenomenon, which motivates the results presented below.

Consider a Schrödinger operator on the half-line endowed with a mixed boundary condition at 0, with Robin parameter $\eta \in [0,\pi)$,

$$\begin{aligned} H_0 u &= -u'' + qu, \\ u \in D(H_0) &= \{u \in L^2(\mathbb{R}_+) : u, u' \in \mathrm{AC_{loc}}[0,\infty), -u'' + qu \in L^2(\mathbb{R}_+) \\ &\qquad \cos(\eta)u(0) = \sin(\eta)u'(0)\}. \end{aligned} \tag{1.5}$$

Assume that q is real-valued, locally integrable in $[0,\infty)$ and eventually periodic, that is, there exists A_0, $a > 0$ such that

$$\forall x > A_0 : \quad q(x+a) = q(x). \tag{1.6}$$

These assumptions allow for the application of the powerful tools of Floquet theory and ensure that H_0 is self-adjoint[3].

Typically, $\sigma_e(H_0)$ may have a band gap structure and H_0 may have eigenvalues in the spectral gaps. For this reason, this operator is an ideal model for investigating spectral pollution in differential operators, and methods to overcome it.

In order to directly numerically discretise H_0 with a finite-difference or Galerkin method, the first step is to perform a *domain truncation*. The simplest truncated Schrödinger operators $H_{0,X}$, $X > 0$, take the form

$$H_{0,X} u = -u'' + qu, \qquad u \in D(H_{0,X}) = \{u|_{[0,X]} : u \in D(H_0),\, u(X) = 0\}.$$

That is, we impose an artificial Dirichlet boundary condition at X. For each $X > 0$, $H_{0,X}$ is self-adjoint and has a purely discrete spectrum which can generally be reliably numerically computed [115].

The truncated operators $H_{0,X}$ approximate the limit operator H_0 in the strong sense and in fact in the strong resolvent sense[4] [7]. Invoking the self-adjointness of H_0 and $H_{0,X}$, classical results tell us that therefore every point in the spectrum of H_0 is approximated by the eigenvalues of $H_{0,X}$ [118, Chapter VIII.7]. This is formulated precisely as follows.

Proposition 1.2. *Let $(X_n)_{n\in\mathbb{N}} \subset \mathbb{R}_+$ such that $X_n \to \infty$ as $n \to \infty$. Then, for every $\mu \in \sigma(H_0)$, there exists a sequence of eigenvalues $\lambda_n(\mu) \in \sigma_d(H_{0,X_n})$, $n \in \mathbb{N}$, such that $\lambda_n(\mu) \to \mu$ as $n \to \infty$.*

If the essential spectrum of H_0 is non-empty with a band structure, it is not hard to show that the simple domain procedure described above produces spectral pollution.

[3] Note that self-adjointness also holds for a much wider class of real potentials.

[4] That is, $(H_{0,X} - \lambda)^{-1} \xrightarrow{s} (H_0 - \lambda)^{-1}$ as $X \to \infty$ for any $\lambda \in \mathbb{C}\backslash\mathbb{R}$.

This renders the spectral approximation of H_0 with the operators $H_{0,X}$ unreliable in general.

Proposition 1.3. [5] *Assume that there exists $-\infty < a < b < \infty$ such that $[a,b] \subset \sigma_e(H_0)$. Then for any $\mu > b$ there exists an arbitrarily large $X > 0$ such that $\mu \in \sigma_d(H_{0,X})$.*

Corollary 1.4. *In addition to the hypotheses of Proposition 1.3, assume that at least one point in (b,∞) lies in the resolvent set $\rho(H_0)$. Then there exist $(X_n)_{n\in\mathbb{N}} \subset \mathbb{R}_+$ with $\lim_{n\to\infty} X_n = \infty$ such that the set of spectral pollution of $(H_{0,X_n})_{n\in\mathbb{N}}$ with respect to H_0 is non-empty.*

Now, consider a perturbation of H_0 by a dissipative barrier and its truncation,

$$H_R := H_0 + i\gamma\chi_{[0,R]}, \qquad H_{R,X} := H_{0,X} + i\gamma\chi_{[0,R]}, \qquad R, X > 0. \tag{1.7}$$

In [104], Marletta and Scheichl have shown that, not only may the eigenvalues of H_R be rapidly approximated using domain truncation methods, but in fact any spectral pollution incurred must lie on the real line.

Theorem 1.5 ([104, Theorems 5 and 6])**.** *For any eigenvalue μ_R of H_R, there exists $X_0 > 0$, eigenvalues $\lambda_{R,X}$ of $H_{R,X}$, $X > X_0$, and $C_1, C_2 > 0$ such that*

$$|\mu_R - \lambda_{R,X}| \leqslant C_1 \exp(-C_2 X), \qquad \textit{for all} \qquad X > X_0.$$

Furthermore, for any compact set $K \subset \rho(H_R)\backslash\mathbb{R}$, there exists $X_K > 0$ such that

$$\sigma(H_{R,X}) \cap K = \emptyset \qquad \textit{for all} \qquad X > X_K.$$

Let $\lambda \in \mathbb{C}$ be an eigenvalue of H_R with corresponding L^2-normalised eigenfunction u. Multiplying both sides of the eigenvalue equation by $\overline{u}$ and integrating by parts, we have

$$\int_0^\infty |u'(x)|^2 \mathrm{d}x + \int_0^\infty q(x)|u(x)|^2 \mathrm{d}x + i\gamma \int_0^R |u(x)|^2 \mathrm{d}x = \lambda \int_0^\infty |u(x)|^2 \mathrm{d}x = \lambda.$$

Taking the imaginary part of both sides of the above equality, noting that q is real-valued, we obtain

$$\mathrm{Im}\lambda = i\gamma \int_0^R |u(x)|^2 \mathrm{d}x > 0.$$

[5] *Proof.* For any $X > 0$, let $\lambda_n(H_X)$ denote the n^{th} eigenvalue of $H_{0,X}$. Let $X_0 > 0$. Since the eigenvalues of H_{0,X_0} accumulate at $+\infty$ there exists $n \in \mathbb{N}$ such that the $\lambda_n(H_{0,X_0}) > \mu$. By the hypothesis and Proposition 1.2, there exists $X_1 > X_0$ such that $\lambda_n(H_{0,X_1}) < b < \mu$. The result follows from the continuity of $X \mapsto \lambda_n(H_{0,X})$ [89, Th. 3.1].

We conclude that all eigenvalues of H_R lie strictly away from the real-line. Consequently, Theorem 1.5 effectively demonstrates that the eigenvalues may be reliably computed.

1.1.2 Dissipative Barrier Method

The dissipative barrier method is a strategy to avoid problems of spectral pollution in the numerical computation for a self-adjoint operator H_0. The discussion in the previous section brings us to the main idea of this method, which may be summarised as follows.

1. Approximate $\sigma(H_0)+i\gamma$ by the eigenvalues of H_R.
2. Numerically approximate the eigenvalues of H_R.

In this way, we could numerically approximate $\sigma(H_0)+i\gamma$ (at least in a compact subset of $\mathbb{C}$), from which a numerical approximation of $\sigma(H_0)$ may be immediately recovered. We focus entirely on Step 1, that is, the spectral approximation of the limit operator $H_0+i\gamma$ by the perturbed operators H_R for large R. This is poorly understood compared to Step 2, which has been justified by various results, such as Theorem 1.5.

Let us now present our first result. In the following theorem, and throughout this subsection, H_R denotes perturbed Schrödinger operators on the half line with eventually periodic background potential q, as defined by (1.5), (1.6) and (1.7).

Theorem 1.6 (Theorems 2.23 and 2.33). *For any eigenvalue μ_d of $\sigma_d(H_0)$, there exists $R_1>0$, eigenvalues $\lambda_R(\mu_d)\in\sigma_d(H_R)$, $R>R_1$, and $C_1,C_2>0$ such that*

$$|(\mu_d+i\gamma)-\lambda_R(\mu_d)|\leqslant C_1\exp(-C_2R) \qquad \textit{for all} \qquad R>R_1.$$

Furthermore, for any $\mu_e\in\sigma_e(H_0)$, there exists $R_2>0$ and eigenvalues $\lambda_R(\mu_e)\in\sigma_d(H_R)$, $R>R_2$, such that

$$\lambda_R(\mu_e)\to\mu_e+i\gamma \qquad \textit{as} \qquad R\to\infty.$$

For $\mu_e\in\sigma_e(H_0)$ lying outside of a certain set of isolated points corresponding to the embedded resonances of H_0 (see Definition 2.36), there exists $C_3>0$ such that

$$|(\mu_e+i\gamma)-\lambda_R(\mu_e)|\leqslant\frac{C_3}{R} \qquad \textit{for all} \qquad R>R_2. \tag{1.8}$$

Remark 1.7. In Chapter 2, this result is formulated in a more general way and we also treat background potentials satisfying other hypotheses. For the special case $q(x)=0$,

$x > A_0$, an analogous result has been proven in [55]. The approximation of shifted eigenvalues $\sigma_d(H_0) + i\gamma$ has been partially treated in [104] and [84], although their results do not fully cover the first part of the above theorem (and certainly do not cover the second).

Figure 1.1 illustrates the effect of adding a dissipative barrier to a real, eventually periodic background potential. Note that the eigenvalues in this figure are in fact numerically computed[6].

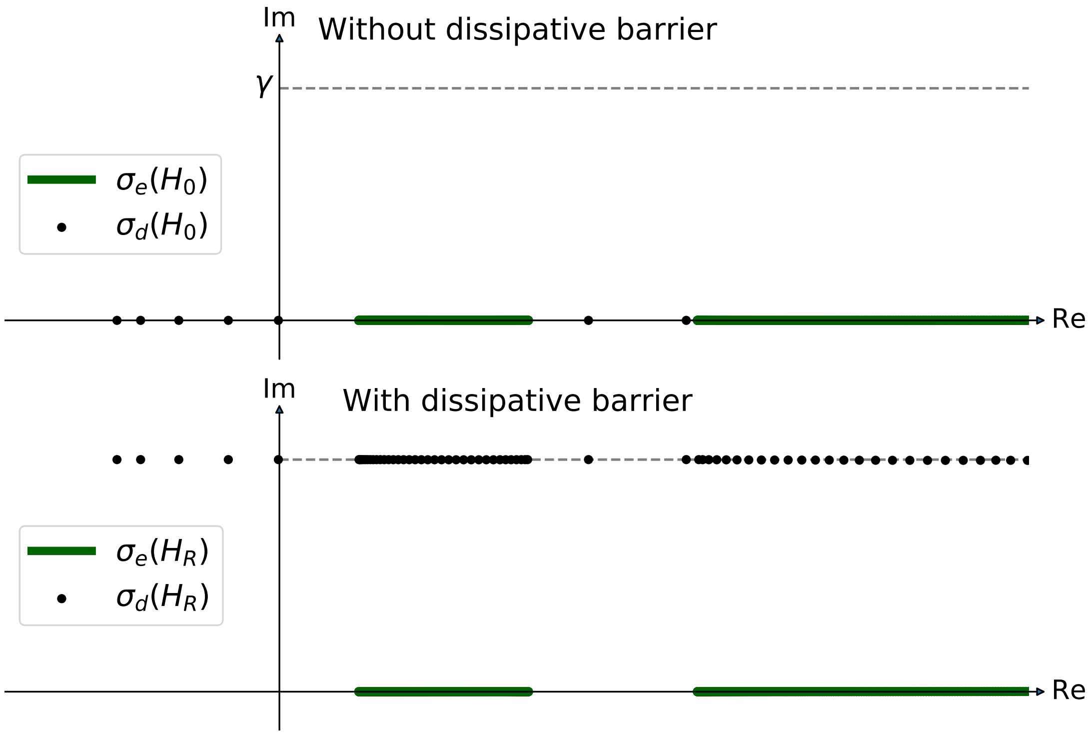

Figure 1.1 The effect of adding a dissipative barrier.

Embedded resonances. In Theorem 1.6, we do not have a rate of convergence for points $\mu_e + i\gamma$, where $\mu_e \in \sigma_e(H_0)$ is an embedded resonance. As explained in Remark 2.37, the eigenvalues of H_0 can be expressed as the zeros of a certain analytic function. This function admits an analytic continuation past the essential spectrum $\sigma_e(H_0)$, revealing new zeros which we refer to as resonances. Embedded resonances are those lying exactly on $\sigma_e(H_0)$. Interestingly, numerical evidence indicates that the eigenvalues of H_R behave in an exceptional way near shifted embedded resonances (see Figure 2.3).

[6]For $q(x) = -10\chi_{[0,5]}(x) + \sum_{n=0}^{\infty} 20\chi_{[0.8,1)}(x-n)$, $\gamma = 30$ and $R = 40$.

Spectral pollution. Note that Theorem 1.6 does not say anything about spectral pollution incurred by the dissipative barrier, that is, the set of spectral pollution of $(H_{R_n})_{n\in\mathbb{N}}$ with respect to $H_0+i\gamma$, for sequences $(R_n)_{n\in\mathbb{N}}\subset\mathbb{R}_+$. Since $\sigma_e(H_0)$ is a subset of $\sigma(H_R)$ for all R, it belongs to this set of spectral pollution, for any $(R_n)_{n\in\mathbb{N}}$. In Chapter 2, we construct an analytic function whose zero set encloses any point of spectral pollution outside of $\sigma_e(H_0)$ (for the case that $R_n-R_{n-1}=a$). Numerical evidence suggests that, in general, there may be spectral pollution outside $\sigma_e(H_0)$ (see Figure 2.4).

1.1.3 Abstract results

One appealing aspect of the dissipative barrier method is that the ideas apply to very general classes of operators. Throughout this subsection, we consider a sequence of operators

$$T_n = T_0 + i\gamma s_n, \qquad n\in\mathbb{N}, \tag{1.9}$$

on a separable Hilbert space, where $\gamma>0$ is fixed. We assume that

$$T_0 \text{ is self-adjoint}, \qquad s_n \xrightarrow{s} I \quad \text{as} \quad n\to\infty \qquad \text{and} \qquad \sup_{n\in\mathbb{N}}\|s_n\|<\infty. \tag{1.10}$$

The next result states that the shifted eigenvalues $\sigma_d(T_0)+i\gamma$ are approximated by the eigenvalues of T_n as $n\to\infty$ for two classes of barrier operators s_n. Furthermore, enclosures are provided for the set of spectral pollution induced by such perturbations. It is proven in Section 2.2 by utilising the notion of *limiting essential spectrum* for unbounded operators [18].

Theorem 1.8 (Theorem 2.12)**.** *Assume that the operators defined by (1.9) and (1.10) satisfy one of the following hypotheses.*

(a) *s_n is a projection operator for all n, that is, $s_n^2=s_n$. In this case, let*

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

(b) *For any sequence $(u_n)_{n\in\mathbb{N}}\subset D(T_0)$ with $\sup_n\|u_n\|<\infty$ and $\sup_n\|T_0u_n\|<\infty$, we have*

$$\langle s_nu_n, T_0u_n\rangle - \langle T_0u_n, s_nu_n\rangle \to 0 \quad \textit{as} \quad n\to\infty.$$

In this case, let

$$\Gamma_b := \sigma_e(T_0) + i[0,\gamma].$$

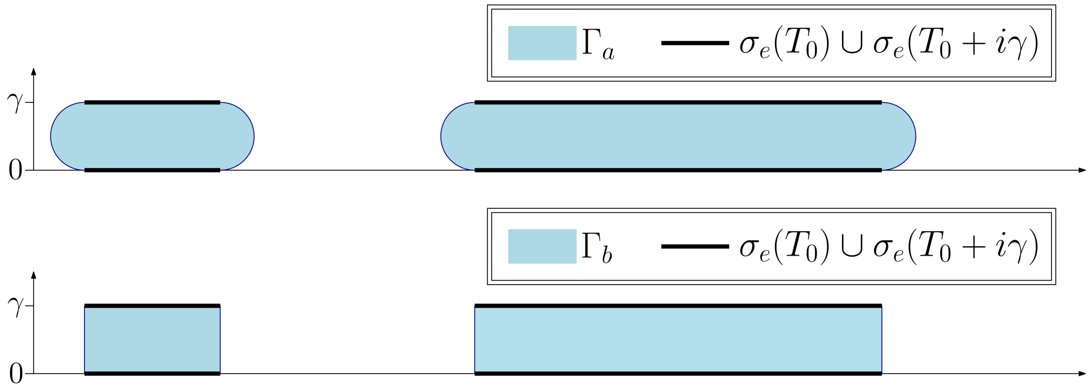

Figure 1.2 An illustration of the sets Γ_a and Γ_b.

Then, for any $\mu \in \sigma_d(T_0)$, there exists $n_0 \in \mathbb{N}$ and eigenvalues $\lambda_n(\mu) \in \sigma_d(T_n)$, $n \geqslant n_0$ such that

$$\lambda_n(\mu) \to \mu + i\gamma \qquad \textit{as} \qquad n \to \infty.$$

Furthermore, the set of spectral pollution of $(T_n)_{n\in\mathbb{N}}$ with respect to $T_0 + i\gamma$ is contained in Γ_a or Γ_b respectively.

Both hypotheses (a) and (b) can be verified in a variety of interesting concrete settings, for instance, partial differential operators and infinite matrices. For the case of operators on $L^2(\mathbb{R}_+)$, "barrier" operators s_n satisfying these hypotheses can be constructed as follows.

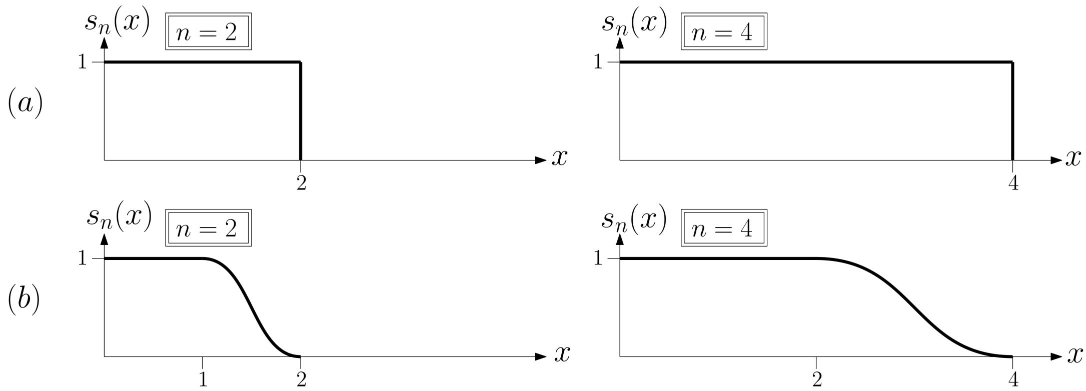

Figure 1.3 An illustration of the multiplication operators s_n constructed in Example 1.9.

Example 1.9. (a) Let s_n be a multiplication operator on $L^2(\mathbb{R}_+)$ defined for any $u \in L^2(\mathbb{R}_+)$ by

$$(s_n u)(x) = \chi_{[0,n]}(x)u(x), \qquad x \in \mathbb{R}_+.$$

Then s_n satisfies hypothesis (a) of Theorem 1.8.

(b) Let $\varphi : \mathbb{R}_+ \to [0,1]$ be any smooth function such that $\operatorname{supp}\varphi \subset [0,1]$ and $\varphi \equiv 1$ on $[0,\frac{1}{2}]$. Let s_n be a multiplication operator on $L^2(\mathbb{R}_+)$ defined for any $u \in L^2(\mathbb{R}_+)$ by

$$(s_n u)(x) = \varphi(x/n)u(x), \qquad x \in \mathbb{R}_+.$$

Then, s_n satisfies hypothesis (b) of Theorem 1.8.

A consequence of Theorem 1.8 is that, any eigenvalue of T_n outside of Γ_a or Γ_b must be near to an eigenvalue of $T_0 + i\gamma$ for large n, or more precisely,

$$\forall \varepsilon > 0 : \exists n_0 \in \mathbb{N} : \forall n \geqslant n_0 : \forall \lambda_n \in \sigma_d(T_n) \cap \Gamma^c : \quad \operatorname{dist}(\lambda_n, \sigma_d(T_0) + i\gamma) < \varepsilon \quad (1.11)$$

where $\Gamma = \Gamma_a$ or Γ_b respectively. Returning to the numerical analysis point of view, suppose that we know the essential spectrum $\sigma_e(T_0)$. In this case, we could compute Γ_a or Γ_b, and restrict our attention to the eigenvalues of T_n in $\mathbb{C}\backslash\Gamma$. Then (1.11) indicates that these eigenvalues can be taken as an approximation for the shifted discrete spectrum $\sigma_d(H_0) + i\gamma$.

1.1.4 Eigenvalue bounds

Spectral enclosures. Any eigenvalue λ of a Dirichlet Schrödinger operator on the half-line with a complex-valued potential $q \in L^1(\mathbb{R}_+)$ (i.e. the operator (1.20)) is contained in a closed ball of radius $\|q\|_{L^1}^2$,

$$|\lambda|^{1/2} \leqslant \|q\|_{L^1}. \quad (1.12)$$

This inequality may be shown to be sharp[7] by, essentially, considering a potential of the form $q(x) = c\delta(x-b)$, where $c \in \mathbb{C}$, $b \in \mathbb{R}$ and δ is the Dirac delta distribution [69, Theorem 1.1].

Now consider a Dirichlet Schrödinger operator of the form

$$H_R = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q + i\gamma\chi_{[0,R]} \qquad \text{on} \qquad L^2(\mathbb{R}_+) \quad (1.13)$$

where $q \in L^1(\mathbb{R}_+)$ may be complex-valued, $\gamma > 0$. Informally speaking, a potential that can be decomposed into the form $q + i\gamma\chi_{[0,R]}$ for large R looks very different from a Dirac delta distribution, in the sense that its mass is spread over a large region. This raises the question:

[7] In fact (1.12) can be improved to $|\lambda|^{1/2} \leqslant g(\theta)\|q\|_{L^1}$ where $g(\theta)$ is a function depending on the complex argument θ of λ, and taking values in [1/2,1].

Q: Does (1.12) (with q replaced by $q + i\gamma\chi_{[0,R]}$) give a good enclosure for the eigenvalues of H_R for large R? Can it be improved for this case?

Asymptotically, (1.12) gives the estimate $|\lambda_R|^{1/2} = O(R)$ as $R \to \infty$. Our next result not only gives a logarithmic improvement for this estimate, but also states that eigenvalues of H_R are bounded independently of R along any ray other than $\mathbb{R}_+$.

Theorem 1.10 (Theorem 3.4)**.** *There exists* $X = X(\gamma, q) > 0$ *such that*

$$\sigma_d(H_R) \subset B_X(0) \cup \Gamma_\gamma,$$

where H_R *refers to the operator (1.13) and*

$$\Gamma_\gamma := (0, \infty) + i(0, \gamma).$$

Furthermore, there exists $R_0 = R_0(\gamma, q) > 0$ *such that any eigenvalue* λ *of* H_R*,* $R \geqslant R_0$*, satisfies*

$$|\lambda - i\gamma|^{1/2} \leqslant \frac{5\gamma R}{\log R}. \tag{1.14}$$

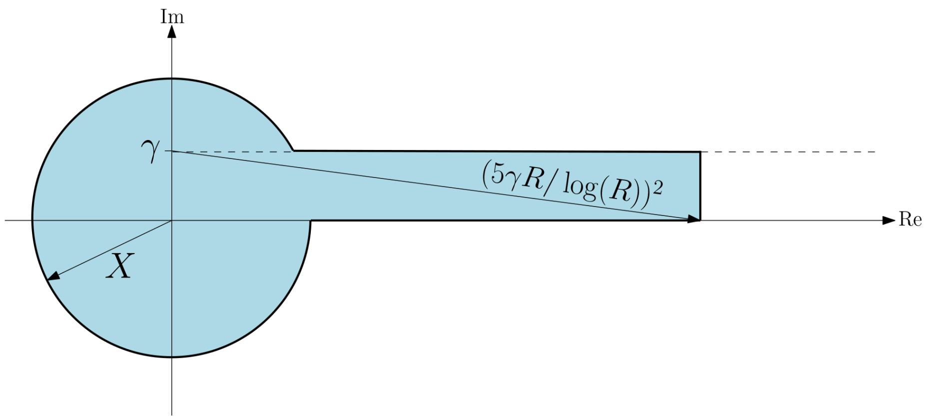

Figure 1.4 An illustration of the spectral enclosure provided by Theorem 1.10.

Number of eigenvalues. Now consider the case that the background potential q satisfies one of the following two assumptions:

(i) q is compactly supported,

(ii) (Naimark condition) There exists $c > 0$ such that

$$\int_0^\infty e^{cx} |q(x)| \, \mathrm{d}x < \infty. \tag{1.15}$$

Note that first condition is stronger, since compactly supported potentials satisfy the Naimark condition, and we obtain stronger results for this case accordingly.

By a classical result of Naimark [108], if the background potential satisfies assumption (i) or (ii) above, then the number of eigenvalues (counting algebraic multiplicities) $N(H_R)$ of H_R is finite.

In Section 2.4, we prove that, under assumption (i) or (ii) above, every point in $i\gamma+\mathbb{R}_+$ is approximated by the eigenvalues of H_R. As a consequence, it must hold that

$$N(H_R) \to \infty \quad \text{as} \quad R \to \infty.$$

A natural question to ask is:

Q: How fast does $N(H_R)$ tend to ∞?

We first address upper bounds for $N(H_R)$. A lower bound shall later be also provided for the case $q \equiv 0$.

In [68], Frank, Laptev and Safronov provided a quantitative upper bound for the number of eigenvalues of Schrödinger operators with potentials satisfying the Naimark condition. It is shown in Section 3.1 that, applied to perturbed operators H_R such that q satisfies the Naimark condition, their result gives the asymptotic estimate

$$N(H_R) = O(R^4) \quad \text{as} \quad R \to \infty.$$

More recently, Korotyaev has proven a bound specific to compactly supported potentials [90]. This bound gives a improved asymptotic bound for perturbed operators H_R such that q is compactly supported,

$$N(H_R) = O(R^2) \quad \text{as} \quad R \to \infty.$$

Note that this asymptotic improvement extends beyond operators of the specific form H_R to more general semiclassical Schrödinger operators with compactly supported potentials (such operators are considered in Remark 4.10 for instance). The next result shows that further improvements are possible for the operators H_R, even when the background potential is not compactly supported (in which case Korotyaev's result does not apply).

Theorem 1.11 (Theorems 3.10 and 3.14). *Consider the perturbed Dirichlet Schrödinger operator (1.13) with a background potential $q \in L^1(\mathbb{R}_+)$ and $\gamma > 0$.*

(a) If q is compactly supported, then there exists $R_0 = R_0(q,\gamma) > 0$ such that

$$N(H_R) \leqslant \frac{11}{\log 2}\frac{\gamma R^2}{\log R}, \qquad R \geqslant R_0.$$

(b) If q satisfies the Naimark condition, then there exists $R_0 = R_0(q,\gamma) > 0$ such that

$$N(H_R) \leqslant 10^5 \frac{\sqrt{X}+c}{c^2}\frac{\gamma^2 R^3}{(\log R)^2}, \qquad R \geqslant R_0,$$

where $X > 0$ is the constant from Theorem 1.10 and $c > 0$ is the constant appearing in (1.15).

While the above bound (a) is based on an application of Jensen's formula, the proof of (b) involves proving a customised complex analysis estimate (see Proposition 3.12) adapted to the problem at hand. It is possible that elements of the proof could be useful in the future to prove more general bounds for the number of eigenvalues of Schrödinger operators. An interesting feature of both bounds (a) and (b) is the logarithmic improvement, which happens to come directly from the logarithm in the magnitude bound (1.14).

Free barrier. In the case of trivial background potential $q \equiv 0$, we denote the perturbed Dirichlet Schrödinger operators H_R studied above as

$$L_{\gamma,R} := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + i\gamma\chi_{[0,R]}, \qquad \gamma, R > 0. \tag{1.16}$$

Despite its simplicity, this family of operators is at the centre of a variety of crucial counter-examples in the theory of Lieb-Thirring-type inequalities. Such counter examples are studied in Chapter 4 and discussed in Section 1.2.

Compared to upper bounds such as Theorems 1.10 and 1.11, lower bounds for properties of the eigenvalues (e.g. the maximum magnitude) are often harder to prove. This is due to the requirement of proving *existence* of complex eigenvalues with given properties. This is especially true in the case of lower bounds for the number of eigenvalues, or sums of eigenvalues, where we are required to prove the existence of large families of eigenvalues.

The next result allows us to prove such lower bounds for $L_{\gamma,R}$. Let $\sqrt{\cdot}$ denote the branch of the square root function such that $\operatorname{Im}\sqrt{z} > 0$ for $z \in \mathbb{C}\backslash\mathbb{R}_+$.

Theorem 1.12 (Proposition 4.16 and Lemma 4.17). *Suppose that* $R \geqslant 600(\gamma^{3/4} + \gamma^{-3/4})$. *Then there exist distinct eigenvalues*

$$\lambda_j \in \sigma_d(L_{\gamma,R}), \qquad 1 \leqslant j \leqslant \left\lfloor \frac{1}{32\pi} \frac{\gamma R^2}{\log R} \right\rfloor,$$

which satisfy

$$\mathrm{Re}(\lambda_j) \geqslant 0, \qquad \frac{\gamma}{2} \leqslant \mathrm{Im}(\lambda_j) \leqslant \gamma$$

and

$$\sqrt{\lambda_j - i\gamma} = \frac{i}{2R}\left[\log\left(\frac{\sqrt{\lambda_j - i\gamma} - \sqrt{\lambda_j}}{\sqrt{\lambda_j - i\gamma} + \sqrt{\lambda_j}}\right) + 2\pi i j\right]. \tag{1.17}$$

An immediate consequence of this is that there exists $C > 0$ such that for all large enough R,

$$N(L_{\gamma,R}) \geqslant C\frac{R^2}{\log R}; \tag{1.18}$$

This demonstrates that Theorem 1.11 (a) gives an order sharp large R estimate.

Although (1.17) is not explicitly resolved in terms of λ_j, it still gives detailed information about the location of the individual eigenvalues λ_j since the logarithm term can often be effectively estimated. A consequence of Theorem 1.12 is Proposition 4.19, which implies that there exists $C > 0$ such that for all large enough R,

$$\sup_{\lambda \in \sigma_d(L_{\gamma,R})} |\lambda|^{1/2} \geqslant C\frac{R}{\log R}, \tag{1.19}$$

proving that inequality (1.14) in Theorem 1.10 gives an order sharp large R estimate.

1.2 Critical case Lieb–Thirring inequalities

Schrödinger operators with real-valued potentials form the central object in non-relativistic quantum mechanics. When the potentials are allowed to be complex, the theory drastically changes since the operators become non-self-adjoint. As well as the applications in numerical analysis described in the previous section, complex potentials appear in the study of systems with energy loss or gain, such as open quantum systems and the damped wave equation [63, 126].

In this section, we give an overview of the results of Chapter 4, which describe the eigenvalues of Dirichlet Schrödinger operators on the half-line with complex potentials $q \in L^1(\mathbb{R}_+)$,

$$H_q u = -u'' + qu, \qquad u \in D(H_q) = \left\{u \in H_0^1(\mathbb{R}_+) : -u'' + qu \in L^2(\mathbb{R}_+)\right\}. \tag{1.20}$$

For such operators, we have $\sigma_e(H_q) = [0,\infty)$ and the spectrum may be decomposed as

$$\sigma(H_q) = \{\lambda_n\}_{n=1}^N \cup [0,\infty), \qquad \text{where} \quad \lambda_n \in \sigma_d(H_q) \quad \text{satisfy} \quad |\lambda_n|^{1/2} \leqslant \|q\|_{L^1}$$

and $N \in \mathbb{N}_0 \cup \{\infty\}$ [69]. Note that eigenvalues of higher algebraic multiplicity are repeated accordingly in $\{\lambda_n\}_{n=1}^N$. It is known that the number of eigenvalues N may be infinite, in which case the eigenvalues λ_n must accumulate to a point in $[0,\infty)$.

We focus on studying sums of the form,

$$S_\varepsilon(H_q) := \sum_{n=1}^N \frac{\operatorname{dist}(\lambda_n, \mathbb{R}_+)}{|\lambda_n|^{(1-\varepsilon)/2}}, \qquad \varepsilon \geqslant 0 \tag{1.21}$$

which describe the distribution of the eigenvalues with respect to the essential spectrum $\mathbb{R}_+$ and the origin of the complex plane. Lieb-Thirring sums, and the corresponding inequalities, originally arose out of the theory of self-adjoint Schrödinger operators and quantum mechanics, where they play a crucial role in the proof of stability of matter. Here, we are concerned with generalisations for non-self-adjoint operators. Sums of this form also arise out of the complex analysis underlying the problem and represent an interesting connection between complex function theory and spectral theory. Note that our results also apply to a wider class of Lieb–Thirring sums (see Proposition 4.23).

When q is real-valued, H_q is self-adjoint and the isolated eigenvalues are strictly negative, $\lambda_n < 0$. In this case, the distribution of the eigenvalues is described by the classical Lieb-Thirring inequality,

$$\sum_{n=1}^N |\lambda_n|^{(1+\varepsilon)/2} \leqslant C(\varepsilon) \int_0^\infty q_-(x)^{1+\varepsilon} \mathrm{d}x, \qquad \varepsilon \geqslant 0 \tag{1.22}$$

where $C(\varepsilon) > 0$ and $q_-(x)$ denotes the negative part of $q(x)$. For negative eigenvalues λ_n, we have $\operatorname{dist}(\lambda_n, \mathbb{R}_+) = |\lambda_n|$ so the sum $S_\varepsilon(H_q)$ coincides with the sums in (1.22).

In both (1.21) and (1.22), $\varepsilon = 0$ corresponds to a critical case. As shall be further explained, the isolated eigenvalues can be expressed in a very natural way as

$$\lambda_n = z_n^2, \qquad z_n \in \mathbb{C}_+,$$

where $\{z_n\}_{n=1}^N$ are the zeros of a certain analytic function in the upper half plane. Then the sum $S_0(H_q)$ is equivalent to the sum

$$J(H_q) := \sum_{n=1}^N \operatorname{Im} z_n \tag{1.23}$$

in the sense that $J(H_q) \leqslant S_0(H_q) \leqslant 2J(H_q)$ (see (4.8)). The sums $J(H_q)$, which we refer to as Jensen sums, arise in Jensen's formula from complex analysis as well as in the Blaschke condition for the upper-half-plane (see Remark 4.13).

1.2.1 Main results

The novelty of the results in Chapter 4 lies in the fact that they provide a detailed description of the critical case $\varepsilon = 0$ alongside the non-critical case $\varepsilon > 0$, for non-self-adjoint operators. Namely, we provide upper bounds for $S_\varepsilon(H_q)$ for all $\varepsilon \geqslant 0$ and corresponding lower bounds show the optimality of the results in various senses.

Upper bound for non-critical case. Our first result is a quantitative upper bound for the sums $S_\varepsilon(H_q)$ in the case $\varepsilon > 0$. A key difference between our result and the classical Lieb–Thirring inequality (1.22) is that our bound is valid for complex-valued L^1 potentials, whereas the right hand side of (1.22) may be infinite for certain real-valued L^1 potentials.

Theorem 1.13 (Theorem 4.5)**.** *For any $\varepsilon > 0$, there exists $C(\varepsilon) > 0$ such that*

$$S_\varepsilon(H_q) \leqslant C(\varepsilon)\|q\|_{L^1}^{1+\varepsilon}.$$

For $\varepsilon > 1$, this result was previously proved by R. Frank and J. Sabin in [70]. R. Frank later proved the case $\varepsilon = 1$ [66].

The Jensen sum cannot be bounded by the L^1 norm. The next result shows that Theorem 1.13 provides the best possible result in terms of range of ε. That is, it shows that the inequality $S_0(H_q) \leqslant C\|q\|_{L^1}$ cannot hold.

Theorem 1.14 (Theorem 4.21)**.** *For all large enough R, we have*

$$S_0(L_{\gamma,R}) \geqslant \frac{\gamma R}{16\pi}\log R \tag{1.24}$$

where $L_{\gamma,R}$ denotes the operator (1.16). Consequently, we have

$$\sup_{q\in L^1(\mathbb{R}_+)} \frac{S_0(H_q)}{\|q\|_{L^1}} = \infty. \tag{1.25}$$

The proof of this theorem is based on an application of Theorem 1.12. A similar result for Schrödinger operators on $\mathbb{R}$ has previously been obtained by S. Bögli and F. Štampach in [22].

Upper bound for critical case. While the previous result shows that $S_0(H_q)$ cannot be bounded by the L^1 norm, it is nonetheless possible to prove a general upper bound. Our idea is to introduce a pair of continuous, monotonically increasing weight functions $a, \hat{a} : \mathbb{R}_+ \to \mathbb{R}_+$ such that

$$a(x)\hat{a}(x) = x. \tag{1.26}$$

We then define a weighted L^1 norm as

$$\|q\|_a := \int_0^\infty |q(x)|a(x)\mathrm{d}x. \tag{1.27}$$

The consideration of such weighted norms does not necessarily imply a loss of generality since, for any $q \in L^1(\mathbb{R}_+)$, it is possible to construct a weight function a growing slowly enough so that $\|q\|_a < \infty$.

Most generally, our upper bound takes the following form.

Theorem 1.15 (Theorem 4.8)**.** *Assume that the following holds.*

(i) $\hat{a}$ is strictly monotonically increasing, $\hat{a}(0) = 0$ and $\hat{a}(\infty) = \infty$.

(ii) a satisfies

$$\int_1^\infty \frac{\mathrm{d}x}{xa(x)} < \infty.$$

Then there exists $K(a, \|q\|_a) > 0$ such that for all $q \in L^1(\mathbb{R}_+)$ satisfying $\|q\|_a < \infty$, we have

$$S_0(H_q) \leqslant K(a, \|q\|_a). \tag{1.28}$$

In particular, (1.28) ensures that $S_0(H_q)$ is finite. An explicit expression for $K(a, \|q\|_a)$ is given in Theorem 4.8.

The purpose of Assumption (i) is to ensure that $\hat{a}$ is invertible. It imposes a restriction on how fast a can grow, since $\hat{a}(\infty) = \infty$ implies that $a(x) = o(x)$ as $x \to \infty$.

Assumption (ii) necessitates that $\lim_{x\to\infty} a(x) = \infty$ and imposes a restriction on how slowly a can grow. For example, if $a(x) = \log^\alpha(x-2)$ for the some $\alpha > 0$, then the assumption is satisfied when $\alpha > 1$ but not when $\alpha \leqslant 1$. As a result of this assumption, Theorem 1.15 is *not* valid for arbitrary L^1 potential, although the restriction it imposes is of a logarithmic nature.

Applied to compactly supported potentials, Theorem 1.15 gives the following bound.

Corollary 1.16 (Corollary 4.12)**.** *Suppose the potential $q \in L^1(\mathbb{R}_+)$ is compactly supported. Then, for every $R > 1$ with $\operatorname{supp}(q) \subset [0,R]$, we have*

$$S_0(H_q) \le 7\left[\frac{1}{R} + \|q\|_1\Big(1 + \log(1+\|q\|_1) + \log R\Big)\right]. \tag{1.29}$$

This bound gives the order sharp large R estimate for dissipative barrier potentials

$$S_0(L_{\gamma,R}) = O(R\log R) \quad \text{as} \quad R \to \infty. \tag{1.30}$$

Applied to potentials which decay in a polynomial sense, Theorem 1.15 gives the following bound.

Corollary 1.17 (Corollary 4.9)**.** *Let $p \in (0,1)$ and $a(x) = 1 + x^p$. Then for each potential $q \in L^1(\mathbb{R}_+)$ with $\|q\|_a < \infty$, we have*

$$S_0(H_q) \leqslant \tfrac{4}{\pi}\|q\|_a \log(1+\|q\|_a) + \tfrac{9}{p}\|q\|_a + 2. \tag{1.31}$$

Upper bounds for the sum $S_0(H_q)$ for potentials satisfying $\|(1+x^p)q\|_{L^1} < \infty$, $p \in (0,1)$, have also previously been obtained by Safronov in [123]. Comparatively, our bound gives an improved asymptotic estimate for semi-classical Schrödinger operators.

An L^1 potential with divergent Jensen sum. The final result of Chapter 4 addresses the question of whether it is possible to obtain any upper bound at all for $S_0(H_q)$ that is valid for arbitrary $q \in L^1(\mathbb{R}_+)$. The following theorem shows that this is not possible and consequently Theorem 1.15 cannot be extended to arbitrary $q \in L^1(\mathbb{R}_+)$.

Theorem 1.18. *There exists $q_\infty \in L^1(\mathbb{R}_+)$ such that $S_0(H_{q_\infty}) = \infty$.*

To the best of our knowledge, this result is the first which demonstrates the divergence of a Lieb–Thirring type sum for non-self-adjoint Schrödinger operators.

1.2.2 Some ideas of proofs

Our approach is based on expressing the eigenvalues as zeros of an analytic function on the upper half plane. Firstly, it is well known that there exists a unique solution $e_+(\cdot,z)$ of $-u'' + qu = z^2 u$ on $\mathbb{R}_+$, known as the *Jost solution*, such that

$$e_+(x,z) \sim e^{izx} \qquad \text{as} \qquad x \to \infty.$$

We define the *Jost function* as $e_+(z) := e_+(0,z)$. Then we have

$$\lambda = z^2 \in \sigma_d(H_q) \qquad \Longleftrightarrow \qquad e_+(z) = 0$$

and the algebraic multiplicity of the eigenvalue coincides with the corresponding zero multiplicity. References are provided in Section 4.1 of Chapter 4.

Non-critical upper bound. First, we recall the following well known estimate for the Jost function,

$$|e_+(z)-1| \leqslant \exp\left(\frac{\|q\|_{L^1}}{|z|}\right)-1, \qquad z\in\mathbb{C}_+. \tag{1.32}$$

Note that (1.32) not only gives an upper bound for $|e_+(z)|$ but also a lower bound.

The next step is to move from the upper half plane $\mathbb{C}_+$ to the unit disk $\mathbb{D}$. We use the following complex change of variables

$$w=w(z)=\frac{z-i}{z+i}, \qquad z=z(w)=i\frac{1+w}{1-w}, \qquad z\in\mathbb{C}_+, \qquad w\in\mathbb{D}. \tag{1.33}$$

An analytic function f on the unit disk is defined as

$$f(w):=\frac{e_+(yz(w))}{e_+(iy)}, \qquad y:=\frac{\|q\|_{L^1}}{\kappa}, \qquad \kappa:=\log\frac{3}{2}. \tag{1.34}$$

The zeros of f have a bijective correspondence to the zeros of e_+. Furthermore, the estimate (1.32) for e_+, as well as the definition of f, ensure that

$$|f(0)|=1 \qquad \text{and} \qquad \log|f(w)|\leqslant\frac{2}{|1+w|}, \qquad w\in\mathbb{D}. \tag{1.35}$$

We then apply a complex analysis result of Borichev, Golinskii and Kupin to the function f. In a simplified form, this result reads as follows.

Theorem 1.19 ([24, Theorem 0.1]). *Consider an analytic function f on the unit disk $\mathbb{D}$ such that $|f(0)|=1$ and*

$$\log|f(w)|\leqslant\frac{D}{|1+w|} \tag{1.36}$$

for some $D>0$. Then for every $\varepsilon>0$, there exists $C(\varepsilon)>0$ such that

$$\sum_{w\in Z(f)}(1-|w|)|1+w|^{\varepsilon}\leqslant C(\varepsilon)D \tag{1.37}$$

where $Z(f)$ denotes the set of zeros of f and zeros of higher multiplicity are repeated accordingly in the sum.

We obtain Theorem 1.13 from (1.37) by going back to the upper half plane using (1.34); the factor $(1-|w|)$ corresponds to the factor $\operatorname{dist}(\lambda,\mathbb{R}_+)/|\lambda|^{1/2}$ in the summand of $S_\varepsilon(H_q)$ and the factor $|1+w|^\varepsilon$ corresponds to the factor $|\lambda|^{\varepsilon/2}$.

Critical upper bound. Observe that the singularity $\frac{1}{|z|}$ in (1.32) (as well as the corresponding singularity $\frac{1}{|1+w|}$ in (1.36)) is not integrable. This is the reason that the result of [24] needed to be applied instead of more elementary complex analysis results and the reason that the factor $|1+w|^{\varepsilon}$ in (1.37) is necessary.

A *key idea* in Chapter 4 is to use weight functions to obtain improved estimates for Jost functions, of the form,

$$|e_+(z)-1| \leqslant \exp\left(\hat{a}\left(\frac{1}{|z|}\right)\|q\|_a\right)-1, \qquad z \in \mathbb{C}_+. \tag{1.38}$$

The assumption that a satisfies condition (ii) of Theorem 1.15 ensures that the singularity $\hat{a}(\frac{1}{|z|})$ is integrable.

We define an analytic function f on $\mathbb{D}$ in a similar way to (1.34). Since $\hat{a}\left(\frac{1}{|z|}\right)$ is integrable, we can apply Jensen's formula,

$$\sum_{w\in Z(f)}(1-|w|) \leqslant \sum_{w\in Z(f)} \log\left(\frac{1}{|z|}\right) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \log|f(e^{i\theta})|\mathrm{d}\theta - \log|f(0)|. \tag{1.39}$$

We obtain the upper bound for $S_0(H_q)$ by estimating the right hand side of (1.39) and going back to the upper half-plane in a similar way as in the non-critical case.

Divergent Jensen sum. Finally, we discuss the ideas of the proof of Theorem 1.18. We utilise in an essential way some ideas of Bögli, which were used in [17] to construct complex potentials with eigenvalues accumulating to every point in the essential spectrum $[0,\infty)$.

The potential $q_\infty \in L^1(\mathbb{R}_+)$ takes the form

$$q_\infty(x) = \sum_{n=1}^{\infty} \gamma_n \chi_{[-R_n,R_n]}(x-X_n) \tag{1.40}$$

where $\gamma_n, R_n, X_n > 0$. Roughly (and non-rigorously) speaking, the idea in [17] is to make each $X_n > 0$ large enough (i.e. separating out the supports of the bumps) so that

$$\sigma_d(H_{q_\infty}) \approx \bigcup_{n=1}^{\infty} \sigma_d(\mathscr{L}_{\gamma_n,R_n})$$

where $\mathscr{L}_{\gamma,R} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + i\gamma\chi_{[-R,R]}$ are Schrödinger operators on $L^2(\mathbb{R})$. More concretely, we are able to set each $X_n > 0$ large enough so that

$$S_0(H_{q_\infty}) \geqslant \frac{1}{2}\sum_{n=1}^{\infty} S_0(\mathscr{L}_{\gamma_n,R_n}). \tag{1.41}$$

Furthermore, Theorem 1.14 gives a lower bound for the rhs of (1.41). The point is then that we are able to set γ_n and R_n such that simultaneously $\|q_\infty\|_{L^1} < \infty$ and the rhs of (1.41) is infinite.

1.3 Rough boundaries

Given a domain $\mathscr{O} \subset \mathbb{R}^2$, (i.e. a non-empty, open, connected set) the corresponding Dirichlet Laplacian is a self-adjoint operator on $L^2(\mathscr{O})$ defined by

$$H_{\mathscr{O}} u = -\Delta u, \qquad u \in D(H_{\mathscr{O}}) = \{u \in H_0^1(\mathscr{O}) : \Delta u \in L^2(\mathscr{O})\}$$

where Δu is understood as a distribution and $H_0^1(\mathscr{O})$ is defined as the closure of $C_c^\infty(\mathscr{O})$ (i.e. smooth functions compactly supported in $\mathscr{O}$) with respect to the H^1 norm (which is defined by (5.5)). The Laplace operator is of fundamental importance since it encodes the dynamics of the wave equation, the free particle Schrödinger equation and the heat equation.

We are interested in the case that the domain $\mathscr{O}$ is bounded. In this case, the spectrum is purely discrete and positive,

$$\sigma(H_{\mathscr{O}}) = \sigma_d(H_{\mathscr{O}}) = \{\lambda_k(\mathscr{O})\}_{k\in\mathbb{N}} \subset \mathbb{R}_+.$$

If $\mathscr{O}$ is sufficiently regular, if it is polygonal for instance, there exist very reliable numerical methods for computing these eigenvalues to arbitrary precision [100]. On the other hand, observe that the boundary of an arbitrary bounded planar domain may be truly pathological; it may be a fractal, it may not be locally connected and it may even have non-zero area. Intuitively, the eigenvalues for such domains, are much harder, perhaps impossible, to numerically approximate.

The underlying motivation of Chapter 5 is to understand for which classes of bounded domains the eigenvalues $\lambda_k(\mathscr{O})$, $k \in \mathbb{N}$, repeated according to geometric multiplicity, are *computable*. This question is addressed rigorously in the powerful framework of *Solvability Complexity Indices (SCI)*. Roughly speaking, our results show that:

1. It is not possible to construct a numerical method able to compute the eigenvalues of an arbitrary bounded domain.

2. There exists such a numerical method for a large sub-class of bounded domains, which we explicitly specify. Domains in this class may have fractal boundaries and cusps, but must be topologically regular, i.e. $\mathscr{O} = \operatorname{int}(\overline{\mathscr{O}})$.

In this section, we focus on presenting the spectral theoretic results at the heart of the second statement. These provide an answer to the following question:

Q: Given a sequence of bounded domains $\mathcal{O}_n \subset \mathbb{R}^2$, $n \in \mathbb{N}$, and a limit domain $\mathcal{O} \subset \mathbb{R}^2$, under what conditions does it hold that

$$\forall k \in \mathbb{N}: \quad \lambda_k(\mathcal{O}_n) \to \lambda_k(\mathcal{O}) \qquad \text{as} \qquad n \to \infty?$$

Rigorous statements of the computational results are postponed until Chapter 5, where SCI theory is properly introduced.

1.3.1 Main spectral approximation result

We now state our main spectral approximation result in a simplified form. We require a number of basic geometric notions. Recall that:

- A Jordan curve is the image of a continuous, injective map $\iota : S^1 \to \mathbb{R}^2$, where $S^1 \subset \mathbb{R}^2$ denotes the unit circle.
- A closed set $K \subset \mathbb{R}^d$ is locally connected if for all $x \in K$, there exists an open neighbourhood U of x such that $K \cap U$ is connected.
- The Hausdorff distance between two non-empty sets $A, B \subset \mathbb{R}^d$ is defined as

$$\operatorname{dist}_H(A,B) = \max\left\{\sup_{x\in A}\operatorname{dist}(x,B), \sup_{x\in B}\operatorname{dist}(x,A)\right\}.$$

We let $\mu_{\text{leb}}(K)$ denote the Lebesgue outer measure of a set $K \subset \mathbb{R}^2$ and, as above, $\lambda_k(\mathcal{O})$ denotes the k^{th} eigenvalue of the Dirichlet Laplacian $H_{\mathcal{O}}$.

Theorem 1.20 (Theorem 5.3, Example 5.4 and Lemma 5.2). *Let $\mathcal{O} \subset \mathbb{R}^2$ be a bounded, open, connected set such that $\partial\mathcal{O}$ is a Jordan curve with $\mu_{\text{leb}}(\partial\mathcal{O}) = 0$. Let $\mathcal{O}_n \subset \mathbb{R}^2$, $n \in \mathbb{N}$, be a sequence of open, bounded sets such that $\partial\mathcal{O}_n$ is locally connected for each $n \in \mathbb{N}$, and*

$$\operatorname{dist}_H(\mathcal{O},\mathcal{O}_n) + \operatorname{dist}_H(\partial\mathcal{O},\partial\mathcal{O}_n) \to 0 \qquad \text{as} \qquad n \to \infty.$$

Then it holds that

$$\lambda_k(\mathcal{O}_n) \to \lambda_k(\mathcal{O}) \qquad \text{as} \qquad n \to \infty.$$

The novelty of this result lies in the generality of the class of admissible domains $\mathcal{O}$. Although the domains $\mathcal{O}$ in Theorem 1.20 are simply connected, this is not essential. A more general version of this theorem is stated in Chapter 5, which allows for domains $\mathscr{O}$ with holes. In fact, the only conditions on $\mathscr{O}$ we impose there are $\mu_{\text{leb}}(\partial\mathscr{O}) = 0$ along with a collection of purely topological hypotheses.

Nevertheless, the hypotheses of Theorem 1.20 capture the essence of the type of domains we allow. Jordan curves are certainly *not* required to be locally the graph of a continuous map and admit a wide variety of fractals. However, domains with cracks, such as $B_1(0)\backslash[0,1)$, are not allowed, since the interior of a Jordan curve must be topologically regular $\mathscr{O} = \text{int}(\overline{\mathscr{O}})$.

The recent papers [33, 85] obtain results which effectively cover Theorem 1.20 in the particular case that $\mathscr{O}$ is a thick domain in the sense of Triebel or an (ε,∞)-domain. Such classes of domains also allow for domains with fractal boundaries, however our hypotheses are more topological in nature and allow for geometric features not allowed in these classes, such as cusps (see the discussion in subsection 5.2.1).

Pixelated domains

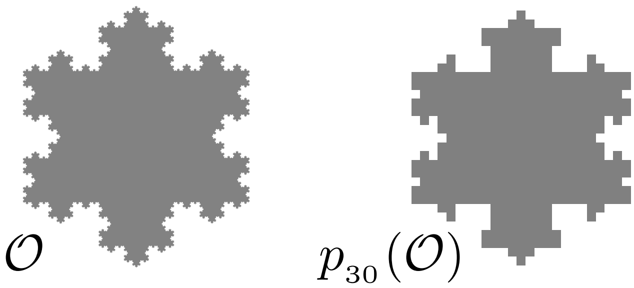

Figure 1.5 An illustration of a pixelated domain approximation.

A connection between the above result and numerical analysis is provided by the following geometric approximation scheme.

Definition 1.21. For an open set $\mathscr{O} \subset \mathbb{R}^2$, the corresponding *pixelated domains* $p_n(\mathscr{O})$ are the open subsets of $\mathbb{R}^2$ defined by

$$p_n(\mathscr{O}) := \text{int}\left(\bigcup_{j\in L_n(\mathscr{O})} (j+[-\tfrac{1}{2n},\tfrac{1}{2n}]^2)\right)$$

where

$$L_n(\mathscr{O}) := \left\{j \in (n^{-1}\mathbb{Z})^2 : j \in \mathscr{O}\right\}.$$

In other words, the closure of a pixelated domain is the union of boxes around the points in the grid $(n^{-1}\mathbb{Z})^2$ which lie in $\mathscr{O}$. Note that the notation $p_n(\mathscr{O})$ is not used in Chapter 5. Pixelated domains are an ideal basis for a general numerical scheme since:

- $p_n(\mathscr{O})$ can be constructed solely from the knowledge of whether or not a finite number of points lie in $\mathscr{O}$, provided $\mathscr{O}$ is bounded[8].
- $p_n(\mathscr{O})$ may be easily triangulated.

In Proposition 5.42, we prove that, provided $\mathscr{O}$ is a bounded, topologically regular domain with $\mu_{\text{leb}}(\partial\mathscr{O}) = 0$, it holds that

$$l(n) := \text{dist}_H(\mathscr{O}, p_n(\mathscr{O})) + \text{dist}_H(\partial\mathscr{O}, \partial p_n(\mathscr{O})) \to 0 \qquad \text{as} \qquad n \to \infty. \tag{1.42}$$

Consequently, the eigenvalues for pixelated domains converge,

$$\forall k \in \mathbb{N}: \qquad \lambda_k(p_n(\mathscr{O})) \to \lambda_k(\mathscr{O}) \qquad \text{as} \qquad n \to \infty.$$

Poincaré-type inequality

As we explain in the next subsection, the following auxiliary result plays a fundamental role in the proof of Theorem 1.20. We have not managed to find another Poincaré-type inequality of this form in the literature, although certain Hardy-type inequalities bear some resemblance (see the discussion in Subsection 5.2.2).

Intuitively, the following inequality gives a precise manner in which functions $u \in H_0^1(\mathscr{O})$ become small near the boundary $\partial\mathscr{O}$. For $r > 0$, we define a family of boundary neighbourhoods as follows

$$\partial^r\mathscr{O} := \{x \in \mathscr{O} : \text{dist}(x, \partial\mathscr{O}) < r\}.$$

The path components of a set are defined as the equivalence classes under the relation $x \sim y \iff x$ connected by a path to y.

Theorem 1.22 (Theorem 5.6)**.** *Let $r_0 := (4\sqrt{2})^{-1} Q(\partial\mathscr{O})$, where*

$$Q(\partial\mathscr{O}) := \inf\{\text{diam}(\Gamma) : \Gamma \subset \partial\mathscr{O} \text{ is a path component}\}.$$

Then, for any $r \in (0, r_0)$ and $u \in H_0^1(\mathscr{O})$,

$$\|u\|_{L^2(\partial^r\mathscr{O})} \leqslant 5r\|\nabla u\|_{L^2(\partial^{2\sqrt{2}r}\mathscr{O})}.$$

1.3.2 Mosco convergence and structure of the proof

The main notion that we utilise in order to prove Theorem 1.20 is that of Mosco convergence for H_0^1 Sobolev spaces.

[8] More accurately, $\mathscr{O} \subset B_X(0)$, where $X > 0$ is known.

Definition 1.23. We have convergence $\mathscr{O}_n \xrightarrow{\mathrm{M}} \mathscr{O}$ in the Mosco sense as $n \to \infty$ if:

(i) For all $u \in H_0^1(\mathscr{O})$, there exists $u_n \in H_0^1(\mathscr{O}_n)$, $n \in \mathbb{N}$, such that $u_n \to u$ in H^1 as $n \to \infty$.

(ii) For any subsequence $H_0^1(\mathscr{O}_{n_j})$, $j \in \mathbb{N}$, and any $u_j \in H_0^1(\mathscr{O}_{n_j})$, $j \in \mathbb{N}$, such that $u_j \rightharpoonup u$ in H^1 as $j \to \infty$ for some $u \in H^1(\mathbb{R}^2)$, we have $u \in H_0^1(\mathscr{O})$.

Mosco convergence can be thought of as a notion of convergence for the H_0^1 spaces themselves and is often denoted as $H_0^1(\mathscr{O}_n) \xrightarrow{\mathrm{M}} H_0^1(\mathscr{O})$ as $n \to \infty$ in the literature.

If $\mathscr{O}$ is bounded, then we have the following chain of implications [118, Chapter VIII.7]

$$\begin{aligned} \mathscr{O}_n \xrightarrow{\mathrm{M}} \mathscr{O} \quad &\Rightarrow \quad \|H_{\mathscr{O}_n}^{-1} - H_{\mathscr{O}}^{-1}\|_{L^2 \to L^2} \to 0 \\ &\Rightarrow \quad \|\mathbb{P}_{(a,b)}(H_{\mathscr{O}_n}) - \mathbb{P}_{(a,b)}(H_{\mathscr{O}})\|_{L^2 \to L^2} \to 0 \\ &\Rightarrow \quad \lambda_k(\mathscr{O}_n) \to \lambda_k(\mathscr{O}) \end{aligned}$$

where all the limits are as $n \to \infty$ and $\mathbb{P}_{(a,b)}(H)$, $a, b \in \mathbb{R}$, $a < b$, denote the spectral projections for a self-adjoint operator H. In other words, Mosco convergence not only implies convergence of the eigenvalues, but also of the associated eigenspaces and of the solutions of Poisson equations.

In particular, this chain of implications shows that in order to prove Theorem 1.20, it suffices to prove that $\mathscr{O}_n \xrightarrow{\mathrm{M}} \mathscr{O}$ as $n \to \infty$ for the domains satisfying the hypotheses. Indeed, the result is formulated in terms of Mosco convergence in Chapter 5. Our first step to proving Mosco convergence is to reduce the problem to the verification of certain uniform Poincaré-type inequalities for the sequence of domains $\mathscr{O}_n$, $n \in \mathbb{N}$, as well as for the limit domain $\mathscr{O}$.

Proposition 1.24. *Assume the hypotheses of Theorem 1.20. Suppose that there exists a sequence $\varepsilon(n) \geqslant 2l(n)$, $n \in \mathbb{N}$, with $\varepsilon(n) \to 0$ as $n \to \infty$ and constants $C, \alpha > 0$ independent of n such that*

$$\|u\|_{L^2(\partial^{\varepsilon(n)}\mathscr{O})} \leqslant C\varepsilon(n)\|\nabla u\|_{L^2(\partial^{\alpha\varepsilon(n)}\mathscr{O})}, \tag{1.43}$$

$$\|v\|_{L^2(\partial^{\varepsilon(n)}\mathscr{O}_n)} \leqslant C\varepsilon(n)\|\nabla v\|_{L^2(\partial^{\alpha\varepsilon(n)}\mathscr{O}_n)} \tag{1.44}$$

for all $n \in \mathbb{N}$, $u \in H_0^1(\mathscr{O})$ and $v \in H_0^1(\mathscr{O}_n)$. Then, $\mathscr{O}_n \xrightarrow{\mathrm{M}} \mathscr{O}$ as $n \to \infty$.

The proof of this proposition involves explicitly constructing appropriate cut-off functions. For instance, to show Definition 1.23 (i), the cut-off functions χ_n are supported in $\mathscr{O}_n$, so that $u_n := \chi_n u \in H_0^1(\mathscr{O}_n)$. The Poincaré-type inequalities (1.43) and (1.44) then allow the convergence criteria to be established.

Inequality (1.43) for a single domain $\mathscr{O}$, follows directly from Theorem 1.22. Therefore, the final ingredient required for Mosco convergence is inequality (1.44) for the sequence $\mathscr{O}_n$, $n \in \mathbb{N}$.

Under the hypotheses of Theorem 1.20, in particular the convergence condition $l(n) \to 0$ for $\mathscr{O}_n$ to $\mathscr{O}$ (see (1.42)), we can provide a geometric characterisation of $\mathscr{O}_n$ for large n. More precisely, it follows from Proposition 5.38 that there exists a sequence $\varepsilon(n)$ as in Proposition 1.24 such that, for all large enough n, $\partial\mathscr{O}_n$ has a path-connected subset Γ_n whose diameter exceeds $\mathrm{diam}(\partial\mathscr{O}) - \varepsilon(n)$ and such that any other point in $\partial\mathscr{O}_n$ lies within a distance $\varepsilon(n)$ to Γ_n. As it turns out, by applying Theorem 1.22 to the domain $\mathscr{V}_n = \Gamma_n^c$, we are able to verify inequality (1.44) with $C = 10$ and $\alpha = 4\sqrt{2}$.

1.3.3 Ideas in the proof of the Poincaré-type inequality

In this final subsection, we give an introduction to some of the main ideas in the proof of the Poincaré-type inequality Theorem 1.22.

The first thing to notice is that, since $C_c^\infty(\mathscr{O})$ is dense in $H_0^1(\mathscr{O})$, it suffices to show that there exist numerical constants $C, \alpha > 0$ and $r_0 = r_0(\mathscr{O}) > 0$ such that

$$\|u\|_{L^2(\partial^r\mathscr{O})} \leqslant Cr\|\nabla u\|_{L^2(\partial^{\alpha r}\mathscr{O})}, \qquad r \in (0, r_0), \qquad u \in C_c^\infty(\mathscr{O}). \tag{1.45}$$

Therefore, we can restrict our attention to functions $u \in C_c^\infty(\mathscr{O})$, for which the point values $u(p)$, $p \in \mathscr{O}$, are well defined.

Fix $u \in C_c^\infty(\mathscr{O})$. Since u vanishes on $\partial\mathscr{O}$, we can express the point values $u(p)$ as path integrals to the boundary. Let $\gamma_p : [0, l_p] \to \mathbb{R}^2$, $p \in \partial^r\mathscr{O}$, be an arbitrary family of piecewise smooth maps representing a bundle of paths, where, for each $p \in \partial^r\mathscr{O}$, $l_p > 0$ denotes the length of the path γ_p. The precise choice for γ_p shall be further specified later. Assume that

- $\gamma_p(0) \in \partial\mathscr{O}$, $\gamma_p(l_p) = p$,
- γ_p has unit speed, that is, $|\frac{\mathrm{d}}{\mathrm{d}t}\gamma_p(t)| = 1$ for all $t \in [0, l_p]$ and
- $\sup_{p \in \partial^r\mathscr{O}} l_p < \infty$.

Then we have

$$u(p) = \int_0^{l_p} \tfrac{\mathrm{d}}{\mathrm{d}t} u(\gamma_p(t))\mathrm{d}t. \tag{1.46}$$

Inserting this path integral expression into an L^2 norm, we get

$$\int_{\partial^r\mathscr{O}} |u(p)|^2 \mathrm{d}p \leqslant \int_{\partial^r\mathscr{O}} \left(\int_0^{l_p} |\tfrac{\mathrm{d}}{\mathrm{d}t} u(\gamma_p(t))| \mathrm{d}t \right)^2 \mathrm{d}p \leqslant \int_{\partial^r\mathscr{O}} \left(\int_0^{l_p} |\nabla u(\gamma_p(t))| \mathrm{d}t \right)^2 \mathrm{d}p$$

where the fact that γ_p is unit speed was used in the last line along with the chain rule. Furthermore, by the Cauchy-Schwarz inequality,

$$\int_0^{l_p} \left|\nabla u(\gamma_p(t))\right| \mathrm{d}t \leqslant l_p^{1/2} \left(\int_0^{l_p} \left|\nabla u(\gamma_p(t))\right|^2 \mathrm{d}t \right)^{1/2}$$

hence

$$\int_{\partial^r \mathscr{O}} |u(p)|^2 \mathrm{d}p \leqslant \left(\sup_{p \in \partial^r \mathscr{O}} l_p \right) \int_{\partial^r \mathscr{O}} \int_0^{l_p} |\nabla u(\gamma_p(t))|^2 \mathrm{d}t \, \mathrm{d}p. \tag{1.47}$$

Sufficient bundle of paths

Inequality (1.47) gives rise to sufficient conditions for γ_p, $p \in \partial^r \mathscr{O}$, in order for the Poincaré-type inequality (1.45) to hold true. These should be verified for all $r \in (0, r_0)$.

The first condition is perhaps not surprising since every point in $\partial^r \mathscr{O}$ is a distance less than r away from $\partial \mathscr{O}$.

(A) There exists a numerical constant $C_1 > 0$ such that

$$\sup_{p \in \partial^r \mathscr{O}} l_p \leqslant C_1 r. \tag{1.48}$$

The second condition should be verified after the first and requires that the bundle of paths does not “concentrate” too much at any given point.

(B) There exists a constant $C_2 > 0$ such that for any positive, continuous function $\phi \in L^1(\mathscr{O})$, we have

$$\int_{\partial^r \mathscr{O}} \int_0^{l_p} \phi(\gamma_p(t)) \mathrm{d}t \, \mathrm{d}p \leqslant C_2 r \int_{\partial^{\alpha r} \mathscr{O}} \phi(p) \mathrm{d}p. \tag{1.49}$$

The proof of Theorem 1.22 essentially consists in explicitly constructing γ_p, $p \in \partial^r \mathscr{O}$, satisfying these two conditions for any domain $\mathscr{O} \subset \mathbb{R}^2$ with $Q(\partial \mathscr{O}) > 0$ and any small enough $r > 0$. Note that we do not use the notation γ_p and l_p in Chapter 5.

To help understand condition (B), and motivate the geometric constructions in Section 5.3, let us now look at some examples.

Example 1: Half-plane

Suppose that $\mathscr{O} = \mathbb{R}_{>0} \times \mathbb{R}$ and fix any $r > 0$. Then we can define a family of paths satisfying the above conditions by

$$\gamma_p(t) := (t, y), \qquad p = (x, y). \tag{1.50}$$

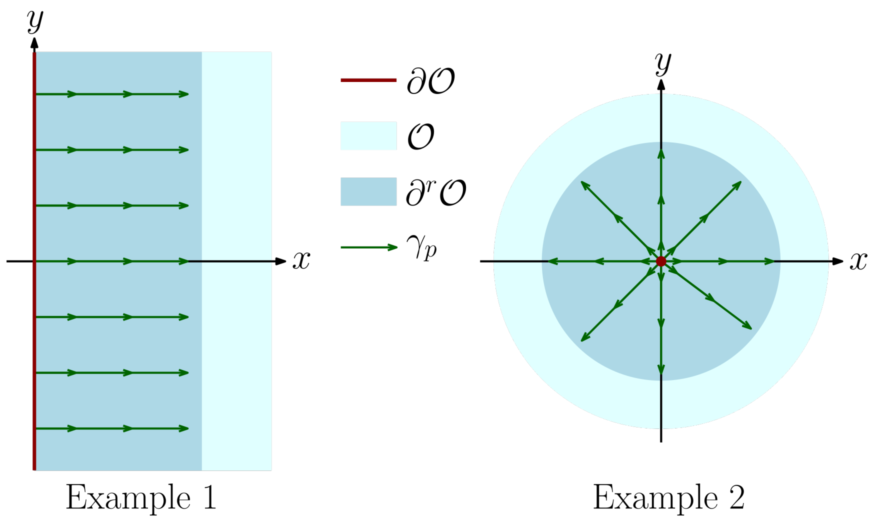

Figure 1.6 (left) An illustration of the paths γ_p from Example 1 for a sample of points $p \in \partial^r \mathscr{O}$. (right) An illustration of one possible family of paths γ_p for the domain in Example 2 and a sample of points $p \in \partial^r \mathscr{O}$.

Then $\gamma_p(0) = (0,y) \in \partial\mathscr{O}$, γ_p is unit speed and, setting $l_p := x$, we have $\gamma_p(l_p) = p$. For $p = (x,y) \in \partial^r \mathscr{O}$, we have $l_p = x \leqslant r$, so condition (A) is satisfied. Condition (B) can be seen to be satisfied by again using $x \leqslant r$,

$$\begin{aligned}\int_{\partial^r\mathscr{O}} \int_0^{l_p} \phi(\gamma_p(t))\mathrm{d}t\,\mathrm{d}p &= \int_{-\infty}^{\infty}\int_0^r \int_0^x \phi(t,y)\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}y \\ &\leqslant r\int_{-\infty}^{\infty}\int_0^r \phi(t,y)\mathrm{d}t\,\mathrm{d}y = r\int_{\partial^r\mathscr{O}} \phi(p)\mathrm{d}p.\end{aligned}$$

Example 2: Concentrating paths

Suppose that $\mathscr{O} = \mathbb{R}^2 \backslash \{0\}$ and fix any $r > 0$. We claim that there does not exist a family of paths γ_p, $p \in \partial^r \mathscr{O}$ satisfying the above conditions.

Assume otherwise, for contradiction. Then, $\gamma_p(0) = 0$ for all $p \in \partial^r \mathscr{O}$ and γ_p has unit speed, so

$$|\gamma_p(\varepsilon)| \leqslant \varepsilon \quad \text{for all} \quad \varepsilon \in (0, l_p].$$

For any $\varepsilon > 0$, let ϕ_ε be any smooth, positive function on $\mathbb{R}^2$ such that

$$\operatorname{supp}\phi_\varepsilon \subset B_\varepsilon(0) \qquad \text{and} \qquad \phi_\varepsilon \equiv 1 \quad \text{on} \quad B_{\varepsilon/2}(0).$$

Then, for any $\varepsilon \in (0, l_p]$,

$$\int_{\partial^r\mathscr{O}} \int_0^{l_p} \phi_\varepsilon(\gamma_p(t))\mathrm{d}t\,\mathrm{d}p \geqslant \int_{\partial^r\mathscr{O}} \int_0^{\varepsilon/2} \phi_\varepsilon(\gamma_p(t))\mathrm{d}t\,\mathrm{d}p \geqslant \frac{\pi r^2 \varepsilon}{2}$$

and, for any $\alpha > 0$,

$$\int_{\partial^{\alpha r}} \phi_\varepsilon(p)\mathrm{d}p \leqslant \pi\varepsilon^2,$$

from which it can be readily seen that condition (B) cannot hold for any fixed $r > 0$.

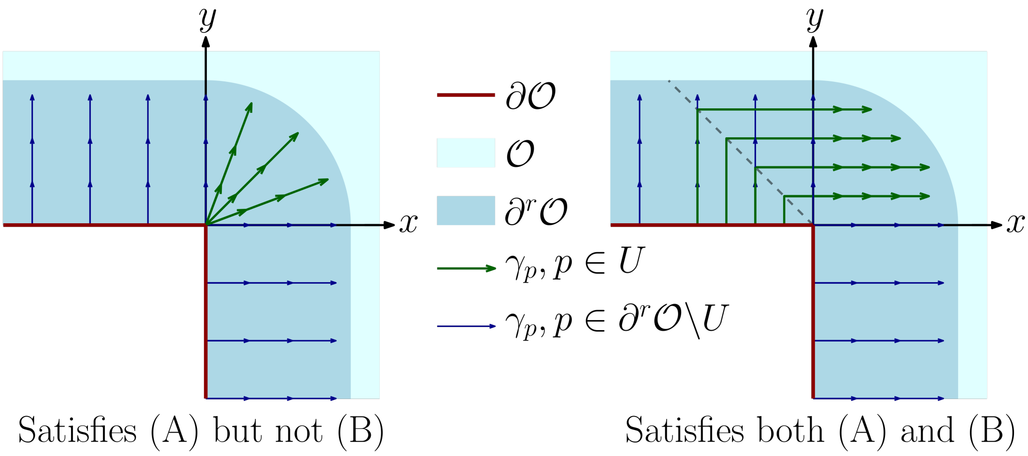

Figure 1.7 (left) An illustration of an incompatible family of paths for the domain in Example 3. (right) An illustration of the compatible family of paths described in Example 3.

Example 3: Turning the corner

Consider the domain $\mathscr{O} = \mathbb{R}^2 \backslash (\mathbb{R}_{\leqslant 0} \times \mathbb{R}_{\leqslant 0})$ and fix any $r > 0$. Then $\mathscr{O}$ has a reentrant corner at the point (0,0). Focus on the problem of constructing a family paths γ_p from $\partial\mathscr{O}$ to points in the region $U = (\mathbb{R}_{>0} \times \mathbb{R}_{>0}) \cap \partial^r\mathscr{O}$.

Suppose that we construct γ_p as illustrated in the left part of Figure 1.7, so that $\gamma_p(0) = (0,0)$ for all $p \in U$. Then the paths γ_p, $p \in U$, concentrate in a similar way to the previous example and condition (B) cannot hold by similar reasoning.

Nevertheless, it is possible to construct a family of paths γ_p, $p \in \partial^r\mathscr{O}$, satisfying both conditions (A) and (B) above. For $p = (x,y) \in U$, we let

$$\gamma_p(t) := \begin{cases} (-y,t) & \text{if} \quad t \in [0,y] \\ (-2y+t,y) & \text{if} \quad t \in (y, 2y+x]. \end{cases} \tag{1.51}$$

On the other hand, for $p \in \partial^r\mathscr{O}$, for $p \in \partial^r\mathscr{O}\backslash U$, define γ_p analogously to (1.50), as illustrated in the right part of Figure 1.7.

Clearly, $l_p = 2y + x \leqslant 3r$ for $p \in U$, and $l_p = r$ otherwise, so condition (A) is satisfied. Since $x, y \leqslant r$ for $p = (x,y) \in U$, we have

$$\int_U \int_0^{l_p} \phi(\gamma_p(t))\mathrm{d}t\,\mathrm{d}p \leqslant \int_0^r \int_0^r \left(\int_0^y \phi(-y,t)\mathrm{d}t + \int_y^{3r} \phi(-2y+t,y)\mathrm{d}t \right) \mathrm{d}x\,\mathrm{d}y$$
$$= r \int_0^r \int_{-r}^r \phi(x,y)\mathrm{d}x\,\mathrm{d}y \leqslant r \int_{\partial^{\sqrt{2}r}\mathscr{O}} \phi(p)\mathrm{d}p.$$

The reasoning of Example 1 shows that the analogous inequality for $\partial^r\mathscr{O}\backslash U$ also holds so condition (B) is satisfied.

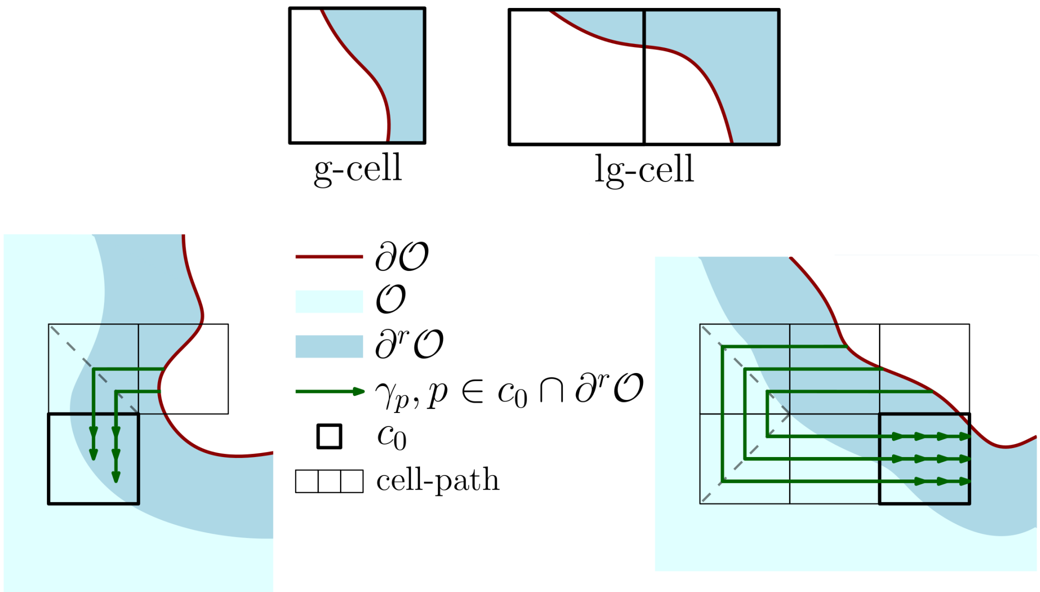

Figure 1.8 (top) An illustration of a g-cell and an lg-cell. (left) An illustration of a construction of a bundle of paths from a nearby g-cell. (right) An illustration of a construction of a bundle of paths from a nearby lg-cell.

Cell-paths, g-cells and lg-cells

In Section 5.3, we construct a similar bundle of paths for an arbitrary open set $\mathscr{O} \subset \mathbb{R}^2$ with $Q(\partial\mathscr{O}) > 0$ and $r \in (0, r_0)$ where $r_0 = (4\sqrt{2})^{-1}Q(\partial\mathscr{O})$. Roughly speaking, the construction can be summarised as follows.

1. Decompose $\mathbb{R}^2$ into a union of closed boxed (which we call cells), of size $r > 0$.
2. Consider an arbitrary cell c_0 such that $c_0 \cap \partial^r\mathscr{O} \neq \emptyset$.
3. A g-cell (or an lg-cell) is a cell (or a pair of cells resp.) such that the boundary bisects the cell(s) as shown in the top part of Figure 1.8. Find a g-cell or an lg-cell near to c_0 (see Lemma 5.27).

4. Find an appropriate path of adjacent cells (a cell-path) from c_0 to the g-cell or lg-cell (see Lemma 5.28).

5. Construct a bundle paths γ_p, $p \in c_0 \cap \partial^r \mathscr{O}$ from $\partial \mathscr{O}$ to each point in c_0 within the cell path (see Proposition 5.26).

Chapter 2

The Dissipative Barrier Method

Declaration:
This chapter appears in a similar form in the published article [130].

2.1 Introduction

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

$$T_R = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q + i\gamma\chi_{[0,R]} \qquad \text{on } L^2(0,\infty), \tag{2.1}$$

endowed with a complex mixed boundary condition at 0, where χ is the characteristic function and q is a possibly complex-valued multiplication operator. 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) [18].

It is well known that the numerical approximation of the spectra of linear operators is often complicated by the possible presence of *spectral pollution* [16, 51, 91, 116]. The primary motivation for this chapter 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 [38, 39, 72], in the computation of resonances in quantum chemistry [119, 128, 139] and in the study of resonances in quantum chaos [109, 110].

2.1.1 Spectral inclusion and pollution

Let us now introduce the abstract notions of spectral inclusion and pollution. Suppose that we are interested in approximating the spectrum of a (linear) operator H on a Hilbert space $\mathscr{H}$ with domain $D(H)$. Let (H_n) be a sequence of operators on $\mathscr{H}$ 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

$$\sigma((H_n)) = \{\lambda \in \mathbb{C} : \exists I \subseteq \mathbb{N} \text{ infinite}, \exists \lambda_n \in \sigma(H_n), n \in I \text{ with } \lambda_n \to \lambda\}. \tag{2.2}$$

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

$$\sigma(H) \cap \Omega \subseteq \sigma((H_n)). \tag{2.3}$$

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

$$\sigma_{\text{poll}}((H_n)) = \{\lambda \in \sigma((H_n)) : \lambda \notin \sigma(H)\}. \tag{2.4}$$

In order to reliably approximate the spectrum of H in $\Omega \subseteq \mathbb{C}$ 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 H and H_n are self-adjoint, 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 [26, 51, 82, 97, 98, 138]. 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 [104].

2.1.2 Dissipative Barrier Method

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

$$T_n = T_0 + i\gamma s_n \qquad (n \in \mathbb{N}), \tag{2.5}$$

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 [4, 102–104, 133]. 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 [21]). 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 $i\gamma + I \subseteq i\gamma + \mathbb{R}$, then in principle one can reliably numerically compute the spectrum of T_0 in I.

2.1.3 Analysis of expanding barriers

The aim of this chapter is to provide spectral inclusion and spectral pollution results for sequences of operators of the form (2.5).

In Section 2.2, we work in an abstract setting, utilising the limiting essential spectrum $\sigma_e((T_n))$ [18], 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 chapter [84] 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 2.2 are far simpler than those of [84], owing to the use of the limiting essential spectrum.

The remainder of the chapter is devoted to a more precise analysis for the case of Sturm-Liouville operators on the half-line. Our results in Sections 2.3 and 2.4 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 (2.1) with the background potential q either in L^1 or real eventually periodic. In Section 2.3, 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 [104, Theorem 10], but only for γ sufficiently small. In Section 2.4 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 2.3 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 2.2 and 2.3 in Section 2.5, 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 2.4 in Section 2.5 shows how spectral pollution may occur in this second case.

2.1.4 Summary of results

Limiting essential spectrum and spectral pollution

In Section 2.2, we consider a self-adjoint operator T_0 on Hilbert space $\mathscr{H}$. It is assumed that the operators s_n ($n \in \mathbb{N}$) on $\mathscr{H}$ are self-adjoint, tend strongly to the identity operator as $n \to \infty$ and are bounded independently of n. For $\gamma > 0$, we define the perturbed operators T_n ($n \in \mathbb{N}$) by (2.5) 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 [18] 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)

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

[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.

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 (2.11)) satisfy $s_- - \varepsilon \leqslant s_n \leqslant s_+ + \varepsilon$ for any $\varepsilon > 0$ and large enough n.

The main results of Section 2.2 are non-convex enclosures for $\sigma_e((T_n))$ complementing the enclosure provided by $W_e((T_n))$.

(A) (Theorem 2.12) 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

$$\Gamma_a := \Big\{\lambda \in \mathbb{C} : \mathrm{Im}(\lambda) \in [0,\gamma],\, \mathrm{dist}(\mathrm{Re}(\lambda), \sigma_e(T_0)) \leqslant \sqrt{\mathrm{Im}(\lambda)(\gamma - \mathrm{Im}(\lambda))}\Big\}.$$

Alternatively, if for any sequence $(u_n) \subset D(T_0)$ bounded in $\mathscr{H}$ with $(T_0 u_n)$ bounded in $\mathscr{H}$ 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 2.11) then $\sigma_e((T_n)) \cup \sigma_e((T_n^*))^* \subset \Gamma_b = \Gamma_b(\sigma_e(T_0), \gamma, s_\pm)$, where

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

In particular, if s_n are projection operators or if Assumption 2.11 is satisfied then

(T_n) is spectrally exact for T 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 2.1. Assumption 2.11 is verified for a class of perturbations for Schrödinger operators on Euclidean domains in Example 2.14.

Second order operators on the half-line

In Section 2.3, 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 2.2. 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 $\mathrm{Im}k > 0$ and with $\tilde{\psi}_{\pm}(\cdot,\lambda)$ bounded. A similar decomposition is required for $\psi'_{\pm}$ - see Assumption 2.15 for the precise statement.

The perturbed operators in Section 2.3 are defined by

$$T_R = T_0 + i\gamma\chi_{[0,R]} \qquad (R \in \mathbb{R}_+) \tag{2.6}$$

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 (2.42)) and prove the following:

(B) (Theorems 2.23 and 2.24) 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 large enough) 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

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

The proofs utilise Rouché's theorem applied to an analytic function (Lemma 2.19) 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 2.15 is verified in two cases:

- (Examples 2.17 and 2.25) T_0 is a Schrödinger operator with an L^1 potential. In this case, $S_{\mathfrak{p}}((R_n)) = \emptyset$.
- (Examples 2.18 and 2.26) 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 (2.51)). It is also proved that $S_{\mathfrak{p}}((R_n)) \subset \sigma_e((T_n))$.

Inclusion for the essential spectrum

In Section 2.4, we let T_0 be a Sturm-Liouville operator satisfying Assumption 2.15, as described above. In addition, we require that $\sigma_e(T_0) \subseteq \mathbb{R}$ 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 2.27 for the precise statement.

The perturbed operators T_R and the limit operator in Section 2.4 are defined by (2.6) and $T = T_0 + i\gamma$ respectively, as in Section 2.3. We construct a set $S_\mathfrak{r} \subseteq i\gamma + \mathbb{R}$ (equation (2.65)) and prove that:

(C) (Theorem 2.33) 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 large enough) 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 2.30) whose zeros are the eigenvalues of T_R. In the case that

- (Examples 2.28 and 2.38) T_0 is a Schrödinger operator with an L^1 potential satisfying the Naimark condition or a dilation analyticity condition, or,
- (Examples 2.29 and 2.39) $\gamma > 0$ 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 2.27 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 (2.79) 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 2.33 with Theorem 2.24 and the characterisation of $S_\mathfrak{p}((R_n))$ to conclude that

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

Notation and conventions

Recall the notations and conventions given at the beginning of Chapter 1. In addition, in Sections 2.3 and 2.4, $\psi'(x,z) := \frac{\mathrm{d}}{\mathrm{d}x}\psi(x,z)$. Also, for sets $\Omega \subset \mathbb{C}$, we define

$$\Omega^* = \{\bar{z} : z \in \Omega\}.$$

2.2 Limiting essential spectrum and spectral pollution

In this section, we study spectral exactness for sequences of abstract operators (T_n) of the form (2.5). In Section 2.2.1, we briefly review the notions of limiting essential spectrum and essential numerical range. We refer the reader to [18] and [21] for a more detailed exposition. In Section 2.2.2, we discuss the application of limiting essential spectrum and essential numerical range to (T_n). In Section 4.4.4, we prove enclosures for the limiting essential spectrum of (T_n).

2.2.1 Limiting essential spectrum and numerical range

Throughout this subsection, let H and H_n ($n \in \mathbb{N}$) be closed, densely-defined operators acting on $\mathscr{H}$.

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

$$\sigma_e((H_n)) = \left\{ \lambda \in \mathbb{C} : \begin{array}{c} \exists I \subseteq \mathbb{N} \text{ infinite}, \exists u_n \in D(H_n), n \in I \text{ with} \\ \|u_n\| = 1,\, u_n \rightharpoonup 0,\, \|(H_n - \lambda)u_n\| \to 0 \end{array} \right\}. \tag{2.7}$$

Note that the terminology "limiting essential spectrum" is a slight misnomer since in general we cannot be certain that the limiting essential spectrum is a subset of the limiting spectrum (see Theorem 2.3, noting that the set of spectral pollution $\sigma_{\mathrm{poll}}((H_n))$ is a subset of the limiting spectrum $\sigma((H_n))$).

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

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

Theorem 2.3 ([18, Theorem 2.3])**.** *If $H_n \xrightarrow{\mathrm{sr}} H$ and $H_n^* \xrightarrow{\mathrm{sr}} H^*$ then*

$$\sigma_{\mathrm{poll}}((H_n)) \subset \sigma_e((H_n)) \cup \sigma_e((H_n^*))^* \tag{2.8}$$

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

$$W_e((H_n)) = \left\{ \lambda \in \mathbb{C} : \begin{array}{c} \exists I \subseteq \mathbb{N} \text{ infinite}, \exists u_n \in D(H_n), n \in I \text{ with} \\ \|u_n\| = 1,\, u_n \rightharpoonup 0,\, \langle H_n u_n, u_n \rangle \to \lambda \end{array} \right\}. \tag{2.9}$$

Proposition 2.6 ([21, Proposition 5.6])**.** *The limiting essential numerical range of (H_n) is closed and convex with*

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

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

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

2.2.2 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 $\mathscr{H}$. Let $\gamma > 0$ and define the perturbed operators, as in the introduction, by

$$T_n = T_0 + i\gamma s_n. \qquad (n \in \mathbb{N}) \tag{2.10}$$

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 strongly to T.

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, $\sigma_{\text{poll}}((T_n)) \subset \sigma_e((T_n)) \cup \sigma_e((T_n^*))^*$ 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 [61]. $\square$

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 (2.10), 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 $\mathscr{H}$ is defined as the union of $\sigma_e(H)$ with $+\infty$ and/or $-\infty$ if H is unbounded from above and/or below respectively.

Throughout the remainder of the section, let

$$s_- := \liminf_{n\to\infty} \inf_{u\in\mathscr{H}:\|u\|=1} \langle s_n u, u\rangle \quad \text{and} \quad s_+ := \limsup_{n\to\infty} \sup_{u\in\mathscr{H}:\|u\|=1} \langle s_n u, u\rangle. \tag{2.11}$$

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

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

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 $\langle (T_0 - \mathrm{Re}(\lambda))u_n, u_n\rangle \to 0$ which implies that

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

where we used [21, Theorem 3.8] in the equality. Finally, $\mathrm{Im}\langle (T_n - \lambda)u_n, u_n\rangle \to 0$ implies that $\mathrm{Im}(\lambda) = \gamma\langle s_n u_n, u_n\rangle + o(1) \in \gamma[s_-, s_+]$. □

2.2.3 Main abstract results

In the main result of this section, Theorem 2.12, 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 2.11, is given below. An example of a class of perturbations for Schrödinger operators satisfying this assumption is provided in Example 2.14. The enclosures are illustrated in Figure 2.1.

Lemma 2.10. *Let H be a self-adjoint operator on $\mathscr{H}$. 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*

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

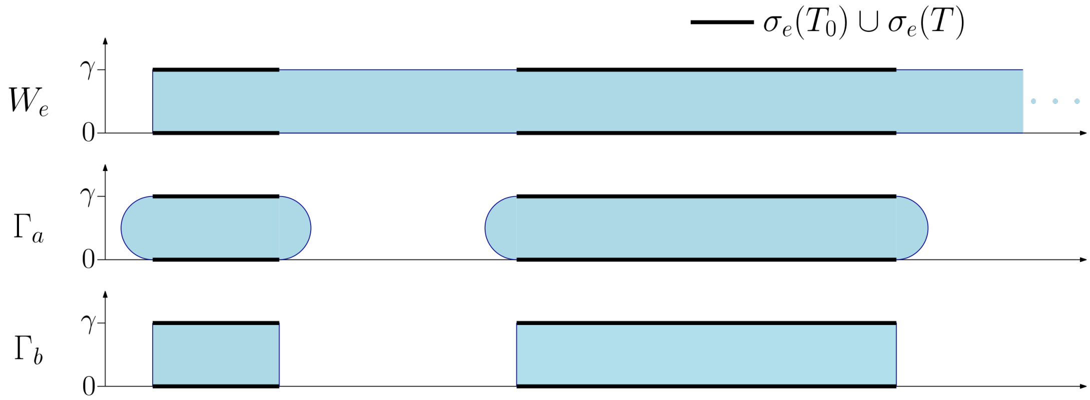

Figure 2.1 Illustration of various enclosures for the limiting essential spectrum: the limiting essential numerical range $W_e = W_e((T_n))$, the enclosure $\Gamma_a = \Gamma_a(\sigma_e(T_0), \gamma)$ of Theorem 2.12 (a) and the enclosure $\Gamma_b = \Gamma_b(\sigma_e(T_0), \gamma, s_\pm)$ of Theorem 2.12 (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.

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 [76, 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 2.11. If $(u_n) \subset D(T_0)$ is bounded in $\mathscr{H}$ with $(T_0 u_n)$ bounded in $\mathscr{H}$ 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 2.12. (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*

$$\Gamma_a := \left\{\lambda \in \mathbb{C} : \mathrm{Im}(\lambda) \in [0,\gamma],\, \mathrm{dist}(\mathrm{Re}(\lambda), \sigma_e(T_0)) \leqslant \sqrt{\mathrm{Im}(\lambda)(\gamma - \mathrm{Im}(\lambda))}\right\}. \tag{2.12}$$

(b) *If Assumption 2.11 holds then $\sigma_e((T_n)) \cup \sigma_e((T_n^*))^* \subset \Gamma_b = \Gamma_b(\sigma_e(T_0), \gamma, s_\pm)$ where*

$$\Gamma_b := \sigma_e(T_0) + i\gamma[s_-, s_+]. \tag{2.13}$$

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

$$\langle T_0 u_n, u_n\rangle = \mathrm{Re}(\lambda) + o(1) \quad \text{and} \quad \gamma\langle s_n u_n, u_n\rangle = \mathrm{Im}(\lambda) + o(1). \tag{2.14}$$

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

$$\|T_0 u_n\|^2 - \mathrm{Re}(\lambda)\langle T_0 u_n, u_n\rangle - \gamma \mathrm{Im}\langle s_n u_n, T_0 u_n\rangle = o(1). \tag{2.15}$$

The first equation in (2.14) gives

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

which, combined with (2.15), yields,

$$\|(T_0 - \mathrm{Re}(\lambda))u_n\|^2 = \gamma \mathrm{Im}\langle s_n u_n, T_0 u_n\rangle + o(1). \tag{2.16}$$

(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 (2.14),

$$\forall n \in I : \langle s_n u_n, u_n\rangle \in [0,1] \quad \Rightarrow \quad \mathrm{Im}(\lambda) \in [0,\gamma]. \tag{2.17}$$

Focusing now on $\mathrm{Re}(\lambda)$, 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 (2.14) gives,

$$\begin{aligned}\mathrm{Im}\langle s_n u_n, T_0 u_n\rangle &= \gamma\|s_n u_n\|^2 - \mathrm{Im}(\lambda)\langle s_n u_n, u_n\rangle + o(1) \\ &= (\gamma - \mathrm{Im}(\lambda))\frac{\mathrm{Im}(\lambda)}{\gamma} + o(1).\end{aligned} \tag{2.18}$$

Combining (2.16) and (2.18), we have

$$\|(T_0 - \mathrm{Re}(\lambda))u_n\| = \sqrt{(\gamma - \mathrm{Im}(\lambda))\mathrm{Im}(\lambda)} + o(1), \tag{2.19}$$

which by Lemma 2.10 implies that

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

(b) In this case, by the definitions of $s_\pm$ in (2.11), a similar reasoning as in (2.17) yields $\mathrm{Im}(\lambda) \in \gamma[s_-, s_+]$. Assumption 2.11 implies that

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

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

$\square$

Remark 2.13. It is interesting to note that Lemma 2.10 is not required in case (b) of Theorem 2.12. This is because Assumption 2.11 ensures that the following holds:

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

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 $\mathrm{Re}(\lambda) \in \sigma_e(T_0)$.

Example 2.14. Suppose that $T_0 = -\Delta + q$ is a self-adjoint Schrödinger operator on $\mathscr{H} = L^2(\Omega)$, where $\Omega \subset \mathbb{R}^d$ is some open set and q is a real function on Ω. Assume that T_0 is endowed with Dirichlet boundary conditions on $\partial\Omega$ and that q is bounded below. 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

$$(s_n u)(x) = \varphi\left(\frac{\langle x\rangle}{R_n}\right)u(x) \qquad (u \in L^2(\Omega),\ x \in \Omega) \tag{2.20}$$

where $\langle x\rangle := (1+|x|^2)^{\frac{1}{2}}$. Then s_n is uniformly bounded, $s_n \xrightarrow{s} I$ and Assumption 2.11 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 ($s_n \xrightarrow{s} I$). 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 $n \in \mathbb{N}$,

$$\|(s_n - I)u\| \leqslant \|\varphi(\langle\cdot\rangle/R_n) - 1\|_{L^\infty(\Omega\cap B_{X_n}(0))}\|u\| + (\|s_n\|+1)\|u\|_{L^2(\Omega\setminus B_{X_n}(0))}. \tag{2.21}$$

By Morrey's inequality, φ is continuous, so, since $\varphi(0) = 1$, the first term on the right hand side of (2.21) 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 2.11). Let $(u_n) \subset D(T_0)$ be any sequence which is bounded in $\mathscr{H}$ such that $(T_0 u_n)$ is bounded in $\mathscr{H}$. Then,

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

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,

$$|\langle s_n u_n, T_0 u_n\rangle - \langle T_0 u_n, s_n u_n\rangle| \leqslant 2\|\nabla\varphi_n\|_{L^\infty(\Omega)}\|\nabla u_n\|\|u_n\|. \tag{2.22}$$

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 $\mathscr{H}$ by hypothesis. (∇u_n) can be seen to be bounded in $\mathscr{H}$ 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 (2.22) tends to zero as $n\to\infty$ hence Assumption 2.11 is satisfied. □

2.3 Second order operators on the half-line

Consider the differential expression

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

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 $q, 1/p, r \in L^1_{\mathrm{loc}}[0,\infty)$. 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 $u, pu' \in AC_{\mathrm{loc}}[0,\infty)$. 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,

$$BC[u] := \cos(\eta)u(0) - \sin(\eta)pu'(0) = 0 \tag{2.23}$$

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

$$
\begin{aligned}
&T_0 u = \tilde{T}_0 u \\
&D(T_0) = \{u \in L^2_r(0,\infty) : u, pu' \in AC_{\mathrm{loc}}[0,\infty), \tilde{T}_0 u \in L^2_r(0,\infty), BC[u] = 0\}.
\end{aligned}
\tag{2.24}
$$

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

$$
T_R u = T_0 u + i\gamma\chi_{[0,R]}u,\ D(T_R) = D(T_0) \qquad (R \in \mathbb{R}_+) \tag{2.25}
$$

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 2.15. 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 $\tilde{\psi}^d_\pm : [0,\infty) \times \mathbb{C}\backslash\sigma_e(T_0) \to \mathbb{C}$ such that:

(i) k is analytic and satisfies $\mathrm{Im}k > 0$.

(ii) $\tilde{\psi}_\pm(x,\cdot)$ and $\tilde{\psi}^d_\pm(x,\cdot)$ are analytic for all x and satisfy

$$
\|\tilde{\psi}_\pm(\cdot,z)\|_{L^\infty(0,\infty)} < \infty, \quad \|\tilde{\psi}^d_\pm(\cdot,z)\|_{L^\infty(0,\infty)} < \infty \tag{2.26}
$$

for all z.

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

$$
\begin{aligned}
\psi_\pm(x,z) &:= e^{\pm ik(z)x}\tilde{\psi}_\pm(x,z) \\
\psi'_\pm(x,z) &:= e^{\pm ik(z)x}\tilde{\psi}^d_\pm(x,z).
\end{aligned}
\tag{2.27}
$$

Remark 2.16 (See [30])**.** The conditions of Assumption 2.15 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

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

where $\overline{\mathrm{co}}$ denotes the closed convex hull, and that $\tilde{T}_0$ is in Sims case I (as defined in [30]).

Example 2.17 (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 [60, 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

$$\psi_\pm(x,z) = e^{\pm i\sqrt{z}x}(1+E_\pm(x,z)) \tag{2.28}$$

$$\psi'_\pm(x,z) = \pm i\sqrt{z}e^{\pm i\sqrt{z}x}\left(1+E^d_\pm(x,z)\right) \tag{2.29}$$

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 $\mathrm{Im}k > 0$ 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 2.15 is satisfied in this case.

Example 2.18 (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 2.15 are met in this case. See, for example, [59] 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

$$\phi_1(X,z) = 1,\ \phi'_1(X,z) = 0 \text{ and } \phi_2(X,z) = 0,\ \phi'_2(X,z) = 1. \tag{2.30}$$

The *discriminant* is defined by

$$\tilde{D}(z) = \phi_1(X+a,z) + \phi'_2(X+a,z). \tag{2.31}$$

The essential spectrum of T_0 is

$$\sigma_e(T_0) = \{z \in \mathbb{R} : |\tilde{D}(z)| \leqslant 2\}. \tag{2.32}$$

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

$$\rho_\pm(z) = \frac{1}{2}\left(\tilde{D}(z) \pm i\sqrt{\tilde{D}(z)^2 - 4}\right). \tag{2.33}$$

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

$$k(z) = -\frac{i}{a}\log(\rho_+(z)). \tag{2.34}$$

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

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

$$\psi_\pm(x,z) = -\phi_2(X+a,z)\phi_1(x,z) + (\phi_1(X+a,z) - \rho_\pm(z))\phi_2(x,z) \tag{2.35}$$

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

$$\begin{aligned}\psi_\pm(x_0+na,z) &= e^{\pm ik(z)na}\psi_\pm(x_0,z)\\ \psi'_\pm(x_0+na,z) &= e^{\pm ik(z)na}\psi'_\pm(x_0,z)\end{aligned} \tag{2.36}$$

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

$$B_{\mathrm{ends}} = \{z \in \mathbb{R} : |\tilde{D}(z)| = 2\}. \tag{2.37}$$

For any $z_0 \in \sigma_e(T_0)\backslash B_{\mathrm{ends}}$, $\rho_\pm$ 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 2.15 can be satisfied by setting

$$\tilde{\psi}_\pm(x,z) = \begin{cases} e^{\mp ik(z)x}\psi_\pm(x,z) & \text{if } x \in [0,X) \\ e^{\mp ik(z)x_0(x)}\psi_\pm(x_0(x),z) & \text{if } x \in [X,\infty) \end{cases} \tag{2.38}$$

and

$$\tilde{\psi}^d_\pm(x,z) = \begin{cases} e^{\mp ik(z)x}\psi'_\pm(x,z) & \text{if } x \in [0,X) \\ e^{\mp ik(z)x_0(x)}\psi'_\pm(x_0(x),z) & \text{if } x \in [X,\infty) \end{cases} \tag{2.39}$$

where $x_0(x) := X + (x-X)\mathrm{mod}\, a$.

Throughout the remainder of the section, let

$$S := \sigma_e(T_0) \cup (i\gamma + \sigma_e(T_0)) \tag{2.40}$$

and suppose that the conditions of Assumption 2.15 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 (2.23).

Lemma 2.19. *$\lambda \in \mathbb{C}\backslash S$ 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

$$(\tilde{T}_0 + i\gamma\chi_{[0,R]})u = \lambda u,\ BC[u] = 0,\ u \in L^2_r(0,\infty), \tag{2.41}$$

on $[0,\infty)$. Any solution to (2.41) 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 (2.41) 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

$$\begin{aligned}&(BC[\psi_-(\cdot,\lambda-i\gamma)]\psi_+(R,\lambda-i\gamma)-BC[\psi_+(\cdot,\lambda-i\gamma)]\psi_-(R,\lambda-i\gamma))\tilde{\psi}_+^d(R,\lambda)\\&-\left(BC[\psi_-(\cdot,\lambda-i\gamma)]\psi_+'(R,\lambda-i\gamma)-BC[\psi_+(\cdot,\lambda-i\gamma)]\psi_-'(R,\lambda-i\gamma)\right)\tilde{\psi}_+(R,\lambda)\end{aligned}$$

which in turn is equivalent to $f_R(\lambda)=0$. The analyticity claim follows from Assumptions 2.15 (i) and (ii). □

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 2.23 and 2.24. We now define a subset of the complex plane capturing such regions.

Definition 2.20. Define subset $S_\mathfrak{p}((R_n))$ of $\mathbb{C}$ by

$$S_\mathfrak{p}((R_n))=\left\{z\in\mathbb{C}\backslash S:\liminf_{n\to\infty}|\Lambda(R_n,z)|=0\right\} \tag{2.42}$$

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

$$\Lambda(R,\lambda)=\tilde{\psi}_+(R,\lambda)\tilde{\psi}_-^d(R,\lambda-i\gamma)-\tilde{\psi}_+^d(R,\lambda)\tilde{\psi}_-(R,\lambda-i\gamma). \tag{2.43}$$

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 2.2. We shall show in Theorems 2.23 and 2.24 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 2.21. *$S\cup S_\mathfrak{p}((R_n))$ is a closed subset of $\mathbb{C}$.*

Proof. By Assumption 2.15 (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 $\overline{B_\varepsilon(\lambda)} \subseteq \mathbb{C}\backslash S$. 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,

$$\Lambda(R_{n_k},\lambda) - \Lambda(R_{n_k},\lambda_k) = \frac{1}{2\pi i}\oint_{\partial B_\varepsilon(\lambda)} \frac{\lambda_k - \lambda}{(z-\lambda)(z-\lambda_k)}\Lambda(R_{n_k},z)\mathrm{d}z \to 0 \tag{2.44}$$

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 2.22. *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 (2.25) such that T_0 satisfies Assumption 2.15. Recall that S is defined by equation (2.40), $S_{\mathfrak{p}}((R_n))$ is defined by (2.42) and $(R_n) \subset \mathbb{R}_+$ is an arbitrary sequence such that $R_n \to \infty$.

Theorem 2.23. *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 large enough) and constants $C_0 = C_0(T_0,\gamma,\mu) > 0$ and $\beta = \beta(T_0,\gamma,\mu) > 0$ such that*

$$|\lambda_n - (\mu + i\gamma)| \leqslant C_0 e^{-\beta R_n} \tag{2.45}$$

for all large enough n.

Proof. Let $C > 0$ denote an arbitrary constant independent of λ and n. Let $C_1, C_2, C_3, N_0 > 0$ denote constants independent of λ and n.

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 2.22 guarantees the existence of an open neighbourhood U of $\mu + i\gamma$ such that $\overline{U} \subseteq \mathbb{C}\backslash S$ 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 2.15 guarantees that $|\alpha_+(R_n,\lambda)| \leqslant C$ ($\lambda \in U, n \in \mathbb{N}$) and $\mathrm{Im}k(\lambda - i\gamma) \geqslant C$ ($\lambda \in U$). Combined with the bound below for Λ, this implies that

$$|\tilde{f}_n(\lambda) - \tilde{f}(\lambda)| = \left| e^{2ik(\lambda - i\gamma)R_n}\frac{\alpha_+(R_n,\lambda)}{\Lambda(R_n,\lambda)}\right| \leqslant C_1 e^{-C_2 R_n} \qquad (\lambda \in U, n \geqslant N_0) \quad (2.46)$$

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

$$|\tilde{f}(\lambda)| \geqslant C_3 |\lambda - (\mu + i\gamma)|^{\nu} \qquad (\lambda \in B_\varepsilon(\mu + i\gamma)) \qquad (2.47)$$

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 (2.46) and (2.47), 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 (2.45). □

The next result concerns spectral pollution - the set of spectral pollution is defined by equation (2.4).

Theorem 2.24. *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*

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

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 $BC[\psi_+(\cdot,\mu-i\gamma)] \neq 0$,

$$|\alpha_-(R_n,\mu)| = |BC[\psi_+(\cdot,\mu-i\gamma)]\Lambda(R_n,\mu)| \geqslant C \tag{2.48}$$

for large enough n. Let $\varepsilon > 0$ be small enough so that $\overline{B_\varepsilon(\mu)} \subseteq \mathbb{C}\backslash S$. Then by Assumption 2.15 we have

$$|\alpha_\pm(R_n,\lambda)| \leqslant C \text{ and } \mathrm{Im}k(\lambda-i\gamma) \geqslant C \qquad (\lambda \in B_\varepsilon(\mu), n \in \mathbb{N}) \tag{2.49}$$

Using Cauchy's integral formula as in (2.44), and making $\varepsilon > 0$ small enough, we have

$$|\alpha_\pm(R_n,\lambda) - \alpha_\pm(R_n,\mu)| \leqslant C|\lambda-\mu| \qquad (\lambda \in B_\varepsilon(\mu), n \in \mathbb{N}). \tag{2.50}$$

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 (2.50) we have

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

Using (2.48) and (2.49) we have

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

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 2.17, $S_{\mathfrak{p}}((R_n))$ can be easily shown to be the empty set.

Example 2.25 (Schrödinger operators with L^1 potentials, continued)**.** Consider again the case $p = r = 1$ with $q \in L^1(0,\infty)$. Then, using expression (2.43) for Λ and the expressions for $\tilde{\psi}_\pm$, $\tilde{\psi}^d_\pm$ in Example 2.17 (ii), Λ satisfies

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

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 2.18, the computation of $S_{\mathfrak{p}}((R_n))$ is more involved.

Example 2.26 (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 (2.38) and (2.39) for $\tilde{\psi}_\pm$ and $\tilde{\psi}^d_\pm$ as well as the definition of $S_{\mathfrak{p}}((R_n))$ in equation (2.42), we infer that $\lambda \in S_{\mathfrak{p}}((R_n))$ if and only if

$$\psi_+(x_0,\lambda)\psi_-'(x_0,\lambda - i\gamma) - \psi_+'(x_0,\lambda)\psi_-(x_0,\lambda - i\gamma) = 0. \tag{2.51}$$

$\psi_\pm(x_0,\cdot)$ 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

$$S_{\mathfrak{p}}((R_n)) \subseteq \sigma_e((T_{R_n})). \tag{2.52}$$

Proof of inclusion (2.52). 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 (2.36) of the Floquet solutions, (2.51) implies that,

$$\psi_+(R_n,\lambda)\psi_-'(R_n,\lambda - i\gamma) - \psi_+'(R_n,\lambda)\psi_-(R_n,\lambda - i\gamma) = 0 \tag{2.53}$$

for all n. (2.53) ensures that there exists $C_{1,n}, C_{2,n} \in \mathbb{C}\backslash\{0\}$ independent of x such that

$$u_n(x) := \begin{cases} C_{1,n}\psi_-(x,\lambda - i\gamma) & \text{if } x \in [0,R_n) \\ C_{2,n}\psi_+(x,\lambda) & \text{if } x \in [R_n,\infty) \end{cases} \tag{2.54}$$

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 (2.36) of the Floquet solutions

$$\|\psi_-'(\cdot,\lambda - i\gamma)\|^2_{L^2(0,R_n)} \leqslant C\|\psi_-(\cdot,\lambda - i\gamma)\|^2_{L^2(0,R_n)} \tag{2.55}$$

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

$$\|u_n\|_{L^2} \leqslant C\|u_n\|_{L^2(\frac{1}{2}R_n,\infty)} \leqslant C\|\tilde{\chi}_n u_n\|_{L^2}. \tag{2.56}$$

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 (2.55) and (2.56). Consequently, by the definition of limiting essential spectrum (see Definition 2.1), we have $\lambda \in \sigma_e((T_{R_n}))$.

$\square$

2.4 Inclusion for the essential spectrum

Consider the Sturm-Liouville operator T_0 introduced in Section 2.3. Suppose that the conditions of Assumption 2.15 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 2.15 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 2.27. T_0 is such that $\sigma_e(T_0) \subseteq \mathbb{R}$. 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

$$\mathrm{Im}\kappa_u(z), -\mathrm{Im}\kappa_l(z) \begin{cases} > 0 & \text{if } z \in \mathbb{C}_+ \cap V_\mu \\ = 0 & \text{if } z \in \mathbb{R} \cap V_\mu \\ < 0 & \text{if } z \in \mathbb{C}_- \cap V_\mu \end{cases}. \tag{2.57}$$

(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

$$\|\tilde{\varphi}_j(\cdot,z)\|_{L^\infty(0,\infty)}, \|\tilde{\varphi}_j^d(\cdot,z)\|_{L^\infty(0,\infty)} < \infty \qquad (j = u \text{ or } l) \tag{2.58}$$

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

$$\varphi_j(x,z) := e^{i\kappa_j(z)x}\tilde{\varphi}_j(x,z), \qquad (j = u \text{ or } l), \tag{2.59}$$

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

$$\varphi_j'(x,z) = e^{i\kappa_j(z)x}\tilde{\varphi}_j^d(x,z). \qquad (j = u \text{ or } l) \tag{2.60}$$

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

Example 2.28 (Schrödinger operators with L^1 potentials, continued)**.** Consider again the case $p = r = 1$ with $q \in L^1(0,\infty)$, introduced in Example 2.17. Recall that $k(\lambda) = \sqrt{\lambda}$ so Assumption 2.27 (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 2.27 (ii) and (iii) hold in this case it suffices to show that for any $\mu \in \operatorname{int}(\sigma_e(T_0))$ 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

$$\varphi(x,z) := e^{i\sqrt{z}x}(1 + E(x,z)) \tag{2.61}$$

satisfies

$$\varphi'(x,z) = i\sqrt{z}e^{i\sqrt{z}x}\Big(1 + E^d(x,z)\Big), \tag{2.62}$$

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 (2.61) and (2.62). Additional conditions on the potential q are required to ensure that this holds. Two such conditions are:

(a) (Naimark condition [131, Lemma 1]) There exists $a > 0$ such that

$$\int_0^\infty e^{ax}|q(x)|\mathrm{d}x < \infty. \tag{2.63}$$

(b) (Dilation analyticity [29]) 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

$$|q(z)| \leqslant C_0|z|^{-\beta} \tag{2.64}$$

for all $z \in U$.

Example 2.29 (Eventually periodic Schrödinger operators, continued)**.** Consider again the case $p = r = 1$ with q eventually real periodic, introduced in Example 2.18. As mentioned in Example 2.18, for any $\mu \in \operatorname{int}(\sigma_e(T_0)) = \sigma_e(T_0) \backslash B_{\text{ends}}$ 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 (2.33) 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 (2.57).

(ii) The analytic continuations of $\tilde{\psi}_+(x, \cdot)$ and $\tilde{\psi}_+^d(x, \cdot)$ satisfy the L^∞ estimates (2.58) by their definitions (2.38) and (2.39).

(iii) The analytic continuations with respect to z of $\psi_+(\cdot, z)$ solve the Schrödinger equation $-\psi'' + q\psi = z\psi$ since by (2.35) they are linear combinations of the solutions $\phi_1(\cdot, z)$ and $\phi_2(\cdot, z)$. Expressions (2.59) and (2.60) 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 $\mu \in \operatorname{int}(\sigma_e(T_0))$ and suppose that the conditions of Assumption 2.27 are satisfied. Also, assume without loss of generality that $(i\gamma + V_\mu) \cap \mathbb{R} = \emptyset$.

Lemma 2.30. *$\lambda \in i\gamma + V_\mu$ 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

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

and

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

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

Proof. The proof is similar to the proof of Lemma 2.19.

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 $\mathrm{span}_{\mathbb{C}}\{u_1(\cdot,\lambda)\}$, 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^2_r 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 $g_R(\lambda) = 0$. $\square$

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

$$S_\mathfrak{r} = \left\{ \lambda \in i\gamma + V_\mu \cap \mathbb{R} : \liminf_{R\to\infty} |\beta_j(R,\lambda)| = 0,\ j = u \text{ or } l \right\}. \tag{2.65}$$

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 2.32. *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 2.27 (i) implies that any $z \in \partial B_\varepsilon(\mu)$ satisfies

$$\arg\left(\frac{h}{|h|}(z)\right) = \arg(h(z)) \in \begin{cases} (0,\pi) & \text{if } z \in \mathbb{C}_+ \cap V_\mu \\ \{0,\pi\} & \text{if } z \in \mathbb{R} \cap V_\mu \\ (\pi, 2\pi) & \text{if } z \in \mathbb{C}_- \cap V_\mu \end{cases}. \tag{2.66}$$

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 [81, pg. 110]. (2.66) 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 2.33. *Assume that $\mu \in \operatorname{int}(\sigma_e(T_0))$ is such that $\mu + i\gamma \notin S_\mathfrak{r}$. There exists eigenvalues λ_R of T_R (R large enough) 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 (2.26) of Assumption 2.15 (ii) and the L^∞ estimates (2.58) of Assumption 2.27 (ii), there exists $C_1, C_2 > 0$ independent of R such that $\beta_{u,R}$ and $\beta_{l,R}$ satisfy

$$C_1 \leqslant |\beta_{j,R}| \leqslant C_2 \qquad (j = u \text{ or } l) \tag{2.67}$$

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

$$(\kappa_u - \kappa_l)(\lambda - i\gamma) = -\frac{i}{R}\left(\log\left(\frac{\beta_{l,R}}{\beta_{u,R}}\right) + 2\pi i n\right) =: \tilde{\kappa}(n) \tag{2.68}$$

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 $\mathrm{Im} w_0 = 0$ by Assumption 2.27. Using (2.67),

$$|\tilde{\kappa}(n(R)) - w_0| \leqslant \frac{1}{R}\left|\log\left(\frac{\beta_{l,R}}{\beta_{u,R}}\right)\right| + \left|\frac{2\pi n(R)}{R} - w_0\right| \leqslant \frac{C}{R} \tag{2.69}$$

for large enough R. By Lemma 2.32, 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

$$\lambda_R^\infty = (\kappa_u - \kappa_l)^{-1}(\tilde{\kappa}(n(R))) + i\gamma \qquad (R \geqslant R_0). \tag{2.70}$$

Then $g_R^\infty(\lambda_R^\infty) = 0$ and, by the analyticity of $(\kappa_u - \kappa_l)^{-1}$ as well as (2.69),

$$|\lambda_R^\infty - (\mu + i\gamma)| \leqslant C|\tilde{\kappa}(n(R)) - w_0| \leqslant \frac{C}{R} \tag{2.71}$$

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

$$\ell_R(\theta) = (\kappa_u - \kappa_l)^{-1}(\tilde{\kappa}(n(R)) + \frac{\delta}{R}e^{i\theta}) + i\gamma. \tag{2.72}$$

By the analyticity of $(\kappa_u - \kappa_l)^{-1}$ and estimate (2.71), we have that

$$|\ell_R(\theta) - (\mu + i\gamma)| \leqslant |\ell_R(\theta) - \lambda_R^\infty| + |\lambda_R^\infty - (\mu + i\gamma)| \leqslant \frac{C}{R} \tag{2.73}$$

for large enough R.

By a direct computation, we have

$$e^{i\kappa_u(\ell_R(\theta) - i\gamma)R} = \frac{\beta_{l,R}}{\beta_{u,R}} e^{i\delta e^{i\theta}} e^{i\kappa_l(\ell_R(\theta) - i\gamma)R}. \tag{2.74}$$

By Assumption 2.27 (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 (2.44) and using (2.73),

$$|\beta_j(R, \ell_R(\theta)) - \beta_j(R, \mu + i\gamma)| \leqslant C|\ell_R(\theta) - (\mu + i\gamma)| \leqslant \frac{C}{R} \qquad (j = u \text{ or } l) \tag{2.75}$$

for large enough R. Using (2.67), (2.74) and (2.75),

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

for large enough R. Similarly,

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

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. □

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

$$
\Lambda_u(R,\lambda) = \tilde{\varphi}_u(R,\lambda - i\gamma)\tilde{\psi}_+^d(R,\lambda) - \tilde{\varphi}_u^d(R,\lambda - i\gamma)\tilde{\psi}_+(R,\lambda) \tag{2.76}
$$

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

$$
\Lambda_l(R,\lambda) = \tilde{\psi}_+(R,\lambda)\tilde{\varphi}_l^d(R,\lambda - i\gamma) - \tilde{\psi}_+^d(R,\lambda)\tilde{\varphi}_l(R,\lambda - i\gamma). \tag{2.77}
$$

By the definition of β_u and β_l in Theorem 2.30,

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

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

Corollary 2.35. *$S_\mathfrak{r}$ can be decomposed as*

$$
S_\mathfrak{r} = (i\gamma + S_{\mathfrak{r},0}) \cup S_{\mathfrak{r},u} \cup S_{\mathfrak{r},l} \tag{2.78}
$$

where
$$S_{\mathfrak{r},0} := \left\{z \in V_\mu \cap \mathbb{R} : BC[\varphi_u(\cdot,z)] = 0 \text{ or } BC[\varphi_l(\cdot,z)] = 0\right\} \tag{2.79}$$
and
$$S_{\mathfrak{r},j} := \left\{\lambda \in i\gamma + V_\mu \cap \mathbb{R} : \liminf_{R\to\infty} |\Lambda_j(R,\lambda)| = 0\right\} \qquad (j = u \text{ or } l). \tag{2.80}$$

Definition 2.36. We refer to the zeros z of $BC[\varphi_u(\cdot,z)]$ and $BC[\varphi_l(\cdot,z)]$ as the *resonances* of T_0. Therefore, the elements of $S_{\mathfrak{r},0}$ are precisely the resonances of T_0 in $V_\mu \cap \mathbb{R}$. We refer to resonances that are located in the essential spectrum of T_0 as *embedded resonances*.

Remark 2.37. Since φ_u and φ_l are analytic continuations of the solution ψ_+ from Assumption 2.15, the functions $z \mapsto BC[\varphi_u(\cdot,z)]$ and $z \mapsto BC[\varphi_l(\cdot,z)]$ are analytic continuations of the function $z \mapsto BC[\psi_+(\cdot,z)]$. The zeros z of $BC[\psi_+(\cdot,z)]$ are eigenvalues of T_0, therefore, by our convention, eigenvalues are also resonances.

Example 2.38 (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 2.27 holds, as discussed in Example 2.28. In this case, since the functions $E_\pm(R,\lambda)$ and $E^d_\pm(R,\lambda)$ 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 2.39 (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 2.29, Assumption 2.27 is satisfied. The sets $S_{\mathfrak{r},u}$ and $S_{\mathfrak{r},l}$ satisfy
$$S_{\mathfrak{r},u} = S_{\mathfrak{r},l} = \emptyset. \tag{2.81}$$

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 (2.81). We will only prove (2.81) 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 (2.38) and (2.39) 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,

$$\varphi_u(x_0, \lambda - i\gamma)\psi_+'(x_0, \lambda) - \varphi_u'(x_0, \lambda - i\gamma)\psi_+(x_0, \lambda) = 0. \tag{2.82}$$

Noting that the solutions $\phi_1(\cdot, \lambda - i\gamma)$ and $\phi_2(\cdot, \lambda - i\gamma)$ defined by (2.30) 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 (2.35) 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,

$$\varphi_l(x_0, \lambda - i\gamma)\overline{\psi_+'}(x_0, \lambda) - \varphi_l'(x_0, \lambda - i\gamma)\overline{\psi_+}(x_0, \lambda) = 0. \tag{2.83}$$

By (2.82) and (2.83), 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

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

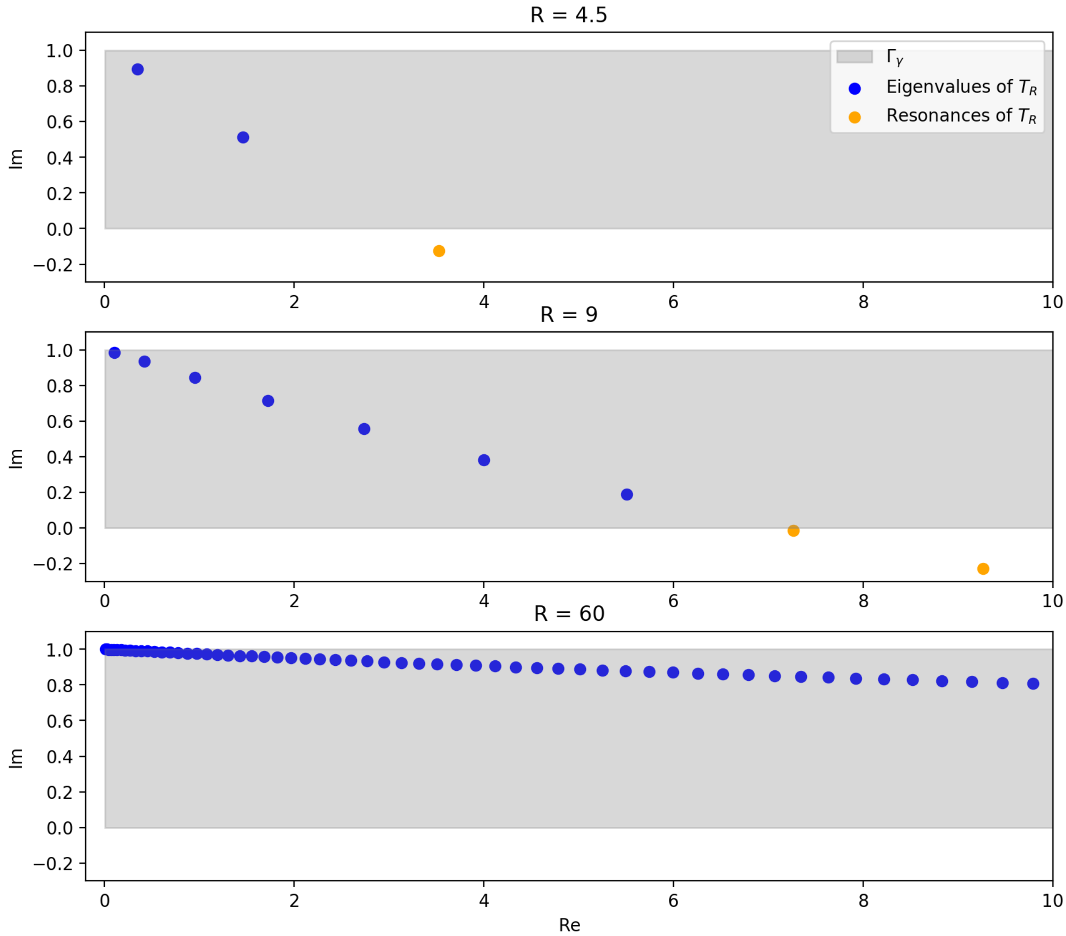

Figure 2.2 Plot of the eigenvalues and resonances of the operator T_R defined by (2.84).

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,

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

which is the desired contradiction. $\square$

2.5 Numerical examples

In this section, we illustrate the results from Sections 2.3 and 2.4 with numerical examples.

Example 2.40. Consider perturbed operators of the form

$$T_R = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + i\chi_{[0,R]}(x) \qquad (R \in \mathbb{R}_+) \tag{2.84}$$

endowed with Dirichlet boundary conditions at 0. This corresponds to the case $p = r = 1$, $q = 0$, $\eta = 0$ and $\gamma = 1$ in Sections 2.3 and 2.4.

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

$$f_R(\lambda) = i\sqrt{\lambda}\sin(R\sqrt{\lambda - i}) - \sqrt{\lambda - i}\cos(R\sqrt{\lambda - i}) = 0. \tag{2.85}$$

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 (2.85), any λ in the lower right quadrant of the complex plane is a resonance of T_R if and only if $f_R(\lambda) = 0$.

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 [52]. The results are illustrated in Figure 2.2.

For small enough $R > 0$, T_R has no eigenvalues [68]. 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

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

of T_0 accumulating to $\sigma_e(T) = i\gamma + [0,\infty)$, as expected by Theorem 2.33.

Example 2.41. Consider perturbed operator of the form

$$T_R = T_0 + i\chi_{[0,R]}(x) = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + i\chi_{[0,R_0]}(x) + i\chi_{[0,R]}(x) \qquad (R \in \mathbb{R}_+) \tag{2.86}$$

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 2.3 and 2.4.

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

$$\begin{aligned} f_R(\lambda) = i\sqrt{\lambda - i}&\left[e^{-2i\sqrt{\lambda-i}(R-R_0)} - \frac{\sqrt{\lambda - i} - \sqrt{\lambda}}{\sqrt{\lambda - i} + \sqrt{\lambda}}\right]\sin(\sqrt{\lambda - 2i}R_0) \\ - \sqrt{\lambda - 2i}&\left[e^{-2i\sqrt{\lambda-i}(R-R_0)} + \frac{\sqrt{\lambda - i} - \sqrt{\lambda}}{\sqrt{\lambda - i} + \sqrt{\lambda}}\right]\cos(\sqrt{\lambda - 2i}R_0) = 0 \end{aligned} \tag{2.87}$$

As before, by suitably analytically continuing the square root function in (2.87), 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 2.3. 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 2.23 and 2.33.

Recall that Example 2.39 guarantees that the rate of convergence of eigenvalues of T_R to $\mu \in \operatorname{int}(\sigma_e(T)) = i\gamma + (0,\infty)$ 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 2.42. Consider perturbed operators of the form

$$T_R = T_0 + \frac{i}{4}\chi_{[0,R]}(x) = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \sin(x) + \frac{i}{4}\chi_{[0,R]}(x) \qquad (R \in \mathbb{R}_+) \tag{2.88}$$

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 2.3 and 2.4. The essential spectrum of T_0 has a band gap structure - the first spectral band, which we denote by B, is approximately $[-0.3785, -0.3477]$ [104, 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 [37] and [104]).

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 2.4. 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 2.4, 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 $B + i(0,\gamma)$. If this is indeed the case then by Bolzano-Weiestrass we expect that there is spectral pollution in $B + i(0,\gamma)$.

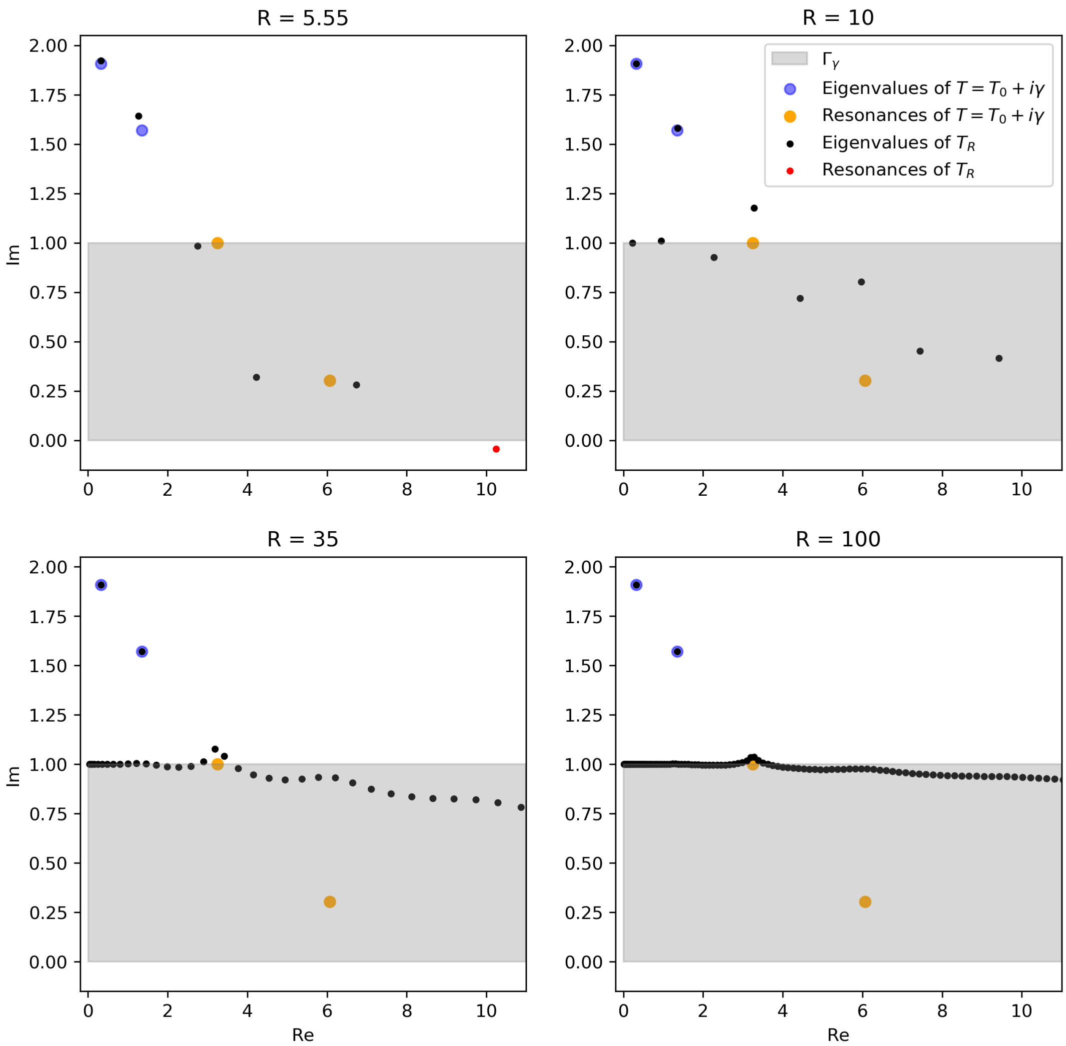

Figure 2.3 Plot of eigenvalues and resonances of the operators T_R and $T = T_0 + i\gamma$ defined by (2.86), with $R_0 = 4.7$. Note that the definition of resonances for T_R falls under Definition 2.36 since the dissipative barrier $i\gamma\chi_{[0,R]}$ is compactly supported. Furthermore, a complex number λ is a resonances of $T_0 + i\gamma$ if $\lambda - i\gamma$ is a resonance of T_0.

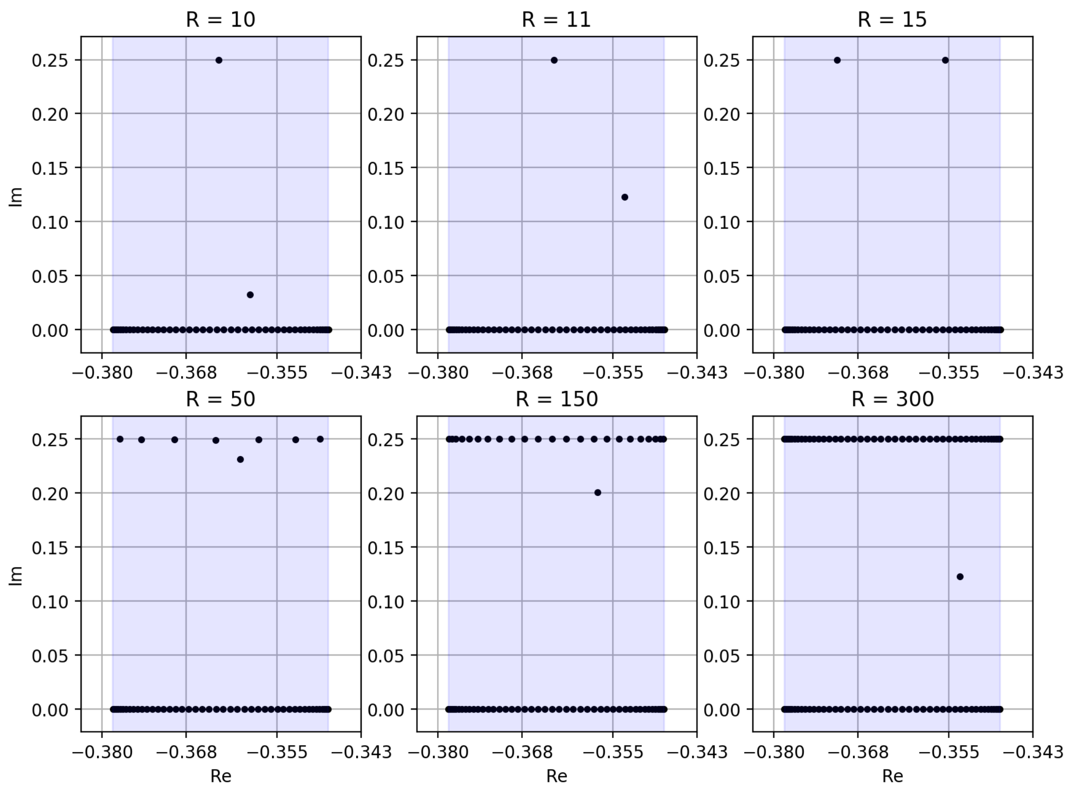

Figure 2.4 Plot of eigenvalues of the domain truncation and finite difference approximation $T_{R,X,h}$ of the operator T_R defined by (2.88). $h = 0.05$ and $X - R = 300$ are fixed. The region $B + i\mathbb{R}$ is shaded in light blue.

Chapter 3

Bounds for Schrödinger operators perturbed by dissipative barriers

Declaration:
This chapter appears in a similar form in the published article [129].

3.1 Introduction

There has recently been a surge of interest concerning bounds for the magnitude of eigenvalues and the number of eigenvalues of Schrödinger operators with complex potentials. In this chapter, we consider Schrödinger operators of the form

$$H_R = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q + i\gamma\chi_{[0,R]} \quad \text{on} \quad L^2(0,\infty) \qquad (R > 0), \tag{3.1}$$

endowed with a Dirichlet boundary condition at 0, where $\gamma > 0$ and the *background potential* $q \in L^1(0,\infty)$ (which may be complex-valued) are regarded as fixed parameters. Perturbations of the form $i\gamma\chi_{[0,R]}$ are referred to as *dissipative barriers* and arise in spectral approximation, where they can be utilised as part of numerical schemes for the computation of eigenvalues [104, 130, 4, 102, 103, 133]. Our aim is to prove estimates for the magnitude and number of eigenvalues of H_R for large R.

3.1.1 Existing bounds for the magnitude and number of eigenvalues

Let us first discuss some relevant existing results concerning the eigenvalues of (non-self-adjoint) Schrödinger operators and apply them to operators of the form H_R.

In [1], Abramov, Aslanyan and Davies investigated bounds for complex eigenvalues of Schrödinger operators, in particular obtaining a bound [1, Theorem 4] for

	Literature	Our Results
Magnitude Bound	$\sqrt{\lvert\lambda_R\rvert} = O(R)$ Frank, Laptev, Seiringer (2011)	$\sqrt{\lvert\lambda_R\rvert} = O(R/\log R)$ Theorem 3.4
Number of Eigenvalues (Compact Support)	$N(H_R) = O(R^2)$ Korotyaev (2020)	$N(H_R) = O(R^2/\log R)$ Theorem 3.10
Number of Eigenvalues (Naimark Condition)	$N(H_R) = O(R^4)$ Frank, Laptev, Safronov (2016)	$N(H_R) = O(R^3/(\log R)^2)$ Theorem 3.14

Table 3.1 A summary of the large R asymptotic estimates for the eigenvalues of H_R implied by our results compared to estimates obtained by applying various results in the literature.

Schrödinger operator on $L^2(\mathbb{R})$ with a potential $V \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})$. Such magnitude bounds were later generalised to include more general potentials, higher dimensions and more general geometries [43, 50, 62, 65, 66, 71, 80, 92, 94, 122]. The work most relevant to this chapter was undertook by Frank, Laptev and Seiringer [69], where they show that any eigenvalue λ of a Schrödinger operator $-\mathrm{d}^2/\mathrm{d}x^2 + V$ on $L^2(\mathbb{R}_+)$, endowed with a Dirichlet boundary condition at 0, satisfies

$$\sqrt{|\lambda|} \leqslant \|V\|_{L^1}. \tag{3.2}$$

Note that the right hand side of the bound presented in [69] depends on $\arg\lambda$ and is sharper than (3.2). An application of this result to operators of the form H_R gives an estimate $\sqrt{|\lambda_R|} = O(R)$ as $R \to \infty$ for any eigenvalue λ_R of H_R.

Proving bounds for the number of eigenvalues of a Schrödinger operator is often regarded a more difficult problem. A sufficient condition for the potential V to ensure that the number of eigenvalues of a Schrödinger operator on $L^2(\mathbb{R}_+)$ is finite is the *Naimark condition* [108]:

$$\exists a > 0 : \int_0^\infty e^{at} |V(t)| \mathrm{d}t < \infty. \tag{3.3}$$

There exist other such sufficient conditions and it is known that the number of eigenvalues may not be finite for certain potentials decaying only sub-exponentially [112, 113].

Quantitative bounds for the number of eigenvalues of a Schrödinger operator on $L^2(\mathbb{R}^d)$ were proved by Stepin in [131, 132] for dimensions $d = 1,3$. Bounds for arbitrary odd dimensions were later proved by Frank, Laptev and Safronov in [68], which give better large R estimates when applied to operators H_R of the form (3.1). [68, Theorem 1.1] states that the number of eigenvalues N (counting algebraic multiplicity) of a Schrödinger operator $-\mathrm{d}^2/\mathrm{d}x^2 + V$ on $L^2(\mathbb{R}_+)$ endowed with a Dirichlet boundary condition at 0 satisfies

$$N \leqslant \frac{1}{\varepsilon^2}\left(\int_0^\infty e^{\varepsilon t}|V(t)|\mathrm{d}t\right)^2. \tag{3.4}$$

for any $\varepsilon > 0$. With the assumption that the background potential q satisfies the Naimark condition, applying this inequality to H_R with $\varepsilon = 1/R$ gives an estimate $N(H_R) = O(R^4)$ as $R \to \infty$ for the number of eigenvalues (counting algebraic multiplicities) $N(H_R)$ of H_R.

Additionally, Korotyaev has proved in [90, Theorem 1.6] a bound specific to Schrödinger operators with compactly supported potentials: the number of eigenvalues N of a Schrödinger operator $-\mathrm{d}^2/\mathrm{d}x^2 + V$ on $L^2(\mathbb{R}_+)$ endowed with a Dirichlet boundary condition at 0, with $V \in L^1(\mathbb{R}_+)$ and $\operatorname{supp} V \subseteq [0,Q]$, satisfies

$$N \leqslant C_1 + C_2 Q \|V\|_{L^1} \tag{3.5}$$

where $C_1, C_2 > 0$ are some numerical constants. With the assumption that the background potential q is compactly supported, applying this inequality to H_R gives an estimate $N(H_R) = O(R^2)$ as $R \to \infty$. We mention also other estimates for numbers of eigenvalues in [23, 86, 127].

3.1.2 Summary of results

Table 3.1 summarises our results for the large R behaviour of the eigenvalues of H_R and compares them to the application of the existing results to operators of the form H_R.

Let $H_R^{(0)}$ denote the operator H_R for the case $q \equiv 0$. The semi-infinite strip

$$\Gamma_\gamma := (0,\infty) + i(0,\gamma) \subset \mathbb{C} \tag{3.6}$$

plays an important role throughout the chapter and has the property that its closure $\overline{\Gamma}_\gamma$ is equal to the numerical range of the operator $H_R^{(0)}$ for any $R > 0$. An open ball in $\mathbb{C}$ of radius $r > 0$ about a point $z_0 \in \mathbb{C}$ is denoted by $B_r(z_0)$. Note that in this chapter we make no attempt to optimise numerical constants.

Our first result gives a uniform in R enclosure for the eigenvalues of H_R:

(A) (Theorem 3.4 (a)) There exists $X = X(q,\gamma) > 0$ such that, for any $R > 0$, the eigenvalues of H_R lie in $B_X(0) \cup \Gamma_\gamma$.

In particular, the imaginary and negative real parts of the eigenvalues are bounded independently of R.

Our next result is a bound for the magnitude of eigenvalues of H_R for sufficiently large R. The bound gives the estimate $\sqrt{|\lambda_R|} = O(R/\log R)$ as $R \to \infty$ for any eigenvalue λ_R of H_R providing a logarithmic improvement to the application of the result [69] of Frank, Laptev and Seiringer to this system.

(B) (Theorem 3.4 (b)) There exists $R_0 = R_0(q,\gamma) > 0$ such that for every $R \geqslant R_0$, any eigenvalue λ of H_R in Γ_γ satisfies

$$\sqrt{|\lambda - i\gamma|} \leqslant \frac{5\gamma R}{\log R}. \tag{3.7}$$

(B) is obtained by considering an analytic function whose zeros are the eigenvalues of H_R and applying large-$|\lambda|$ Levinson asymptotics.

The fact that large eigenvalues of H_R for large R must be contained in the numerical range of $H_R^{(0)}$ and the right hand side of inequality (3.7) is independent of q indicates that the effect of the background potential q on the large eigenvalues is dominated by effect of the dissipative barrier $i\gamma\chi_{[0,R]}$ for large R.

Our first estimate for the number of eigenvalues $N(H_R)$ for H_R is for the case that the background potential q is compactly supported. It gives the estimate $N(H_R) = O(R^2/\log R)$ as $R \to \infty$, which offers a logarithmic improvement to the application of the result [90, Theorem 1.6] of Korotyaev to this system.

(C) (Theorem 3.10) If q is compactly supported then there exists $R_0 = R_0(q,\gamma) > 0$ such that for every $R \geqslant R_0$,

$$N(H_R) \leqslant \frac{11}{\log 2} \frac{\gamma R^2}{\log R}.$$

The proof consists in an application of Jensen's formula.

The case in which the background potential q merely satisfies the Naimark condition requires more sophisticated techniques compared to the compactly supported case. Our result gives the estimate $N(H_R) = O(R^3/(\log R)^2)$ as $R \to \infty$, providing a more significant improvement to the application of the result [68, Theorem 1.1] of Frank, Laptev and Safronov to this system, which gives $N(H_R) = O(R^4)$. The reasons for the more significant improvement are discussed below.

(D) (Theorem 3.14) If there exists $a > 0$ such that

$$\int_0^\infty e^{4at}|q(t)|\mathrm{d}t < \infty.$$

then there exists $R_0 = R_0(q,\gamma) > 0$ such that for every $R \geqslant R_0$,

$$N(H_R) \leqslant C\frac{\sqrt{X}+a}{a^2}\frac{\gamma^2 R^3}{(\log R)^2} \tag{3.8}$$

where $X = X(q,\gamma) > 0$ is the constant appearing in (A) and $C = 88788$.

The proof of (D) involves first obtaining a bound which counts the number of zeros in a strip for an arbitrary analytic function in the upper half plane (Proposition 3.12). This bound can be applied to the estimation of $N(H_R)$ thanks to the uniform in R enclosure (A), which implies that the square-roots of the eigenvalues of H_R are contained in a strip, uniformly in R. Without the uniform enclosure, we would have to use the magnitude bound (B) in place of the uniform enclosure with which the best we could obtain is inequality (3.8) with $\sqrt{X}$ replaced by $O(R/\log R)$, giving the large R estimate $N(H_R) = O(R^4/(\log R)^3)$. This indicates that the more significant improvement in (D) is due to the combination of a bound for the quantity $\mathrm{Im}\sqrt{\lambda}$ of the eigenvalues λ with the bound Proposition 3.12 for analytic functions.

Operators of the form $H_R^{(0)}$, corresponding to the special case $q = 0$, have been studied by Bögli and Štampach in [22], by Golinskii in [77] and by Cuenin in [44]. As discussed in Chapter 1, lower bounds for $H_R^{(0)}$ show that Theorem 3.4 (b) and Theorem 3.10 provide optimal large R estimates.

3.1.3 Notations and conventions

Throughout the chapter, $C > 0$ denotes a constant, whose dependencies are generally indicated, that may change from line to line. $\psi'(x,\lambda)$ will denote $\frac{\mathrm{d}}{\mathrm{d}x}\psi(x,\lambda)$ throughout. The branch cut of $\sqrt{\cdot}$ is made along $\sigma_e(H_R) = [0,\infty)$, so that $\mathrm{Im}\sqrt{z} \geqslant 0$ for all $z \in \mathbb{C}$. $N(H_R)$ shall denote the number of eigenvalues of H_R, counting algebraic multiplicities (as above). Finally, note that f_R will always denote an analytic function but will be redefined in each section.

3.2 Magnitude bound

Since $q \in L^1(0,\infty)$, we can employ Levinson's asymptotic theorem which states that the solution space of the Schrödinger equation $-u'' + qu = \lambda u$ on $[0,\infty)$ is spanned by solutions ψ_+ and ψ_-, which admit the decomposition [107, Appendix II, Theorems 1 and 3] [60, Theorem 1.3.1]:

$$\begin{aligned} \psi_\pm(x,\lambda) &= e^{\pm i\sqrt{\lambda}x}(1+E_\pm(x,\lambda)) \\ \psi'_\pm(x,\lambda) &= \pm i\sqrt{\lambda}e^{\pm i\sqrt{\lambda}x}(1+E^d_\pm(x,\lambda)) \end{aligned} \qquad (x\in[0,\infty),\lambda\in\mathbb{C}\backslash\{0\}). \tag{3.9}$$

Here, $E_\pm$ and $E^d_\pm$ are some functions such that,

$$|E_\pm(x,\lambda)|+|E^d_\pm(x,\lambda)|\to 0 \quad \text{as} \quad x\to\infty \tag{3.10}$$

for all $\lambda\in\mathbb{C}\backslash\{0\}$, and

$$|E_\pm(x,\lambda)|+|E^d_\pm(x,\lambda)|\leqslant \frac{C(q)}{\sqrt{|\lambda|}} \tag{3.11}$$

for all $x\in[0,\infty)$ and $\lambda\in\mathbb{C}$ with $|\lambda|\geqslant 1$.

While the error $E_+(x,\lambda)$ tends to 0 as $x\to\infty$ uniformly for $\lambda\in\mathbb{C}\backslash B_\delta(0)$, $\delta>0$, the error E_- does not have this property. For this reason, we will need to utilise large-$|\lambda|$ asymptotics of $\psi_\pm$ in this section.

Lemma 3.1. $\lambda\in\mathbb{C}\backslash[0,\infty)$ *with* $\lambda\neq i\gamma$ *is an eigenvalue of* H_R *if an only if* $f_R(\lambda)=0$*, where*

$$\begin{aligned} f_R(\lambda) := {}&\psi_-(0,\lambda-i\gamma)\Big(\sqrt{\lambda}-\sqrt{\lambda-i\gamma}+\mathscr{E}_1(R,\lambda)\Big)e^{i\sqrt{\lambda-i\gamma}R} \\ &-\psi_+(0,\lambda-i\gamma)\Big(\sqrt{\lambda}+\sqrt{\lambda-i\gamma}+\mathscr{E}_2(R,\lambda)\Big)e^{-i\sqrt{\lambda-i\gamma}R}. \end{aligned}$$

Here, $\mathscr{E}_1,\mathscr{E}_2$ *are defined, for any* $R>0$ *and* $\lambda\in\mathbb{C}\backslash\{0,i\gamma\}$*, by*

$$\begin{aligned} \mathscr{E}_1(R,\lambda) = {}&\sqrt{\lambda}\Big(E_+(R,\lambda-i\gamma)+E^d_+(R,\lambda)+E_+(R,\lambda-i\gamma)E^d_+(R,\lambda)\Big) \\ &-\sqrt{\lambda-i\gamma}\Big(E^d_+(R,\lambda-i\gamma)+E_+(R,\lambda)+E^d_+(R,\lambda-i\gamma)E_+(R,\lambda)\Big), \end{aligned} \tag{3.12}$$

$$\begin{aligned} \mathscr{E}_2(R,\lambda) = {}&\sqrt{\lambda}\Big(E^d_+(R,\lambda)+E_-(R,\lambda-i\gamma)+E^d_+(R,\lambda)E_-(R,\lambda-i\gamma)\Big) \\ &+\sqrt{\lambda-i\gamma}\Big(E_+(R,\lambda)+E^d_-(R,\lambda-i\gamma)+E_+(R,\lambda)E^d_-(R,\lambda-i\gamma)\Big) \end{aligned} \tag{3.13}$$

and, for some $\mathscr{C}_1=\mathscr{C}_1(q,\gamma)>0$*, satisfy*

$$|\mathscr{E}_1(R,\lambda)|+|\mathscr{E}_2(R,\lambda)|\leqslant\mathscr{C}_1 \tag{3.14}$$

for all $R > 0$ and all $\lambda \in \mathbb{C}$ with $|\lambda| \geqslant 1+\gamma$. Furthermore, f_R, $\mathscr{E}_1(R,\cdot)$ and $\mathscr{E}_2(R,\cdot)$ are analytic on $\mathbb{C}\backslash([0,\infty)\cup(i\gamma+[0,\infty)))$.

Proof. Let $\lambda \in \mathbb{C}\backslash[0,\infty)$ with $\lambda \neq i\gamma$. λ is an eigenvalue of H_R if and only if there a solution to the boundary value problem

$$-\psi''+(q+i\gamma\chi_{[0,R]})\psi = \lambda\psi \text{ on } [0,\infty),\ \psi(0)=0,\ \psi \in L^2(0,\infty). \tag{3.15}$$

Any solution to (3.15) on $[0,R]$ must be of the form $C_1\psi_1(\cdot,\lambda)$, where

$$\psi_1(x,\lambda) := \psi_-(0,\lambda-i\gamma)\psi_+(x,\lambda-i\gamma)-\psi_+(0,\lambda-i\gamma)\psi_-(x,\lambda-i\gamma) \tag{3.16}$$

and $C_1 \in \mathbb{C}$ is independent of x. Any solution to the boundary value problem (3.15) 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

$$x \mapsto \begin{cases} C_1\psi_1(x,\lambda) & \text{if } x \in [0,R) \\ C_2\psi_+(x,\lambda) & \text{if } x \in [R,\infty) \end{cases}$$

is continuously differentiable which holds if and only if

$$if_R(\lambda)e^{i\sqrt{\lambda}R} \equiv \psi_1(R,\lambda)\psi_+'(R,\lambda)-\psi_1'(R,\lambda)\psi_+(R,\lambda)=0. \tag{3.17}$$

The required expression for f_R holds by a direct computation, using expressions (3.9) for $\psi_\pm$.

For $\lambda \in \mathbb{C}$ with $|\lambda| \geqslant 1+\gamma$ we have $|\lambda| \geqslant 1$ and $|\lambda - i\gamma| \geqslant 1$. Therefore, estimates (3.11) apply to all the terms in (3.12) and (3.13) involving $E_\pm$ or $E_\pm^d$. The $O(1/\sqrt{|\lambda|})$ decay of the terms involving $E_\pm$ or $E_\pm^d$ as $|\lambda| \to \infty$ cancels the growth of the square roots, hence estimate (3.14) holds. Finally, f_R, $\mathscr{E}_1(R,\cdot)$ and $\mathscr{E}_2(R,\cdot)$ are analytic on $\mathbb{C}\backslash([0,\infty)\cup(i\gamma+[0,\infty)))$ because $\sqrt{\cdot}$, $E_\pm(R,\cdot)$ and $E_\pm^d(R,\cdot)$ are analytic on $\mathbb{C}\backslash[0,\infty)$. $\square$

In the special case $q \equiv 0$, f_R is denoted by $f_R^{(0)}$ and we have that:

$$\lambda \in \mathbb{C}\backslash[0,\infty) \text{ is an eigenvalue of } H_R^{(0)} \text{ if and only if } f_R^{(0)}(\lambda)=0.$$

The terms $E_\pm$ and $E_\pm^d$ in Levinson's asymptotic theorem are simply zero for this case, so

$$f_R^{(0)}(\lambda) = \left(\sqrt{\lambda}-\sqrt{\lambda-i\gamma}\right)e^{i\sqrt{\lambda-i\gamma}R}-\left(\sqrt{\lambda}+\sqrt{\lambda-i\gamma}\right)e^{-i\sqrt{\lambda-i\gamma}R}. \tag{3.18}$$

Lemma 3.2. *There exists a constant $\mathscr{C}_2 = \mathscr{C}_2(q,\gamma) > 0$ such that*

$$|f_R(\lambda) - f_R^{(0)}(\lambda)| \leqslant \mathscr{C}_2 e^{\operatorname{Im}\sqrt{\lambda - i\gamma}R}$$

for all $R > 0$ and all $\lambda \in \mathbb{C}$ with $|\lambda| \geqslant 1+\gamma$.

Proof. By a direct computation, using Lemma 3.1 and the fact that

$$\psi_\pm(0,\lambda - i\gamma) = 1 + E_\pm(0,\lambda - i\gamma),$$

we have

$$\begin{aligned}(f_R(\lambda) - f_R^{(0)}(\lambda))e^{i\sqrt{\lambda-i\gamma}R} &= E_-(0,\lambda - i\gamma)\left[\sqrt{\lambda} - \sqrt{\lambda - i\gamma}\right]e^{2i\sqrt{\lambda-i\gamma}R} \\ &\quad - E_+(0,\lambda - i\gamma)\left[\sqrt{\lambda} + \sqrt{\lambda - i\gamma}\right] \\ &\quad + (1 + E_-(0,\lambda - i\gamma))\mathscr{E}_1(R,\lambda)e^{2i\sqrt{\lambda-i\gamma}R} \\ &\quad - (1 + E_+(0,\lambda - i\gamma))\mathscr{E}_2(R,\lambda).\end{aligned} \tag{3.19}$$

Each term on the right hand side of (3.19) is bounded uniformly for all $R > 0$ and all $\lambda \in \mathbb{C}$ with $|\lambda| \geqslant 1+\gamma$; this follows using the boundedness for $\mathscr{E}_1$ and $\mathscr{E}_2$ proved in Lemma 3.1 as well as the large-$|\lambda|$ asymptotics of $E_\pm(0,\lambda - i\gamma)$ in (3.11). In particular, inequality (3.11) implies that $E_\pm(0,\lambda - i\gamma) = O(1/\sqrt{|\lambda|})$ as $|\lambda| \to \infty$, balancing the growth of the factors $\sqrt{\lambda} \pm \sqrt{\lambda - i\gamma}$ in the first two terms of (3.19). □

Recall that Γ_γ is an open strip defined by equation (3.6). We shall need the following elementary inequalities:

Lemma 3.3. (a) *If $\lambda \in \Gamma_\gamma \cup [0,\infty)$ then*

$$|\sqrt{\lambda} + \sqrt{\lambda - i\gamma}| \leqslant \frac{\gamma}{\sqrt{|\lambda - i\gamma|}} \text{ and } |\sqrt{\lambda} - \sqrt{\lambda - i\gamma}| \geqslant \sqrt{|\lambda - i\gamma|}.$$

(b) *If $\lambda \in \mathbb{C}\backslash\big(\Gamma_\gamma \cup [0,\infty)\big)$ then*

$$|\sqrt{\lambda} + \sqrt{\lambda - i\gamma}| \geqslant \sqrt{|\lambda|} \text{ and } |\sqrt{\lambda} - \sqrt{\lambda - i\gamma}| \leqslant \frac{\gamma}{\sqrt{|\lambda|}}.$$

(c) *If $\lambda \in \Gamma_\gamma$ then*

$$\operatorname{Im}\sqrt{\lambda - i\gamma} \leqslant \frac{1}{\sqrt{2}}\frac{\gamma}{\sqrt{|\lambda - i\gamma|}}.$$

Proof. (a) If $\lambda \in \Gamma_\gamma \cup [0,\infty)$ then

$$\operatorname{sgnRe}\sqrt{\lambda - i\gamma} = -\operatorname{sgnRe}\sqrt{\lambda},\ |\operatorname{Re}\sqrt{\lambda - i\gamma}| \geqslant \operatorname{Im}\sqrt{\lambda - i\gamma} \text{ and } |\operatorname{Re}\sqrt{\lambda}| \geqslant \operatorname{Im}\sqrt{\lambda},$$

so

$$\begin{aligned}|\sqrt{\lambda}-\sqrt{\lambda-i\gamma}|^2 =&(\mathrm{Re}\sqrt{\lambda})^2+(\mathrm{Re}\sqrt{\lambda-i\gamma})^2+(\mathrm{Im}\sqrt{\lambda})^2+(\mathrm{Im}\sqrt{\lambda-i\gamma})^2\\ &-2\mathrm{Re}\sqrt{\lambda}\mathrm{Re}\sqrt{\lambda-i\gamma}-2\mathrm{Im}\sqrt{\lambda}\mathrm{Im}\sqrt{\lambda-i\gamma}\\ \geqslant&|\lambda-i\gamma|.\end{aligned} \tag{3.20}$$

The inequality for $\sqrt{\lambda}+\sqrt{\lambda-i\gamma}$ follows from the identity

$$\sqrt{\lambda}+\sqrt{\lambda-i\gamma}=\frac{i\gamma}{\sqrt{\lambda}-\sqrt{\lambda-i\gamma}}. \tag{3.21}$$

(b) If $\lambda\in i\gamma+\mathbb{C}_+\cup[0,\infty)$ or $\lambda\in\mathbb{C}_-$ then, similarly to (3.20),

$$\mathrm{sgnRe}\sqrt{\lambda}=\mathrm{sgnRe}\sqrt{\lambda-i\gamma}\quad\Rightarrow\quad|\sqrt{\lambda}+\sqrt{\lambda-i\gamma}|^2\geqslant|\lambda|.$$

If $\lambda\in(-\infty,0]+i[0,\gamma]$ then $|\mathrm{Re}\sqrt{\lambda}|\leqslant\mathrm{Im}\sqrt{\lambda}$ and $|\mathrm{Re}\sqrt{\lambda-i\gamma}|\leqslant\mathrm{Im}\sqrt{\lambda-i\gamma}$ so

$$|\sqrt{\lambda}+\sqrt{\lambda-i\gamma}|^2\geqslant|\lambda-i\gamma|+|\lambda|\geqslant|\lambda|,$$

hence the inequality for $\sqrt{\lambda}+\sqrt{\lambda-i\gamma}$ holds. The inequality for $\sqrt{\lambda}-\sqrt{\lambda-i\gamma}$ follows from (3.21).

(c) Let $\lambda\in\Gamma_\gamma$ and let $z=\lambda-i\gamma$. Then $|\mathrm{Im}z|,\leqslant\gamma$ so

$$2(\mathrm{Im}\sqrt{z})^2=|z|-\mathrm{Re}z=\frac{(\mathrm{Im}z)^2}{|z|+\mathrm{Re}z}\leqslant\frac{\gamma^2}{|z|}.$$

□

Using the function f_R for the eigenvalues of H_R, combined with the large-$|\lambda|$ asymptotics of $\psi_\pm$, we can estimate the location of the eigenvalues of H_R:

Theorem 3.4. (a) *There exists $X=X(q,\gamma)>0$ such that, for any $R>0$, the eigenvalues of H_R lie in $B_X(0)\cup\Gamma_\gamma$.*

(b) *There exists $R_0=R_0(q,\gamma)>0$ such that for every $R\geqslant R_0$, any eigenvalue λ of H_R in Γ_γ satisfies*

$$\sqrt{|\lambda-i\gamma|}\leqslant\frac{5\gamma R}{\log R}. \tag{3.22}$$

Proof. (a) Let $R>0$. H_R has no eigenvalues in $[0,\infty)$ (indeed, this follows from the Levinson asymptotic formulas (3.9)) so it suffices to show that any zero of f_R in $\mathbb{C}\setminus\big(\Gamma_\gamma\cup[0,\infty)\big)$ must lie in an open ball in the complex plane, whose radius is independent of R. Let $\lambda \in \mathbb{C}\backslash(\Gamma_\gamma \cup [0,\infty))$ be such that $|\lambda| \geqslant X$, where $X = X(q,\gamma) > 0$ is a large enough constant to be further specified. Let $X > 0$ be large enough so that $|\lambda| \geqslant 1+\gamma$. By the expression for f_R in Lemma 3.1,

$$\begin{aligned}\left|f_R(\lambda)e^{i\sqrt{\lambda-i\gamma}R}\right| \geqslant \Big| &|\psi_+(0,\lambda-i\gamma)(\sqrt{\lambda}+\sqrt{\lambda-i\gamma}+\mathscr{E}_2(R,\lambda))| \\ &-|\psi_-(0,\lambda-i\gamma)(\sqrt{\lambda}-\sqrt{\lambda-i\gamma}+\mathscr{E}_1(R,\lambda))|e^{-2\mathrm{Im}\sqrt{\lambda-i\gamma}R}\Big|.\end{aligned} \tag{3.23}$$

By the boundedness of $\mathscr{E}_1$ and E_- (Lemma 3.1 and estimates (3.11)), as well an inequality in Lemma 3.3 (b), there exists $C_1 = C_1(q,\gamma) > 0$ such that

$$\left|\psi_-(0,\lambda-i\gamma)\Big(\sqrt{\lambda}-\sqrt{\lambda-i\gamma}+\mathscr{E}_1(R,\lambda)\Big)\right|e^{-2\mathrm{Im}\sqrt{\lambda-i\gamma}R} \leqslant C_1. \tag{3.24}$$

Let $\delta > 0$. Recall that $|\mathscr{E}_2(R,\lambda)| \leqslant \mathscr{C}_1$, where $\mathscr{C}_1 > 0$ is the constant appearing in Lemma 3.1. Let $X > 0$ be large enough such that $|\psi_+(0,\lambda-i\gamma)| \geqslant \frac{1}{2}$ and

$$\sqrt{|\lambda|} \geqslant 2(C_1+\delta)+\mathscr{C}_1.$$

Then, using Lemma 3.3 (b),

$$\left|\psi_+(0,\lambda-i\gamma)\Big(\sqrt{\lambda}+\sqrt{\lambda-i\gamma}+\mathscr{E}_2(R,\lambda)\Big)\right| \geqslant \frac{1}{2}\left|\sqrt{|\lambda|}-\mathscr{C}_1\right| \geqslant C_1+\delta. \tag{3.25}$$

Combining (3.23), (3.24) and (3.25), we have

$$|f_R(\lambda)| \geqslant \delta > 0.$$

Consequently, λ is not an eigenvalue of H_R proving that there are no eigenvalues of H_R in $\mathbb{C}\backslash\Gamma_\gamma$ with magnitude greater than X.

(b) Let $R \geqslant R_0$, where $R_0 = R_0(q,\gamma) > 0$ is a large enough constant to be further specified. Let $\lambda \in \Gamma_\gamma$ be such that

$$\sqrt{|\lambda-i\gamma|}\log|\lambda-i\gamma| \geqslant 8\gamma R. \tag{3.26}$$

We aim to prove that λ is not an eigenvalue of H_R.

Using the expression (3.18) for $f_R^{(0)}$,

$$\frac{|f_R^{(0)}(\lambda)|}{|\lambda-i\gamma|^{1/4}}e^{-\mathrm{Im}\sqrt{\lambda-i\gamma}R} \geqslant \left|\frac{|\sqrt{\lambda}-\sqrt{\lambda-i\gamma}|}{|\lambda-i\gamma|^{1/4}}e^{-2\mathrm{Im}\sqrt{\lambda-i\gamma}R}-\frac{|\sqrt{\lambda}+\sqrt{\lambda-i\gamma}|}{|\lambda-i\gamma|^{1/4}}\right|$$

Using the inequality (3.26) and Lemma 3.3 (c), λ satisfies

$$e^{-2\mathrm{Im}\sqrt{\lambda-i\gamma}R} \geqslant e^{-\sqrt{2}\gamma R/\sqrt{|\lambda-i\gamma|}} \geqslant e^{-\frac{\sqrt{2}}{8}\log|\lambda-i\gamma|} = \frac{1}{|\lambda-i\gamma|^{\sqrt{2}/8}}. \tag{3.27}$$

Ensure $R_0>0$ is large enough so that $|\lambda-i\gamma|^{1/4} \geqslant 2|\lambda-i\gamma|^{\sqrt{2}/8}$. Then, using Lemma 3.3 (a),

$$\frac{|\sqrt{\lambda}-\sqrt{\lambda-i\gamma}|}{|\lambda-i\gamma|^{1/4}} \geqslant |\lambda-i\gamma|^{1/4} \geqslant 2|\lambda-i\gamma|^{\sqrt{2}/8}. \tag{3.28}$$

Ensure also that $R_0>0$ is large enough so that $|\lambda-i\gamma| \geqslant \gamma^{4/3}$. Combining (3.28) with (3.27) and using Lemma 3.3 (a) again,

$$\frac{|\sqrt{\lambda}-\sqrt{\lambda-i\gamma}|}{|\lambda-i\gamma|^{1/4}} e^{-2\mathrm{Im}\sqrt{\lambda-i\gamma}R} \geqslant 2 \geqslant 1+\frac{\left|\sqrt{\lambda}+\sqrt{\lambda-i\gamma}\right|}{|\lambda-i\gamma|^{1/4}}.$$

and hence

$$|f_R^{(0)}(\lambda)| \geqslant |\lambda-i\gamma|^{1/4} e^{\mathrm{Im}\sqrt{\lambda-i\gamma}R}. \tag{3.29}$$

In particular, $f_R^{(0)}(\lambda) \neq 0$.

Recall that $\mathscr{C}_2 = \mathscr{C}_2(q,\gamma) > 0$ denotes the constant appearing in Lemma 3.2. Ensure that $R_0>0$ is large enough so that $|\lambda| \geqslant 1+\gamma$ and $|\lambda-i\gamma|^{1/4} \geqslant 2\mathscr{C}_2$. By (3.29) and Lemma 3.2,

$$|f_R(\lambda)-f_R^{(0)}(\lambda)| \leqslant \mathscr{C}_2 e^{\mathrm{Im}\sqrt{\lambda-i\gamma}R} \leqslant \frac{1}{2}|\lambda-i\gamma|^{1/4} e^{\mathrm{Im}\sqrt{\lambda-i\gamma}R} \leqslant \frac{1}{2}|f_R^{(0)}(\lambda)|$$

therefore $f_R(\lambda) \neq 0$ and, consequently, λ is not an eigenvalue of H_R. This proves that any eigenvalue of H_R must satisfy

$$\sqrt{|\lambda-i\gamma|}\log\sqrt{|\lambda-i\gamma|} \leqslant 4\gamma R. \tag{3.30}$$

Let W denote the Lambert-W-function (also known as the product log function). W satisfies

$$W(x) = \log\left(\frac{x}{W(x)}\right) \quad \text{and} \quad y\log y = x \iff y = \frac{x}{W(x)} \qquad (x>0, y>0).$$

Hence (3.30) can be written as

$$\sqrt{|\lambda-i\gamma|} \leqslant \frac{4\gamma R}{W(4\gamma R)} = \frac{4\gamma R}{\log(4\gamma R)-\log(W(4\gamma R))}$$

from which (3.22) follows (note that it is well known that $W(x) = o(x)$ as $x \to \infty$).

□

Remark 3.5. The constant $X = X(q,\gamma) > 0$ in Theorem 3.4 (a) satisfies

$$X = O(\|q\|_{L^1}^3) \quad \text{as} \quad \|q\|_{L^1} \to \infty.$$

This can be seen by noting that $E_\pm(R,\lambda), E_\pm^d(R,\lambda) = O(\|q\|_{L^1})$ (see [60, Chapter 1.4]), $\mathscr{C}_1 = O(\|q\|_{L^1}^2)$ and $C_1 = O(\|q\|_{L^1}^3)$.

3.3 Number of eigenvalues

In this section, we estimate the number of eigenvalues for H_R, for which we necessarily need to add additional assumptions on the background potential q.

3.3.1 Preliminaries

Let $\psi_\pm$ denote the solutions (3.9) for the Schrödinger equation and

$$\varphi(x,z) := \psi_+(x,z^2) \qquad (x \in [0,\infty), z \in \mathbb{C}_+).$$

φ is commonly referred to as the *Jost solution*. For each $R > 0$, define function $f_R : \mathbb{C}_+ \to \mathbb{C}$ by

$$i f_R(z) e^{izR} = \theta(R,z)\varphi'(R,z) - \theta'(R,z)\varphi(R,z) \qquad (z \in \mathbb{C}_+).$$

where, for any $z \in \mathbb{C}$, $\theta(\cdot,z)$ is defined as the solution to the initial value problem

$$-\theta'' + q\theta = (z^2 - i\gamma)\theta,\ \theta(0) = 0, \theta'(0) = 1. \tag{3.31}$$

By the same arguments as in Lemma 3.1, we have the following.

Lemma 3.6. *f_R is analytic on $\mathbb{C}_+$ and any $z \in \mathbb{C}_+$ satisfies*

$$f_R(z) = 0 \quad \Longleftrightarrow \quad z^2 \text{ is an eigenvalue of } H_R. \tag{3.32}$$

φ can be decomposed in a similar way to $\psi_\pm$,

$$\begin{aligned} \varphi(x,z) &= e^{izx}(1 + E(x,z)) \\ \varphi'(x,z) &= ize^{izx}(1 + E^d(x,z)) \end{aligned} \qquad (x \in [0,\infty), z \in \mathbb{C}_+) \tag{3.33}$$

for some functions E and E^d whose properties will be later specified, for the different assumptions on the background potential q that we consider. We shall need the following facts concerning f_R and θ. Note that in Lemma 3.7, $\mathscr{E}_1$ and $\mathscr{E}_2$ are defined in a different way than in Lemma 3.1.

Lemma 3.7. *Suppose that, for each $R > 0$, $\varphi(R,\cdot)$ and $\varphi'(R,\cdot)$ admits an analytic continuation from $\mathbb{C}_+$ into some open $U \subset \mathbb{C}$. Then, f_R admits analytic continuation into U. Furthermore, for each $R > 0$ and $z \in U\backslash\{\pm\sqrt{i\gamma}\}$,*

$$f_R(z)u(z) = \psi_-(0,z^2-i\gamma)\Big(z-\sqrt{z^2-i\gamma}+\mathscr{E}_1(R,z)\Big)e^{i\sqrt{z^2-i\gamma}R} - \psi_+(0,z^2-i\gamma)\Big(z+\sqrt{z^2-i\gamma}+\mathscr{E}_2(R,z)\Big)e^{-i\sqrt{z^2-i\gamma}R} \quad (3.34)$$

where

$$u(z) := \psi_-(0,z^2-i\gamma)\psi_+'(0,z^2-i\gamma) - \psi_+(0,z^2-i\gamma)\psi_-'(0,z^2-i\gamma), \quad (3.35)$$

$$\mathscr{E}_1(R,z) := z\Big(E_+(R,z^2-i\gamma)+E^d(R,z)+E_+(R,z^2-i\gamma)E^d(R,z)\Big) - \sqrt{z^2-i\gamma}\Big(E_+^d(R,z^2-i\gamma)+E(R,z)+E_+^d(R,z^2-i\gamma)E(R,z)\Big) \quad (3.36)$$

and

$$\mathscr{E}_2(R,z) := z\Big(E^d(R,z)+E_-(R,z^2-i\gamma)+E^d(R,z)E_-(R,z^2-i\gamma)\Big) + \sqrt{z^2-i\gamma}\Big(E(R,z)+E_-^d(R,z^2-i\gamma)+E(R,z)E_-^d(R,z^2-i\gamma)\Big). \quad (3.37)$$

Proof. Analytic continuation holds by the fact that $\theta(R,\cdot)$ is entire [135, Lemma 5.7] for each $R > 0$. If $z \neq \pm\sqrt{i\gamma}$ then the functions $\psi_\pm(\cdot,z^2-i\gamma)$ span the solution space of the Schrödinger equation $-\psi''+q\psi = (z^2-i\gamma)\psi$ so

$$\begin{aligned}\theta(R,z) &= \frac{\psi_-(0,z^2-i\gamma)\psi_+(R,z^2-i\gamma)-\psi_+(0,z^2-i\gamma)\psi_-(R,z^2-i\gamma)}{\psi_-(0,z^2-i\gamma)\psi_+'(0,z^2-i\gamma)-\psi_+(0,z^2-i\gamma)\psi_-'(0,z^2-i\gamma)} \\ &= \frac{\psi_1(R,z^2)}{u(z)}\end{aligned}$$

where ψ_1 denotes the function defined by (3.16) in Lemma 3.1. The lemma follows by a direct computation, similar to one in Lemma 3.1. $\square$

Lemma 3.8. *For any $x \in [0,\infty)$ and $z \in \mathbb{C}\backslash\{\pm i\gamma\}$, the solution θ to the initial value problem (3.31) satisfies the inequality*

$$|\theta(x,z)| + |\theta'(x,z)| \leqslant (1+x)e^{|\mathrm{Im}\sqrt{z^2-i\gamma}|x}\exp\left(\int_0^x (1+t)|q(t)|\mathrm{d}t\right).$$

Proof. Let $\mu = \mu(z) := \sqrt{z^2 - i\gamma}$. θ and θ' satisfy the integral equations

$$\theta(x,z) = \frac{\sin(\mu x)}{\mu} + \int_0^x \frac{\sin(\mu(x-t))}{\mu} q(t)\theta(t,z)\mathrm{d}t$$

and

$$\theta'(x,z) = \cos(\mu x) + \int_0^x \cos(\mu(x-t))q(t)\theta(t,z)\mathrm{d}t,$$

hence satisfy the integral inequality

$$|\theta(x,z)| + |\theta'(x,z)| \leqslant (1+x)e^{|\mathrm{Im}\mu|x}\left[1 + \int_0^x e^{-|\mathrm{Im}\mu|t}|q(t)|\big(|\theta(t,z)| + |\theta'(t,z)|\big)\mathrm{d}t\right],$$

where we used the fact that $|\sin(\mu x)||\mu|^{-1} \leqslant xe^{|\mathrm{Im}\mu|x}$ and $|\cos(\mu x)| \leqslant e^{|\mathrm{Im}\mu|x}$. The result follows from an application of Grönwall's Lemma. □

3.3.2 Compactly supported potentials

Assumption 3.9. q is compactly supported, that is, there exists $Q > 0$ such that

$$\mathrm{supp}\, q \subset [0,Q].$$

If Assumption 3.9 holds and then the Jost solution φ satisfies

$$\varphi(R,z) = e^{izR} \qquad (R > Q, z \in \mathbb{C}_+) \tag{3.38}$$

hence, for each $x \in [0,\infty)$, $\varphi(x,\cdot)$ can be analytically continued to $\mathbb{C}$. Consequently, for $R > Q$, f_R can be analytically continued to $\mathbb{C}$ and can be written as

$$f_R(z) = z\theta(R,z) + i\theta'(R,z) \qquad (z \in \mathbb{C}). \tag{3.39}$$

Theorem 3.10. *Suppose that Assumption 3.9 holds. Then there exists $R_0 = R_0(q,\gamma) > 0$ such that for every $R \geqslant R_0$,*

$$N(H_R) \leqslant \frac{11}{\log 2}\frac{\gamma R^2}{\log R}. \tag{3.40}$$

Proof. Let $z_0 \in \mathbb{C}_+$ be such that

$$\psi_+(0, z_0^2 - i\gamma) \neq 0, \quad \operatorname{Im}\sqrt{z_0^2 - i\gamma} \geqslant 1 \quad \text{and} \quad \sqrt{|z_0^2 - i\gamma|} \leqslant 2. \tag{3.41}$$

In fact, by choosing z_0 to be the minimiser of some suitable total order on $\mathbb{C}$ in the set of points that maximise $z \mapsto \psi_+(0, z^2 - i\gamma)$ while satisfying the latter two inequalities of (3.41), z_0 can be determined uniquely by q and γ, $z_0 = z_0(q, \gamma)$. Define $r = r(R) > 0$ by

$$\frac{r}{2} = \gamma^{1/2} + |z_0| + \frac{5\gamma R}{\log R}. \tag{3.42}$$

By the triangle inequality,

$$|z - z_0| \leqslant |z| + |z_0| \leqslant \sqrt{|z^2 - i\gamma| + \gamma} + |z_0| \leqslant \sqrt{|z^2 - i\gamma|} + \gamma^{1/2} + |z_0| \tag{3.43}$$

so,

$$S_R := \left\{ z \in \mathbb{C}_+ : \sqrt{|z^2 - i\gamma|} \leqslant \frac{5\gamma R}{\log R} \right\} \subseteq \overline{B}_{r/2}(z_0). \tag{3.44}$$

Let $R > Q > 0$ be large enough so that estimate (3.22) of Theorem 3.4 (b) holds. Since the zeros of f_R in $\mathbb{C}_+$ have a bijective correspondence with the eigenvalues of H_R, the set S_R contains all the zeros of f_R in $\mathbb{C}_+$ and hence the number of eigenvalues of H_R is bounded by the number of zeros for f_R in the ball $\overline{B}_{r/2}(z_0)$,

$$N(H_R) \leqslant |f_R^{-1}\{0\} \cap \overline{B}_{r/2}(z_0))|. \tag{3.45}$$

Since f_R is entire, Jensen's formula gives us

$$|f_R^{-1}\{0\} \cap \overline{B}_{r/2}(z_0)| \leqslant \frac{1}{\log 2} \log \left| \frac{1}{f_R(z_0)} \sup_{|z - z_0| = r} |f_R(z)| \right|. \tag{3.46}$$

Since $R > Q$, the terms $\mathscr{E}_1(R, z)$ and $\mathscr{E}_1(R, z)$, defined by (3.36) and (3.37) respectively, vanish. Hence, by Lemma 3.7 and the fact that $\operatorname{Im}\sqrt{z_0^2 - i\gamma} \geqslant 1$,

$$\begin{aligned} |f_R(z_0)u(z_0)| \geqslant |\psi_+(0, z_0^2 - i\gamma)(z_0 + \sqrt{z_0^2 - i\gamma})|e^R \\ - |\psi_-(0, z_0^2 - i\gamma)(z_0 - \sqrt{z_0^2 - i\gamma}))|e^{-R}. \end{aligned}$$

Note that $\mathrm{Im}\sqrt{z_0^2 - i\gamma} \geqslant 1$ implies that $z_0 \neq \pm\sqrt{i\gamma}$ so Lemma 3.7 is indeed applicable here. Then, since $\psi_+(0, z_0^2 - i\gamma) \neq 0$, $\sqrt{|z_0^2 - i\gamma|} \leqslant 2$ and $z_0 = z_0(q,\gamma)$,

$$|f_R(z_0)| \geqslant C(q,\gamma) \tag{3.47}$$

for large enough R.

By expression (3.39) for f_R and the estimates in Lemma 3.8 for θ and θ', for all $z \in \partial B_r(z_0)$,

$$|f_R(z)| \leqslant C(q)(1+R)(1+|z|)e^{|\sqrt{z^2 - i\gamma}|R}. \tag{3.48}$$

Furthermore, by the triangle inequality and expression (3.42) for r, for all $z \in \partial B_r(z_0)$,

$$\sqrt{|z^2 - i\gamma|} \leqslant |z - z_0| + |z_0| + \gamma^{1/2} = 3\gamma^{1/2} + 3|z_0| + \frac{10\gamma R}{\log R}. \tag{3.49}$$

Noting that for $z \in \partial B_r(z_0)$, the factor $(1+|z|)$ in (3.48) is $o(R)$, combining (3.45) - (3.49) gives us

$$N(H_R) \leqslant \frac{1}{\log 2}\left(\log o(R^2) + \left(3\gamma^{1/2} + 3|z_0|\right)R + \frac{10\gamma R^2}{\log R}\right)$$

as $R \to \infty$. Estimate (3.40) follows. □

3.3.3 Exponentially decaying potentials

Assumption 3.11 (Naimark Condition)**.** There exists $a > 0$ such that

$$\int_0^\infty e^{4at}|q(t)|\mathrm{d}t < \infty.$$

If Assumption 3.11 is satisfied then for each $x > 0$ the functions $\varphi(x,\cdot)$ and $\varphi'(x,\cdot)$ admit analytic continuations from $\mathbb{C}_+$ into $\{\mathrm{Im}z > -2a\}$. For each $x > 0$, the functions E and E^d appearing in the decomposition (3.33) of the Jost solution φ satisfy

$$|E(x,z)| + |E^d(x,z)| \leqslant C(q) \quad \text{if} \quad \mathrm{Im}z \geqslant -a \tag{3.50}$$

and

$$|E(x,z)| + |E^d(x,z)| \leqslant \frac{C(q)}{|z|} \quad \text{if} \quad \mathrm{Im}z \geqslant -a \text{ and } |z| \geqslant 1. \tag{3.51}$$

See [108, Theorem 2.6.1] and [131, Lemma 1] for proofs of the above claims.

The next proposition allows us to utilise the uniform enclosure of Theorem 3.4 (a) in the estimation of the number of eigenvalues of H_R.

Proposition 3.12. *Suppose that f is an analytic function defined on an open neighbourhood of the closed semi-disc $D_r := \overline{B}_r(0) \cap \overline{\mathbb{C}}_+$ for some $r > 0$. Let α and β be any numbers in the interval $(0,1)$ satisfying*

$$\beta \left(\frac{1-\alpha}{\alpha+\beta} \right)^2 > \frac{Y}{\eta} \tag{3.52}$$

and let $N(\alpha r)$ denote the number of zeros of f in the region

$$D_{\alpha r,\eta,Y} := \{z \in \mathbb{C} : \eta \leqslant \operatorname{Im} z \leqslant Y, \, |z| \leqslant \alpha r\} \tag{3.53}$$

where $Y, \eta > 0$ are given parameters satisfying $\eta < Y < r$. Then,

$$N(\alpha r) \leqslant \frac{2}{\log \Lambda(r)} \log \left(\frac{1}{\min\{\beta, 1-\beta\}} \frac{\sup_{z \in \partial D_r} |f(z)|}{|f(i\beta r)|} \right) \tag{3.54}$$

where

$$\Lambda(r) := \frac{1 + \frac{4\beta\eta}{(\alpha+\beta)^2} \frac{1}{r}}{1 + \frac{4Y}{(1-\alpha)^2} \frac{1}{r}}. \tag{3.55}$$

Remark 3.13. One can always guarantee that condition (3.52) for α and β is satisfied by choosing, for instance,

$$\alpha = \beta = \frac{1}{4} \frac{\eta}{2Y + \eta}. \tag{3.56}$$

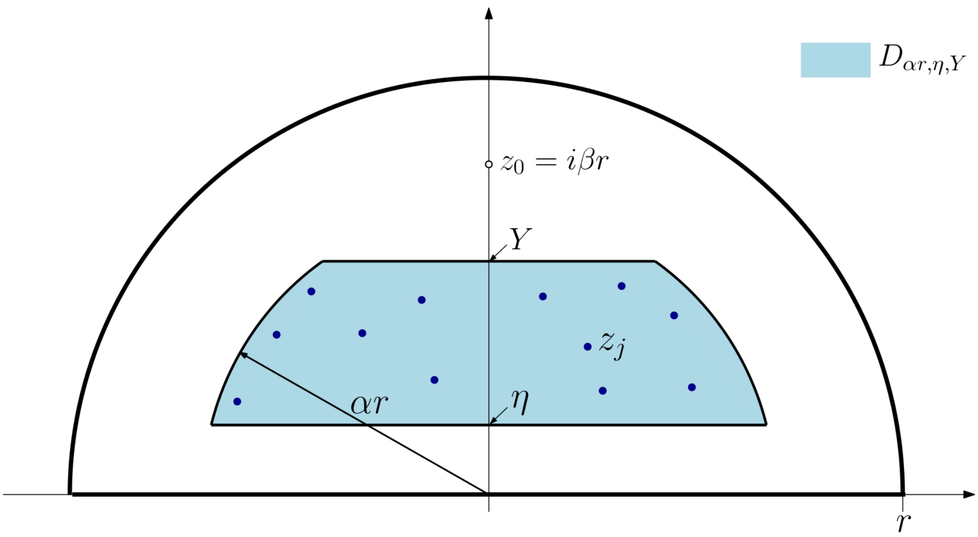

Figure 3.1 Illustration for the setup of Proposition 3.12.

Proof of Proposition 3.12. Let $\{z_j\}_{j=1}^{N(\alpha r)}$ denote the set of zeros of f in the set $D_{\alpha r,\eta,Y}$ and consider the Blaschke product

$$b(z) := \prod_j \frac{z-\bar{z}_j}{z-z_j} \equiv \prod_j b_j(z).$$

Note that higher multiplicity zeros of f are repeated in the set $\{z_j\}$ accordingly. Let $z_0 := i\beta r$. The function $f(z)b(z)$ is analytic on an open neighbourhood of D_r so by Cauchy's formula,

$$\frac{1}{2\pi i}\oint_{\partial D_r} \frac{f(z)b(z)}{z-z_0}\mathrm{d}z = f(z_0)b(z_0). \tag{3.57}$$

Observing that $|z-z_0| \geqslant \min\{\beta, 1-\beta\}r$ for all $z \in \partial D_r$, it holds that

$$\frac{1}{2\pi}\oint_{\partial D_r} \frac{|\mathrm{d}z|}{|z-z_0|} \leqslant \frac{1}{\min\{\beta,1-\beta\}},$$

which can be used to estimate the integral in (3.57) to get

$$\prod_j \frac{|b_j(z_0)|}{\sup_{z\in\partial D_r}|b_j(z)|} \leqslant \frac{\sup_{z\in\partial D_r}|f(z)|}{|f(z_0)|}\frac{1}{\min\{\beta,1-\beta\}}. \tag{3.58}$$

By a direct computation, we have

$$|b_j(z)| = \sqrt{1+\frac{4\mathrm{Im}z\mathrm{Im}z_j}{|z-z_j|^2}}.$$

Since

$$\mathrm{Im}z_0 = \beta r, \quad \mathrm{Im}z_j \geqslant \eta, \quad |z_0 - z_j| \leqslant (\alpha+\beta)r,$$

giving us a lower bound for $|b_j(z_0)|$, and since for any $z \in \mathbb{C}$ with $|z| = r$

$$\mathrm{Im}z \leqslant r, \quad \mathrm{Im}z_j \leqslant Y, \quad |z-z_j| \geqslant (1-\alpha)r,$$

giving us an upper bound for $|b_j(z)|$, we have

$$\frac{|b_j(z_0)|}{|b_j(z)|} \geqslant \Lambda(r)^{1/2} \tag{3.59}$$

for any $z \in \partial D_r$ with $|z| = r$. Furthermore, if $z \in \mathbb{R}$ then $|b_j(z)| = 1$ so (3.59) in fact holds for every $z \in \partial D_r$. Combining (3.59) with (3.58) gives us

$$\Lambda(r)^{N(\alpha r)/2} \leqslant \frac{1}{\min\{\beta,1-\beta\}}\frac{\sup_{z\in\partial D_r}|f(z)|}{|f(z_0)|}. \tag{3.60}$$

If hypothesis (3.52) for α and β holds then $\Lambda(r) > 1$ so we can take the logarithm of both sides of (3.60) and rearrange to obtain inequality (3.54). $\square$

Theorem 3.14. *Suppose that Assumption 3.11 holds. Then there exists $R_0 = R_0(q,\gamma) > 0$ such that for every $R \geqslant R_0$,*

$$N(H_R) \leqslant C\frac{\sqrt{X}+a}{a^2}\frac{\gamma^2 R^3}{(\log R)^2} \tag{3.61}$$

where $C = 88788$ and $X = X(q,\gamma) > 0$ is the constant appearing in Theorem 3.4 (a).

Proof. Let $\tilde{f}_R(z) := f_R(z-ia)$ and let $\alpha,\beta > 0$ satisfy equation (3.56) of Remark 3.13 with $\eta = a$ and $Y = \sqrt{X}+a$ where $X = X(q,\gamma)$ is the constant appearing in Theorem 3.4. Then hypothesis (3.52) of Proposition 3.12 is satisfied. Note that with this choice of β we have $\beta < 1/2$, so,

$$\min\{\beta, 1-\beta\} = \beta. \tag{3.62}$$

The zeros of $\tilde{f}_R$ in $\{\mathrm{Im} z > a\}$ have a bijective correspondence to eigenvalues of H_R given by

$$(z-ia)^2 \in \sigma_d(H_R) \qquad \Longleftrightarrow \qquad \mathrm{Im} z > a \text{ and } \tilde{f}_R(z) = 0. \tag{3.63}$$

Assuming without loss of generality that $X \geqslant \gamma$, the square root of any element of $B_X(0) \cup \Gamma_\gamma$ is contained in the strip $\{0 \leqslant \mathrm{Im} w \leqslant \sqrt{X}\} \subset \mathbb{C}$. Then by the uniform enclosure of Theorem 3.4 (a), the zeros of $\tilde{f}_R$ in $\{\mathrm{Im} z > a\}$ are contained in the strip $\{a \leqslant \mathrm{Im} z \leqslant \sqrt{X}+a\}$. By the triangle inequality and the magnitude bound of Theorem 3.4 (b), any zero z of $\tilde{f}_R$ with $\mathrm{Im} z > a$ satisfies

$$|z| \leqslant \gamma^{1/2} + a + \sqrt{|(z-ia)^2 - i\gamma|} \leqslant \alpha r \tag{3.64}$$

where $r = r(R)$ is defined by

$$\alpha r = \gamma^{1/2} + a + \frac{5\gamma R}{\log R}. \tag{3.65}$$

Hence the zeros of $\tilde{f}_R$ in $\{\mathrm{Im} z > a\}$ are contained in $D_{\alpha r,\eta,Y}$.

Applying Proposition 3.12, we get an estimate for the number of eigenvalues of H_R,

$$N(H_R) = |\tilde{f}_R^{-1}\{0\} \cap D_{\alpha r,\eta,Y}| \leqslant \frac{2}{\log \Lambda(r)} \log\left(\frac{1}{\beta}\frac{\sup_{z\in\partial D_r}|\tilde{f}_R(z)|}{|\tilde{f}_R(i\beta r)|}\right), \tag{3.66}$$

where

$$\Lambda(r) = \frac{1+C_1/r}{1+C_2/r} \tag{3.67}$$

for some constants $C_1 > C_2 > 0$ depending only on X and a. The remainder of the proof consists in estimating the right hand side of (3.66).

Let $z_R := i\beta r(R) - ia$. By Lemma 3.7,

$$\begin{aligned} |f_R(z_R)u(z_R)| \geqslant{} & |\psi_+(0, z_R^2 - i\gamma)(z_R + \sqrt{z_R^2 - i\gamma} + \mathscr{E}_2(R, z_R))| \\ & - |\psi_-(0, z_R^2 - i\gamma)(z_R - \sqrt{z_R^2 - i\gamma} + \mathscr{E}_1(R, z_R))| \end{aligned} \tag{3.68}$$

for large enough R. By estimates (3.11) for $E_\pm$ and $E_\pm^d$, and the corresponding estimates (3.51) for E and E^d,

$$|u(z_R)| + |\psi_-(0, z_R^2 - i\gamma)| + |\mathscr{E}_1(R, z_R)| + |\mathscr{E}_2(R, z_R)| \leqslant C(q, \gamma) \tag{3.69}$$

and

$$|\psi_+(0, z_R^2 - i\gamma)| \geqslant C(q, \gamma) \tag{3.70}$$

for large enough R. By Lemma 3.3,

$$\lim_{R\to\infty} |z_R + \sqrt{z_R^2 - i\gamma}| = \infty \quad \text{and} \quad \lim_{R\to\infty} |z_R - \sqrt{z_R^2 - i\gamma}| = 0. \tag{3.71}$$

Combining (3.68) with (3.69), (3.70) and (3.71) gives us

$$|\tilde{f}_R(i\beta r)| = |f_R(z_R)| \geqslant 1 \tag{3.72}$$

for large enough R.

The factor involving $\Lambda(r)$ on the right hand side of (3.66) can be estimated using the expression (3.67) for Λ and the inequality $\log x \geqslant (x-1)/(x+1)$ $(x \geqslant 1)$,

$$\log \Lambda(r) \geqslant \frac{\Lambda(r) - 1}{\Lambda(r) + 1} = \frac{(C_1 - C_2)/r(R)}{2 + (C_1 + C_2)/r(R)} \geqslant \frac{C_1 - C_2}{3r(R)} \tag{3.73}$$

for large enough R.

The function $\tilde{f}_R$ is estimated from above using the bound in Lemma 3.8 for θ and θ' and the uniform bounds (3.50) for $E(R,\cdot)$ and $E^d(R,\cdot)$,

$$|\tilde{f}_R(z)| \leqslant C(q)(1+R)(1+|z|)e^{aR} e^{|\sqrt{(z-ia)^2 - i\gamma}|R} \qquad (z \in \overline{\mathbb{C}}_+). \tag{3.74}$$

Using the expression (3.65) for r, for any $z \in \partial D_r$ we have

$$\sqrt{|(z-ia)^2 - i\gamma|} \leqslant \gamma^{1/2} + a + |z| \leqslant O(1) + \frac{5\gamma R}{\alpha \log R} \tag{3.75}$$

as $R \to \infty$. Combining (3.66) with (3.72), (3.73), (3.74) and (3.75), noting that $|z| = o(R)$ for $z \in \partial D_R$ and $\beta^{-1} = O(1)$, gives

$$N(H_R) \leqslant \frac{6}{C_1 - C_2}\left(O(1) + \frac{5\gamma R}{\alpha \log R}\right)\left(O(R) + \frac{5\gamma R^2}{\alpha \log R}\right)$$

as $R \to \infty$ and so

$$N(H_R) \leqslant \frac{151\gamma^2 R^3}{(C_1 - C_2)\alpha^2 (\log R)^2} \tag{3.76}$$

for large enough R.

Finally, we put the constant into a more illuminating form. By the definition (3.55) of Λ in Proposition 3.12,

$$C_1 = \frac{\eta}{\alpha} \quad \text{and} \quad C_2 = \frac{4Y}{(1-\alpha)^2}. \tag{3.77}$$

Since $\frac{\eta}{12Y} \leqslant \alpha \leqslant \frac{\eta}{8Y}$, we have

$$(C_1 - C_2)\alpha^2 = \eta\alpha - \frac{4Y\alpha^2}{(1-\alpha)^2} \geqslant \frac{\eta^2}{12Y} - \frac{4Y\alpha^2}{(1-\frac{\eta}{8Y})^2} \tag{3.78}$$

and since $0 \leqslant \eta/Y \leqslant 1$, we have

$$\frac{\alpha^2}{(1-\frac{\eta}{8Y})^2} = \frac{\eta^2}{64Y^2}\frac{1}{(1+\frac{\eta}{2Y})^2(1-\frac{\eta}{8Y})^2} \leqslant \frac{\eta^2}{49Y^2} \tag{3.79}$$

Combining (3.78) and (3.79), we have

$$(C_1 - C_2)\alpha^2 \geqslant \frac{1}{588}\frac{\eta^2}{Y}. \tag{3.80}$$

which gives estimate (3.61) when substituted into (3.76), with $Y = \sqrt{X} + a$ and $\eta = a$.
$\square$

Chapter 4

Lieb–Thirring and Jensen sums

Declaration and acknowledgements:
This chapter is joint work with **Leonid Golinskii** and appears in a similar form in the preprint [79]. We thank S. Bögli and J.-C. Cuenin for helpful discussions and R. Frank for enlightening comments which motivated us to include Proposition 4.23.

4.1 Introduction

There is a vast literature on the spectral theory of self-adjoint Schrödinger operators, motivated by their numerous applications in various areas of mathematical physics. One of the highlights of this theory is the seminal Lieb–Thirring inequality for operators on $L^2(\mathbb{R}^d)$, $d \in \mathbb{N}$, which describes the discrete spectrum of such operators. For the case of real line $d = 1$ it reads [99]

$$\sum_{\lambda \in \sigma_d(H)} |\lambda|^\mu \leqslant C(\mu) \int_{-\infty}^{\infty} [q_-(x)]^{\mu+1/2} dx, \qquad \mu \geqslant \frac{1}{2}, \tag{4.1}$$

where $C(\mu) > 0$ depends only on μ, H denotes a Schrödinger operator on $\mathbb{R}$ with real-valued potential q and $q_-(x) = \max(0, -q(x))$.

By comparison, the non-self-adjoint theory is in its youth. The results obtained in the last two decades have revealed new phenomena and demonstrated crucial differences between SA and NSA theories. Among the problems which have attracted attention, let us mention spectral enclosure results and bounds on the number of complex eigenvalues [1, 50, 92, 65, 71, 68, 20]. Another active area of interest is non-self-adjoint generalisations of Lieb–Thirring inequalities for Schrödinger operators [67, 53, 70, 123, 78, 66, 19], as well as for other types of operators [54, 124, 57, 58, 28]. Still, many questions remain unanswered.

The main object under consideration in the present chapter is a Schrödinger operator

$$H = H_q := -\frac{d^2}{dx^2} + q \qquad \text{on} \qquad L^2(\mathbb{R}_+) \tag{4.2}$$

endowed with a Dirichlet boundary condition at 0, where the potential $q \in L^1(\mathbb{R}_+)$ may be complex-valued. As is well known, the set of discrete eigenvalues $\sigma_d(H)$ (i.e., eigenvalues of finite algebraic multiplicity in $\mathbb{C}\backslash\mathbb{R}_+$) may be countably infinite and may accumulate only to $\mathbb{R}_+$. Lieb–Thirring-type inequalities give information on the distribution of the eigenvalues and, in particular, on the rate of accumulation to points in $\mathbb{R}_+$.

In this chapter, we study sums of eigenvalues of the form

$$S_\varepsilon(H) := \sum_{\lambda \in \sigma_d(H)} \frac{\operatorname{dist}(\lambda, \mathbb{R}_+)}{|\lambda|^{(1-\varepsilon)/2}}, \qquad \varepsilon \geqslant 0. \tag{4.3}$$

Here, eigenvalues of higher algebraic multiplicity are repeated in the sums accordingly. We refer to $S_\varepsilon(H)$ as the *Lieb–Thirring sums*. Note that, in the case when q is real, the eigenvalues of H_q are all negative, so $S_\varepsilon(H_q)$ coincides with the classical Lieb–Thirring sum in (4.1), with $\mu = (1+\varepsilon)/2$. In this chapter, we use the following shorthand notation for the L^1 norm,

$$\|q\|_1 := \int_0^\infty |q(x)|dx, \qquad q \in L^1(\mathbb{R}_+). \tag{4.4}$$

By [69], the spectral enclosure $|\lambda| \leq \|q\|_1^2$ holds for every $\lambda \in \sigma_d(H)$. So, there is a simple relation between the Lieb–Thirring sums with different ε

$$S_{\varepsilon_2}(H_q) \leq \|q\|_1^{\varepsilon_2 - \varepsilon_1} S_{\varepsilon_1}(H_q), \qquad 0 \leq \varepsilon_1 < \varepsilon_2. \tag{4.5}$$

We also study the sums

$$J(H) := \sum_{\lambda \in \sigma_d(H)} \operatorname{Im} \sqrt{\lambda}, \tag{4.6}$$

$\sqrt{\cdot}$ denotes the branch of the square root such that $\operatorname{Im}\sqrt{z} > 0$ for all $z \in \mathbb{C}\backslash\mathbb{R}_+$, and we refer to $J(H)$ as the *Jensen sums*. Notably, $J(H)$ arises naturally from Jensen's formula in complex analysis. It follows immediately from the inequality [53, Lemma 1]

$$|\lambda|^{1/2} |\operatorname{Im}\sqrt{\lambda}| \leq \operatorname{dist}(\lambda, \mathbb{R}_+) \leq 2|\lambda|^{1/2} |\operatorname{Im}\sqrt{\lambda}|, \tag{4.7}$$

that $J(H)$ is equivalent to $S_0(H)$

$$J(H) \leqslant S_0(H) \leqslant 2J(H). \tag{4.8}$$

The aim of the chapter is two-fold. On one hand, we shall establish upper bounds for the sums $S_\varepsilon(H)$, $\varepsilon \geqslant 0$, and $J(H)$. While the upper bounds for the sums $S_\varepsilon(H)$, $\varepsilon > 0$, (i.e., the non-critical case) hold for arbitrary integrable potentials, the upper bounds for the sums $J(H)$ (i.e., the critical case) are only valid for sub-classes of integrable potentials. On the other hand, corresponding lower bounds shall be proven for specific potentials, demonstrating optimality of our upper bounds in various senses. Moreover, in Section 3 we shall construct an integrable potential such that the sum $J(H) = \infty$.

Summary of main results

Our analysis is based on identifying the square roots of eigenvalues of the Schrödinger operator H (4.2) with the zeros of an analytic function in the upper-half of the complex plane $\mathbb{C}_+$. The idea of using methods of complex analysis in the theory of non-self-adjoint Schrödinger operator on the half-line goes back to the pioneering papers of Naimark [108] and Levin [96], and reaches its culmination in the famous series of papers by Pavlov [112–114], who found the threshold between finitely and infinitely many eigenvalues in the case of a complex potential.

Let us first recall the notion of a Jost function, which will be useful for describing the basic ideas of the proofs, and then proceed to give an account of our main results.

Jost functions

Recall that it is well known [108, Theorems 2.2.1 and 2.3.1] that for any $z \in \mathbb{C}_+$, the Schrödinger equation on $\mathbb{R}_+$

$$-y'' + q(x)y = z^2 y, \qquad q \in L^1(\mathbb{R}_+) \tag{4.9}$$

has a unique solution $e_+(\cdot, z)$ with the property that $e_+(x, \cdot)$ is analytic on $\mathbb{C}_+$ for all $x \geqslant 0$ and

$$e_+(x,z) = e^{ixz}\big(1 + o(1)\big), \quad \text{as} \quad x \to \infty \tag{4.10}$$

uniformly on compact subsets of $\mathbb{C}_+$. $e_+(\cdot, z)$ is referred to as the *Jost solution*. The *Jost function* is defined as $e_+(z) := e_+(0,z)$, $z \in \mathbb{C}_+$, and has the property that

$$\lambda = z^2 \in \sigma_d(H) \qquad \Longleftrightarrow \qquad e_+(z) = 0. \tag{4.11}$$

Moreover, the algebraic multiplicity (i.e., the rank of the Riesz projection) of z^2 as an eigenvalue of H coincides with the multiplicity of z as a zero of e_+ (see, for instance, [74, Theorem 5.4 and Lemma 6.2]).

Upper bound for the non-critical case

Our first result concerns a bound from above for the Lieb-Thirring sums $S_\varepsilon(H)$ in the non-critical case $\varepsilon > 0$. It is valid for Schrödinger operators with arbitrary integrable potentials.

Theorem 4.1 (= Theorem 4.5)**.** *For every $\varepsilon > 0$, there exists a constant $K(\varepsilon) > 0$ depending only on ε, such that for any potential $q \in L^1(\mathbb{R}_+)$, we have*

$$S_\varepsilon(H_q) = \sum_{\lambda \in \sigma_d(H_q)} \frac{\operatorname{dist}(\lambda, \mathbb{R}_+)}{|\lambda|^{(1-\varepsilon)/2}} \leqslant K(\varepsilon) \|q\|_1^{1+\varepsilon}. \tag{4.12}$$

Given a pair (α, β) of positive parameters, we define a generalised Lieb–Thirring sum $S_{\alpha,\beta}(H_q)$ by

$$S^{2\alpha}_{\alpha,\beta}(H_q) := \sum_{\lambda \in \sigma_d(H_q)} |\lambda|^\alpha \left[\frac{\operatorname{dist}(\lambda, \mathbb{R}_+)}{|\lambda|}\right]^\beta = \sum_{\lambda \in \sigma_d(H_q)} \frac{\operatorname{dist}^\beta(\lambda, \mathbb{R}_+)}{|\lambda|^{\beta-\alpha}}. \tag{4.13}$$

In terms of such sums, Theorem 4.1 takes the form

$$S_{\alpha,1}(H_q) \le C_\alpha \|q\|_1, \qquad \forall \alpha > \frac{1}{2}. \tag{4.14}$$

We study such generalised Lieb–Thirring sums in more detail in Proposition 4.23.

The proof of Theorem 4.1 is based on the application of a result of Borichev, Golinskii and Kupin [24] concerning the Blaschke-type conditions on zeros of analytic functions on the unit disk $\mathbb{D}$ satisfying appropriate growth conditions at the boundary. An analytic function on $\mathbb{D}$ is constructed from the Jost function e_+ using a certain conformal mapping, and the growth conditions are verified by applying classical estimates for e_+.

Upper bounds for the critical case

Let us address upper bounds for the Jensen sums $J(H)$. We proceed by embarking on a study of sub-classes of $L^1(\mathbb{R}_+)$.

To begin with, we introduce a pair of positive, continuous functions a and $\hat{a}$ on $\mathbb{R}_+$, such that

$$\hat{a}(x) = \frac{x}{a(x)}, \qquad a(x) = \frac{x}{\hat{a}(x)}, \qquad x \in \mathbb{R}_+. \tag{4.15}$$

We will refer to a and $\hat{a}$ as weight functions. We require that:

- a is monotonically increasing.
- $\hat{a}$ is strictly monotonically increasing, $\hat{a}(0) = 0$ and $\hat{a}(\infty) = \infty$.

Introduce the norm

$$\|q\|_a := \int_0^\infty a(x)|q(x)|dx, \tag{4.16}$$

which agrees with (4.4) for $a \equiv 1$. We consider sub-classes of $L^1(\mathbb{R}_+)$ of the form

$$Q_a := \{q \in L^1(\mathbb{R}_+) : \|q\|_a < \infty\}. \tag{4.17}$$

In its most general form, our upper bound for the Jensen sum reads as follows.

Theorem 4.2 (= Theorem 4.8)**.** *Let a and $\hat{a}$ be a pair of weight functions as described above. Assume also that*

$$\int_1^\infty \frac{dx}{xa(x)} < \infty. \tag{4.18}$$

Then, for each potential $q \in Q_a$ and each $\delta \in (0,1)$, we have

$$J(H_q) \leq y \log \frac{1+\delta}{(1-\delta)^2} + \frac{4}{\pi} \|q\|_a \int_{\frac{1}{y}}^\infty \frac{dx}{xa(x)}, \tag{4.19}$$

where $y = y(\delta, a, \|q\|_a) > 0$ is uniquely determined by

$$\hat{a}\left(\frac{1}{y}\right) \|q\|_a = \log(1+\delta). \tag{4.20}$$

We emphasise that this upper bound is not applicable for arbitrary potentials $q \in L^1(\mathbb{R}_+)$. Loosely speaking, the conditions $\|q\|_a < \infty$ and (4.18) may contradict each other, as far as the growth of a goes. An instructive family of integrable potentials is considered in Remark 4.11, namely,

$$q(x) = \frac{i}{x \log^\alpha(x)} \chi_{[e,\infty)}(x), \qquad \alpha > 1, \quad x \in \mathbb{R}_+, \tag{4.21}$$

where χ denotes the indicator function. For $\alpha > 2$, there exists an appropriate weight function a, and Theorem 4.2 is applicable to q. For $1 < \alpha \leqslant 2$, such a weight function a does not exist.

We do not claim that $J(H_q) = \infty$ for the potentials q in (4.21) with $1 < \alpha \leqslant 2$. In Theorem 4.30, we construct an example of a potential for which the Jensen sum diverges, showing that Theorem 4.2 cannot be extended to all integrable potentials.

Theorem 4.2 is applied to obtain upper bounds for $J(H)$ valid for two important specific classes of potentials.

(A) (See Corollary 4.9) *Let* $p \in (0,1)$ *and* $a(x) = 1 + x^p$. *Then for each potential* $q \in Q_a$, *we have*

$$J(H_q) \leqslant \tfrac{4}{\pi}\|q\|_a \log\left(1 + \|q\|_a\right) + \tfrac{9}{p}\|q\|_a + 2. \tag{4.22}$$

In [123], Safronov has also obtained a bound for the Jensen sum $J(H)$, valid for potentials $q \in L^1(\mathbb{R}_+)$ satisfying $\|x^p q\|_1 < \infty$ for some $p \in (0,1)$. Comparatively, the above result (A) offers an improved asymptotic estimate for semiclassical Schrödinger operators (see Remark 4.10).

(B) (See Corollary 4.12) *Suppose the potential* $q \in L^1(\mathbb{R}_+)$ *is compactly supported. Then, for every* $R > 1$ *with* $\operatorname{supp}(q) \subset [0,R]$, *we have*

$$J(H_q) \leq 7\left[\frac{1}{R} + \|q\|_1\Big(1 + \log(1 + \|q\|_1) + \log R\Big)\right]. \tag{4.23}$$

As we will see below, this bound is optimal in a certain asymptotic sense.

The proof of Theorem 4.2 centers around establishing improved estimates for the Jost function e_+ corresponding to potentials in a given sub-class Q_a. These improved estimates are obtained by combining the arguments for the classical case with the following simple principle:

$$0 < A \leqslant \min(X_1, X_2) \;\Rightarrow\; A = a(A)\hat{a}(A) \leqslant a(X_1)\hat{a}(X_2). \tag{4.24}$$

The bound (4.19) of Theorem 4.2 is proven by using these improved estimates for e_+ in conjunction with Jensen's formula. The proofs of Corollaries 4.9 and 4.12 amount to appropriate choices for a and δ.

Lower bounds for dissipative barrier potentials

The optimality of the above upper bounds can be addressed by studying corresponding lower bounds for Schrödinger operators with so-called *dissipative barrier potentials*. Precisely, for $\gamma, R > 0$, we consider the Schrödinger operator

$$L_{\gamma,R} := -\frac{d^2}{dx^2} + i\gamma\chi_{[0,R]} \qquad \text{on} \qquad L^2(\mathbb{R}_+) \tag{4.25}$$

endowed with a Dirichlet boundary condition at 0. The dissipative barrier potentials find applications in the numerical computation of eigenvalues, where they are considered as a perturbation of a fixed background potential [104, 130]. We focus on establishing our estimates for large enough R. Observe that $\|i\gamma\chi_{[0,R]}\|_1 = \gamma R$.

Theorem 4.3 (= Theorem 4.21)**.** *Suppose that* $R \geqslant 600(\gamma^{3/4} + \gamma^{-3/4})$.

(i) *We have the following lower bound*

$$2J(L_{\gamma,R}) \geqslant S_0(L_{\gamma,R}) \geqslant \frac{\gamma R}{16\pi} \log R. \tag{4.26}$$

(ii) *Let* $0 < \varepsilon < 1$. *Under the stronger assumption on R:*

$$R \geq \frac{4}{e^2\gamma}(64\pi)^{2/\varepsilon} + 1, \tag{4.27}$$

we have the lower bound

$$S_\varepsilon(L_{\gamma,R}) \geqslant \frac{1}{256\pi\varepsilon} \frac{(\gamma R)^{1+\varepsilon}}{\log^\varepsilon R}. \tag{4.28}$$

The estimate (4.26) shows that

$$\sup_{0 \neq q \in L^1(\mathbb{R}_+)} \frac{S_0(H_q)}{\|q\|_1} = +\infty.$$

An analogous, but slightly less explicit, result for Schrödinger operators on the whole real line has appeared in [22] (cf. Remark 4.22). Notably, our proofs seem to use rather different methods.

The main ideas in the proof of Theorem 4.3 are as follows. Starting from the Jost function of $L_{\gamma,R}$, we construct a countable family of equations, each of which is in the form of a fixed point equation. We are able to use the contraction mapping principle to prove that each equation has a unique solution corresponding to exactly one zero of the Jost function e_+ (or, more precisely, one zero of the analytic continuation of e_+ to $\mathbb{C}$).

As it turns out, each equation has a convenient form that allows us to gain quantitative information about its solution, hence about an individual zero of e_+. Estimates for the different equations can be combined to obtain lower bounds for the sums $J(L_{\gamma,R})$ and $S_\varepsilon(L_{\gamma,R})$ as well as other quantities, such as the number of eigenvalues (see Corollary 4.18).

Finally, note that, when applied to the Schrödinger operators $L_{\gamma,R}$ (4.25), the upper bound (4.23) gives the optimal asymptotic estimate (see Proposition 4.24)

$$J(L_{\gamma,R}) = O(R \log R), \quad \text{as} \quad R \to \infty. \tag{4.29}$$

Divergent Jensen sum

As mentioned, while Theorem 4.2 provides an upper bound for $J(H)$ for a wide range of potentials, there exist integrable potentials to which it does not apply. It is therefore natural to ask whether or not it is possible to extend this upper bound to arbitrary integrable potentials. Our final result show that this is impossible.

Theorem 4.4 (=Theorem 4.30)**.** *There exists a potential $q \in L^1(\mathbb{R}_+)$ such that $J(H_q) = \infty$.*

The proof of this result uses two crucial ingredients. The first is an idea of Bögli [17], which allows one to construct a Schrödinger operator whose eigenvalues approximate the union of the eigenvalues of a given sequence of Schrödinger operators $\mathscr{L}_n$, $n \in \mathbb{N}$. The second is the lower bound of Theorem 4.3 for the Jensen sum $J(L_{\gamma,R})$. Indeed, the given sequence of Schrödinger operators $\mathscr{L}_n$ in our case shall have dissipative barrier potentials. Note that the explicit condition $R \geqslant 600(\gamma^{3/4} + \gamma^{-3/4})$ in Theorem 4.3 plays an important role in Theorem 4.4.

Remark. ($\mathbb{R}_+$ vs $\mathbb{R}$). Given a potential $q \in L^1(\mathbb{R}_+)$, denote by Q its even extension on the whole line. By Proposition 4.26 below, there is inclusion $\sigma_d(H_q) \subset \sigma_d(H_Q)$, counting multiplicities, for the discrete spectra of Dirchlet Schrödinger operator H_q on $L^2(\mathbb{R}_+)$ and Schrödinger operator H_Q on $L^2(\mathbb{R})$. Hence, the inequality

$$\sum_{\lambda \in \sigma_d(H_q)} \Phi(\lambda) \leqslant \sum_{\lambda \in \sigma_d(\mathscr{H}_Q)} \Phi(\lambda), \qquad q \in L^1(\mathbb{R}_+), \tag{4.30}$$

holds with an arbitrary nonnegative function Φ on the complex plane. Thereby, upper bounds, such as (4.12), for H_q can be derived from the corresponding results for the operator H_Q. As an example, the spectral enclosure [69] mentioned above is a direct consequence of the result for the whole line [1, Theorem 4].

Several inequalities of Lieb–Thirring-type for Schrödinger operators with complex potentials on $L^2(\mathbb{R})$ are known nowadays, but neither covers completely the main results of the chapter. The result of Frank and Sabin [70, Theorem 16] in dimension one is (4.12) with $\varepsilon > 1$. The case $\varepsilon = 1$ is a consequence of [66, Theorem 1.3]. The result of Demuth, Hansmann and Katriel [53, Corollary 3] in dimension one reads

$$\sum_{\lambda \in \sigma_d(\mathscr{H}_Q)} \frac{\operatorname{dist}^{p+\varepsilon}(\lambda, \mathbb{R}_+)}{|\lambda|^{\frac{1}{2}+\varepsilon}} \leqslant C(p,\varepsilon)\|Q\|^p_{L^p(\mathbb{R})}, \qquad p \geq \frac{3}{2}, \quad \varepsilon \in (0,1).$$

Recently, Bögli [19] has extended this result considerably by including a much wider class of sums. The results of both DHK and Bögli are not applicable for arbitrary L^1 potentials, hence do not imply Theorem 4.1.

We believe that the results for Schrödinger operators with complex potentials on $L^2(\mathbb{R})$, analogous to our upper bounds, can be obtained along the same line of reasoning by using similar methods. The study of this problem should be carried out elsewhere.

Outline of the chapter

In Section 1, we focus on upper bounds for the Lieb–Thirring sums with an arbitrary potential $q \in L^1(\mathbb{R}_+)$, and for the Jensen sums with potentials $q \in Q_a$. Section 2 is devoted to the spectral analysis of Schrödinger operators with dissipative barrier potentials and to the lower bounds for the Lieb-Thirring and Jensen sums with such potentials. In Section 3 we prove Theorem 4.4.

4.2 Classes of potentials and inequalities for sums of eigenvalues

As we mentioned earlier in the introduction, a complex number $\zeta \in \mathbb{C}_+$ belongs to the zero set $Z(e_+)$ of the Jost function if and only if $\lambda = \zeta^2 \in \sigma_d(H)$, and the zero multiplicity coincides with the algebraic multiplicity of the corresponding eigenvalue. Therefore, the divisor $Z(e_+)$ (zeros counting multiplicities) has a precise spectral interpretation. In this section, we study this divisor using various results from complex analysis and hence obtain bounds for sums of Lieb-Thirring and Jensen types. Throughout the section, we shall let

$$\mathbb{C}_+^0 := \{z \in \mathbb{C} : \operatorname{Im} z \geq 0,\ z \neq 0\}.$$

4.2.1 Bounds for Lieb–Thirring sums

Recall that the Lieb–Thirring sum for a Dirchlet Schrödinger operator H is given by

$$S_\varepsilon(H) = \sum_{\lambda \in \sigma_d(H)} \frac{\operatorname{dist}(\lambda, \mathbb{R}_+)}{|\lambda|^{\frac{1-\varepsilon}{2}}}, \qquad 0 \leq \varepsilon < 1.$$

Our first result gives an upper bound for $S_\varepsilon(H)$ in the non-critical case of $\varepsilon > 0$ and arbitrary $q \in L^1(\mathbb{R}_+)$.

Theorem 4.5 (= Theorem 4.1). *For every $\varepsilon > 0$, there exists a constant $K(\varepsilon) > 0$, depending only on ε, such that*

$$S_\varepsilon(H_q) \leq K(\varepsilon) \|q\|_1^{1+\varepsilon}. \tag{4.31}$$

Proof. A key ingredient of the proof is the following well-known inequality for the Jost function (see, e.g., [131, Lemma 1])

$$|e_+(z)-1| \le \exp\left\{\frac{\|q\|_1}{|z|}\right\} - 1, \qquad z \in \mathbb{C}_+^0. \tag{4.32}$$

Let

$$y := \frac{\|q\|_1}{\kappa} > 0, \qquad \kappa := \log\frac{3}{2}.$$

By (4.32),

$$|e_+(iy)-1| \le \frac{1}{2}, \qquad |e_+(iy)| \ge \frac{1}{2}.$$

Consider the function

$$g(z) := \frac{e_+(yz)}{e_+(iy)}, \quad z \in \mathbb{C}_+, \qquad g(i) = 1.$$

By the definition of y, we have

$$\begin{aligned} |g(z)| &\le 2|e_+(yz)| \le 2\exp\left\{\frac{\|q\|_1}{y|z|}\right\} = 2\exp\left\{\frac{\kappa}{|z|}\right\}, \\ \log|g(z)| &\le \log 2 + \frac{\kappa}{|z|} < \log 2\,\frac{1+|z|}{|z|}. \end{aligned}$$

To go over to the unit disk, we introduce a new variable,

$$w = w(z) = \frac{z-i}{z+i} : \mathbb{C}_+ \to \mathbb{D}, \qquad z = z(w) = i\,\frac{1+w}{1-w}. \tag{4.33}$$

Write $f(w) := g(z(w))$. An elementary inequality

$$\frac{2}{1+|z|} \le |1-w(z)| \le \frac{2\sqrt{2}}{1+|z|}, \qquad z \in \mathbb{C}_+,$$

gives the following bound for f

$$\log|f(w)| \le \frac{2\sqrt{2}\log 2}{|1+w|}, \qquad f(0) = 1. \tag{4.34}$$

The Blaschke-type conditions for zeros of such analytic functions in $\mathbb{D}$ are obtained in [24] (see [25] for some advances)

$$\sum_{\eta\in Z(f)} (1-|\eta|)|1+\eta|^{\varepsilon} \le K_1(\varepsilon), \qquad \forall\varepsilon > 0,$$

where $K_1(\varepsilon) > 0$ depends only on ε. Going back to the upper half-plane and using another elementary inequality

$$\frac{\operatorname{Im} z}{1+|z|^2} \le 1 - |w| \le \frac{8 \operatorname{Im} z}{1+|z|^2}, \tag{4.35}$$

we come to the following relation for the divisor $Z(g)$

$$\sum_{\xi \in Z(g)} \frac{\operatorname{Im} \xi}{1+|\xi|^2} \frac{|\xi|^\varepsilon}{|\xi + i|^\varepsilon} \le K_2(\varepsilon).$$

But $\xi \in Z(g)$ is equivalent to $\zeta = y\xi \in Z(e_+)$, so

$$\left(\frac{\kappa}{\|q\|_1}\right)^{1+\varepsilon} \sum_{\zeta \in Z(e_+)} \frac{\operatorname{Im} \zeta \, |\zeta|^\varepsilon}{\left\{1 + \left(\frac{\kappa|\zeta|}{\|q\|_1}\right)^2\right\} \left|\frac{\kappa\zeta}{\|q\|_1} + i\right|^\varepsilon} \le K_2(\varepsilon).$$

The aforementioned spectral enclosure result ensures that $|\zeta| \le \|q\|_1$ for $\zeta \in Z(e_+)$. It follows that both factors in the denominator are bounded from above by some constants depending only on ε. We come to

$$\sum_{\zeta \in Z(e_+)} (\operatorname{Im} \zeta) \, |\zeta|^\varepsilon \le K(\varepsilon) \|q\|_1^{1+\varepsilon}, \tag{4.36}$$

where a positive constant K depends only on ε.

To complete the proof, we employ the inequality (4.7), mentioned in the introduction. So, (4.31) follows. □

4.2.2 Classes of potentials and Jensen sums

In the rest of the section, we study the behavior of the discrete spectrum for Schrödinger operators within special classes of potentials.

Let a be a monotonically increasing and locally integrable, nonnegative function on $\mathbb{R}_+$. Consider the classes of complex-valued potentials

$$Q_a := \{q \in L^1(\mathbb{R}_+) : \int_0^\infty a(x)|q(x)|dx < \infty\}. \tag{4.37}$$

The weight function a is fixed in the sequel, and dependence of constants on a is sometimes omitted.

Define a function $\hat{a}$ on $\mathbb{R}_+$ by

$$\hat{a}(x) := \frac{x}{a(x)}, \qquad x \in \mathbb{R}_+,$$

and put

$$\omega_a(x,z) := \hat{a}\left(\frac{1}{|z|}\right) \int_x^\infty a(t)|q(t)|dt, \qquad x \in \mathbb{R}_+, \quad z \in \mathbb{C}_+^0.$$

Proposition 4.6. *Assume that both a and $\hat{a}$ are monotonically increasing functions on $\mathbb{R}_+$. Then the Jost solution admits the bound*

$$|e^{-izx}e_+(x,z) - 1| \le \exp(\omega_a(x,z)) - 1, \qquad x \in \mathbb{R}_+, \quad z \in \mathbb{C}_+^0. \tag{4.38}$$

Proof. We follow the arguments of M.A. Naimark for the classical case $a \equiv 1$.

The Jost solution is known to satisfy the Schrödinger integral equation

$$e_+(x,z) = e^{ixz} + \int_x^\infty \frac{\sin((t-x)z)}{z} q(t)e_+(t,z)dt.$$

The latter can be resolved by the successive approximations method.

Introduce a new unknown function

$$f(x,z) := e^{-ixz}e_+(x,z) - 1,$$

which satisfies

$$\begin{aligned} f(x,z) &= g(x,z) + \int_x^\infty k(t-x,z)q(t)f(t,z)dt, \\ k(u,z) &:= \frac{\sin uz}{z} e^{iuz}, \quad g(x,z) := \int_x^\infty k(t-x,z)q(t)dt. \end{aligned} \tag{4.39}$$

Let

$$f_1(x,z) := g(x,z), \quad f_{n+1}(x,z) = \int_x^\infty k(t-x,z)q(t)f_n(t,z)dt, \quad n \in \mathbb{N}.$$

In view of an elementary bound for the kernel k

$$|k(u,z)| \le \min\left(u, \frac{1}{|z|}\right),$$

and monotonicity of a and $\hat{a}$, we see that

$$|k(u,z)| = \hat{a}(|k(u,z)|)\, a(|k(u,z)|) \le \hat{a}\left(\frac{1}{|z|}\right) a(u), \tag{4.40}$$

cf. (4.24).

We first estimate f_1. By (4.40),

$$|f_1(x,z)| \le \int_x^\infty |k(t-x,z)||q(t)|dt \le \hat{a}\left(\frac{1}{|z|}\right) \int_x^\infty a(t-x)|q(t)|dt \le \omega_a(x,z).$$

Assume for induction that

$$|f_j(x,z)| \le \frac{\omega_a^j(x,z)}{j!}, \qquad j = 1,2,\dots,n. \tag{4.41}$$

We compute

$$\begin{aligned}\frac{d}{dx}\left[\omega_a^{n+1}(x,z)\right] &= (n+1)\,\omega_a^n(x,z)\,\frac{d}{dx}\left[\omega_a(x,z)\right]\\ &= -(n+1)\,\omega_a^n(x,z)\,\hat{a}\left(\frac{1}{|z|}\right) a(x)|q(x)|,\end{aligned}$$

and so

$$\begin{aligned}|f_{n+1}(x,z)| &\le \int_x^\infty |k(t-x,z)||q(t)|\frac{\omega_a^n(t,z)}{n!}dt\\ &\le \frac{1}{n!}\hat{a}\left(\frac{1}{|z|}\right)\int_x^\infty a(t)|q(t)|\,\omega_a^n(t,z)dt\\ &= -\frac{1}{(n+1)!}\int_x^\infty \frac{d}{dt}\left[\omega_a^{n+1}(t,z)\right]dt = \frac{\omega_a^{n+1}(x,z)}{(n+1)!}.\end{aligned}$$

Hence, (4.41) indeed holds for all $n \in \mathbb{N}$.

It follows that the solution f to (4.39), which is known to be unique, satisfies

$$|f(x,z)| \le \sum_{n=1}^\infty |f_n(x,z)| \le \exp\bigl(\omega_a(x,z)\bigr) - 1$$

(the latter series converges absolutely and uniformly on the compact subsets of $(x \in \mathbb{R}_+, z \in \mathbb{C}_+^0)$). The bound (4.38) follows. $\square$

The above result for $a(x)=x^\alpha$, $\alpha\in[0,1]$, is due to Stepin [131, Lemma 1]. The bound for the Jost function $e_+(z)=e_+(0,z)$ is (4.38) with $x=0$:

$$|e_+(z)-1|\le \exp\left\{\hat{a}\left(\frac{1}{|z|}\right)\|q\|_a\right\}-1, \quad \|q\|_a:=\int_0^\infty a(t)|q(t)|dt. \tag{4.42}$$

The following spectral enclosure result is a simple consequence of (4.42) and the basic property of zeros of e_+.

Corollary 4.7. *Under the hypothesis of Proposition 4.6, define the value*

$$\rho=\rho(a,q):=\inf\Big\{t>0:\ \hat{a}(\sqrt{t})\ge\frac{\log 2}{\|q\|_a}\Big\}.$$

Then the discrete spectrum $\sigma_d(H_q)$ is contained in the closed disk

$$\sigma_d(H_q)\subset B_{\rho^{-1}}(0).$$

The case $\hat{a}(\infty)<\log 2\,\|q\|_a^{-1}$ implies that $\rho=\infty$, and so the discrete spectrum is empty.

As a matter of fact, in view of [69], we have a more precise inclusion

$$\sigma_d(H_q)\subset B_r(0), \qquad r:=\min(\rho^{-1},\,\|q\|_1^2). \tag{4.43}$$

To study the distribution of eigenvalues of H for potentials from the class Q_a, we apply standard tools from complex analysis (the Jensen formula). Recall that the Jensen sum is given by

$$J(H)=\sum_{\lambda\in\sigma_d(H)}\operatorname{Im}\sqrt{\lambda}. \tag{4.44}$$

Here $\sqrt{\cdot}=\mathrm{sq}_+(\cdot)$ is the branch of the square root, which maps $\mathbb{C}\backslash\mathbb{R}_+$ onto the upper half-plane $\mathbb{C}_+$.

Theorem 4.8 (= Theorem 4.2)**.** *In addition to the hypothesis of Proposition 4.6, assume that*

1. *$\hat{a}$ is a continuous, strictly monotonically increasing function, and $\hat{a}(0)=0$, $\hat{a}(\infty)=\infty$,*

2. $$\int_1^\infty\frac{dx}{xa(x)}<\infty.$$

Then, for each potential $q \in Q_a$, and each $\delta \in (0,1)$, the following bound for the Jensen sum holds

$$J(H_q) \le y \log \frac{1+\delta}{(1-\delta)^2} + \frac{4}{\pi} \|q\|_a \int_{\frac{1}{y}}^{\infty} \frac{dx}{xa(x)}, \tag{4.45}$$

where $y = y(\delta, a, \|q\|_a) > 0$ is uniquely determined by

$$\hat{a}\left(\frac{1}{y}\right) \|q\|_a = \log(1+\delta). \tag{4.46}$$

Proof. The argument is similar to that in Theorem 4.5. It follows from (4.42) and (4.46) that

$$|e_+(iy) - 1| \le 1 + \delta - 1 = \delta, \qquad |e_+(iy)| \ge 1 - \delta,$$

so the normalized function

$$g(z) := \frac{e_+(yz)}{e_+(iy)}, \qquad g(i) = 1,$$

satisfies

$$\log|g(z)| \le \log \frac{1}{1-\delta} + \hat{a}\left(\frac{1}{y|z|}\right) \|q\|_a, \qquad z \in \mathbb{C}_+.$$

Introduce a new variable $w \in \mathbb{D}$, related to $z \in \mathbb{C}_+$ by (4.33). For $f(w) := g(z(w))$ one has, as above, $f(0) = 1$ and

$$\log|f(w)| \leqslant \log \frac{1}{1-\delta} + \hat{a}\left(\frac{1}{y}\left|\frac{1-w}{1+w}\right|\right) \|q\|_a, \quad w \in \mathbb{D}.$$

For $w = re^{i\theta}$, $|\theta| \le \pi$, it is easy to calculate

$$\max_{0 \le r \le 1} \left|\frac{1-re^{i\theta}}{1+re^{i\theta}}\right| = \begin{cases} 1, & |\theta| \le \frac{\pi}{2}, \\ \left|\tan\frac{\theta}{2}\right|, & \frac{\pi}{2} < |\theta| < \pi, \end{cases}$$

so

$$\log|f(w)| \le \begin{cases} \log\frac{1+\delta}{1-\delta}, & |\theta| \le \frac{\pi}{2}, \\ \log\frac{1}{1-\delta} + \hat{a}\left(\frac{1}{y}\left|\tan\frac{\theta}{2}\right|\right) \|q\|_a, & \frac{\pi}{2} < |\theta| < \pi. \end{cases}$$

In view of assumption (2), the Jensen formula provides

$$\begin{aligned}\sum_{\eta\in Z(f)}(1-|\eta|) &\le \sum_{\eta\in Z(f)}\log\frac{1}{|\eta|}\\ &\le \frac{1}{2}\log\frac{1+\delta}{(1-\delta)^2}+\frac{\|q\|_a}{\pi}\int_{\pi/2}^{\pi}\hat{a}\left(\frac{1}{y}\Big(\tan\frac{\theta}{2}\Big)\right)d\theta\\ &= \frac{1}{2}\log\frac{1+\delta}{(1-\delta)^2}+\frac{2\|q\|_a}{\pi}\int_1^{\infty}\frac{\hat{a}(y^{-1}t)}{1+t^2}dt,\end{aligned}$$

and hence

$$\begin{aligned}\sum_{\eta\in Z(f)}(1-|\eta|) &\le \frac{1}{2}\log\frac{1+\delta}{(1-\delta)^2}+\frac{2\|q\|_a}{\pi}\int_1^{\infty}\frac{\hat{a}(y^{-1}t)}{t^2}dt\\ &\le \frac{1}{2}\log\frac{1+\delta}{(1-\delta)^2}+\frac{2\|q\|_a}{\pi y}\int_{\frac{1}{y}}^{\infty}\frac{dx}{xa(x)} =: B.\end{aligned}$$

Going back to the function g and the upper half-plane and using (4.35), we come to

$$\sum_{\xi\in Z(g)}\frac{\operatorname{Im}\xi}{1+|\xi|^2}\le B.$$

The relation between $Z(g)$ and $Z(e_+)$ is straightforward

$$\xi\in Z(g)\ \Leftrightarrow\ \zeta=y\xi\in Z(e_+),$$

and, hence,

$$\sum_{\zeta\in Z(e_+)}\frac{\operatorname{Im}\zeta}{1+\left|\frac{\zeta}{y}\right|^2}\le By. \tag{4.47}$$

As it follows from (4.42),

$$\hat{a}\left(\frac{1}{|z|}\right)\|q\|_a<\log 2\ \Rightarrow\ e_+(z)\neq 0.$$

Therefore,

$$\hat{a}\left(\frac{1}{|\zeta|}\right)\|q\|_a\ge\log 2,\qquad \zeta\in Z(e_+),$$

and so (see the choice of y (4.46)), by monotonicity of $\hat{a}$,

$$\hat{a}\left(\frac{1}{|\zeta|}\right)\|q\|_a>\hat{a}\left(\frac{1}{y}\right)\|q\|_a\ \Rightarrow\ \left|\frac{\zeta}{y}\right|<1.$$

We conclude from (4.47), that

$$\sum_{\zeta \in Z(e_+)} \operatorname{Im} \zeta \leq 2By,$$

and (4.45) follows. The proof is complete. □

As a first application of the above result, we study Schrödinger operators H_q with potentials q satisfying $\|(1+x^p)q\|_1 < \infty$ for some $p \in (0,1)$. Taking $a(x) := x^p$ and any fixed $\delta \in (0,1)$ (e.g., $\delta = 1/2$) in Theorem 4.8 easily yields the inequality

$$J(H_q) \leqslant C(p) \left(\int_0^\infty x^p |q(x)| dx \right)^{\frac{1}{1-p}}, \qquad p \in (0,1).$$

The following corollary of Theorem 4.8 offers a refinement of this bound.

Corollary 4.9. *Let $p \in (0,1)$ and $a(x) = 1 + x^p$. Then for each potential $q \in Q_a$, the following inequality holds*

$$J(H_q) \leqslant \tfrac{4}{\pi} \|q\|_a \log(1 + \|q\|_a) + \tfrac{9}{p} \|q\|_a + 2. \tag{4.48}$$

Proof. Put

$$\delta := \exp\Big(\min\big(\tfrac{1}{2}\|q\|_a, \kappa\big)\Big) - 1 \in \big(0, \tfrac{1}{2}\big], \qquad \kappa = \log \tfrac{3}{2}.$$

Then, by (4.46),

$$A_0 := \frac{\log(1+\delta)}{\|q\|_a} = \hat{a}\left(\frac{1}{y}\right) \leqslant \frac{1}{2} \quad \text{and} \quad \log \frac{1+\delta}{(1-\delta)^2} \leqslant \log 6.$$

Since $\hat{a}$ is monotonically increasing, with $\hat{a}(1) = \frac{1}{2}$, we must have $y \geqslant 1$. In particular, this implies that

$$\frac{y^{-1}}{1+y^{-1}} \geqslant \frac{y^{-1}}{1+y^{-p}} = \hat{a}(y^{-1}) = A_0, \qquad \frac{1}{y} \geqslant \frac{A_0}{1-A_0},$$

and so

$$1 \leq y \leq \frac{1-A_0}{A_0} \leq \frac{1}{A_0}. \tag{4.49}$$

If $\|q\|_a \geqslant 2\kappa$, then $\delta = \frac{1}{2}$, so $y \leqslant 3\|q\|_a$. On the other hand, if $\|q\|_a < 2\kappa$, then $A_0 = \frac{1}{2}$, so $y = 1$ ($\hat{a}$ is strictly monotonically increasing). We conclude that

$$y \leqslant 3\|q\|_a + 1. \tag{4.50}$$

The right hand side of (4.45) is the sum of two terms. We bound the first one as

$$A_1 := y \log \frac{1+\delta}{(1-\delta)^2} \leqslant \log 6\,(3\|q\|_a + 1) < 6\|q\|_a + 2.$$

The second (integral) term reads

$$A_2 := \frac{4}{\pi}\,\|q\|_a \int_{1/y}^{\infty} \frac{dx}{x(1+x^p)}.$$

The integral may be computed, and bounded above, as

$$\begin{aligned}\int_{1/y}^{\infty} \frac{dx}{x(1+x^p)} &= \frac{1}{p}\log\left(1+\frac{1}{y^p}\right) + \log y\\ &\leqslant \frac{1}{py^p} + \log y.\end{aligned}$$

Using the upper bound (4.50) and the lower bound (4.49) for y, we obtain

$$\begin{aligned}A_2 &\leqslant \frac{4}{\pi}\,\|q\|_a \left[\log(1+\|q\|_a) + \log 3 + \frac{1}{p}\right]\\ &\leqslant \frac{4}{\pi}\,\|q\|_a \log(1+\|q\|_a) + \frac{3}{p}\,\|q\|_a.\end{aligned}$$

The bound (4.48) follows by combining the bounds for A_1 and A_2. □

Remark 4.10. In [123], Safronov also studies Schrödinger operators H_q on $\mathbb{R}_+$ with potentials q satisfying $\|(1+x^p)q\|_1 < \infty$ for some $p \in (0,1)$, and obtains the estimate

$$J(H_q) \leqslant C(p)\left(\int_0^{\infty} x^p|q(x)|dx \left(\int_0^{\infty} |q(x)|dx\right)^p + \int_0^{\infty} |q(x)|dx\right). \tag{4.51}$$

Consider the following Dirchlet Schrödinger operators on $\mathbb{R}_+$,

$$H_h = -\frac{d^2}{dx^2} + q(xh), \qquad h > 0,$$

where $q \in L^1(\mathbb{R}_+)$ is fixed. A rescaling shows that $h \to 0$ is equivalent to a semiclassical limit. It can be seen that Corollary 4.9 gives

$$J(H_h) = O(h^{-(1+p)} \log(\tfrac{1}{h})) \quad \text{as} \quad h \to 0,$$

while the estimate (4.51) gives

$$J(H_h) = O(h^{-(1+2p)}) \quad \text{as} \quad h \to 0,$$

hence our result offers an improved asymptotic estimate for H_h.

The next example is more delicate. It presents an integrable potential q that is not covered by Theorem 4.8. More precisely, $q \notin Q_a$ for any weight function a satisfying the assumptions of Theorem 4.8.

Example 4.11. Take $\alpha > 1$ and put

$$q(x) := \begin{cases} \frac{i}{x\log^\alpha x}, & x \geq e, \\ 0, & 0 < x < e, \end{cases} \tag{4.52}$$

Then, $q \in L^1(\mathbb{R}_+)$. We distinguish two cases.

1. Assume that $\alpha > 2$. Choose β from $1 < \beta < \alpha - 1$ and denote

$$a(x) := \begin{cases} \log^\beta x, & x \geq e^\beta, \\ \beta^\beta, & 0 < x < e^\beta, \end{cases}$$

so a is a positive, monotonically increasing and continuous function on $\mathbb{R}_+$. Then,

$$\hat{a}(x) = \begin{cases} \frac{x}{\log^\beta x}, & x \geq e^\beta, \\ \beta^{-\beta} x, & 0 < x < e^\beta. \end{cases}$$

Since $\beta > 1$, both assumptions of Theorem 4.8 are met. Clearly, $\|q\|_a < \infty$, so the Jensen sum $J(H_q)$ is finite for this potential.

2. Let now $1 < \alpha \leq 2$. We claim that there is no such weight function a.

Assume on the contrary, that there are a and $\hat{a}$, which satisfy the assumptions of Theorem 4.8, and $\|q\|_a < \infty$. Then, for $t \geq e$,

$$\infty > \int_t^\infty \frac{a(x)}{x\log^\alpha x} dx \geq a(t) \int_t^\infty \frac{dx}{x\log^\alpha x} = \frac{1}{\alpha - 1} \frac{a(t)}{(\log t)^{\alpha-1}},$$

or

$$a(t) \leq C_1 (\log t)^{\alpha-1}, \qquad t \geq e.$$

But $\alpha - 1 \leq 1$, and so

$$\int_1^\infty \frac{dt}{ta(t)} = \infty.$$

A contradiction completes the proof.

Part 2 of the above example by no means claims that $J(H_q) = \infty$ for those potentials.

As a final consequence of Theorem 4.8, we study the Jensen sums for Schrödinger operators with compactly supported potentials.

Corollary 4.12. *For any potential $q \in L^1(\mathbb{R}_+)$ with* $\operatorname{supp}(q) \subset [0,R]$, $R > 1$, *the following inequality holds*

$$J(H_q) \le 7\left[\frac{1}{R} + \|q\|_1\Big(1+\log(1+\|q\|_1)+\log R\Big)\right]. \tag{4.53}$$

Proof. We choose the weight functions

$$a(x) = \begin{cases} 1, & 0 < x \le R, \\ \left(\frac{\log x}{\log R}\right)^2, & x \ge R, \end{cases} \qquad \hat{a}(x) = \begin{cases} x, & 0 < x \le R, \\ x\left(\frac{\log R}{\log x}\right)^2, & x \ge R. \end{cases}$$

Since $\operatorname{supp}(q) \subset [0,R]$, we have $\|q\|_a = \|q\|_1$.

Put

$$\delta := \exp\Big(\min\big(\|q\|_1 R,\ \kappa\big)\Big) - 1 \in \Big(0, \frac{1}{2}\Big], \quad \kappa = \log\frac{3}{2}.$$

Clearly,

$$\log(1+\delta) = \min\big(\|q\|_1 R,\ \kappa\big) \le \|q\|_1 R, \quad \frac{\log(1+\delta)}{\|q\|_1} \le R,$$

and so the quantity y defined in (4.46) is given by

$$y = \frac{\|q\|_1}{\log(1+\delta)}.$$

The right hand side of (4.45) is the sum of two terms, $A = A_1 + A_2$. The first one is

$$\begin{aligned} A_1 &:= y\log\frac{1+\delta}{(1-\delta)^2} = \|q\|_1 + y\log\frac{1}{(1-\delta)^2} \leqslant \|q\|_1\left\{1+\frac{\log 4}{\log(1+\delta)}\right\} \\ &= \|q\|_1\left\{1+\frac{\log 4}{\min\big(\|q\|_1 R,\ \kappa\big)}\right\}. \end{aligned}$$

Hence,

$$A_1 \le \begin{cases} \|q\|_1\left(1+\frac{\log 4}{\kappa}\right) < 5\|q\|_1, & \|q\|_1 R \ge \kappa, \\ \|q\|_1 + \frac{\log 4}{R} = \frac{\|q\|_1 R + \log 4}{R} < \frac{\log 6}{R}, & \|q\|_1 R < \kappa. \end{cases}$$

To estimate the second (integral) term A_2, note that $y^{-1} \le R$, and so $A_2 = A_{21} + A_{22}$ with

$$\begin{aligned} A_{21} &:= \frac{4}{\pi}\|q\|_1 \int_{\frac{1}{y}}^{R} \frac{dt}{t} = \frac{4}{\pi}\|q\|_1 \log\frac{\|q\|_1 R}{\log(1+\delta)}, \\ A_{22} &:= \frac{4}{\pi}\|q\|_1 \log^2 R \int_R^\infty \frac{dt}{t\log^2 t} = \frac{4}{\pi}\|q\|_1 \log R. \end{aligned}$$

Hence,

$$A_2 \le \frac{4}{\pi}\,\|q\|_1 \log R + \frac{4}{\pi}\,\|q\|_1 \log \frac{\|q\|_1 R}{\min\big(\|q\|_1 R,\ \kappa\big)}\,,$$

or

$$A_2 \le \begin{cases} \frac{4}{\pi}\,\|q\|_1 \left(\log R + \log(\|q\|_1 R) + \log \frac{1}{\kappa}\right), & \|q\|_1 R \ge \kappa, \\ \frac{4}{\pi}\,\|q\|_1 \log R, & \|q\|_1 R < \kappa. \end{cases}$$

A combination of the above bounds (with appropriate calculation of the constants) leads to (4.53), as claimed. □

Remark 4.13. The celebrated Blaschke condition for zeros of analytic functions on the upper half-plane reads (see [73, Section II.2, (2.3)])

$$\sum_{z \in Z(f)} \frac{\operatorname{Im} z}{1+|z|^2} < \infty. \tag{4.54}$$

It holds, for instance, for functions of bounded type (ratios of bounded analytic functions). In view of the spectral enclosure $|z| \le \|q\|_1$, the bound $J(H_q) < \infty$ is equivalent to the Blaschke condition for zeros of the Jost function.

4.3 Dissipative barrier potentials

As in the introduction (see (4.25)), let $L_{\gamma,R}$ denote a Dirchlet Schrödinger operator on $\mathbb{R}_+$ with the potential

$$q_{db} := i\gamma\chi_{[0,R]}, \qquad \gamma, R > 0. \tag{4.55}$$

We fix γ throughout this section and shall be interested in large R. The aim of the section is to prove the bounds for the Lieb-Thirring and Jensen sums of the eigenvalues of $L_{\gamma,R}$ for large enough R.

4.3.1 Eigenvalues of Schrödinger operators with dissipative barrier potentials

The value $z^2 \in \sigma_d(L_{\gamma,R})$ if the equation

$$-y'' + i\gamma\chi_{[0,R]}(x)y = z^2 y \tag{4.56}$$

has a solution $y \in L^2(\mathbb{R}_+)$ with $y(0) = 0$. An integration by parts with the normalized eigenfunction gives

$$\begin{aligned} z^2 &= \int_0^\infty |y'(t)|^2 dt + i\gamma \int_0^R |y(t)|^2 dt \in \Gamma_+, \\ \Gamma_+ &:= \{\zeta \in \mathbb{C} : \operatorname{Re}\zeta > 0,\ 0 < \operatorname{Im}\zeta < \gamma\}. \end{aligned} \tag{4.57}$$

It shall be convenient for us to work with two different branches $\mathrm{sq}_\pm$ of the square-root function. $\mathrm{sq}_\pm$ have branch-cuts along $\mathbb{R}_\pm$, respectively, and the corresponding argument functions $\arg_\pm$ satisfy

$$\arg_+(\zeta) \in [0, 2\pi), \quad \arg_-(\zeta) \in [-\pi, \pi), \quad \zeta \in \mathbb{C}; \quad \mathrm{sq}_\pm(\zeta) = \sqrt{|\zeta|}e^{\frac{i}{2}\arg_\pm(\zeta)}.$$

Since the solutions of the equation (4.56) are obviously computable, we may characterise the eigenvalues of $L_{\gamma,R}$ as the zeros of an explicit analytic function. Let

$$\varphi_R(z) := \big(z - \mathrm{sq}_+(z^2 - i\gamma)\big)e^{iR\,\mathrm{sq}_+(z^2 - i\gamma)} - \big(z + \mathrm{sq}_+(z^2 - i\gamma)\big)e^{-iR\,\mathrm{sq}_+(z^2 - i\gamma)}.$$

Lemma 4.14. *For any $R > 0$ and any $z \in \mathbb{C}_+$ with $z^2 \neq i\gamma$,*

$$z^2 \in \sigma_d(L_{\gamma,R}) \quad \Longleftrightarrow \quad \varphi_R(z) = 0.$$

Proof. Let $R > 0$ and $z \in \mathbb{C}_+$ such that $z^2 \neq i\gamma$. Recall that $e_+(\cdot, z)$ denotes the Jost solution. Since $e_+(\cdot, z)$ spans the space of solutions of (4.56) in $L^2(\mathbb{R}_+)$, we have

$$z^2 \in \sigma_d(L_{\gamma,R}) \quad \Longleftrightarrow \quad e_+(0, z) = 0.$$

It suffices to show that $e_+(0, z) = 0$ if and only if $\varphi_R(z) = 0$. Since $z \neq 0$ and $z^2 \neq i\gamma$, e_+ must satisfy

$$e_+(x, z) = \begin{cases} c_1(z)e^{ix\,\mathrm{sq}_+(z^2 - i\gamma)} + c_2(z)e^{-ix\,\mathrm{sq}_+(z^2 - i\gamma)}, & 0 < x < R \\ e^{ixz}, & x \geqslant R, \end{cases}$$

for some $c_j(z) \in \mathbb{C}$, $j = 1, 2$. c_1 and c_2 are determined by imposing the continuity of $e_+(\cdot, z)$ and $\frac{d}{dx}e_+(\cdot, z)$ at the point R,

$$\begin{aligned} c_1(z) &= \frac{\mathrm{sq}_+(z^2 - i\gamma) + z}{2\,\mathrm{sq}_+(z^2 - i\gamma)} e^{-iR\left(\mathrm{sq}_+(z^2 - i\gamma) - z\right)}, \\ c_2(z) &= \frac{\mathrm{sq}_+(z^2 - i\gamma) - z}{2\,\mathrm{sq}_+(z^2 - i\gamma)} e^{iR\left(\mathrm{sq}_+(z^2 - i\gamma) + z\right)}, \end{aligned}$$

and so the expression for the Jost function $e_+(0,z)$ is

$$\begin{aligned}
&e^{-iRz}e_+(0,z)\\
&=\frac{\big(z+\mathrm{sq}_+(z^2-i\gamma)\big)e^{-iR\,\mathrm{sq}_+(z^2-i\gamma)}-\big(z-\mathrm{sq}_+(z^2-i\gamma)\big)e^{iR\,\mathrm{sq}_+(z^2-i\gamma)}}{2\,\mathrm{sq}_+(z^2-i\gamma)}\\
&=\cos\big(R\,\mathrm{sq}_+(z^2-i\gamma)\big)-izR\frac{\sin\big(R\,\mathrm{sq}_+(z^2-i\gamma)\big)}{R\,\mathrm{sq}_+(z^2-i\gamma)}.
\end{aligned}$$

Note that it is clear from this expression that e_+ is an entire function.

Finally, $z^2\neq i\gamma$, so $e_+(0,z)=0$ if and only if

$$\varphi_R(z)=-2\,\mathrm{sq}_+(z^2-i\gamma)e^{-iRz}e_+(0,z)=0.$$

The proof is complete. □

Note that, $\varphi_R(z_0)=0$ for $z_0^2=i\gamma$, but $z_0^2\notin\sigma_d(L_{\gamma,R})$.

Our strategy is to derive a countable family of equations, each of which has a unique solution corresponding to exactly one zero of φ_R. Introduce a new variable w by

$$w:=\mathrm{sq}_+(z^2-i\gamma).$$

For $\operatorname{Re} z>0$, we have $z=\mathrm{sq}_-(z^2)$ and so

$$z=\mathrm{sq}_-(w^2+i\gamma). \tag{4.58}$$

Consider the family of equations

$$w=G_{j,R}(w):=\frac{-B_j(w)+iA(w)}{2R},\qquad j\in\mathbb{N}, \tag{4.59}$$

where

$$A(w):=\log\left|\frac{\mathrm{sq}_-(w^2+i\gamma)-w}{\mathrm{sq}_-(w^2+i\gamma)+w}\right|$$

and

$$B_j(w):=\arg_-\left(\frac{\mathrm{sq}_-(w^2+i\gamma)-w}{\mathrm{sq}_-(w^2+i\gamma)+w}\right)+2\pi j,\qquad j\in\mathbb{N}.$$

Clearly,

$$2\pi\Big(j-\frac{1}{2}\Big)\le B_j(w)<2\pi\Big(j+\frac{1}{2}\Big),\qquad j\in\mathbb{N}. \tag{4.60}$$

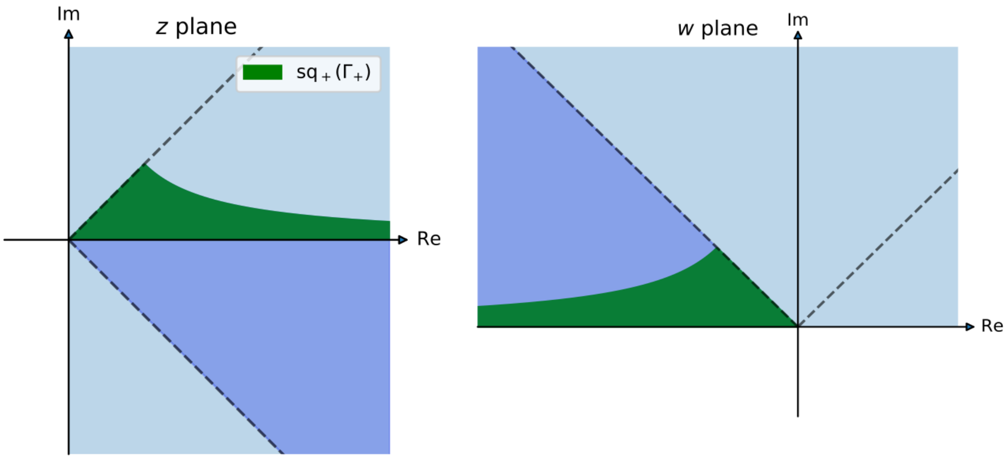

Figure 4.1 An illustration of the new complex variable w. Regions of identical colours are mapped to each other.

Lemma 4.15. *Let $R > 0$. If $w \in \mathbb{C}_+$ solves equation (4.59), and $w^2 + i\gamma \in \mathbb{C}_+$, then $w^2 + i\gamma \in \sigma_d(L_{\gamma,R})$.*

Proof. The equation (4.59) can be written as

$$w = G_{j,R}(w) = \frac{i}{2R}\left(\log_-\left(\frac{\mathrm{sq}_-(w^2+i\gamma)-w}{\mathrm{sq}_-(w^2+i\gamma)+w}\right)+2\pi i j\right) \tag{4.61}$$

where $\log_-$ denote the branch of the logarithm corresponding to $\arg_-$. Rearranging this equation, it holds that

$$\big(\mathrm{sq}_-(w^2+i\gamma)-w\big)e^{iRw} - \big(\mathrm{sq}_-(w^2+i\gamma)+w\big)e^{-iRw} = 0, \tag{4.62}$$

which is equivalent to $\varphi_R(z) = 0$, where z is defined by (4.58). Finally, $w \neq 0$ implies $z^2 \neq i\gamma$, and the hypothesis $w^2 + i\gamma \in \mathbb{C}_+$ ensures that $z \in \mathbb{C}_+$ so, by Lemma 4.14, we have $z^2 = w^2 + i\gamma \in \sigma_d(L_{\gamma,R})$. □

From this point on, we shall restrict our attention to solutions of (4.59) in the angle

$$\begin{aligned} F_\infty &= \{w \in \mathbb{C} : \operatorname{Re} w \leqslant 0 \leqslant \operatorname{Im} w,\ |\operatorname{Re} w| \geqslant 2\operatorname{Im} w\} \\ &= \{re^{i\theta} :\ \pi - \arctan\frac{1}{2} \leq \theta \leq \pi,\ r \geqslant 0\} \end{aligned} \tag{4.63}$$

and its subsets

$$F_j := \{w \in F_\infty : B_j(w) \geqslant 2\,|A(w)|\}, \qquad j \in \mathbb{N}.$$

Since $B_{j+1}(w) = B_j(w) + 2\pi$, the family $\{F_j\}_{j\geq 1}$ is nested

$$F_j \subset F_{j+1}, \qquad \bigcup_{j=1}^{\infty} F_j = F_\infty.$$

As $B_j(w) \geq \pi$ for all $w \in F_\infty$, and $A(0) = 0$, the set F_j is nonempty for all $j \in \mathbb{N}$.

The next result establishes existence and uniqueness of solutions in the regions F_j for each equation (4.59) and large enough R. Precisely, we assume that

$$R \geqslant C_0\left(\gamma^{3/4} + \gamma^{-3/4}\right), \qquad C_0 = 600. \tag{4.64}$$

Proposition 4.16. *For all R satisfying* (4.64) *and all $j \in \mathbb{N}$, the equation* (4.59) *has a unique solution in F_∞ which lies in F_j. For different equations the solutions are different.*

Proof. A key ingredient of the proof is the contraction mapping principle (see, e.g., [118, Theorem V.18]) on the complete metric space $(F_j, |\cdot|)$ with the usual absolute value on $\mathbb{C}$ as a distance.

Fix $j \in \mathbb{N}$. Suppose we can show that for R satisfying (4.64),

(a) $G_{j,R} : F_j \to F_j$,

(b) $G_{j,R}$ is a strict contraction mapping.

Then, the map $G_{j,R} : F_j \to F_j$ has a unique fixed point, and so the equation $w = G_{j,R}(w)$ has a unique solution in F_j. Moreover, there are no solutions for the latter equation outside F_j. Indeed, any solution $w \in F_\infty$ satisfies

$$w = G_{j,R}(w) = \frac{-B_j(w) + iA(w)}{2R} \;\Rightarrow\; B_j(w) \geq 2|A(w)|$$

so $w \in F_j$. So, it suffices to prove the statements (a) and (b) above.

Put

$$w = u + iv, \quad z = \mathrm{sq}_-(w^2 + i\gamma) = x + iy.$$

Let us show first that for each $w \in F_\infty$,

$$x = \mathrm{Re}\,\mathrm{sq}_-(w^2 + i\gamma) \geqslant 0, \quad |y| = \left|\mathrm{Im}\,\mathrm{sq}_-(w^2 + i\gamma)\right| \leqslant x = \mathrm{Re}\,\mathrm{sq}_-(w^2 + i\gamma). \tag{4.65}$$

Indeed, the first inequality follows from the definition of sq_-. As for the second one, since $\mathrm{Re}\,(z^2) = \mathrm{Re}\,(w^2)$ and $|u| \geq 2v$, we have

$$u^2 - v^2 = x^2 - y^2, \quad x^2 = y^2 + u^2 - v^2 \geq y^2 + 3v^2 \;\Rightarrow\; |y| \leq x,$$

as claimed.

Step 1. To prove the statement (a), we show first that the following inequalities hold

1. $\mathrm{Re}\, G_{j,R}(w) < 0 \le \mathrm{Im}\, G_{j,R}(w),\ \ w \in F_\infty,$

2. $|\mathrm{Re}\, G_{j,R}(w)| \ge 2\,\mathrm{Im}\, G_{j,R}(w), \quad w \in F_j.$

In view of the definition of $B_j(w) = -2R\,\mathrm{Re}\, G_{j,R}(w)$, and the bounds (4.60) for B_j, the left inequality in (1) is obvious. To prove the right one, it suffices to show that $A(w) \geqslant 0$ for all $w \in F_\infty$. We write

$$|z \pm w|^2 = |z|^2 + |w|^2 \pm 2\,\mathrm{Re}\,(\bar{w}z) = |z|^2 + |w|^2 \pm 2(ux + vy),$$

and so

$$|z-w|^2 - |z+w|^2 = -4(ux+vy).$$

As we know, $|u| \ge 2v$ for $w \in F_\infty$, and also $x \ge |y|$, by (4.65). Hence,

$$|vy| \le \frac{|u|x}{2} \le |ux|, \quad ux + vy \le ux + |vy| \le ux + |ux| = 0,$$

which implies

$$|z-w|^2 - |z+w|^2 = -4(ux+vy) \ge 0, \quad A(w) = \log\left|\frac{z-w}{z+w}\right| \ge 0,$$

and (1) follows. (2) is just the definition of F_j. So, $G_{j,R} : F_j \to F_\infty$.

Next, we want to check that for R satisfying (4.64),

$$B_j\big(G_{j,R}(w)\big) \ge 2\,|A\big(G_{j,R}(w)\big)|, \qquad w \in F_j, \tag{4.66}$$

or, in other words, $G_{j,R}(w) \in F_j$. It is shown above that, for $w \in F_j$, we have $G_{j,R}(w) \in F_\infty$ and $|A\big(G_{j,R}(w)\big)| = A\big(G_{j,R}(w)\big) \ge 0$. Then,

$$\begin{aligned} A\big(G_{j,R}(w)\big) &= \log \frac{\left|\mathrm{sq}_-(G^2_{j,R}(w) + i\gamma) - G_{j,R}(w)\right|^2}{\gamma} \\ &\le \log \frac{2(4|G_{j,R}(w)|^2 + \gamma)}{\gamma} = \log\left(\frac{8|G_{j,R}(w)|^2}{\gamma} + 2\right). \end{aligned}$$

For $w \in F_j$ one has $2|A(w)| \le B_j(w)$, and so, by (4.60),

$$|G_{j,R}(w)|^2 = \frac{A^2(w) + B_j^2(w)}{4R^2} \le \frac{5B_j^2(w)}{16R^2} \le \frac{5\pi^2}{4R^2}\Big(j + \frac{1}{2}\Big)^2.$$

Hence,

$$A\big(G_{j,R}(w)\big) \le \log\Big(2+\frac{10\pi^2(j+\frac{1}{2})^2}{\gamma R^2}\Big). \tag{4.67}$$

Clearly, $10\pi^2 < \gamma R^2$ for R satisfying (4.64), so we come to

$$A\big(G_{j,R}(w)\big) \le \log\Big(2+\Big(j+\frac{1}{2}\Big)^2\Big) < \log\Big(2\Big(j+\frac{1}{2}\Big)^2\Big), \quad j\in\mathbb{N}. \tag{4.68}$$

Elementary calculus shows that

$$\log 2 + 2\log\Big(j+\frac{1}{2}\Big) < \pi\Big(j-\frac{1}{2}\Big), \quad j\in\mathbb{N},$$

and so $2A\big(G_{j,R}(w)\big) \le B_j\big(G_{j,R}(w)\big)$, which completes the proof of (4.66). The statement (a) is verified.

Step 2. We shall proceed with the statement (b). Let h denote the function

$$h(w) := \frac{\mathrm{sq}_-(w^2+i\gamma)-w}{\mathrm{sq}_-(w^2+i\gamma)+w} = \frac{1}{i\gamma}\big(\mathrm{sq}_-(w^2+i\gamma)-w\big)^2. \tag{4.69}$$

In view of (4.65) and $u=\operatorname{Re} w \le 0$, it is easy to see that for each $w\in F_\infty$,

$$\mathrm{sq}_-(w^2+i\gamma)-w \in G := \{\zeta\in\mathbb{C}:\ \operatorname{Re}\zeta \geqslant 0,\ |\operatorname{Im}\zeta| \le \operatorname{Re}\zeta\},$$

and so $h: F_\infty \to \overline{\mathbb{C}}_-$.

We conclude that the branch $\log_-$ of the logarithm (corresponding to $\arg_-$) is continuously differentiable on $h(F_\infty)$. By the expression for $G_{j,R}$ in (4.61), $G_{j,R}$ is continuously differentiable on F_∞. A direct computation yields

$$\frac{d}{dw}G_{j,R}(w) = \frac{-i}{R\,\mathrm{sq}_-(w^2+i\gamma)}.$$

It is easy to show (see the definition of F_∞ (4.63)) that

$$\min_{w\in F_\infty} |w^2+i\gamma| = C\gamma, \qquad C=\cos\Big(2\arctan\frac{1}{2}\Big) > \frac{1}{2},$$

and so

$$\left|\frac{d}{dw}G_{j,R}(w)\right| < 1, \qquad w\in F_\infty,$$

as long as R satisfies (4.64). Hence, $G_{j,R}: F_j \to F_j$ is a strict contraction mapping for such R, completing the proof. □

4.3.2 The number of eigenvalues and Lieb–Thirring sums for $L_{\gamma,R}$

Now that existence of solutions for the family of equations (4.59) has been established, we may prove lower bounds for Lieb–Thirring sums. Throughout the remainder of the section, we assume that $j \in \mathbb{N}$ and R satisfies (4.64), and we let $w_j = w_j(\gamma,R) \in F_j$ denote the unique solution to the equation $w = G_{j,R}(w)$ in F_j.

As it turns out, one has to impose some restriction on the values j to guarantee that w_j corresponds to an eigenvalue. Precisely, assume that

$$1 \le j \le M_R := \left\lfloor \frac{1}{32\pi} \frac{\gamma R^2}{\log R} \right\rfloor . \tag{4.70}$$

Lemma 4.17. *For R satisfying* (4.64) *and j satisfying* (4.70)*, the inequalities*

$$-\frac{\gamma}{2} \le \operatorname{Im} w_j^2 \le 0 \tag{4.71}$$

hold, so $z_j^2 = w_j^2 + i\gamma \in \mathbb{C}_+$ and $z_j^2 \in \sigma_d(L_{\gamma,R})$.

Proof. Firstly, we claim that for all $\gamma > 0$ and R satisfying (4.64), we have

$$\Phi_\gamma(R) := \frac{\gamma R^2}{\log R} > \frac{C_0^2}{2\log C_0}. \tag{4.72}$$

Since $R \ge 2C_0 > \sqrt{e}$, the function $\Phi_\gamma(R)$ is monotonically increasing and for each $\gamma > 0$

$$\begin{aligned}\Phi_\gamma(R) \ge f(\gamma) &:= C_0^2 \frac{\gamma\left(\gamma^{3/4}+\gamma^{-3/4}\right)^2}{\log C_0 + \log\left(\gamma^{3/4}+\gamma^{-3/4}\right)} \\ &= C_0^2 \frac{\gamma^3 + 2\gamma^{3/2} + 1}{\sqrt{\gamma}\log C_0 + \sqrt{\gamma}\log\left(\gamma^{3/2}+1\right) - \frac{3}{4}\sqrt{\gamma}\log\gamma}.\end{aligned}$$

Since $f(\gamma) \le f(\gamma^{-1})$, $0 < \gamma \le 1$, and $C_0 > e^2$, we see that

$$\min_{\gamma>0} f(\gamma) = \min_{0<\gamma\le 1} f(\gamma) \ge \frac{C_0^2}{\log C_0 + \log 2 + \frac{3}{2e}} > \frac{C_0^2}{\log C_0 + 2} > \frac{C_0^2}{2\log C_0},$$

proving (4.72).

Next, we have

$$M_R > \frac{\Phi_\gamma(R)}{32\pi} - 1 > \frac{1}{32\pi}\frac{C_0^2}{2\log C_0} - 1 \ge 1, \tag{4.73}$$

as long as

$$\frac{C_0^2}{2\log C_0} > 64\pi,$$

which certainly true for the value C_0 in (4.64). By (4.73),

$$\frac{\Phi_\gamma(R)}{32\pi} > 2, \qquad \frac{\Phi_\gamma(R)}{96\pi} > \frac{2}{3} > \frac{1}{2}.$$

We assume that $1 \leq j \leq M_R$, so

$$j + \frac{1}{2} \leqslant \frac{\Phi_\gamma(R)}{32\pi} + \frac{1}{2} < \frac{\Phi_\gamma(R)}{24\pi} = \frac{1}{24\pi}\frac{\gamma R^2}{\log R}. \tag{4.74}$$

Since $A(w_j) \geq 0$, $B_j(w_j) > 0$, we have

$$\begin{aligned} w_j^2 = G_{j,R}^2(w_j) &= \frac{B_j^2(w_j) - A^2(w_j) - 2iB_j(w_j)A(w_j)}{4R^2}, \\ \operatorname{Im} w_j^2 &= -\frac{B_j(w_j)A(w_j)}{2R^2} \leq 0. \end{aligned} \tag{4.75}$$

To prove the lower bound in (4.71), we apply (4.68) and (4.74)

$$A(w_j) \leq \log 2 + 2\log\Big(j + \frac{1}{2}\Big) < 2\log\gamma + 4\log R,$$

and hence

$$B_j(w_j)A(w_j) \leq 4\pi\Big(j + \frac{1}{2}\Big)(\log\gamma + 2\log R).$$

But $R > \gamma^{3/4}$, $\log R > \frac{3}{4}\log\gamma$, and so, by (4.74),

$$\log\gamma + 2\log R < \frac{10}{3}\log R, \;\; B_j(w_j)A(w_j) \leq \frac{1}{6}\frac{\gamma R^2}{\log R}\cdot\frac{10}{3}\log R < \gamma R^2.$$

The lower bound in (4.71) follows. The remaining claims follow from an application of Lemma 4.15. The proof is complete. □

The result of Lemma 4.17 immediately implies a lower bound for the number $N(L_{\gamma,R})$ of eigenvalues of $L_{\gamma,R}$, counting algebraic multiplicities.

Corollary 4.18. *For R satisfying* (4.64)*, we have the lower bound*

$$N(L_{\gamma,R}) \geqslant \left\lfloor \frac{1}{32\pi}\frac{\gamma R^2}{\log R} \right\rfloor.$$

The next result amplifies the above corollary and will be used in our study of the sums $S_{\alpha,\beta}(H_q)$ below. An analogous result for Schrödinger operators on the real line has previously been obtained by Cuenin in [44, Theorem 4], by a different method. Let $N(L_{\gamma,R};\Omega)$ denote the number of eigenvalues of $L_{\gamma,R}$ in a given region $\Omega \subset \mathbb{C}$, counting algebraic multiplicities.

Proposition 4.19. *There exists constants $R_0, C_1 > 0$, depending only on γ, such that for the regions*

$$\Sigma_R := \left\{ \lambda \in \mathbb{C} : \tfrac{\gamma}{2} \leqslant \mathrm{Im}\,(\lambda) \leqslant \gamma, \frac{C_1^{-1} R^2}{\log^2 R} \leqslant |\lambda| \leqslant \frac{C_1 R^2}{\log^2 R} \right\} \tag{4.76}$$

and all $R \geqslant R_0$, we have

$$N(L_{\gamma,R};\Sigma_R) \geqslant \frac{1}{128\pi} \frac{\gamma R^2}{\log R}. \tag{4.77}$$

Proof. In this proof, we shall say that a statement holds for large enough R if there exists $R_0 = R_0(\gamma) > 0$ such that the statement holds for all $R \geqslant R_0$. Furthermore, $C = C(\gamma) > 0$ will denote a constant that may change from line to line.

Consider the unique solution $w_j = w_j(\gamma, R)$ of the equation $w = G_{j,R}(w)$ in F_j, which exists for large enough R, with

$$\left\lceil \frac{1}{64\pi} \frac{\gamma R^2}{\log R} \right\rceil \leqslant j \leqslant \left\lfloor \frac{1}{32\pi} \frac{\gamma R^2}{\log R} \right\rfloor. \tag{4.78}$$

By Lemma 4.17, $\lambda_j := w_j^2 + i\gamma$ is an eigenvalue of $L_{\gamma,R}$ with $\frac{\gamma}{2} \leqslant \mathrm{Im}\,(\lambda_j) \leqslant \gamma$.

By (4.67), we have

$$|A(w_j)| = |A(G_{j,R}(w_j))| \leqslant \log\left(2 + \frac{10\pi^2 (j+\frac{1}{2})^2}{\gamma R^2}\right) \leqslant CR$$

for large enough R. Using the inequality $B_j(w_j) \geqslant 2\pi(j - \frac{1}{2})$ and the lower bound in (4.78), we have

$$|\lambda_j| \geqslant |w_j|^2 - \gamma = \frac{|B_j(w_j)|^2 + |A(w_j)|^2}{4R^2} - \gamma \geqslant \frac{CR^2}{\log^2 R}$$

for large enough R. On the other hand, using the inequality $B_j(w_j) \leqslant 2\pi(j + \frac{1}{2})$ and the upper bound in (4.78), we have

$$|\lambda_j| \leqslant \frac{|B_j(w_j)|^2 + |A(w_j)|^2}{4R^2} + \gamma \leqslant \frac{CR^2}{\log^2 R}$$

for large enough R. It follows that $\lambda_j \in \Sigma_R$ for some constant $C_1 = C_1(\gamma) > 0$ and all large enough R. Finally, we have

$$N(L_{\gamma,R};\Sigma_R) \geqslant \left\lfloor \frac{1}{32\pi}\frac{\gamma R^2}{\log R} \right\rfloor - \left\lceil \frac{1}{64\pi}\frac{\gamma R^2}{\log R} \right\rceil \geqslant \frac{1}{128\pi}\frac{\gamma R^2}{\log R}$$

for large enough R, completing the proof. □

Remark 4.20. An upper bound for the number of eigenvalues for Schrödinger operators with potentials of the form $q_R = q + i\gamma\chi_{[0,R]}$, where q is compactly supported, is obtained in [129, Theorem 8]

$$N(H_{q_R}) \leq \frac{11}{\log 2}\frac{\gamma R^2}{\log R} \tag{4.79}$$

for large enough R. Our particular case corresponds to $q \equiv 0$ and demonstrates that (4.79) is optimal.

The result of Theorem 4.5 states that for each $\varepsilon > 0$ there exists a constant $K(\varepsilon) > 0$, independent from q, so that

$$S_\varepsilon(H_q) \leq K(\varepsilon)\, \|q\|_1^{1+\varepsilon}$$

for any integrable potential q. Our goal here is to obtain corresponding lower bounds for the operators $L_{\gamma,R}$ with potentials q_{db} (4.55) and, thereby, to demonstrate the optimal character of this upper bound with respect to ε. Precisely, we will show that the value $S_0(L_{\gamma,R})$ tends to infinity fast enough as $R \to \infty$.

Theorem 4.21 (= Theorem 4.3)**.** *Suppose that R satisfies* (4.64).

(i) *We have the lower bound*

$$S_0(L_{\gamma,R}) \geq \frac{\|q_{db}\|_1}{16\pi}\log R = \frac{\gamma R}{16\pi}\log R. \tag{4.80}$$

(ii) *Let* $0 < \varepsilon < 1$. *Under the stronger assumption on* R

$$R \geq \frac{4}{e^2\gamma}(64\pi)^{2/\varepsilon} + 1, \tag{4.81}$$

we have the lower bound

$$S_\varepsilon(L_{\gamma,R}) \geq \frac{1}{256\pi\varepsilon}\frac{(\gamma R)^{1+\varepsilon}}{\log^\varepsilon R}\,. \tag{4.82}$$

Proof. (i). The bound from below for $S_0(L_{\gamma,R})$ arises when we take a subset of the eigenvalues, precisely, $\lambda_j = z_j^2 = w_j^2 + i\gamma$, with j from (4.70). So, for $\varepsilon = 0$ we have, in view of Lemma 4.17,

$$S_0(L_{\gamma,R}) \geq \sum_{j=1}^{M_R} \frac{\operatorname{Im}(w_j^2 + i\gamma)}{|w_j^2 + i\gamma|^{1/2}} \geq \frac{\gamma}{2} \sum_{j=1}^{M_R} \frac{1}{\sqrt{\gamma} + |w_j|}. \tag{4.83}$$

But, owing to (4.60),

$$|w_j|^2 = |G_{j,R}(w_j)|^2 = \frac{|A(w_j)|^2 + |B_j(w_j)|^2}{4R^2} \leq \frac{5|B_j(w_j)|^2}{16R^2} \leq \frac{5\pi^2}{4R^2}\left(j + \frac{1}{2}\right)^2,$$

and so

$$S_0(L_{\gamma,R}) \geq \frac{\gamma}{2} \sum_{j=1}^{M_R} \frac{1}{\sqrt{\gamma} + \frac{2\pi}{R}(j+1)}.$$

An elementary inequality

$$\sum_{j=1}^{N} \frac{1}{a + b(j+1)} > \int_2^{N+1} \frac{dx}{a+bx} = \frac{1}{b} \log \frac{a + b(N+1)}{a+2b}$$

with $a = \sqrt{\gamma}$, $b = 2\pi R^{-1}$, $N = M_R$, gives

$$S_0(L_{\gamma,R}) \geq \frac{\gamma R}{4\pi} \log \frac{\sqrt{\gamma} + 2\pi R^{-1}(M_R+1)}{\sqrt{\gamma} + 4\pi R^{-1}} \geq \frac{\gamma R}{4\pi} \log \frac{1 + \frac{\sqrt{\gamma}R}{16\log R}}{1 + \frac{4\pi}{\sqrt{\gamma}R}}. \tag{4.84}$$

Let us check that for R satisfying (4.64), one has

$$\frac{1 + \frac{\sqrt{\gamma}R}{16\log R}}{1 + \frac{4\pi}{\sqrt{\gamma}R}} > R^{1/4}, \quad \frac{\sqrt{\gamma}R}{16\log R} + 1 > R^{1/4} + \frac{4\pi}{\sqrt{\gamma}R^{3/4}}.$$

Indeed,

$$\frac{\sqrt{\gamma}R^{3/4}}{16\log R} = \frac{\gamma^{1/2}R^{2/3}}{16} \frac{R^{1/12}}{\log R} > \frac{C_0^{2/3}}{16} \frac{e}{12} > 1$$

as long as

$$C_0 > \left(\frac{192}{e}\right)^{3/2},$$

which is true for C_0 in (4.64) (at this point the value $C_0 = 600$ comes about). Next,

$$\frac{4\pi}{\sqrt{\gamma}R^{3/4}} = \frac{4\pi}{\gamma^{1/2}R^{2/3}R^{1/12}} < \frac{4\pi}{C_0^{2/3}} < 1$$

as long as $C_0 > (4\pi)^{3/2}$. The bound (4.80) follows directly from (4.84).

(ii). We have, as above in (i),

$$S_\varepsilon(L_{\gamma,R}) \geq \frac{\gamma}{2}\sum_{j=1}^{M_R} \frac{1}{\gamma^{\frac{1-\varepsilon}{2}} + |w_j|^{1-\varepsilon}} \geq \frac{\gamma^{\frac{1+\varepsilon}{2}}}{2}\sum_{j=1}^{M_R} \frac{1}{1+\left(\frac{2\pi}{\sqrt{\gamma}R}(j+1)\right)^{1-\varepsilon}}, \tag{4.85}$$

and so

$$S_\varepsilon(L_{\gamma,R}) \geq \frac{\gamma^{1+\frac{\varepsilon}{2}}R}{4\pi}\int_{\beta_1}^{\beta_2} \frac{dy}{1+y^{1-\varepsilon}}, \quad \beta_1 := \frac{4\pi}{\sqrt{\gamma}R}, \quad \beta_2 := \frac{2\pi(M_R+1)}{\sqrt{\gamma}R}.$$

An elementary inequality $1+y^{1-\varepsilon} \leq 2^\varepsilon(1+y)^{1-\varepsilon}$ leads to the bound

$$\begin{aligned} S_\varepsilon(L_{\gamma,R}) &\geq \frac{\gamma^{1+\frac{\varepsilon}{2}}R}{4\pi 2^\varepsilon}\int_{\beta_1+1}^{\beta_2+1} \frac{dt}{t^{1-\varepsilon}} = \frac{\gamma^{1+\frac{\varepsilon}{2}}R}{4\pi\varepsilon 2^\varepsilon}\Big\{(1+\beta_2)^\varepsilon - (1+\beta_1)^\varepsilon\Big\} \\ &= I_1 - I_2. \end{aligned}$$

We apply once again $(1+\beta_2)^\varepsilon \geq 2^{\varepsilon-1}(1+\beta_2^\varepsilon)$ to estimate the first term

$$I_1 \geq \frac{\gamma^{1+\frac{\varepsilon}{2}}R}{8\pi\varepsilon}\left(1+\beta_2^\varepsilon\right) \geq \frac{\gamma^{1+\frac{\varepsilon}{2}}R}{8\pi\varepsilon}\left(\frac{2\pi(M_R+1)}{\sqrt{\gamma}R}\right)^\varepsilon > \frac{(\gamma R)^{1+\varepsilon}}{128\pi\varepsilon}\frac{1}{\log^\varepsilon R}. \tag{4.86}$$

Concerning the second term, note that (4.81) implies $\sqrt{\gamma}R > 8$, and so

$$(1+\beta_1)^\varepsilon = \left(1+\frac{4\pi}{\sqrt{\gamma}R}\right)^\varepsilon < 1+\frac{\pi}{2} < \pi.$$

Then

$$I_2 \leq \frac{\gamma^{1+\frac{\varepsilon}{2}}R}{4\varepsilon 2^\varepsilon} = \frac{(\gamma R)^{1+\varepsilon}}{4\varepsilon 2^\varepsilon}\frac{1}{(\sqrt{\gamma}R)^\varepsilon} < \frac{(\gamma R)^{1+\varepsilon}}{4\varepsilon}\frac{1}{(\sqrt{\gamma}R)^\varepsilon}.$$

But, under assumption (4.81),

$$\frac{\sqrt{\gamma}R}{\log R} = \frac{\sqrt{\gamma}R^{1/2}}{\log R}R^{1/2} \geq \frac{\sqrt{\gamma}e}{2}R^{1/2} \geq (64\pi)^{1/\varepsilon},$$

so

$$\left(\frac{\log R}{\sqrt{\gamma}R}\right)^\varepsilon \leqslant \frac{1}{64\pi}, \qquad \frac{1}{(\sqrt{\gamma}R)^\varepsilon} \leqslant \frac{1}{64\pi\log^\varepsilon R}.$$

Hence,

$$I_2 \leq \frac{(\gamma R)^{1+\varepsilon}}{256\pi\varepsilon\log^\varepsilon R}.$$

Comparing the latter with (4.86), we come to (4.82). The proof is complete. □

Remark 4.22. The same methods lead to lower bounds for more general sums, which were considered in [22]. Let $p \geqslant 1$. A slight modification of the proof of Theorem 4.21 (i) yields

$$\sum_{\lambda \in \sigma_d(L_{\gamma,R})} \frac{\operatorname{dist}^p(\lambda, \mathbb{R}_+)}{|\lambda|^{1/2}} \geqslant \frac{\gamma^p R \log R}{8\pi \cdot 2^p}, \tag{4.87}$$

provided R satisfies (4.64). Indeed, the only place in the proof of Theorem 4.21 (i) that needs to be modified is (4.83), and there we use the inequality

$$\operatorname{Im}(w_j^2 + i\gamma)^p \geqslant (\gamma/2)^p.$$

Furthermore, by the spectral enclosure [69] mentioned in the introduction, we have

$$|\lambda|^{s-1/2} \leqslant \|q_{db}\|_1^{2s-1} = (\gamma R)^{2s-1}, \quad \lambda \in \sigma_d(L_{\gamma,R}), \quad s \geq \frac{1}{2},$$

so it follows from (4.87) that

$$\sum_{\lambda \in \sigma_d(L_{\gamma,R})} \frac{\operatorname{dist}^p(\lambda, \mathbb{R}_+)}{|\lambda|^s} \geqslant \frac{1}{8\pi \cdot 2^p} \frac{\gamma^p R \log R}{(\gamma R)^{2s-1}}. \tag{4.88}$$

Now take $R = n$ and $\gamma = n^{-1}$ for $n \in \mathbb{N}$. Then, R satisfies (4.64), and so (4.88) holds, for large enough n. Noting that $\|q_{db}\|^p_{L^p(\mathbb{R}_+)} = \gamma^p R$ and $\gamma R = 1$, and taking the limit $n \to \infty$, we conclude that

$$\sup_{0 \neq q \in L^p(\mathbb{R}_+) \cap L^1(\mathbb{R}_+)} \frac{1}{\|q\|^p_{L^p(\mathbb{R}_+)}} \sum_{\lambda \in \sigma_d(H_q)} \frac{\operatorname{dist}^p(\lambda, \mathbb{R}_+)}{|\lambda|^s} = \infty. \tag{4.89}$$

In view of Proposition 4.26 below, the statement (4.88) holds analogously for Schrödinger operators on $L^2(\mathbb{R})$ with symmetric potentials $i\gamma\chi_{[-R,R]}$, hence (4.89) holds for Schrödinger operators on $L^2(\mathbb{R})$, which implies [22, Theorem 9].

Recall that the generalised Lieb–Thirring sum $S_{\alpha,\beta}(H_q)$ is defined by (4.13). The problem we are interested in now is the range of positive parameters (α, β) for which

$$\mathscr{S}_{\alpha,\beta} := \sup_{0 \neq q \in L^1(\mathbb{R}_+)} \frac{S_{\alpha,\beta}(H_q)}{\|q\|_1} < \infty.$$

The results are illustrated in Figure 4.2.

Proposition 4.23. *We have*

$$\mathscr{S}_{\alpha,\beta} < \infty, \qquad \text{for } \alpha > \frac{1}{2}, \ \beta \geq 1, \tag{4.90}$$

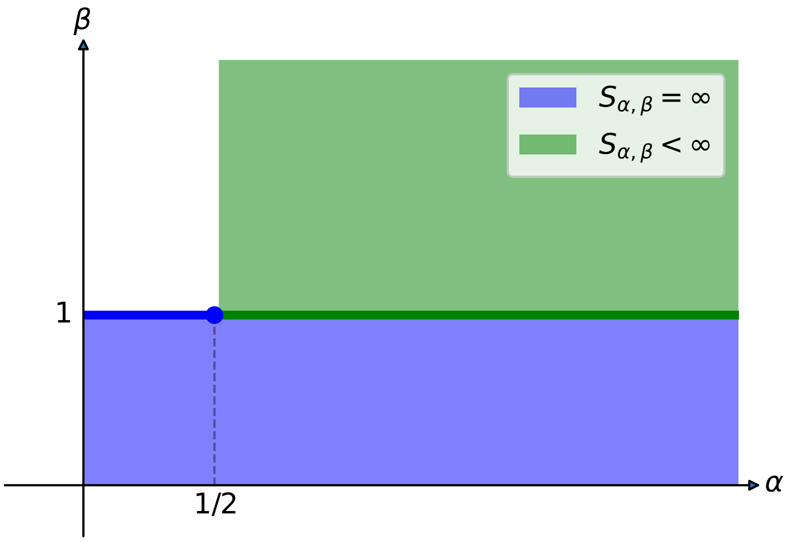

Figure 4.2 An illustration of Proposition 4.23.

and

$$\mathscr{S}_{\alpha,\beta} = \infty, \qquad \text{for } \ \alpha > 0,\ 0 < \beta < 1, \ \text{ and } \ 0 < \alpha \leq \frac{1}{2},\ \beta = 1. \tag{4.91}$$

Proof. Theorem 4.5 implies that we have $\mathscr{S}_{\alpha,1} < \infty$ for $\alpha > \frac{1}{2}$. Furthermore, by $\operatorname{dist}(\lambda, \mathbb{R}_+) \leqslant |\lambda|$, the function $f(\beta) = S_{\alpha,\beta}(H_q)$ is monotone decreasing for fixed α, from which (4.90) follows.

By Proposition 4.19, for $\alpha > 0$ and $0 < \beta < 1$, we have

$$\begin{aligned} S_{\alpha,\beta}^{2\alpha}(H_q) &\geqslant N(L_{\gamma,R};\Sigma_R) \inf_{\lambda \in \Sigma_R} \left(\frac{\operatorname{dist}(\lambda, \mathbb{R}_+)}{|\lambda|} \right)^{\beta} |\lambda|^{\alpha} \\ &\geqslant \frac{1}{128\pi} \frac{\gamma R^2}{\log R} \left(\frac{\gamma}{2} \right)^{\beta} \left(\frac{\min\left\{C_1, C_1^{-1}\right\} R^2}{\log^2 R} \right)^{\alpha-\beta} \\ &= C \frac{R^{2(1-\beta)}}{(\log R)^{1+2\alpha-2\beta}} (\gamma R)^{2\alpha} \end{aligned}$$

for some constant $C = C(\gamma) > 0$ and all large enough R. The first statement in (4.91) follows by considering the limit $R \to \infty$.

By (4.88) with $p = \beta = 1$ and $s = 1 - \alpha \geqslant \frac{1}{2}$, we have

$$S_{\alpha,\beta}^{2\alpha}(L_{\gamma,R}) = \sum_{\lambda \in \sigma_d(L_{\gamma,R})} \frac{\operatorname{dist}(\lambda, \mathbb{R}_+)}{|\lambda|^{1-\alpha}} \geqslant \frac{1}{16\pi} (\gamma R)^{2\alpha} \log R$$

for large enough R. The second statement in (4.91) follows by again considering the limit $R \to \infty$. $\square$

We are in a position now to obtain a two-sided bound for the Jensen sums $J(L_{\gamma,R})$. Recall that $\|q_{db}\|_1 = \gamma R$.

Proposition 4.24. *For all R satisfying* (4.64)*, the following two-sided inequality holds*

$$\frac{1}{32\pi} \le \frac{J(L_{\gamma,R})}{\gamma R \log R} \le 42. \tag{4.92}$$

Proof. The lower bound is a direct consequence of (4.80) and (4.8). To prove the upper bound, we apply Corollary 4.12, so

$$J(L_{\gamma,R}) \le 7\left[\frac{1}{R} + \gamma R + \gamma R \log R + \gamma R \log(1+\gamma R)\right].$$

Note that (4.64) implies $R > e$ and $R^2 > \gamma + \gamma^{-1} + 1$. Hence,

$$\frac{1}{R} < \gamma R \log R, \quad \gamma R < \gamma R \log R, \quad \log(1+\gamma R) < 3 \log R,$$

and inequality (4.92) follows. $\square$

4.4 An integrable potential with divergent Jensen sum

The aim of this section is to construct a potential $q_\infty \in L^1(\mathbb{R}_+)$ such that $J(H_{q_\infty}) = \infty$. We shall begin, in Sections 4.4.1 and 4.4.2, by collecting some well-known facts about Schrödinger operators on both the half-line and the full real line. We shall then proceed to prove two spectral approximation lemmas in Section 4.4.3. These will give us information on the eigenvalues of Schrödinger operators on the half-line, for potentials consisting of a sum of compactly supported functions whose supports are separated from one another by large enough distances. The consideration of Schrödinger operators on the full real line is required in order to formulate one of these lemmas. With these tools at hand, the potential q_∞ is constructed in Section 4.4.4.

4.4.1 Case of the half-line

Consider the following differential equation on the positive half-line $\mathbb{R}_+$

$$h[y] := -y'' + q(x)y = z^2 y, \qquad q \in L^1(\mathbb{R}_+), \quad z \in \mathbb{C}_+, \tag{4.93}$$

where the potential q may be complex-valued. There exists a unique pair of solutions $e_\pm(\cdot,z;q)$ of (4.93), such that $e_\pm(x,\cdot;q)$ are analytic on the upper half-plane $\mathbb{C}_+$, and

$$\begin{aligned} e_+(x,z;q) &= e^{ixz}(1+o(1)), & e'_+(x,z;q) &= ize^{ixz}(1+o(1)), \\ e_-(x,z;q) &= e^{-ixz}(1+o(1)), & e'_-(x,z;q) &= -ize^{-ixz}(1+o(1)), \end{aligned} \tag{4.94}$$

as $x \to +\infty$, uniformly on compact subsets of $\mathbb{C}_+$ (see, e.g., [108, Sections 2.2 and 2.3]). The Wronskian satisfies

$$W(z,q) = W(e_+,e_-) = -2iz. \tag{4.95}$$

Recall that $H = H_q$ denotes the Dirchlet Schrödinger operator on $L^2(\mathbb{R}_+)$.

4.4.2 Case of the real line

Consider the following differential equation on the real line $\mathbb{R}$

$$\mathfrak{h}[y] := -y'' + q(x)y = z^2 y, \qquad q \in L^1(\mathbb{R}), \quad z \in \mathbb{C}_+, \tag{4.96}$$

where the potential q may be complex-valued.

The result below is likely to be well known. We provide the proof for the sake of completeness.

Proposition 4.25. *There exists a unique pair of solutions $\mathfrak{e}_\pm(\cdot,z;q)$ of* (4.96)*, known as the Jost solutions, such that $\mathfrak{e}_\pm(x,\cdot;q)$ are analytic on the upper half-plane $\mathbb{C}_+$,*

$$\mathfrak{e}_+(x,z;q) = e^{izx}(1+o(1)), \quad \mathfrak{e}'_+(x,z;q) = ize^{izx}(1+o(1)) \tag{4.97}$$

as $x \to +\infty$, and

$$\mathfrak{e}_-(x,z;q) = e^{-izx}(1+o(1)), \quad \mathfrak{e}'_-(x,z;q) = -ize^{-izx}(1+o(1)) \tag{4.98}$$

as $x \to -\infty$, uniformly on compact subsets of $\mathbb{C}_+$.

$\lambda = z^2$ is the eigenvalue of the corresponding Schrödinger operator $\mathscr{H}_q$ on $L^2(\mathbb{R})$ if and only if $\mathfrak{e}_+$ and $\mathfrak{e}_-$ are proportional, that is, the Wronskian

$$\mathcal{W}(z,q) := \mathfrak{e}_+(0,z;q)\mathfrak{e}'_-(0,z;q) - \mathfrak{e}_-(0,z;q)\mathfrak{e}'_+(0,z;q) = 0.$$

The algebraic multiplicity $\nu(\lambda,\mathscr{H}_q)$ of the eigenvalue $\lambda = z^2$ equals the multiplicity of the corresponding zero of $\mathcal{W}(\cdot,q)$.

Proof. The first statement, regarding the existence and analytic properties of the Jost solutions, may be seen by extending appropriate Jost solutions on the half-line. Indeed, let $s(x,z)$ and $c(x,z)$ denote the solutions of (4.96) such that

$$s(0,z) = c'(0,z) = 0, \qquad s'(0,z) = c(0,z) = 1.$$

We define

$$\begin{aligned} e_+(x,z;q) &= c(x,z)e_+(0,z;q_+) + s(x,z)e_+'(0,z;q_+) \\ e_-(x,z;q) &= c(x,z)e_+(0,z;q_-) - s(x,z)e_+'(0,z;q_-), \end{aligned}$$

where $q_\pm$ are potentials on the half-line such that

$$q_\pm(x) := q(\pm x), \qquad x \in \mathbb{R}_+.$$

Notice that the functions $e_\pm(\pm x,z;q)$, $x \in \mathbb{R}_+$, solve the Schrödinger equations (4.93) with $q = q_\pm$. By computing the boundary conditions of $e_\pm(\pm x,z;q)$ at $x = 0$, we see that

$$\begin{aligned} e_+(x,z;q) &= e_+(x,z;q_+), \qquad && x \in \mathbb{R}_+, \\ e_-(x,z;q) &= e_+(-x,z;q_-), \qquad && x \in \mathbb{R}_-. \end{aligned}$$

The asymptotic relations (4.97) and (4.98) follow. The analyticity statement follows from the fact that $s(x,\cdot)$ and $c(x,\cdot)$ are entire functions (see, for instance, [135, Lemma 5.7]) as well as the analyticity of $e_+(0,\cdot;q_\pm)$ and $e_+'(0,\cdot;q_\pm)$ on $\mathbb{C}_+$.

Next, we prove the second statement, characterising the eigenvalues of $\mathscr{H}_q$. If the Jost solutions $e_\pm$ are proportional, the eigenfunction exists, and so z^2 is the eigenvalue. Conversely, assume that e_+ and e_- are linearly independent. The limit case on each half-line (cf. (4.94)) means that $e_\pm \notin L^2(\mathbb{R}_\mp)$. Hence, all solutions of (4.96) from $L^2(\mathbb{R}_\pm)$ are of the form $c_\pm\, e_\pm$. If $z^2 \in \sigma_d(\mathscr{H}_q)$, there is a solution $e \in L^2(\mathbb{R})$ of (4.96) with

$$e(x,z;q) = \begin{cases} c_+ e_+(x,z;q), & x \in \mathbb{R}_+, \\ c_- e_-(x,z;q), & x \in \mathbb{R}_-, \end{cases}$$

and so e_+ and e_- are proportional. A contradiction completes the proof.

The final statement follows from [93, Theorem 28]. □

In what follows, we shall suppress indication of z dependence where appropriate.

Compactly supported potentials

Assume that q is compactly supported,
$\operatorname{supp} q \subset [-a,a]$, $a>0$. Then

$$e_-(x,q) = e^{-izx}, \qquad e_-'(x,q) = -ize^{-izx}, \qquad x \leqslant -a. \tag{4.99}$$

Also, there exist $A_\pm(z)$ such that

$$\begin{aligned} e_+(x,q) &= A_+(z)e^{izx} + A_-(z)e^{-izx}, \\ e_+'(x,q) &= iz\Big(A_+(z)e^{izx} - A_-(z)e^{-izx}\Big), \quad x \leq -a. \end{aligned} \tag{4.100}$$

We can easily calculate the Wronskian. For $x \leq -a$,

$$\begin{aligned} W(e_+,e_-) = {}& \Big(A_+(z)e^{izx} + A_-(z)e^{-izx}\Big)\Big(-ize^{-izx}\Big) \\ & - iz\Big(A_+(z)e^{izx} - A_-(z)e^{-izx}\Big)e^{-izx} = -2izA_+(z) \end{aligned}$$

and so

$$W(z,q) = W(e_+,e_-) = -2izA_+(z). \tag{4.101}$$

Note that equations analogous to (4.99), (4.100) and (4.101) also hold for the opposite half-line $x \geqslant a$.

Shifted potentials

Next, consider a shifted equation

$$\hbar_X[y] := -y'' + q(x-X)y = z^2 y, \qquad X > 0. \tag{4.102}$$

All its solutions are shifts of the corresponding solutions of (4.96). In particular, the Jost solutions satisfy

$$e_\pm(x, q(\cdot - X)) = e^{\pm izX}\, e_\pm(x-X, q). \tag{4.103}$$

Symmetrisation of potentials

The following result will allow us to apply the lower bounds of Section 4.3 to even extensions of dissipative barrier potentials. We mentioned it in the introduction, see (4.30).

Proposition 4.26. *Given a potential $q \in L^1(\mathbb{R}_+)$, let q_e be its even extension on the line*

$$q_e(-x) = q_e(x), \quad x \in \mathbb{R}; \qquad q_e|_{\mathbb{R}_+} = q.$$

Then $\sigma_d(H_q) \subset \sigma_d(\mathscr{H}_{q_e})$, and moreover, for each $\lambda \in \sigma_d(H_q)$,

$$\nu(\lambda, H_q) \leqslant \nu(\lambda, \mathscr{H}_{q_e}). \tag{4.104}$$

Proof. It is clear from the definition, that

$$e_-(x,z;q_e) = e_+(-x,z;q_e), \quad e'_-(x,z;q_e) = -e'_+(-x,z;q_e), \qquad x \in \mathbb{R}.$$

Hence, $W(z,q_e) = -2e_+(0,z;q_e)\,e'_+(0,z;q_e)$. But $q_e|_{\mathbb{R}_+} = q$, so

$$e_+(x,z;q_e) = e_+(x,z;q), \quad x \in \mathbb{R}_+; \quad W(z,q_e) = -2e_+(0,z;q)\,e'_+(0,z;q).$$

The result now follows from Proposition 4.25. □

4.4.3 Auxillary spectral approximation results

Large shifts

The following lemma and its corollary are crucial for the proof of Theorem 4.30. A more general, but slightly less precise, version of this result has been proven in [17, Lemma 4] by invoking the abstract notion of limiting essential spectrum (cf. [18]). In contrast to that result, it is important for us to account for algebraic multiplicities, and our proof only relies on basic ODE theory and complex analysis.

Lemma 4.27. *Let $q \in L^1(\mathbb{R}_+)$ and $\mathsf{q} \in L^1(\mathbb{R})$ be potentials with compact supports. For any $X > 0$, denote*

$$q(x,X) := q(x) + \mathsf{q}(x-X), \qquad x \in \mathbb{R}_+.$$

Then $q(\cdot,X) \in L^1(\mathbb{R}_+)$ for all $X > 0$, and

$$\lim_{X\to\infty} e_+(0,z;q(\cdot,X)) = -\frac{e_+(0,z;q)\,W(z,\mathsf{q})}{2iz} = e_+(0,z;q)\frac{W(z,\mathsf{q})}{W(z,\mathsf{q})} \tag{4.105}$$

uniformly on compact subsets of $\mathbb{C}_+$.

Proof. Assume that

$$\operatorname{supp} q \subset [0,b], \qquad \operatorname{supp} \mathsf{q} \subset [-a,a], \qquad a,b > 0,$$

so that $\operatorname{supp} q(\cdot - X) \subset [X-a, X+a]$. Assume also that X is so large that

$$b < \frac{X}{2} := Y < X - a.$$

Then $\operatorname{supp} q(\cdot - X) \subset \mathbb{R}_+$, and the supports of q and $q(\cdot - X)$ are disjoint. For the Jost solution, we have

$$e_+(x, q(\cdot, X)) = \begin{cases} c_+ e_+(x,q) + c_- e_-(x,q), & 0 \le x \le Y \\ e_+(x, q(\cdot - X)) = e^{izX} e_+(x-X, q), & x > Y, \end{cases} \tag{4.106}$$

for some $c_\pm = c_\pm(X,z) \in \mathbb{C}$. The adjustment conditions at Y yield

$$\begin{aligned} c_+ e_+(Y,q) + c_- e_-(Y,q) &= e^{izX} e_+(-Y,q), \\ c_+ e'_+(Y,q) + c_- e'_-(Y,q) &= e^{izX} e'_+(-Y,q), \end{aligned}$$

or, in matrix form,

$$\begin{bmatrix} e_+(Y,q) & e_-(Y,q) \\ e'_+(Y,q) & e'_-(Y,q) \end{bmatrix} \begin{bmatrix} c_+ \\ c_- \end{bmatrix} = e^{izX} \begin{bmatrix} e_+(-Y,q) \\ e'_+(-Y,q) \end{bmatrix}.$$

A matrix inversion yields

$$\begin{bmatrix} c_+ \\ c_- \end{bmatrix} = \frac{e^{izX}}{W(z,q)} \begin{bmatrix} e'_-(Y,q) & -e_-(Y,q) \\ -e'_+(Y,q) & e_+(Y,q) \end{bmatrix} \begin{bmatrix} e_+(-Y,q) \\ e'_+(-Y,q) \end{bmatrix}.$$

We can now calculate the Jost function from the upper relation in (4.106), taking into account (4.94) and (4.95)

$$\begin{aligned} & e_+(0, q(\cdot, X)) = c_+ e_+(0,q) + c_- e_-(0,q) \\ &= -\frac{e^{izY}}{2iz} \begin{bmatrix} e_+(0,q) & e_-(0,q) \end{bmatrix} \begin{bmatrix} -iz + o(1) & -1 + o(1) \\ e^{izX}(-iz + o(1)) & e^{izX}(1 + o(1)) \end{bmatrix} \begin{bmatrix} e_+(-Y,q) \\ e'_+(-Y,q) \end{bmatrix} \\ &= -\frac{e^{izY}}{2iz} \begin{bmatrix} e_+(0,q) & e_-(0,q) \end{bmatrix} \begin{bmatrix} f_+(X,q) \\ f_-(X,q) \end{bmatrix}, \end{aligned}$$

where

$$\begin{aligned} f_+(X,q) &:= (-iz + o(1)) e_+(-Y,q) + (-1 + o(1)) e'_+(-Y,q), \\ f_-(X,q) &:= e^{izX} \left\{ (-iz + o(1)) e_+(-Y,q) + (1 + o(1)) e'_+(-Y,q) \right\}, \ Y = \frac{X}{2}. \end{aligned}$$

Since $Y > a$, then, by (4.100),

$$e^{izY} f_+(X,q) = (-iz + o(1))\big(A_+ + A_- e^{izX}\big) + (-iz + o(1))\big(A_+ - A_- e^{izX}\big)$$
$$= -2izA_+ + o(1), \qquad X \to \infty,$$

uniformly on compact subsets of $\mathbb{C}_+$. It is clear from (4.100), that

$$e^{izY} f_-(X,q) = o(1), \qquad X \to \infty,$$

also uniformly on compact subsets of $\mathbb{C}_+$. The relation (4.101) completes the proof. □

Before we move on, let us clarify what we shall mean by a collection of eigenvalues. When we say that there exists a collection of $N \in \mathbb{N}$ eigenvalues $\lambda_1, \dots, \lambda_N$ of an operator T, we mean that:

1. λ_j is an eigenvalue of T for each $j \in \{1, \dots, N\}$, and
2. if λ is repeated ν times in the collection $\lambda_1, \dots, \lambda_N$, then λ is an eigenvalue of T with algebraic multiplicity at least ν.

An integer-valued function $\nu(\cdot, T)$ is said to be an algebraic multiplicity with respect to a linear operator T, if $\nu(\lambda, T)$ equals the algebraic multiplicity of λ in case when $\lambda \in \sigma_d(T)$, and $\nu(\lambda, T) = 0$ otherwise.

Corollary 4.28. *Let the potentials q and $\mathfrak{q}$ be defined as above. Given $\lambda \in \mathbb{C} \backslash \mathbb{R}_+$, put*

$$\nu = \nu(\lambda) := \nu(\lambda, H_q) + \nu(\lambda, \mathscr{H}_{\mathfrak{q}}). \tag{4.107}$$

Then $\lambda \in \sigma_d(H_q) \cup \sigma_d(\mathscr{H}_{\mathfrak{q}})$, if and only if there exists a collection of ν eigenvalues $\lambda_X^{(1)}$, ..., $\lambda_X^{(\nu)}$ of $H_{q(\cdot,X)}$, $X > 0$ large enough, such that

$$\lim_{X \to \infty} \lambda_X^{(j)} = \lambda, \qquad j = 1, 2, \dots, \nu.$$

Proof. By Proposition 4.25 (and similar property of the Jost function $e_+(0, \cdot; q)$), $\lambda = z^2 \in \sigma_d(H_q) \cup \sigma_d(\mathscr{H}_{\mathfrak{q}})$ if and only if $z \in \mathbb{C}_+$ is a root of the right-hand side (4.105) with multiplicity equal to $\nu(\lambda)$ (4.107). The rest is a direct consequence of Lemma 4.27 and Hurwitz's theorem. □

In particular, note that if $\nu(\mu, H_q) = \nu(\mu, \mathscr{H}_{\mathfrak{q}}) = 0$, then μ is separated from the discrete spectra $\sigma_d(H_{q(\cdot,X)})$ for all large enough X.

Truncation

Given a potential $q \in L^1(\mathbb{R}_+)$, we define its truncation at the level $X > 0$ as

$$q_X(x) := \begin{cases} q(x), & 0 \le x \le X; \\ 0, & x > X. \end{cases} \tag{4.108}$$

Let $(X_n)_{n\in\mathbb{N}}$ be a sequence of positive numbers such that $\lim_{n\to\infty} X_n = \infty$. Put

$$q_n := q_{X_n}, \qquad H_n := H_{q_n}.$$

Lemma 4.29. *In the above notation, the limit relation*

$$\lim_{X\to\infty} e_+(0,z;q_X) = e_+(0,z;q) \tag{4.109}$$

holds uniformly on compact subsets of $\mathbb{C}_+$. *In particular,* $\lambda \in \mathbb{C}\backslash\mathbb{R}_+$ *is an eigenvalue of* $H = H_q$ *of algebraic multiplicity* ν *if and only if there exists a collection of eigenvalues* $\lambda_n^{(1)}, \dots, \lambda_n^{(\nu)}$ *of* H_n *such that*

$$\lim_{n\to\infty} \lambda_n^{(j)} = \lambda, \qquad j = 1,2,\dots,\nu.$$

Proof. The argument is similar to one above. We have

$$e_+(x,q_X) = \begin{cases} c_+e_+(x,q) + c_-e_-(x,q), & 0 \le x < X; \\ e^{izx}, & x \ge X, \end{cases}$$

$c_\pm = c_\pm(X,z)$. The adjustment conditions at X yield

$$c_+e_+(X,q) + c_-e_-(X,q) = e^{izX},$$
$$c_+e'_+(X,q) + c_-e'_-(X,q) = iz\,e^{izX},$$

or in matrix form

$$\begin{bmatrix} e_+(X,q) & e_-(X,q) \\ e'_+(X,q) & e'_-(X,q) \end{bmatrix} \begin{bmatrix} c_+ \\ c_- \end{bmatrix} = e^{izX} \begin{bmatrix} 1 \\ iz \end{bmatrix}$$

The matrix inversion gives

$$\begin{bmatrix} c_+ \\ c_- \end{bmatrix} = -\frac{e^{izX}}{2iz} \begin{bmatrix} e'_-(X,q) & -e_-(X,q) \\ -e'_+(X,q) & e_+(X,q) \end{bmatrix} \begin{bmatrix} 1 \\ iz \end{bmatrix},$$

and so

$$c_+(X,z) = -\frac{e^{izX}}{2iz}\Big[e'_-(X,q) - ize_-(X,q)\Big],$$
$$c_-(X,z) = -\frac{e^{izX}}{2iz}\Big[-e'_+(X,q) + ize_+(X,q)\Big].$$

Finally,

$$e_+(0,q_X) =$$
$$-\frac{e^{izX}}{2iz}\Big\{\Big[e'_-(X,q) - ize_-(X,q)\Big]e_+(0,q) + \Big[-e'_+(X,q) + ize_+(X,q)\Big]e_-(0,q)\Big\},$$

and (4.109) follows from the asymptotic relations (4.94).

The second statement is clear thanks to Hurwitz's theorem. □

4.4.4 Main result

We are in a position now to prove the main result of the section.

Theorem 4.30. *There exists a potential $q_\infty \in L^1(\mathbb{R}_+)$ with infinite Jensen sum.*

Proof. Let $(\gamma_n)_{n\in\mathbb{N}}, (R_n)_{n\in\mathbb{N}}, (X_n)_{n\in\mathbb{N}} \subset \mathbb{R}_+$, to be further specified. Define a sequence of Schrödinger operators on the line

$$\mathscr{L}_n y := -y'' + \ell_n y, \qquad \ell_n(x) := i\gamma_n \chi_{[-R_n,R_n]}(x) \in L^1(\mathbb{R}), \quad n \in \mathbb{N}. \tag{4.110}$$

Let $(N_n)_{n\in\mathbb{N}_0}$ be defined such that $N_0 = 0$ and, for $n \geqslant 1$, $N_n - N_{n-1}$ equals the number of eigenvalues of $\mathscr{L}_n$, counting algebraic multiplicity. We place all the eigenvalues $(\lambda_j)_{j\in\mathbb{N}}$ of all operators $\mathscr{L}_n$ in a single sequence in such a way that

$$\{\lambda_{N_{n-1}+1}, \dots, \lambda_{N_n}\} = \sigma_d(\mathscr{L}_n), \qquad n \in \mathbb{N}.$$

Define consecutively a sequence of potentials

$$q_n(x) := q_{n-1}(x) + i\gamma_n \chi_{[X_n, X_n+2R_n]}(x) = q_{n-1}(x) + \ell_n(x - X_n - R_n), \quad n \in \mathbb{N},$$

$q_0 \equiv 0$, or, in other words,

$$q_n(x) = \sum_{k=1}^{n} i\gamma_k \chi_{[X_k, X_k+2R_k]}(x). \tag{4.111}$$

We assume that $X_{k+1} > X_k + 2R_k$, so the intervals $[X_k, X_k + 2R_k]$, $k \in \mathbb{N}$, are disjoint.

Let M_n denote the cardinality of the discrete spectrum $\sigma_d(H_{q_n})$, counting algebraic multiplicity

$$\sigma_d(H_{q_n}) = \{\lambda_{j,n}\}_{j=1}^{M_n}.$$

In view of Corollary 4.28, we see that for large enough X_n,

$$M_{n-1} + N_n - N_{n-1} \leq M_n, \qquad N_n - N_{n-1} \leq M_n - M_{n-1},$$

and, as $M_0 = N_0 = 0$, it follows $N_n \leq M_n$ for all $n \in \mathbb{N}$.

By Corollary 4.28, for each $n \in \mathbb{N}$, we can set X_n large enough such that the collection of eigenvalues $\lambda_{j,n}$, $j = 1,...,N_n$, of H_{q_n} (note that $N_n \leq M_n$) satisfy

$$\begin{gathered}|\lambda_{j,n} - \lambda_j| + |\mathrm{Im}\sqrt{\lambda_{j,n}} - \mathrm{Im}\sqrt{\lambda_j}| \leq \frac{3}{(\pi n)^2}\,\mathrm{Im}\sqrt{\lambda_j},\\ j = N_{n-1}+1,\ldots,N_n, \quad n \in \mathbb{N},\end{gathered} \tag{4.112}$$

and

$$\begin{gathered}|\lambda_{j,n} - \lambda_{j,n-1}| + |\mathrm{Im}\sqrt{\lambda_{j,n}} - \mathrm{Im}\sqrt{\lambda_{j,n-1}}| \leq \frac{3}{(\pi n)^2}\,\mathrm{Im}\sqrt{\lambda_j},\\ j = 1,\ldots,N_{n-1}, \quad n = 2,3,\ldots.\end{gathered} \tag{4.113}$$

For each fixed $j \in \mathbb{N}$, $\lambda_{j,n}$ exists for all $n \geqslant m$, where $m \in \mathbb{N}$ is such that $\lambda_j \in \sigma_d(\mathscr{L}_m)$. The sequence $(\lambda_{j,n})_{n \geqslant m}$ is Cauchy, so there exists

$$\mu_j := \lim_{n\to\infty} \lambda_{j,n}.$$

Next, putting $\lambda_{j,m-1} := \lambda_j$, we have for any $k \geqslant m+1$

$$\sum_{n=m}^{k}\left(\mathrm{Im}\sqrt{\lambda_{j,n}} - \mathrm{Im}\sqrt{\lambda_{j,n-1}}\right) = \mathrm{Im}\sqrt{\lambda_{j,k}} - \mathrm{Im}\sqrt{\lambda_j},$$

so

$$\begin{aligned}&\left|\mathrm{Im}\sqrt{\lambda_{j,k}} - \mathrm{Im}\sqrt{\lambda_j}\right| \leq \sum_{n=m}^{k}\left|\mathrm{Im}\sqrt{\lambda_{j,n}} - \mathrm{Im}\sqrt{\lambda_{j,n-1}}\right|\\ &= \left|\mathrm{Im}\sqrt{\lambda_{j,m}} - \mathrm{Im}\sqrt{\lambda_j}\right| + \sum_{n=m+1}^{k}\left|\mathrm{Im}\sqrt{\lambda_{j,n}} - \mathrm{Im}\sqrt{\lambda_{j,n-1}}\right|\\ &\leq \frac{3\,\mathrm{Im}\sqrt{\lambda_j}}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2} = \frac{1}{2}\,\mathrm{Im}\sqrt{\lambda_j},\end{aligned}$$

whence it follows, as $k \to \infty$, that

$$\operatorname{Im}\sqrt{\mu_j} \geq \frac{1}{2}\operatorname{Im}\sqrt{\lambda_j}, \qquad j \in \mathbb{N}, \tag{4.114}$$

and in particular, $\mu_j \in \mathbb{C}\backslash\mathbb{R}_+$.

Set

$$\begin{aligned} \gamma_n &= \frac{1}{(n\log^2(n+2))^4} < 1, \\ R_n &= 1200\,\gamma_n^{-3/4} = 1200\,(n\log^2(n+2))^3, \quad n \in \mathbb{N}. \end{aligned} \tag{4.115}$$

Define a potential on $\mathbb{R}_+$

$$q_\infty := \sum_{n=1}^{\infty} i\gamma_n \chi_{[X_n, X_n+2R_n]}. \tag{4.116}$$

Then,

$$\|q_\infty\|_1 = 2\sum_{n=1}^{\infty} \gamma_n R_n = 2400\sum_{n=1}^{\infty} \frac{1}{n\log^2(n+2)} < \infty,$$

so $q_\infty \in L^1(\mathbb{R}_+)$.

The partial sums (4.111) can be viewed as truncations of q_∞ at the level $X_n + 2R_n$. Lemma 4.29 implies that for each $j \in \mathbb{N}$, μ_j is an eigenvalue of H_{q_∞} with algebraic multiplicity greater than or equal to the number of times it appears in the sequence $(\mu_k)_{k\in\mathbb{N}}$. It follows that

$$J(H_{q_\infty}) \geqslant \sum_{j=1}^{\infty} \operatorname{Im}\sqrt{\mu_j} \geqslant \frac{1}{2}\sum_{j=1}^{\infty} \operatorname{Im}\sqrt{\lambda_j} = \frac{1}{2}\sum_{n=1}^{\infty} J(\mathscr{L}_n).$$

Recall that $L_n := L_{\gamma_n, R_n}$ is defined in (4.25) as the Schrödinger operator on $L^2(\mathbb{R}_+)$ with potential $i\gamma_n\chi_{[0,R_n]}$. By Proposition 4.26, any eigenvalue of L_n is also an eigenvalue of $\mathscr{L}_n$, and (4.104) holds. Hence, employing the left inequality in Proposition 4.24, we have

$$J(\mathscr{L}_n) \geqslant J(L_n) \geqslant \frac{1}{32\pi}\gamma_n R_n \log R_n, \qquad R_n \geqslant 600(\gamma_n^{3/4} + \gamma_n^{-3/4}). \tag{4.117}$$

The latter inequality is true for all $n \in \mathbb{N}$ due to the choice of R_n (4.115) and $\gamma_n < 1$. Consequently,

$$J(H_{q_\infty}) \geqslant \frac{1}{64\pi}\sum_{n=1}^{\infty} \gamma_n R_n \log R_n = \frac{600}{32\pi}\sum_{n=1}^{\infty} \frac{\log R_n}{n\log^2(n+2)}. \tag{4.118}$$

Since $\log R_n \sim 3\log n$ as $n \to \infty$, the sum on the right hand side of (4.118) diverges. We conclude that the Jensen sum $J(H_{q_\infty}) = \infty$, completing the proof. $\square$

Chapter 5

Spectral approximation for the Laplacian on rough domains

Declaration and acknowledgements:
This chapter is joint work with **Frank Rösler** and appears in a similar form in the preprint [121]. We thank Victor Burenkov for his helpful comments on the Poincaré-type inequality.

5.1 Introduction

The purpose of this chapter is to investigate numerical methods for computing Dirichlet eigenvalues of bounded domains with extremely rough, possibly fractal, boundaries and to develop analytical tools for dealing with such problems. Following [14], we utilise the framework of *Solvability Complexity Indices (SCI)* [83] and consider sequences of *arithmetic algorithms* $(\Gamma_n)_{n\in\mathbb{N}}$ intended to approximate the spectrum $\sigma(-\Delta_{\mathscr{O}})$ of the Dirichlet Laplacian as $n\to\infty$ on any domain $\mathscr{O}\subset\mathbb{R}^2$ in a specified *primary set* $\Omega\subset 2^{\mathbb{R}^2}$ (recall 2^A = power set of set A). The sole input to each arithmetic algorithm Γ_n is the information of whether or not a chosen finite number of points lie in the domain $\mathscr{O}$ and the output is a closed subset of $\mathbb{C}$ which should approximate $\sigma(-\Delta_{\mathscr{O}})$ in an appropriate metric. Each Γ_n obtains its output from the input via a finite number of arithmetic operations, in a consistent way - the rigorous formulation will be given in Sections 5.2.3 and 5.2.4.

The question we ask is: what is the “largest” primary set Ω of bounded domains we can identify such that there exists a single sequence of arithmetic algorithms computing the Dirichlet eigenvalues of any domain in Ω?

Our first finding shows that there is no hope of constructing a single sequence of arithmetic algorithms capable of computing the Dirichlet eigenvalues of every bounded domain (cf. Proposition 5.14). The problem of proving the existence of sequences of arithmetic algorithms that do converge is approached via explicit construction. We shall introduce an approximation $\mathscr{O}_n$ for a domain $\mathscr{O}$ which we refer to as a *pixelated domain* for $\mathscr{O}$ (cf. Definition 5.16). Each pixelated domain $\mathscr{O}_n$ is constructed solely from the information of which points in the grid $(\frac{1}{n}\mathbb{Z})^2$ lie in $\mathscr{O}$. Utilising computable error bounds for the finite element method and matrix computations, we construct a sequence of arithmetic algorithms intended to compute the spectrum of the Dirichlet Laplacian. These arithmetic algorithms are then shown to converge on any domain for which the corresponding pixelated domains converge in the *Mosco sense* (cf. Definition 5.1).

The problem is thus reduced to the study of Mosco convergence, which we approach in a general way. This notion ensures convergence of Dirichlet eigenvalues and of solutions to the Poisson equation. In Section 5.4.3, we prove that if the Hausdorff convergence condition

$$\mathrm{d}_H(\mathscr{O},\mathscr{O}_n)+\mathrm{d}_H(\partial\mathscr{O},\partial\mathscr{O}_n)\to 0 \quad \text{as} \quad n\to\infty, \tag{5.1}$$

holds and a collection of mild geometric conditions (such as topological regularity of $\mathscr{O}$) are satisfied, then $\mathscr{O}_n$ converges to $\mathscr{O}$ in the Mosco sense (cf. Theorem 5.3). This result, which is valid for arbitrary sequences of domains, is applied to pixelated domains thus concluding the identification of a large primary set Ω_1 of bounded domains for which there exists a corresponding sequence of arithmetic algorithms (cf. Theorem 5.15). These arithmetic algorithms describe a simple numerical method that is guaranteed to converge on a very wide class of rough domains.

An intermediate step in the proof of our Mosco convergence result is the reduction of Mosco convergence $\mathscr{O}_n \xrightarrow{\mathrm{M}} \mathscr{O}$ to the establishment of a uniform Poincaré-type inequality of the form

$$\exists C,\alpha,r_0>0:\forall r<r_0:\forall u\in H_0^1(\mathscr{O}): \quad \|u\|_{L^2(\partial^r\mathscr{O})}\leqslant Cr\|\nabla u\|_{L^2(\partial^{\alpha r}\mathscr{O})} \tag{5.2}$$

where

$$\partial^r\mathscr{O}:=\{x\in\mathscr{O}:\mathrm{dist}(x,\partial\mathscr{O})<r\},$$

as well as an analogous sequence of inequalities verified uniformly over the sequence $\mathscr{O}_n$ (cf. Proposition 5.30). A Poincaré-type inequality of the form (5.2), for a single domain $\mathscr{O}$, is proved in Section 5.3 via a geometric method involving the construction of a bundle of paths from every point in $\partial^r\mathscr{O}$ to $\partial\mathscr{O}$ (cf. Theorem 5.6). The corresponding inequalities for the sequence of domains $\mathscr{O}_n$ are established by combining Theorem 5.6 with a characterisation of the geometry of $\partial\mathscr{O}_n$ for large n (cf. Proposition 5.38).

Organisation of the chapter

In Section 5.2, we state our main results and provide preliminaries. In Section 5.3, we prove an explicit Poincaré-type inequality. Section 5.4 is dedicated to proving Mosco convergence results as well as a geometric convergence result for pixelated domains. In Section 5.5, we apply our analytical results to the theory of Solvability Complexity Indices. In Section 5.6, we illustrate our results with a numerical investigation for the Dirichlet Laplacian on a filled Julia set.

Notation and conventions

We shall adopt the following notation, which is not necessarily standard and which will be used frequently throughout the chapter.

- For any $r>0$ and any set $A\subset\mathbb{R}^d$, the *r-collar neighbourhood* $\partial^r A$ is defined (as above) by
$$\partial^r A := \{x\in A : \mathrm{dist}(x,\partial A) < r\}. \tag{5.3}$$
- For any set $A\subset\mathbb{R}^d$, we let $\#_c(A)\in\mathbb{N}_0\cup\{\infty\}$ denote the number of connected components of A.
- For any $r>0$ and any set $A\subset\mathbb{R}^d$, we define the set $\mathrm{dil}_r(A)$ by
$$\mathrm{dil}_r(A) := \{x\in\mathbb{R}^d : \mathrm{dist}(x,A) < r\}. \tag{5.4}$$
- $\sigma(\mathscr{O})$ shall denote the spectrum of the Dirichlet Laplacian $-\Delta_{\mathscr{O}}$ on $L^2(\mathscr{O})$.

We shall also use the following notation.

- For every $A\subset\mathbb{R}^d$, $\mu_{\mathrm{leb}}(A)$ denotes the d-dimensional Lebesgue outer measure.
- As usual, for any open set $U\subseteq\mathbb{R}^d$,
$$H^1(U) := \{u\in L^2(U) : \|\nabla u\|_{L^2(U)} < \infty\},$$
$$\|\cdot\|_{H^1(U)} := (\|\cdot\|^2_{L^2(U)} + \|\nabla\cdot\|^2_{L^2(U)})^{1/2} \tag{5.5}$$
and $H^1_0(U)$ is defined as the closure of $C^\infty_c(U)$ in $H^1(U)$.
- For any non-empty, bounded sets $A,B\subset\mathbb{R}^d$, the Hausdorff distance between A and B is defined by
$$\mathrm{d}_H(A,B) := \max\left\{\sup_{x\in A}\mathrm{dist}(x,B), \sup_{x\in B}\mathrm{dist}(x,A)\right\}. \tag{5.6}$$

We define $\mathrm{d}_H(\emptyset, A) = \infty$ for any non-empty bounded open set $A \subset \mathbb{R}^d$ and $\mathrm{d}_H(\emptyset, \emptyset) = 0$.

- We let $B_r(x) \subset \mathbb{R}^d$ denote an open ball of radius $r > 0$ about $x \in \mathbb{R}^d$.
- The diameter of a set $A \subset \mathbb{R}^d$ is denoted by

$$\operatorname{diam}(A) := \sup_{x\in A} \sup_{y\in A} |x - y| \in [0, \infty) \cup \{\infty\}. \tag{5.7}$$

5.2 Preliminaries and overview of results

This section is devoted to providing preliminaries, stating our main results and reviewing some closely related literature. In Sections 5.2.1 and 5.2.2 we present our analytical results on Mosco convergence and Poincaré-type inequalities respectively. An introduction to the theory of Solvability Complexity Indices is given in Section 5.2.3 and we state our results on the computational complexity of the eigenvalue problem in Section 5.2.4.

5.2.1 Mosco Convergence

The question of whether a given approximation for a domain gives a reliable spectral approximation for the Dirichlet Laplacian leads us to study *Mosco convergence*. We shall give the definition for H_0^1 Sobolev spaces on Euclidean domains (as in [47, Defn. 1.1]) but the notion can be more generally formulated for convex subsets of Banach spaces [106].

Definition 5.1. The sequence of open sets $\mathscr{O}_n \subseteq \mathbb{R}^d$, $n \in \mathbb{N}$, converges to an open set $\mathscr{O} \subseteq \mathbb{R}^d$ in the *Mosco sense*, denoted by $\mathscr{O}_n \xrightarrow{\mathrm{M}} \mathscr{O}$ as $n \to \infty$, if:

1. Any weak limit point u of a sequence $u_n \in H_0^1(\mathscr{O}_n)$, $n \in \mathbb{N}$, satisfies $u \in H_0^1(\mathscr{O})$.
2. For every $u \in H_0^1(\mathscr{O})$ there exists $u_n \in H_0^1(\mathscr{O}_n)$ such that $u_n \to u$ as $n \to \infty$ in $H^1(\mathbb{R}^d)$.

Note that a function $u \in H_0^1(\mathscr{O})$ may be realised as a function in $H^1(\mathbb{R}^d)$ via extension by zero.

For an arbitrary open set $\mathscr{O} \subset \mathbb{R}^d$, one may realise the Dirichlet Laplacian $-\Delta_{\mathscr{O}}$ as a positive, self-adjoint operator on $L^2(\mathscr{O})$ [61, Th. VI.1.4]. In the case that $\mathscr{O}$ is bounded, the Dirichlet Laplacian has compact resolvent, hence, purely discrete spectrum.

Provided the open sets $\mathscr{O} \subset \mathbb{R}^d$ and $\mathscr{O}_n \subset \mathbb{R}^d$, $n \in \mathbb{N}$, are bounded, Mosco convergence $\mathscr{O}_n \xrightarrow{\mathrm{M}} \mathscr{O}$ as $n \to \infty$ implies that $-\Delta_{\mathscr{O}_n}$ converges to $-\Delta_{\mathscr{O}}$ in the norm-resolvent sense as $n \to \infty$ [47, Th. 3.3 and 3.5]. In turn, norm-resolvent convergence implies spectral convergence [118, Th. VIII.23].

Lemma 5.2. *If $\mathscr{O} \subset \mathbb{R}^d$ and $\mathscr{O}_n \subset \mathbb{R}^d$, $n \in \mathbb{N}$, are open and bounded, and $\mathscr{O}_n \xrightarrow{\mathrm{M}} \mathscr{O}$ as $n \to \infty$, then for every bounded $S \subset \mathbb{C}$,*

$$\mathrm{d}_H(\sigma(\mathscr{O}_n) \cap S, \sigma(\mathscr{O}) \cap S) \to 0 \quad as \quad n \to \infty.$$

An open set $\mathscr{O} \subset \mathbb{R}^d$ is said to be *regular* if

$$\mathscr{O} = \mathrm{int}(\overline{\mathscr{O}}). \tag{5.8}$$

For a bounded open set $\mathscr{O} \subset \mathbb{R}^d$, the quantity $Q(\partial\mathscr{O}) > 0$ is defined by

$$Q(\partial\mathscr{O}) := \inf\{\mathrm{diam}(\Gamma) : \Gamma \subseteq \partial\mathscr{O} \text{ path-connected component of } \partial\mathscr{O}\}. \tag{5.9}$$

Recall that $\#_c$ denotes the number of connected components. Recall that a set $A \subset \mathbb{R}^d$ is *locally connected* if for every $x \in A$, there exists an open neighbourhood $U \subset \mathbb{R}^d$ of x such that $U \cap A$ is connected. In Section 5.4.3, we shall prove the following result, which provides geometric hypotheses ensuring Mosco convergence for domains in $\mathbb{R}^2$.

Theorem 5.3. *Suppose that $\mathscr{O} \subset \mathbb{R}^2$ is a bounded, connected, regular open set such that $\mu_{\mathrm{leb}}(\partial\mathscr{O}) = 0$, $Q(\partial\mathscr{O}) > 0$ and $\#_c\mathrm{int}(\mathscr{O}^c) = \#_c(\mathscr{O}^c) < \infty$. Suppose that $\mathscr{O}_n \subset \mathbb{R}^2$, $n \in \mathbb{N}$, is a collection of bounded, open sets such that $\partial\mathscr{O}_n$ is locally connected for all $n \in \mathbb{N}$ and such that*

$$\mathrm{d}_H(\mathscr{O}, \mathscr{O}_n) + \mathrm{d}_H(\partial\mathscr{O}, \partial\mathscr{O}_n) \to 0 \quad as \quad n \to \infty. \tag{5.10}$$

Then, $\mathscr{O}_n$ converges to $\mathscr{O}$ in the Mosco sense as $n \to \infty$.

The condition $Q(\partial\mathscr{O}) > 0$ in the above theorem can be replaced by the condition that each connected component of $\partial\mathscr{O}$ is path-connected (cf. Remark 5.40). In turn, the latter condition satisfied if $\partial\mathscr{O}$ is locally connected [105, §16]. A sufficient condition for the hypothesis $\mu_{\mathrm{leb}}(\partial\mathscr{O}) = 0$ is $\dim_H(\partial\mathscr{O}) < 2$ where $\dim_H$ denotes the Hausdorff dimension [64]. The condition $\#_c\mathrm{int}(\mathscr{O}^c) = \#_c(\mathscr{O}^c) < \infty$ intuitively states that $\mathscr{O}$ has a finite number of holes, which neither touch each other nor the outer boundary component of the domain.

Examples

The following classes of domains satisfy the hypotheses of Theorem 5.3. The first example includes the classical Koch snowflake domain. One could also modify this example to allow for domains with holes.

Example 5.4 (Interior of a Jordan curve)**.** Let $C \subset \mathbb{R}^2$ be any Jordan curve with $\mu_{\text{leb}}(C) = 0$. By the Jordan curve theorem, $\mathbb{R}^2 \backslash C$ is a disjoint union of two open, connected sets - a bounded interior $\mathscr{O}$ and an unbounded exterior S_{ext}. Then, $\mathscr{O}$ satisfies the hypotheses of Theorem 5.3.

Proof. It is known that $\partial\mathscr{O} = C$, hence it holds that $\mu_{\text{leb}}(\partial\mathscr{O}) = 0$ and $Q(\partial\mathscr{O}) > 0$. It is also known that $\partial(S_{\text{ext}}) = C$, hence any open set $U \subset \mathbb{R}^2$ satisfies either $U \subset \mathscr{O}$ or $U \cap S_{\text{ext}} \neq \emptyset$. From this it follows that $\text{int}(\overline{\mathscr{O}}) = \mathscr{O}$, that is, $\mathscr{O}$ is regular. Similarly, we have that $\text{int}(\mathscr{O}^c) = S_{\text{ext}}$ so $\#_c\text{int}(\mathscr{O}^c) = \#_c(\mathscr{O}^c) = 1$. □

The second example is a concrete special case of the above class of domains and is the object study in a numerical investigation in Section 5.6. We naturally identify $\mathbb{C} \cong \mathbb{R}^2$.

Example 5.5 (Filled Julia sets with connected interior)**.** Let $f_c(z) := z^2 + c$, where $c \in \mathbb{C}$ satisfies $|c| < \frac{1}{4}$. Consider the *filled Julia set*

$$K(f_c) := \{z \in \mathbb{C} : (f_c^{\circ n}(z))_{n\in\mathbb{N}} \text{ bounded}\} \tag{5.11}$$

where $f^{\circ n}(z) := \underbrace{f \circ \cdots \circ f}_{n \text{ times}}(z)$. The domain $\mathscr{O} = \text{int}(K(f_c))$ satisfies the hypotheses of Theorem 5.3.

Proof. Firstly, $K(f_c)$ is compact and $\partial\mathscr{O} = \partial K(f_c) = J(f_c)$, where $J(f_c)$ is the so-called *Julia set* for f_c [105, Lem. 17.1]. The Julia set can be thought of as the set of $z \in \mathbb{C}$ for which the dynamics of $f^{\circ n}(z)$ is chaotic. Since $|c| < \frac{1}{4}$, it is known that $J(f_c)$ is a Jordan curve [64, Th. 14.16]. By Example 5.4, it suffices that $\mu_{\text{leb}}(J(f_c)) = 0$.

One may show that $B_{1/4}(0) \subset K(f_c)$ [64, Ex. 14.3], hence, $|f_c'(z)| > 0$ for every $z \in J(f_c)$, that is, there are no critical points on the Julia set. It turns out that this is enough to ensure that the Lebesgue measure of the Julia set vanishes (cf. [31, pg. 2] and references therein). □

On the other hand, consider the *Mandelbrot set*

$$M := \{c \in \mathbb{C} : (f_c^{\circ n}(0))_{n\in\mathbb{N}} \text{ bounded}\}. \tag{5.12}$$

Then, the domains $\mathscr{O} = \mathrm{int}(M)$ and $\mathscr{O} = B_X(0)\backslash M$ (where $X > \mathrm{diam}(M)$) do *not* satisfy the hypotheses of Theorem 5.3, since $\#_c\mathrm{int}(M) = \infty$. The questions of whether $\mu_{\mathrm{leb}}(\partial M) = 0$ and ∂M is path connected are major open problems, the latter being implied by the famous MLC conjecture (MLC = Mandelbrot set locally connected) [56].

Comparison to known results

Let us now discuss some related results in the literature. Firstly, it is known that nested approximations converge in the Mosco sense, that is, for $\mathscr{O} \subseteq \mathbb{R}^d$ and $\mathscr{O}_n \subseteq \mathbb{R}^d$, $n \in \mathbb{N}$, open we have [48, Prop. 5.4.1]

$$\forall n \in \mathbb{N} : \mathscr{O}_n \subseteq \mathscr{O}_{n+1} \subseteq \mathscr{O} \quad \text{and} \quad \mathscr{O} = \bigcup_{n=1}^{\infty} \mathscr{O}_n \quad \Rightarrow \quad \mathscr{O}_n \xrightarrow{\mathrm{M}} \mathscr{O} \quad \text{as} \quad n \to \infty.$$

For non-nested approximations, such as those we consider in our study of the computational eigenvalue problem, Mosco convergence is more difficult to prove.

An open set $\mathscr{O} \subset \mathbb{R}^d$ is said to be *stable* if [48, Defn. 5.4.1]

$$H_0^1(\mathscr{O}) = H_0^1(\overline{\mathscr{O}}) := \{u|_{\mathscr{O}} : u \in H^1(\mathbb{R}^d), u = 0 \text{ a.e. on } \overline{\mathscr{O}}^c\}.$$

This notion allows for the application of powerful spectral and Mosco convergence results [117, 47, 46]. In particular, if a sequence of bounded domains $\mathscr{O}_n \subset \mathbb{R}^d$ converges to a bounded, stable domain $\mathscr{O} \subset \mathbb{R}^d$ in the sense that there exists "inner" and "outer" domains $\mathscr{O}'_n \subset \mathbb{R}^d$, $n \in \mathbb{N}$, and $\mathscr{O}^\dagger_n \subset \mathbb{R}^d$, $n \in \mathbb{N}$, such that for all $n \in \mathbb{N}$,

$$\mathscr{O}'_n \subseteq \mathscr{O}_n \subseteq \mathscr{O}^\dagger_n,$$

$$\mathscr{O}'_n \subseteq \mathscr{O}'_{n+1} \subseteq \mathscr{O}, \quad \bigcup_{k=1}^{\infty} \mathscr{O}'_k = \mathscr{O}$$

and

$$\mathscr{O} \subseteq \mathscr{O}^\dagger_{n+1} \subseteq \mathscr{O}^\dagger_n, \quad \bigcap_{k=1}^{\infty} \mathscr{O}^\dagger_k \subseteq \overline{\mathscr{O}},$$

then $\mathscr{O}_n \xrightarrow{\mathrm{M}} \mathscr{O}$ as $n \to \infty$.[1]

Stability may be characterised in terms of stability of the Dirichlet problems [5] and in terms of capacities [47][2, Ch. 11]. A sufficient geometric condition that ensures that a domain is stable is that it is bounded and the boundary is locally the

[1] Indeed, we have $\mathscr{O}'_n \xrightarrow{\mathrm{M}} \mathscr{O}$ by [48, Prop. 5.4.1] and $\mathscr{O}^\dagger_n \xrightarrow{\mathrm{M}} \mathscr{O}$ by [48, Prop 5.4.4]. Then, by the "sandwich" lemma [36, Lemma 2.3], it follows that $\mathscr{O}_n \xrightarrow{\mathrm{M}} \mathscr{O}$.

image of a continuous map [5, Prop. 2.2]. Another sufficient condition, which allows for certain domains with fractal boundaries has been proven in [33] and is discussed below.

Spectral convergence results, with convergence rates, have also been obtained for the Laplacian on Reifenberg-flat domains [95] and for more general non-negative, elliptic, self-adjoint operators [49, 32] . As far as we are aware these results are not applicable to non-nested approximations of domains with fractal boundary.

Recently, domains with fractal boundaries have also been studied. In [33, Corollary 4.13], the authors proved that E-thick domains $\mathscr{O}$ with $\mu_{\mathrm{leb}}(\partial\mathscr{O}) = 0$ are stable. Furthermore, in [85, Theorem 8], the authors proved a related type of Mosco convergence result for quadratic functionals on (ε,∞)-domains. Note that there exist domains satisfying the hypotheses of Theorem 5.3 that are neither E-thick, nor (ε,∞)-domains, for instance, domains with reentrant cusps like the interior of a standard cardioid (see [136, Figure 3.3 and Remark 3.7] for an illustration and discussion of such cusps). Also, for $\mathscr{O}$ to be an (ε,∞)-domain, it is necessary and sufficient that $\partial\mathscr{O}$ is a quasi-circle, that is, the corresponding map $\iota : S^1 \to \mathbb{R}^2$ (such that $\iota(S^1) = \partial\mathscr{O}$) is the restriction of a quasi-conformal map [87, Theorem C].

5.2.2 An explicit Poincaré-type Inequality

A key ingredient for the proof of Theorem 5.3 is a Poincaré-type inequality for collar neighbourhoods of the boundary of a domain. Theorem 5.6 provides a bound with an explicit constant which is independent of the particular domain $\mathscr{O}$. As far as the authors are aware, this is the first Poincaré-type inequality of its form to be reported. The proof is given in Section 5.3.4. Recall that $Q(\partial\mathscr{O})$ is defined by (5.9).

Theorem 5.6. *Let $\mathscr{O} \subseteq \mathbb{R}^2$ be any open set. If $Q(\partial\mathscr{O}) > 0$ and $r > 0$ satisfies $4\sqrt{2}r < Q(\partial\mathscr{O})$, then*

$$\|u\|_{L^2(\partial^r\mathscr{O})} \leqslant 5r\|\nabla u\|_{L^2(\partial^{2\sqrt{2}r}\mathscr{O})} \tag{5.13}$$

for all $u \in H_0^1(\mathscr{O})$.

Comparison to known results

Precise bounds have recently been obtained in terms of *Hardy inequalities* (see [8, 9, 88, 27, 137] and the references therein). These are bounds on the L^p norm of u/η in terms of ∇u, where $u \in W_0^{1,p}(\mathscr{O})$ and $\eta(x) = \mathrm{dist}(x,\partial\mathscr{O})$. Classically, the domain $\mathscr{O}$ is assumed to be of class C^1, but relaxations are possible (see [8, 137] for an overview). Hardy-type inequalities have also been studied in connection with questions of spectral convergence [49].

We mention the following result from [88][137, Th. 3.4.8].

If $d \geqslant 2$ and $\mathscr{O} \subset \mathbb{R}^d$ is open, connected, such that $\mathbb{R}^d \setminus \mathscr{O}$ is connected and unbounded, then there exists $C > 0$ such that for all $u \in W_0^{1,d}(\mathscr{O})$

$$\left\| \frac{u}{\eta} \right\|_{L^d(\mathscr{O})} \leqslant C \, \|\nabla u\|_{L^d(\mathscr{O})} . \tag{5.14}$$

The connectedness assumption on $\mathbb{R}^d \setminus \mathscr{O}$ can be replaced by the weaker, technical condition of so-called *uniform m-fatness* (cf. [88, Th. 4.1]) Applying inequality (5.14) to the case $d = 2$ immediately yields the bound $\|u\|_{L^2(\partial^r \mathscr{O})} \leqslant Cr\|\nabla u\|_{L^2(\mathscr{O})}$ for a r-collar neighbourhood of $\partial\mathscr{O}$. Note that this statement is weaker than Theorem 5.6 in two ways: first, the constant C is neither explicit, nor independent of $\mathscr{O}$ and second, the L^2-norm of ∇u is over the entire domain $\mathscr{O}$, rather than a neighbourhood of $\partial\mathscr{O}$. These differences are key for application to our proof of Theorem 5.3.

5.2.3 Computational problems and arithmetic algorithms

The theory of the Solvability Complexity Index (SCI) hierarchy was developed in [11, 83, 12]. Broadly speaking, it studies the question *Given a class Ω of computational problems, can the solutions always be computed by an algorithm?* In order to give a rigorous formulation of this question, it is necessary to introduce precise definitions of the terms "computational problem" and "algorithm" (the reader may think of a Turing machine for the time being). We will give a brief review of the central elements of the theory here and refer to [11] for further details.

Definition 5.7 (Computational problem)**.** A *computational problem* is a quadruple $(\Omega, \Lambda, \mathscr{M}, \Xi)$, where

(A) Ω is a set, called the *primary set*,

(B) Λ is a set of complex-valued functions on Ω, called the *evaluation set*,

(C) $\mathscr{M}$ is a metric space,

(D) $\Xi : \Omega \to \mathscr{M}$ is a map, called the *problem function*.

Intuitively, elements of the primary set Ω are the objects giving rise to the computational problems, the evaluation set Λ represents the information available to an algorithm, the metric space $\mathscr{M}$ is the output of an algorithm and the problem function Ξ represents the true solutions of the computational problems.

Example 5.8. An instructive example of a computational problem in the sense of Definition 5.7 is given by the following data. Let $\Omega = \mathscr{B}(\ell^2(\mathbb{N}))$, the bounded operators on the space of square summable sequences, $\Lambda = \{A \mapsto \langle Ae_i, e_j\rangle_{\ell^2} : i, j \in \mathbb{N}\}$ the set of matrix elements in the canonical basis, $\mathscr{M} = (\mathrm{comp}(\mathbb{C}), d_{\mathrm{H}})$ the compact subsets of $\mathbb{C}$, together with the Hausdorff distance d_{H}, and finally $\Xi(A) = \sigma(A)$, the spectrum of an operator. In words, this computational problem reads "Compute the spectrum of a bounded operator on $\ell^2(\mathbb{N})$ using its matrix entries as an input."

Now we are in position to define the notion of an arithmetic algorithm. The definition here differs slightly from the one in [11, Definition 6.3] as it is convenient for us to explicitly indicate the evaluation set Λ.

Definition 5.9 (Arithmetic algorithm)**.** Let $(\Omega, \Lambda, \mathscr{M}, \Xi)$ be a computational problem. An *arithmetic algorithm with input* Λ is a map $\Gamma : \Omega \to \mathscr{M}$ such that for each $T \in \Omega$ there exists a finite subset $\Lambda_\Gamma(T) \subset \Lambda$ such that

(i) the action of Γ on T depends only on $\{f(T)\}_{f\in\Lambda_\Gamma(T)}$,

(ii) (consistency) for every $S \in \Omega$ with $f(T) = f(S)$ for all $f \in \Lambda_\Gamma(T)$ one has $\Lambda_\Gamma(S) = \Lambda_\Gamma(T)$,

(iii) the action of Γ on T consists of performing only finitely many arithmetic operations[2] on $\{f(T)\}_{f\in\Lambda_\Gamma(T)}$.

Arithmetic algorithms give a notion of computability. We shall deem a computational problem $(\Omega, \Lambda, \mathscr{M}, \Xi)$ to be computable if

$$\exists \text{ arithmetic algorithms } \left\{ \begin{matrix} \Gamma_n : \Omega \to \mathscr{M}, n \in \mathbb{N}, \\ \text{with input } \Lambda \end{matrix} \right\} \text{ s.t. } \lim_{n\to\infty} d_{\mathscr{M}}(\Gamma_n(T), \Xi(T)) = 0 \, \forall T \in \Omega, \tag{5.15}$$

where $\mathrm{d}_{\mathscr{M}}$ denote the metric for the metric space $\mathscr{M}$.

Example 5.10 (Example 5.8 continued)**.** The solvability of the computational problem defined in Example 5.8 is thus equivalent to the existence of a sequence of arithmetic algorithms $(\Gamma_n)_{n\in\mathbb{N}}$, where $\Gamma_n : \mathscr{B}(\ell^2(\mathbb{N})) \to \mathrm{comp}(\mathbb{C})$ such that (i)-(iii) of Definition 5.9 are satisfied and $d_{\mathrm{H}}(\Gamma_n(A), \sigma(A)) \to 0$ as $n \to \infty$ for all $A \in \mathscr{B}(\ell^2(\mathbb{N}))$. In particular, for each fixed $n \in \mathbb{N}$, the image $\Gamma_n(A)$ must be computable from finitely many matrix elements of A in finitely many arithmetic operations.

[2] Recall that the arithmetic operations are $+, -, \times, \div$, as well as exponentiation and complex conjugation. Arithmetic comparisons are also allowed, that is, given $a, b \in \mathbb{R}$ we may test whether $a < b$, $b > a$ or $a = b$. A more precise (but less transparent) definition may also be given in terms of BSS machines [15] [12, Definition 6.6].

In [83], Hansen showed that it *is* possible to compute $\sigma(A)$ for $A \in \mathscr{B}(\ell^2(\mathbb{N}))$ as above. However, rather than having algorithms Γ_n with a single index $n \in \mathbb{N}$, *three* indices were required, satisfying $\sigma(A) = \lim_{n_3\to\infty} \lim_{n_2\to\infty} \lim_{n_1\to\infty} \Gamma_{n_1,n_2,n_3}(A)$. The algorithms Γ_{n_1,n_2,n_3} are given explicitly, and can be implemented numerically. In [11] it was proved that this is optimal: this computation cannot be performed with fewer than 3 limits, and hence we say that this problem has an SCI value of 3.

We formalise the foregoing example with the following definitions:

Definition 5.11 (Tower of arithmetic algorithms)**.** Let $(\Omega, \Lambda, \mathscr{M}, \Xi)$ be a computational problem. A *tower of algorithms* of height k for Ξ is a family

$$\{\Gamma_{n_1,n_2,\dots,n_k} : \Omega \to \mathscr{M} | n_j \in \mathbb{N}, j = 1, \dots, k\}$$

of arithmetic algorithms such that for all $T \in \Omega$

$$\Xi(T) = \lim_{n_k\to\infty} \cdots \lim_{n_1\to\infty} \Gamma_{n_1,n_2,\dots,n_k}(T).$$

Definition 5.12 (SCI)**.** A computational problem $(\Omega, \Lambda, \mathscr{M}, \Xi)$ is said to have a *Solvability Complexity Index* (SCI) of k if k is the smallest integer for which there exists a tower of algorithms of height k for Ξ. If a computational problem has solvability complexity index k, we write

$$\mathrm{SCI}(\Omega, \Lambda, \mathscr{M}, \Xi) = k.$$

With this new terminology, condition (5.15) is equivalent to $\mathrm{SCI}(\Omega, \Lambda, \mathscr{M}, \Xi) = 1$. Definition 5.12 naturally places computational problems into a *hierarchy*: the higher the SCI of a problem, the more limits are needed to solve it, thus the higher its computational complexity.

A refinement of the SCI hierarchy (as described above) has been proposed in [11] based on whether Γ_n approximates Ξ from above or from below (in an appropriate sense) and whether explicit error control is possible. We shall not dive any deeper into these refinements here and refer the interested reader to [11, Def. 6.11].

Several kinds of computational (spectral and other) problems have been classified in the SCI hierarchy in recent years, not just in the abstract bounded setting of Example 5.8, but also in more applied PDE problems. Recent results include classification of abstract spectral problems [11, 40], spectral problems for PDE on $\mathbb{R}^d$ [11, 41, 42, 120], resonance problems for potential scattering [13] and obstacle scattering [14]. The computability of spectral problems on domains in $\mathbb{R}^d$ and its relation to boundary regularity has not yet been studied as far as the authors are aware.

5.2.4 Computational eigenvalue problem for the Laplacian

Now we describe our contribution to the SCI hierarchy.

Statement of SCI results

We shall consider the following computational problem.

(A) The primary set Ω is a subset of the set of domains

$$\Omega_0 := \{\mathscr{O} \subset \mathbb{R}^2 : \mathscr{O} \text{ open, bounded and connected}\}.$$

(B) The evaluation set is

$$\Lambda_0 := \{\mathscr{O} \mapsto \chi_{\mathscr{O}}(x) : x \in \mathbb{R}^2\}$$

where χ is the characteristic function.

(C) The metric space is $\mathscr{M} := (\mathrm{cl}(\mathbb{C}), \mathrm{d_{AW}})$, where $\mathrm{cl}(\mathbb{C})$ denotes the set of closed, nonempty subsets of $\mathbb{C}$ and $\mathrm{d_{AW}}$ denotes the Attouch-Wets metric. Note that the spectrum of the Dirichlet Laplacian on a bounded domain is always closed and nonempty by classical results. Recall that the Attouch-Wets metric is defined by

$$\mathrm{d_{AW}}(A,B) := \sum_{j=1}^{\infty} 2^{-j} \min\left\{1, \sup_{|x|\leqslant j} |\mathrm{dist}(x,A) - \mathrm{dist}(x,B)|\right\}$$

for any subsets $\emptyset \neq A, B \subseteq \mathbb{C}$ (cf. [10, Ch. 3]). Note that for bounded sets $A, B \subset \mathbb{C}$, $\mathrm{d_{AW}}$ is equivalent to the Haussdorff distance $\mathrm{d_H}$ [10, Th. 3.2.3].

(D) The problem function $\Xi_\sigma : \Omega \to \mathscr{M}$ is defined by $\Xi_\sigma(\mathscr{O}) := \sigma(\mathscr{O})$, where recall that $\sigma(\mathscr{O})$ denotes the spectrum of the Dirichlet Laplacian $-\Delta_{\mathscr{O}}$ on $L^2(\mathscr{O})$.

Remark 5.13. In addition to Λ_0 we shall always assume that the n^{th} arithmetic algorithm $\Gamma_n(\mathscr{O})$ has access to the information that it is the n^{th} in the sequence, i.e., the map $\mathscr{O} \mapsto n$ is also in the evaluation set. For notational brevity, we do not explicitly indicate this.

The following result follows immediately from Proposition 5.48. The proof is based on the construction of a certain counter-example which “fools" a sequence of arithmetic algorithms aiming to compute the spectrum on an arbitrary domain in Ω_0.

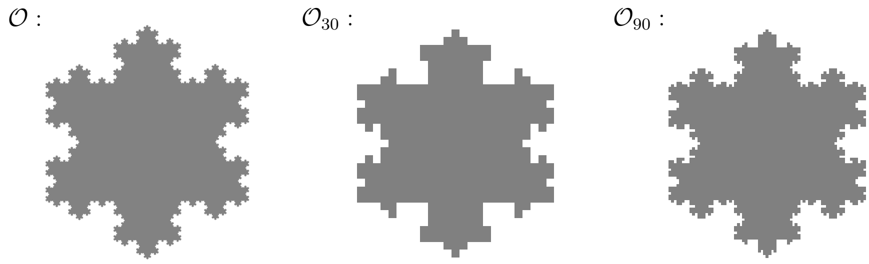

Figure 5.1 Sketch of a domain $\mathscr{O}$ and its pixelated analogue $\mathscr{O}_n$

Proposition 5.14. *There does not exist a sequence of arithmetic algorithms* $\Gamma_n : \Omega_0 \to \mathrm{cl}(\mathbb{C})$ *with input* Λ_0 *which satisfy*

$$\mathrm{d_{AW}}\left(\Gamma_n(\mathscr{O}), \sigma(\mathscr{O})\right) \to 0 \quad \textit{as} \quad n \to \infty \qquad \textit{for all} \qquad \mathscr{O} \in \Omega_0.$$

That is,

$$\mathrm{SCI}(\Omega_0, \Lambda_0, \mathscr{M}, \Xi_\sigma) \geqslant 2.$$

Our final result is an explicit construction of a sequence of arithmetic algorithms, describing a simple numerical method for the computation of eigenvalues of the Dirichlet Laplacian on a large class of bounded domains. Recall that $Q(\partial\mathscr{O})$ is defined by (5.9) and $\#_c$ is the number of connected components.

Theorem 5.15. *Let*

$$\Omega_1 := \left\{ \mathscr{O} \in \Omega_0 \ : \ \begin{array}{c} \mathscr{O} = \mathrm{int}(\overline{\mathscr{O}}),\, \mu_{\mathrm{leb}}(\partial\mathscr{O}) = 0,\, Q(\partial\mathscr{O}) > 0, \text{ and} \\ \#_c \mathrm{int}(\mathscr{O}^c) = \#_c(\mathscr{O}^c) < \infty \end{array} \right\}. \tag{5.16}$$

There exists a sequence of arithmetic algorithms $\Gamma_n : \Omega_1 \to \mathrm{cl}(\mathbb{C})$ *with input* Λ_0 *such that*

$$\mathrm{d_{AW}}\left(\Gamma_n(\mathscr{O}), \sigma(\mathscr{O})\right) \to 0 \quad \textit{as} \quad n \to \infty \qquad \textit{for all} \qquad \mathscr{O} \in \Omega_1,$$

that is,

$$\mathrm{SCI}(\Omega_1, \Lambda_0, \mathscr{M}, \Xi_\sigma) = 1.$$

Note that any domain described in Example 5.4 or 5.5 lies in Ω_1.

The arithmetic algorithms in the above theorem are based on the following approximation for a Euclidean domain.

Definition 5.16. For any open set $\mathscr{O} \subseteq \mathbb{R}^d$, the *pixelated domains* for $\mathscr{O}$ are the open sets $\mathscr{O}_n \subseteq \mathbb{R}^d$, $n \in \mathbb{N}$, defined by

$$\mathscr{O}_n := \mathrm{int}\left(\bigcup_{j \in L_n} \left(j + [-\tfrac{1}{2n}, \tfrac{1}{2n}]^d\right) \right),$$

where
$$L_n := \left\{ j \in \mathbb{Z}_n^d : j \in \mathscr{O} \right\} \quad \text{and} \quad \mathbb{Z}_n^d := (n^{-1}\mathbb{Z})^d.$$

The basic idea behind the construction of the algorithm is to combine pixelation approximations of the domain with computable error bounds for the finite-element method and matrix eigenvalue problem. The algorithm of Theorem 5.15 can be summarised as:

Step 1 Approximate $\mathscr{O}$ by a corresponding pixelated domain $\mathscr{O}_n$.

Step 2 Approximate the eigenvalues of $\mathscr{O}_n$ to an error $1/n$ (in the Attouch-Wets metric) by the eigenvalues of a matrix pencil, using computable error bounds for the finite element method on a uniform triangulation of $\mathscr{O}_n$.

Step 3 Compute the eigenvalues of the matrix pencil to an error $1/n$ (in the Attouch-Wets metric) using the Jacobi method combined with a-posteriori error bounds for the associated matrix pencils.

The computable error bounds for the finite element method that we employ are those of Liu and Oishi [100], but similar bounds have also been obtained in [34, 35]. The matrix pencil a-posteriori estimates we utilise are due to Oishi [111].

In Proposition 5.46, this algorithm is shown to converge on any bounded domains for which the pixelation approximations converge in the Mosco sense, that is, for any domain in

$$\Omega_M := \left\{ \mathscr{O} \subset \mathbb{R}^2 : \mathscr{O} \text{ open, bounded and } \mathscr{O}_n \xrightarrow{\mathrm{M}} \mathscr{O} \text{ where } \mathscr{O}_n \text{ pixelated domains for } \mathscr{O} \right\}.$$

In Proposition 5.42, we show that if $\mathscr{O}_n$ are the pixelated domains for a bounded, open set $\mathscr{O} \subset \mathbb{R}^d$ satisfying $\mathscr{O} = \mathrm{int}(\overline{\mathscr{O}})$ and $\mu_{\mathrm{leb}}(\partial \mathscr{O}) = 0$, then

$$\mathrm{d}_H(\mathscr{O}_n, \mathscr{O}) + \mathrm{d}_H(\partial \mathscr{O}_n, \partial \mathscr{O}) \to 0 \quad \text{as} \quad n \to \infty.$$

Theorem 5.15 therefore follows by an application of our Mosco convergence result Theorem 5.3.

Remark 5.17. We believe that use of computable error bounds in Step 2 may not be strictly necessary. As mentioned, Mosco convergence can also be defined for more general Hilbert spaces. In particular, we can makes sense of statements like $V_0^n(\mathscr{O}_n) \xrightarrow{\mathrm{M}} H^1(\mathscr{O})$ as $n \to \infty$, where $V_0^n(\mathscr{O}_n)$ is a P1 finite element space corresponding to a triangulation of $\mathscr{O}_n$. Such techniques have application to finding conditions under which finite element error may be linked with geometric approximation error [36].

5.3 An explicit Poincaré-type inequality

This section is devoted to the proof of the Poincaré-type inequality Theorem 5.6 on the collar neighbourhood $\partial^r\mathscr{O}$ of a domain $\mathscr{O} \subset \mathbb{R}^2$. Our approach is inspired by the simple proof of the Poincaré inequality in the textbook of Adams and the Fournier [3, Theorem 6.30]. The method consists in expressing the value of a function in $H_0^1(\mathscr{O})$ at a given point $x \in \partial^r\mathscr{O}$ as an integral over a path from x to the boundary $\partial\mathscr{O}$. We shall explicitly construct these paths. This must be done in a way such that the bundle of paths corresponding to the different points in $\partial^r\mathscr{O}$ do not "concentrate" too much at any given point on the boundary. This is made possible by the assumption $Q(\partial\mathscr{O}) > 0$ (cf. (5.9)). In fact, this assumption is necessary, as the following example shows.

Example 5.18. Let $1 > \varepsilon > 0$ and consider the domain $\mathscr{O} := B_1(0) \setminus B_\varepsilon(0) \subset \mathbb{R}^2$ (hence $Q(\partial\mathscr{O}) = 2\varepsilon$). In polar coordinates, define the function $f_\varepsilon(r) = \frac{\log(\varepsilon)-\log(r)}{\log(\varepsilon)}$. An explicit calculation shows

$$\|f_\varepsilon\|^2_{L^2(\mathscr{O})} = 2\pi\left(\frac{1}{2} + \frac{1}{2\log(\varepsilon)} + \frac{1-\varepsilon^2}{4\log^2(\varepsilon)}\right)$$
$$\|\nabla f_\varepsilon\|^2_{L^2(\mathscr{O})} = -\frac{2\pi}{\log(\varepsilon)}$$

And thus

$$\frac{\|f_\varepsilon\|^2_{L^2(\mathscr{O})}}{\|\nabla f_\varepsilon\|^2_{L^2(\mathscr{O})}} \geqslant C|\log(\varepsilon)|$$

as $\varepsilon \to 0$. Since $f_\varepsilon(x) \to 1$ as $x \to \partial B_1(0)$, f can be extended to a H_0^1 function on any domain that contains $\overline{B_1(0)} \setminus B_\varepsilon(0)$. This example shows that no uniform Poincaré inequality can hold on domains with arbitrarily small holes. Similar statements can be proved in higher dimensions (cf. [117, Lemma 4.5]).

Throughout the section, let $\mathscr{O} \subset \mathbb{R}^2$ be an arbitrary open set and fix the value $r > 0$, corresponding to the size of the collar neighbourhood $\partial^r\mathscr{O}$.

5.3.1 Some geometric notions

The construction of the bundle of paths shall be assisted by the introduction of a grid of boxes covering $\mathbb{R}^2$. We choose the boxes to have edge of length $r > 0$ - exactly the size of the collar neighbourhood $\partial^r\mathscr{O}$. We shall introduce, for the purpose of the proof, various notions such as *cell-paths*, *g-cells* and *lg-cells*. Cell-paths can be thought of a higher level structure within which the bundles of paths shall be constructed. Then, g-cells and lg-cells (good cells and long good cells) are cells which $\partial\mathcal{O}$ intersects in a way such that a bundle of paths can be terminated at that cell.

Definition 5.19. (a) A *cell* is a closed box $j+[0,r]^2$ for some $j\in(r\mathbb{Z})^2$.

(b) An *edge* of a cell is one of the 4 connected, closed straight line segments whose union comprises the boundary of the cell.

Definition 5.20. A *g-cell* is a cell c_0 such that two distinct, parallel edges e_1 and e_2 of c_0 are connected by a path-connected segment of $\partial\mathcal{O}$ in c_0, that is,

$$\exists\Gamma\subseteq\partial\mathcal{O}\cap c_0:\Gamma\text{ path-connected},\Gamma\cap e_1\neq\emptyset\text{ and }\Gamma\cap e_2\neq\emptyset.$$

The two edges of c_0 other than e_1 and e_2 are called the *normal edges*.

Definition 5.21. (a) A *long-cell* is a set of two cells $\{c_1,c_2\}$ such that c_1 and c_2 share a common edge.

(b) An *edge* of a long-cell $\{c_1,c_2\}$ is one of the 4 connected, closed straight line segments whose union comprises the boundary of the set $c_1\cup c_2$.

(c) A *short-edge* of the long-cell is an edge of the long cell which is also the edge of a cell.

(d) A *long-edge* of a long-cell is an edge of the long-cell which is not a short-edge.

Definition 5.22. An *lg-cell* is a long cell $\{c_1,c_2\}$ for which there exist distinct long-edges e_1 and e_2 connected by a path-connected segment of $\partial\mathcal{O}$ in c_0, that is,

$$\exists\Gamma\subseteq\partial\mathcal{O}\cap(c_1\cup c_2):\Gamma\text{ path-connected},\Gamma\cap e_1\neq\emptyset\text{ and }\Gamma\cap e_2\neq\emptyset.$$

The *normal edges* of a lg-cell refers to its short edges. We shall often say that an lg-cell $\{c_1,c_2\}$ is contained in a set A to mean that $c_1\cup c_2\subseteq A$.

Definition 5.23. A *cell path* from a cell c_0 to a g-cell c_n (or to an lg-cell $\{c_n,c_{n+1}\}$) is a sequence of cells $(c_1,...,c_{n-1})$ such that

1. if $n\geqslant 2$, then c_j shares a common edge with c_{j-1} for each $j\in\{1,...,n-1\}$,
2. if $n\geqslant 1$, then there exists an edge of c_{n-1} which is also a normal edge of the g-cell c_n (or of the lg-cell $\{c_n,c_{n+1}\}$ resp.) and
3. $(c_0,...,c_n)$ (or $(c_0,...,c_{n+1})$ resp.) consists of distinct elements.

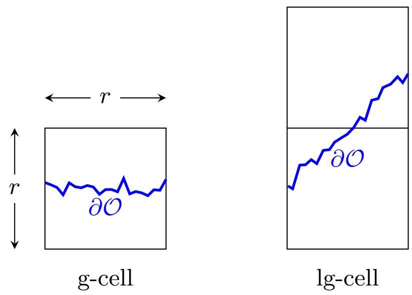

Figure 5.2 Illustration for Definitions 5.20 and 5.22.

Here, we allow the possibility that $n = 1$, corresponding to the case that there exists an edge of c_0 which is also a normal edge of the g-cell c_n (or of the lg-cell $\{c_n, c_{n+1}\}$ resp.) and we allow the possibility that $n = 0$, corresponding to the case that c_0 is itself a g-cell (or in an lg-cell resp.). In both of these cases, the cell-path is empty.

Definition 5.24. (a) The *1-cell neighbourhood* $D_1[c_0]$ of a cell c_0 is the union of all cells sharing an edge or a corner with c_0, that is,

$$D_1[c_0] = \bigcup \{c : c \text{ is a cell and } c \cap c_0 \neq \emptyset\}.$$

(b) The *2-cell neighbourhood* $D_2[c_0]$ of a cell c_0 is the union of all cells sharing an edge or a corner with $D_1[c_0]$, that is,

$$D_2[c_0] = \bigcup \{c : c \text{ is a cell and } c \cap D_1[c_0] \neq \emptyset\}.$$

Definition 5.25. (a) A *filled cell* is a cell c such that $c \cap \partial\mathscr{O} \neq \emptyset$.

(b) A *covering cell* is a cell c which shares an edge or a corner with a filled cell c_f, i.e. $c \cap c_f \neq \emptyset$.

5.3.2 Poincaré-type inequality for cell-paths

Given a cell c_0 and a cell-path from c_0 to either a g-cell or an lg-cell, one may express the value of a function $u \in C_0^\infty(c_0)$ any point in c_0 as a line integral over a path within the cell path from that point to the boundary (cf. equation (5.19)). With this representation for u, one may proceed in a way similar to the proof of [3, Theorem 6.30] to obtain a Poincaré-type inequality for c_0. Note that, throughout the chapter, we shall always regard functions in $H_0^1(\mathscr{O})$ as being defined on the whole of $\mathbb{R}^2$ via extension by zero.

Lemma 5.26. *Let c_0 be a cell and let $(c_1,...,c_{n-1})$ be a cell path from c_0 to a g-cell c_n or an lg-cell $\{c_n,c_{n+1}\}$. Then, for any $u \in H_0^1(\mathscr{O})$,*

$$\|u\|_{L^2(c_0)}^2 \leqslant r^2 \sum_{j=0}^{n+1} \|\nabla u\|_{L^2(c_j)}^2. \tag{5.17}$$

In (5.17)*, c_{n+1} is considered to be the empty set in the case of a cell path to a g-cell.*

Proof. Assume without loss of generality that $c_0 = [0,r]^2$. In the case of a cell path to an lg-cell, assume without loss of generality that c_n shares an edge with c_{n-1}. We first deal with the case that $n \geqslant 1$, so that $c_0 \neq c_n$ (or $c_0 \notin \{c_n,c_{n+1}\}$ in the case of a cell-path to an lg-cell). The easier case $n = 0$ will be treated separately.

For each $j \in \{0,...,n-1\}$, let e_j denote the unique edge shared by c_j and c_{j+1} (note that $c_j \neq c_{j+1}$ by the definition of a cell path). Assume without loss of generality that $e_0 = [0,r] \times \{0\}$. Let us parameterise each of the edges e_j by $(e_j(s))_{s\in[0,r]}$ such that the path $s \mapsto e_j(s)$ has unit speed. It suffices to specify the point $e_j(0)$ or the point $e_j(r)$ in order to define the entire parameterisation $(e_j(s))_{s\in[0,r]}$.

1. Define $(e_0(s))_{s\in[0,r]}$ by $e_0(0) = (0,0)$, so that $e_0(s) = (s,0)$.

If $n = 1$, then we are done. If $n \geqslant 2$, then the parameterisations are defined recursively as follows. Note that for each $j \in \{1,...,n-1\}$, we have $c_{j-1} \neq c_{j+1}$ by the definition of a cell-path and so $e_j \neq e_{j-1}$.

(2) For $j \in \{1,...,n-1\}$, if e_{j-1} is parallel to e_j, then we call c_j a *straight tile*. In this case, define $(e_j(s))_{s\in[0,r]}$ by the condition that $e_j(0)$ is connected by an edge of c_j to $e_{j-1}(0)$, so that $e_j(r)$ is connected by an edge of c_j to $e_{j-1}(r)$.

(3) For $j \in \{1,...,n-1\}$, if e_{j-1} is perpendicular to e_j, then we call c_j an *corner tile*. If e_j and e_{j-1} share the point $e_{j-1}(0)$, then c_j is said to be *positively oriented*. In this case, define $(e_j(s))_{s\in[0,r]}$ by the condition that $e_j(0) = e_{j-1}(0)$. On the other hand, if e_j and e_{j-1} share the point $e_{j-1}(r)$, then c_j is said to be *negatively oriented*. In this case, define $(e_j(s))_{s\in[0,r]}$ by the condition that $e_j(r) = e_{j-1}(r)$.

Next, we construct a family of isometries $(\iota_j : \mathbb{R}^2 \to \mathbb{R}^2)_{j\in\{1,...,n\}}$ each of which maps $[0,r]^2$ to the cell c_j. The purpose of this is to simplify the later construction of paths within each cell. Recall that any composition of translations, rotations and reflections in the plane is an isometry. This, along with the fact that $e_j \neq e_{j-1}$ for all $j \in \{1,...,n-1\}$, is what guarantees the existence of isometries satisfying the below conditions.

1. For $j \in \{1,...,n-1\}$, if c_j is a straight tile, then choose ι_j such that $\iota_j(s,0) = e_j(s)$ and $\iota_j(s,r) = e_{j-1}(s)$.

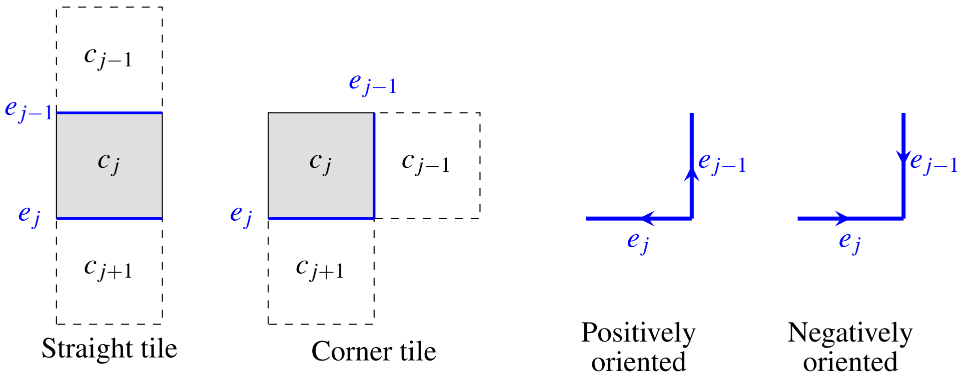

Figure 5.3 Sketch of the different types of tiles and orientation.

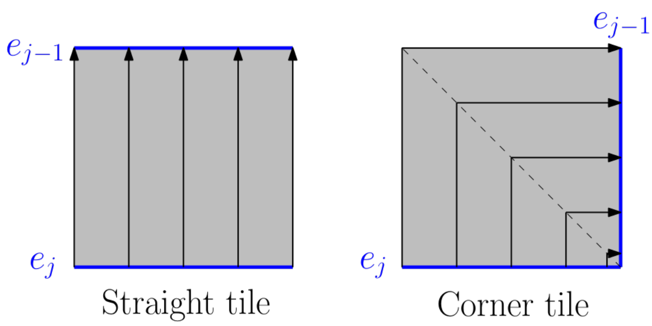

Figure 5.4 Sketch of the integration paths for straight and corner tiles.

2. For $j \in \{1, \ldots, n-1\}$, if c_j is a positively oriented corner tile, then choose ι_j so that $\iota_j(r-s, 0) = e_j(s)$ and $\iota_j(r, s) = e_{j-1}(s)$.
3. For $j \in \{1, \ldots, n-1\}$, if c_j is a negatively oriented corner tile, then choose ι_j so that $\iota_j(s, 0) = e_j(s)$ and $\iota_j(r, r-s) = e_{j-1}(s)$.
4. Choose ι_n so that $\iota_n(s, r) = e_{n-1}(s)$ and $\iota_n([0, r]^2) = c_n$. In the case of a cell-path to an lg-cell, this implies that $\iota_n([0, r] \times [-r, 0]) = c_{n+1}$.

By the density of $C_c^\infty(\mathscr{O})$ in $H_0^1(\mathscr{O})$, it suffices to show that (5.17) holds for all $u \in C_c^\infty(\mathscr{O})$. Hence, let $u \in C_c^\infty(\mathscr{O})$.

By Definitions 5.20 and 5.22 for a g-cell and an lg-cell respectively, there exists a function $w : [0, r] \to [-r, r]$ such that $u \circ \iota_n(s, w(s)) = 0$ for all $s \in [0, r]$. Note that in the case of a cell-path to a g-cell, w only takes values in $[0, r]$.

Firstly, for any $s \in [0, r]$,

$$u(e_{n-1}(s)) = u \circ \iota_n(s, r) = \int_{w(s)}^{r} \frac{\partial}{\partial t} u \circ \iota_n(s, t) \mathrm{d}t =: I_g(s).$$

Let $j \in \{1,...,n-1\}$. If c_j is a straight tile, then for any $s \in [0,r]$,

$$u(e_{j-1}(s)) - u(e_j(s)) = u \circ \iota_j(s,r) - u \circ \iota_j(s,0) = \int_0^r \frac{\partial}{\partial t} u \circ \iota_j(s,t) \mathrm{d}t =: I_j(s).$$

If c_j, is an corner tile, then let

$$\tilde{I}_j(s) := \int_0^s \frac{\partial}{\partial t} u \circ \iota_j(r-s,t) \mathrm{d}t + \int_{r-s}^r \frac{\partial}{\partial t} u \circ \iota_j(t,s) \mathrm{d}t.$$

If c_j is a positively oriented corner tile, then for any $s \in [0,r]$,

$$u(e_{j-1}(s)) - u(e_j(s)) = u \circ \iota_j(r,s) - u \circ \iota_j(r-s,0) = \tilde{I}_j(s) =: I_j(s).$$

If c_j is a negatively oriented corner tile, then for any $s \in [0,r]$,

$$u(e_{j-1}(s)) - u(e_j(s)) = u \circ \iota_j(r,r-s) - u \circ \iota_j(s,0) = \tilde{I}_j(r-s) =: I_j(s).$$

We can now express the value of u at any point in $c_0 = [0,r]^2$ as sum of line integrals. For any $x,y \in [0,r]$,

$$u(x,y) = u(e_0(x)) + \int_0^y \frac{\partial}{\partial t} u(x,t) \mathrm{d}t = I_g(x) + \sum_{j=1}^{n-1} I_j(x) + \int_0^y \frac{\partial}{\partial t} u(x,t) \mathrm{d}t \tag{5.18}$$

hence

$$\begin{aligned} \|u\|_{L^2(c_0)}^2 &= \int_0^r \int_0^r |u(x,y)|^2 \mathrm{d}x \mathrm{d}y \\ &\leqslant r \left[\int_0^r |I_g(x)|^2 \mathrm{d}x + \sum_{j=1}^{n-1} \int_0^r |I_j(x)|^2 \mathrm{d}x + \int_0^r \left(\int_0^r \left| \frac{\partial}{\partial t} u(x,t) \right| \mathrm{d}t \right)^2 \mathrm{d}x \right]. \end{aligned} \tag{5.19}$$

Focusing on the final term in the square brackets of (5.19) and applying Cauchy-Schwarz,

$$\int_0^r \left(\int_0^r \left| \frac{\partial}{\partial t} u(x,t) \right| \mathrm{d}t \right)^2 \mathrm{d}x \leqslant r \int_0^r \int_0^r \left| \frac{\partial}{\partial t} u(x,t) \right|^2 \mathrm{d}x \mathrm{d}t \leqslant r \|\nabla u\|_{L^2(c_0)}^2. \tag{5.20}$$

To estimate the remaining terms, we need to use the fact that

$$\left| \frac{\partial}{\partial t} u \circ \iota_j(x,t) \right| \leqslant \left| \nabla u(\iota_j(x,t)) \right| \left| \frac{\partial \iota_j}{\partial t}(x,t) \right| \leqslant \left| \nabla u(\iota_j(x,t)) \right|,$$

where the final inequality holds since ι_j is an isometry, and similarly,

$$\left|\frac{\partial}{\partial t}u\circ\iota_j(t,y)\right|\leqslant\left|\nabla u(\iota_j(t,y))\right|.$$

Focusing on the middle terms in the square brackets of (5.19), let $j\in\{1,...,n-1\}$. If c_j is a straight tile, then

$$\begin{aligned}\int_0^r|I_j(x)|^2dx\leqslant\int_0^r\left(\int_0^r\left|\nabla u(\iota_j(x,t))\right|\mathrm{d}t\right)^2\mathrm{d}x\leqslant r\int_0^r\int_0^r\left|\nabla u(\iota_j(x,t))\right|^2\mathrm{d}x\mathrm{d}t\\=r\|\nabla u\|^2_{L^2(c_j)}.\end{aligned}\tag{5.21}$$

If c_j is an corner tile, then

$$\begin{aligned}\int_0^r|\tilde{I}_j(x)|^2\mathrm{d}x&\leqslant\int_0^r\left(\int_0^x\left|\nabla u(\iota_j(r-x,t))\right|\mathrm{d}t\right)^2\mathrm{d}x+\int_0^r\left(\int_{r-x}^r\left|\nabla u(\iota_j(t,x))\right|\mathrm{d}t\right)^2\mathrm{d}x\\&\leqslant r\left(\int_0^r\int_0^x\left|\nabla u(\iota_j(r-x,t))\right|^2\mathrm{d}t\mathrm{d}x+\int_0^r\int_{r-x}^r\left|\nabla u(\iota_j(t,x))\right|^2\mathrm{d}t\mathrm{d}x\right)\\&=r\|\nabla u\|^2_{L^2(c_j)}.\end{aligned}$$

Hence, if c_j is a positively oriented corner tile, then

$$\int_0^r|I_j(x)|^2\mathrm{d}x=\int_0^r|\tilde{I}_j(x)|^2\mathrm{d}x\leqslant r\|\nabla u\|^2_{L^2(c_j)}\tag{5.22}$$

and, similarly, if c_j is a negatively oriented corner tile, then

$$\int_0^r|I_j(x)|^2\mathrm{d}x=\int_0^r|\tilde{I}_j(r-x)|^2\mathrm{d}x=\int_0^r|\tilde{I}_j(x)|^2\mathrm{d}x\leqslant r\|\nabla u\|^2_{L^2(c_j)}.\tag{5.23}$$

Finally, letting $h=0$ in the case of cell-path to a g-cell and $h=-r$ in the case of a cell-path to an lg-cell, we have

$$\begin{aligned}\int_0^r|I_g(x)|^2\mathrm{d}x&\leqslant\int_0^r\left(\int_{w(x)}^r|\nabla u(\iota_n(x,t))|\mathrm{d}t\right)^2\mathrm{d}x\\&\leqslant\int_0^r\left(\int_0^r|\nabla u(\iota_n(x,t))|\mathrm{d}t\right)^2\mathrm{d}x+\int_0^r\left(\int_h^0|\nabla u(\iota_n(x,t))|\mathrm{d}t\right)^2\mathrm{d}x\\&\leqslant r\left(\|\nabla u\|^2_{L^2(c_n)}+\|\nabla u\|^2_{L^2(c_{n+1})}\right).\end{aligned}\tag{5.24}$$

where c_{n+1} is considered to the empty set in the case of a cell-path to a g-cell. The proof for the case $n\geqslant 1$ is completed by substituting estimates (5.20)-(5.24) into (5.19).

The case $n = 0$ is similar. Assume that $c_0 = [0,r]^2$ and in the lg-cell case, that $c_1 = [0,r] \times [-r,0]$. Then there exists a function $w : [0,r] \to [-r,r]$ such that

$$u(x,y) = \int_{w(x)}^{y} \frac{\partial}{\partial t} u(x,t) \mathrm{d}t \qquad ((x,y) \in c_0)$$

and the proof proceeds as before. □

5.3.3 Construction of the cell-paths

Next, we need to construct cell paths from any covering cell to a g-cell or an lg-cell. The first step is to show that there is a g-cell or an lg-cell in the 1-cell neighbourhood of a filled cell, provided the path-connected components of $\partial\mathscr{O}$ all have large enough diameter. We shall need the fact that

$$\operatorname{diam}(A) \leqslant 2 \inf_{x \in A} \sup_{y \in A} |x - y|. \tag{5.25}$$

for any bounded set $A \subset \mathbb{R}^d$.

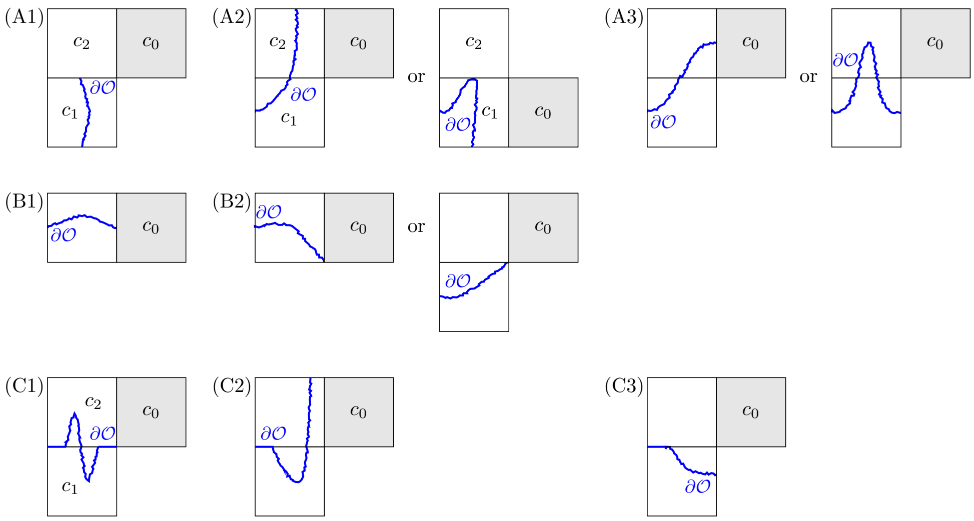

Figure 5.5 Example sketches for some of the cases (A), (B), (C) in the proof of Lemma 5.27

Lemma 5.27. *If $Q(\partial\mathscr{O}) > 4\sqrt{2}r$, then for any filled cell c_0 there exists a g-cell or an lg-cell contained in $D_1[c_0]$.*

Proof. Let c_0 be a filled cell. There exists a path-connected component $\Gamma \subseteq \partial\mathscr{O}$ such that $\Gamma \cap c_0 \neq \emptyset$. Let $x \in \Gamma \cap c_0$. Using (5.25) and the hypothesis on $Q(\partial\mathscr{O})$,

$$2\sqrt{2}r < \frac{1}{2} Q(\partial\mathscr{O}) \leqslant \frac{1}{2} \operatorname{diam}(\Gamma) \leqslant \sup_{y \in \Gamma} |x - y|$$

so there exists $y \in \Gamma$ with $|x-y| > 2\sqrt{2}r$. In particular, $y \in \Gamma$ lies outside of $D_1[c_0]$. Since Γ is path-connected, there exists a continuous path in Γ from y to x. Restricting this path, we deduce there exist a continuous path $\gamma : [0,1] \to D_1[c_0]$ such that

$$\gamma(t) \in \begin{cases} \partial D_1[c_0] & \text{if } t = 0 \\ \mathrm{int} D_1[c_0] \backslash c_0 & \text{if } t \in (0,1) \\ \partial c_0 & \text{if } t = 1 \end{cases} \quad \text{and} \quad \forall t \in [0,1] : \gamma(t) \in \Gamma.$$

Let us fix some notions that will allow us to prove the lemma. Firstly, an edge e is a *zeroth edge* if $\gamma(0) \in e$ and $e \subset \partial D_1[c_0]$. Since we defined an edge to be closed, there may be up to two zeroth edges.

Let

$$t_1 := \inf\{t > 0 : \exists \text{ edge } e \text{ such that } \gamma(t) \in e\} \in [0,1].$$

A *first edge* is defined as any edge e such that $\gamma(t_1) \in e$ and e is not a zeroth edge. If $t_1 \in (0,1)$, then the first edge is unique since $\gamma(t)$ can belong to at most one edge for $t \in (0,1)$. If $t_1 = 1$, then there may be up to four first edges (indeed, this is the case if $\gamma(1)$ lies in a corner of c_0). If $t_1 = 0$, then the first edge is again unique. This is because $\gamma(0)$ must lie in $\partial D_1[c_0]$ and hence can only lie in at most one edge which isn't entirely contained in $\partial D_1[c_0]$ (indeed, an edge containing $\gamma(0)$ which is contained in $\partial D_1[c_0]$ must be a zeroth edge).

If $t_1 < 1$, then there exists a unique first edge e_1 so we can make the following definitions. Let

$$t_2 := \inf\{t > 0 : \exists \text{ edge } e \text{ such that } \gamma(t) \in e \text{ and } e \neq e_1\} \in (t_1, 1].$$

Here, t_2 exists and satisfies $t_2 \leqslant 1$ since $\gamma(1)$ lies in at least one edge which is contained in ∂c_0, hence, which is not the first edge e_1. Also, t_2 satisfies $t_2 > t_1$ since the only edge that $\gamma(t)$ can intersect for $t \in (0, t_1]$ is the first edge e_1. A *second edge* is defined as any edge e such that $\gamma(t_2) \in e$ and $e \neq e_1$. Note that a second edge cannot be a zeroth edge since $t_1 > 0$. Finally, let

$$\tilde{t}_1 := \sup\{t \leqslant t_2 : \gamma(t) \in e_1\}.$$

If $t_1 = 1$, then t_2, the second edges and $\tilde{t}_1$ are not defined.

Let us now proceed onto the main part of the proof, in which we repeatedly use the continuity of the path γ.

(A) Suppose that $t_1 \in (0,1)$. Then, there exists a unique first edge e_1 and a unique cell c_1 containing $\gamma([0,t_1])$ (indeed, note that $\gamma((0,t_1))$ must be contained in the interior of a cell). c_1 must contain e_1 - let c_2 be the other cell containing e_1.

(A1) If there exists a zeroth edge contained in c_1 which is parallel to e_1, then c_1 is a g-cell.

(A2) Suppose there exists a second edge e which is contained in a cell $c \in \{c_1, c_2\}$ and which is parallel to e_1. By the definition of a second edge, $e \neq e_1$. $\gamma([\tilde{t}_1, t_2])$ is contained in c and connects the distinct parallel edges e and e_1 of c, therefore, c is a g-cell.

(A3) In the only other case, there exists a zeroth edge e_0 contained in the cell c_1 and a second edge e_2 contained in a cell $c \in \{c_1, c_2\}$ such that both e_0 and e_2 are perpendicular to the edge e_1. It follows that e_0 and e_2 are distinct, parallel edges. Furthermore, the edges e_0 and e_2 are contained in distinct long edges of the long-cell $\{c_1, c_2\}$, hence the long edges of $\{c_1, c_2\}$ are connected by $\gamma([0,t_2])$. Since $\gamma([0,t_2])$ is contained in $c_1 \cup c_2$, $\{c_1, c_2\}$ is an lg-cell.

We conclude that if $t_1 \in (0,1)$, then there is a g-cell or an lg-cell contained in $D_1[c_0]$.

(B) Suppose that $t_1 = 1$. Then, $\gamma([0,1])$ is contained entirely in one cell since $\gamma(t)$ does not lie in any edge for every $t \in (0,1)$.

(B1) Suppose $\gamma(1)$ is in the interior of an edge e belonging to c_0. Then the unique cell $c \neq c_0$ containing e also contains a zeroth edge parallel to e, as well as $\gamma([0,1])$ in its entirety. In this case, c is a g-cell.

(B2) In the only other case, $\gamma(1)$ is not in the interior an edge so $\gamma(1)$ is a corner of c_0. Then, there are four first edges, each of which is parallel and sharing a cell with exactly one of the four possible zeroth edges. Consequently, in this case the cell containing $\gamma([0,1])$ in its entirety is a g-cell.

We conclude that if $t_1 = 1$, then there is a g-cell contained in $D_1[c_0]$.

(C) Suppose that $t_1 = 0$. In this case, there exists a unique first edge e_1.

(C1) Suppose that $\tilde{t}_1 = t_2$. Let c_1 and c_2 be the cells sharing the edge e_1. In this case $\gamma(0) \in \partial D_1[c_0]$ and $\gamma(t_2) \in \partial c_0$ belong to opposite extremal points of the edge e_1 hence belong to distinct long-edges of the long cell $\{c_1, c_2\}$. Furthermore, since the only edge that $\gamma((0,t_2))$ can intersect is e_1, $\gamma([0,t_2]) \subset c_1 \cup c_2$ hence $\{c_1, c_2\}$ forms an lg-cell.

Suppose, on the other hand, that $\tilde{t}_1 < t_2$. Then, since $\gamma(t)$ does not lie in any edge for $t \in (\tilde{t}_1, t_2)$, there exists a unique cell c_1 containing $\gamma([\tilde{t}_1, t_2])$. c_1 must contain the edge e_1 - let c_2 denote the other cell containing the edge e_1. c_1 must contain at least one second edge so we have the following possibilities.

(C2) If there exists a second edge e contained in c_1 which is parallel to e_1, then c_1 is a g-cell since $\gamma([\tilde{t}_1, t_2])$ connects e_1 and e.

(C3) In the only other possibility, there exists a second edge contained in c_1 which is perpendicular to e_1. In this case, $\gamma(0)$ and $\gamma(t_2)$ are contained in distinct long-edges of the long-cell $\{c_1, c_2\}$, hence $\{c_1, c_2\}$ forms an lg-cell.

We conclude that if $t_1 = 0$, then there exists a g-cell or an lg-cell contained in $D_1[c_0]$.

We have covered every possible case, proving the lemma. $\square$

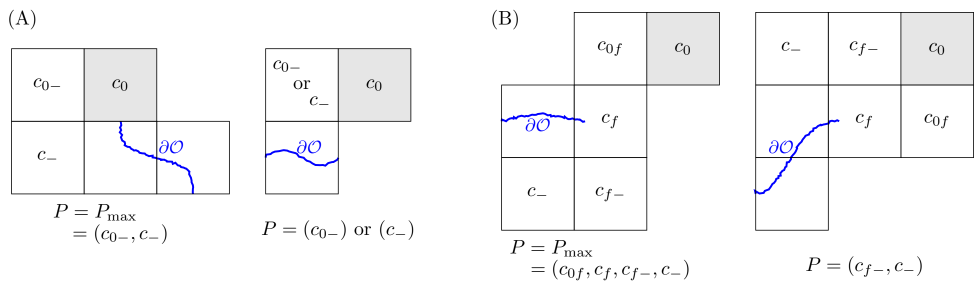

Figure 5.6 Examples of cell-paths for different cases in the proof of Lemma 5.28.

Next we construct a cell-path for each covering cell, using the above lemma as well as the fact that there is a filled cell in the 1-cell neighbourhood of any covering cell.

Lemma 5.28. *For any covering cell c_0, there exists a g-cell c_n (or an lg-cell $\{c_n, c_{n+1}\}$) contained in $D_2[c_0]$ and a cell-path $(c_1, \ldots, c_{n-1})$ from c_0 to c_n (or to $\{c_n, c_{n+1}\}$ resp.) such that c_j is a covering cell contained in $D_2[c_0]$ for all $j \in \{1, \ldots, n-1\}$,*

Proof. Let c_0 be a covering cell. We aim to construct a g-cell c_g (or an lg-cell $\{c_{lg}^{(1)}, c_{lg}^{(2)}\}$) and a cell path P from c_0 to c_g (or to $\{c_{lg}^{(1)}, c_{lg}^{(2)}\}$ resp). If c_0 is a g-cell (or in an lg-cell), then we define P to be empty. We consider the two remaining possible cases.

(A) Suppose first that there exists a g-cell $c_g \subset D_1[c_0]$ (or an lg-cell $\{c_{lg}^{(1)}, c_{lg}^{(2)}\}$ with $c_{lg}^{(j)} \subset D_1[c_0]$ for some $j \in \{1,2\}$). Let $\tilde{c}_g := \mathrm{int}(c_g)$ (or $\tilde{c}_g := \mathrm{int}(c_{lg}^{(1)} \cup c_{lg}^{(2)})$ resp.). There exists a cell $c_- \subset D_1[c_0] \backslash \tilde{c}_g$ which shares a normal edge with c_g

(or with $\{c_{lg}^{(1)}, c_{lg}^{(2)}\}$ resp.). There exists a cell $c_{0-} \subset D_1[c_0]\backslash\tilde{c}_g$ which shares an edge with both c_0 and c_-.

Define P as any length-minimising subsequence of

$$P_{\max} := (c_{0-}, c_-)$$

such that hypotheses (1) and (2) of Definition 5.23 are satisfied. Note that P always exists since $P_{\max}$ satisfies these hypotheses. P cannot contain c_0 or repeated elements since this would yield a shorter such subsequence. P does not contain c_g (or an element of $\{c_{lg}^{(1)}, c_{lg}^{(2)}\}$ resp.) by definition. Consequently, P satisfies hypothesis (3) of Definition 5.23 and is a cell path. c_{0-} and c_0 are contained in $D_1[c_0]$ and share an edge or corner with a g-cell (or an lg-cell respectively) so the elements of P are covering cells contained in $D_1[c_0] \subset D_2[c_0]$.

(B) In the other case, there does not exist a g-cell, or an element of an lg-cell, contained in $D_1[c_0]$. Since c_0 is a covering cell, there exists a filled cell $c_f \subset D_1[c_0]$. There exists a cell $c_{0f} \subset D_1[c_0]$ sharing an edge with both c_0 and c_f. By Lemma 5.27, there exists a g-cell $c_g \subset D_1[c_f]$ (or an lg-cell $\{c_{lg}^{(1)}, c_{lg}^{(2)}\}$ contained in $D_1[c_f]$). Note that, by assumption, c_f and c_{0f} are distinct from c_g (or from both elements of $\{c_{lg}^{(1)}, c_{lg}^{(2)}\}$ resp.). Let $\tilde{c}_g := \mathrm{int}(c_g)$ (or $\tilde{c}_g := \mathrm{int}(c_{lg}^{(1)} \cup c_{lg}^{(2)})$ resp.). There exists a cell $c_- \subset D_1[c_f]\backslash\tilde{c}_g$ which shares a normal edge with c_g (or with $\{c_{lg}^{(1)}, c_{lg}^{(2)}\}$ resp.). There exists a cell $c_{f-} \subset D_1[c_f]\backslash\tilde{c}_g$ which shares an edge with both c_f and c_-.

Define P as any length-minimising subsequence of

$$P_{\max} := (c_{0f}, c_f, c_{f-}, c_-)$$

such that hypotheses (1) and (2) of Definition 5.23 are satisfied. By a similar reasoning as in (A), P is a cell-path and its elements are covering cells contained in $D_2[c_0]$.

□

Finally, we utilise the cell-paths that we have constructed, combined with the Poincaré-type inequality for the cell-paths, to prove the Poincaré-type inequality on $\partial^r\mathscr{O}$.

5.3.4 Proof of Theorem 5.6

Let $\{c_j\}$ be the set of covering cells. Then, $\partial^r\mathscr{O} \subseteq \bigcup_j c_j$.

For each c_j which is not a g-cell or in an lg-cell, fix an integer $n_j \geqslant 1$, an associated g-cell $\mathrm{as}[c_j]_{n_j}$ (or an associated lg-cell $\{\mathrm{as}[c_j]_{n_j}, \mathrm{as}[c_j]_{n_j+1}\}$) and (if $n_j \geqslant 2$) an associated cell-path $(\mathrm{as}[c_j]_1, ..., \mathrm{as}[c_j]_{n_j-1})$ from c_j to $\mathrm{as}[c_j]_{n_j}$ (or to $\{\mathrm{as}[c_j]_{n_j}, \mathrm{as}[c_j]_{n_j+1}\}$ resp.). If c_j is a g-cell itself then there are no associated cells and if c_j is in an lg-cell, let $\mathrm{as}[c_j]_1$ be the other cell in the lg-cell.

For each j, in the case of an associated g-cell, let $N_j := n_j$ and in the case of an associated lg-cell let $N_j := n_j + 1$. Additionally, in the case that c_j is a g-cell, let $N_j = 0$ and in the case that c_j is in an lg-cell, let $N_j = 1$. By Lemma 5.28, we can choose $\mathrm{as}[c_j]_k$ such that for each j and each $k \in \{1, ..., N_j\}$, $\mathrm{as}[c_j]_k$ is a covering cell contained in $D_2[c_j]$ and $(c_j, \mathrm{as}[c_j]_1, ..., \mathrm{as}[c_j]_{N_j})$ consists of distinct elements.

Applying Lemma 5.26, we have,

$$\|u\|^2_{L^2(\partial^r\mathscr{O})} \leqslant \sum_j \|u\|^2_{L^2(c_j)} \leqslant r^2 \sum_j \left(\|\nabla u\|^2_{L^2(c_j)} + \sum_{k=1}^{N_j} \|\nabla u\|^2_{L^2(\mathrm{as}[c_j]_k)} \right) \tag{5.26}$$

where the sum over k is empty in the case $N_j = 0$. Since the associates to a given covering cell are in its 2-cell neighbourhood, each covering cell can be an associate to at most 24 other covering cells (indeed, there are 25 cells in a 2-cell neighbourhood). Furthermore, the associates to a given covering cell are distinct and each associate $\mathrm{as}[c_j]_k$ is a covering cell so it follows from (5.26) that

$$\|u\|^2_{L^2(\partial^r\mathscr{O})} \leqslant 25r^2 \sum_j \|\nabla u\|^2_{L^2(c_j)} \leqslant 25r^2 \|\nabla u\|^2_{L^2(\partial^{2\sqrt{2}r}\mathscr{O})}$$

where the last inequality holds since $\mathrm{int}(\cup_j c_j) \subseteq \partial^{2\sqrt{2}r}\mathscr{O}$.

5.4 Mosco convergence

In this section, we establish a general Mosco convergence theorem and apply it to pixelated domain approximations. We will make use of the notion of an ε-dilation $\mathrm{dil}_\varepsilon(A)$ of a set $A \subset \mathbb{R}^d$ - recall that this is defined by equation (5.4).

5.4.1 From uniform Poincaré-type inequalities to Mosco convergence

The first step is to prove Mosco convergence for sequences of domains $(\mathscr{O}_n)$ which satisfy a Hausdorff convergence condition to a limit domain $\mathscr{O}$ and which verify a certain Poincaré-type inequality uniformly for the whole sequence. Such a uniform Poincaré inequality does not follow immediately from the results of the previous section, but will be established in Section 5.4.2 under suitable hypotheses.

The following fact shall be useful.

Lemma 5.29. *For any non-empty, bounded sets $A, B \subset \mathbb{R}^d$, we have*

$$\sup_{x \in A^c \cap B} \operatorname{dist}(x, \partial B) \leqslant \mathrm{d}_H(A,B) + \mathrm{d}_H(\partial A, \partial B).$$

Proof. This holds because

$$\begin{aligned}\sup_{x \in A^c \cap B} \operatorname{dist}(x, \partial B) &\leqslant \sup_{x \in A^c \cap B} \operatorname{dist}(x, \partial A) + \mathrm{d}_H(\partial A, \partial B) \\ &= \sup_{x \in A^c \cap B} \operatorname{dist}(x, A) + \mathrm{d}_H(\partial A, \partial B) \\ &\leqslant \mathrm{d}_H(A,B) + \mathrm{d}_H(\partial A, \partial B).\end{aligned}$$

□

The proof of the next proposition uses a construction of certain cut-off functions to directly prove that the two conditions in Definition 5.1 for Mosco convergence hold. Note that the regularity of the limit domain $\mathscr{O}$ is not yet required. We do require, however, that the Lebesgue measure of the boundary $\partial\mathscr{O}$ vanishes, which ensures that the Lebesgue measure of the collar neighbourhood $\partial^{\varepsilon}\mathscr{O}$ tends to 0 as $\varepsilon \to 0$.

Proposition 5.30. *Let $\mathscr{O} \subset \mathbb{R}^d$ and $\mathscr{O}_n \subset \mathbb{R}^d$, $n \in \mathbb{N}$, be bounded, open sets such that the following holds:*

(a) $l(n) := \mathrm{d}_H(\mathscr{O}, \mathscr{O}_n) + \mathrm{d}_H(\partial\mathscr{O}, \partial\mathscr{O}_n) \to 0$ *as* $n \to \infty$.

(b) *There exist*

   (i) $(f(n))_{n \in \mathbb{N}}$ *such that* $2l(n) \leqslant f(n)$ *for all* $n \in \mathbb{N}$ *and* $f(n) \to 0$ *as* $n \to \infty$,

   (ii) *constants* $C, \alpha > 0$ *independent of* n *and* u

   such that, if either $V = \mathscr{O}$ or $V = \mathscr{O}_n$ for some large enough $n \in \mathbb{N}$, then for all $u \in H_0^1(V)$ we have

$$\|u\|_{L^2(\partial^{f(n)} V)} \leqslant C f(n) \|\nabla u\|_{L^2(\partial^{\alpha f(n)} V)}. \tag{5.27}$$

(c) $\mu_{\mathrm{leb}}(\partial\mathscr{O}) = 0$.

Then, $\mathscr{O}_n$ converges to $\mathscr{O}$ in the Mosco sense as $n \to \infty$.

Proof. Throughout the proof, let L^p denote $L^p(\mathbb{R}^d)$ for $p = 2, \infty$ and let H^1 denote $H^1(\mathbb{R}^d)$. All limits will be as $n \to \infty$.

Define function $\tilde{\chi} : \mathbb{R}_+ \to [0,1]$ by

$$\tilde{\chi}(t) := \begin{cases} t & \text{if } t \in [0,1) \\ 1 & \text{if } t \in [1,\infty). \end{cases} \tag{5.28}$$

$\tilde{\chi}$ is weakly differentiable with $\|\tilde{\chi}'\|_{L^\infty} = 1$. $\tilde{\chi}$ will be used in the construction of a cut-off function χ_n in both Step 1 and Step 2 below. We shall also require the following two facts. Firstly, for any $A \subset \mathbb{R}^d$ with piecewise smooth boundary, the function $x \mapsto \mathrm{dist}(x,A)$ is continuous and piecewise smooth hence weakly differentiable. Furthermore, since

$$|\mathrm{dist}(x,A) - \mathrm{dist}(y,A)| \leqslant |x-y| \qquad (x,y \in \mathbb{R}^d),$$

the L^∞ norm of $x \mapsto \nabla_x \mathrm{dist}(x,A)$ is bounded by 1.

Step 1 (Mosco convergence condition (1)). Let $u_n \in H_0^1(\mathscr{O}_n)$, $n \in \mathbb{N}$, and suppose that $u_n \rightharpoonup u$ in H^1 for some $u \in H^1$. We aim to show that $u \in H_0^1(\mathscr{O})$.

Let $P : H^1 \to H_0^1(\mathscr{O})$ be the orthogonal projection. If $(w_n) \subset H_0^1(\mathscr{O})$ and $w_n \rightharpoonup u$ in H^1 then

$$\langle u, (1-P)\phi \rangle_{H^1} = \lim_{n\to\infty} \langle w_n, (1-P)\phi \rangle_{H^1} = 0 \qquad (\phi \in H^1)$$

so $u \in H_0^1(\mathscr{O})$. Hence it suffices to show that there exists $w_n \in H_0^1(\mathscr{O})$ such that $w_n \rightharpoonup u$ in H^1.

Assume without loss of generality that $f(n) > 0$ for all $n \in \mathbb{N}$. For each $n \in \mathbb{N}$, let $A_n \subset \mathbb{R}^d$ be an open neighbourhood of $\mathscr{O}^c$ with piecewise smooth boundary such that $A_n \cap \mathscr{O} \subseteq \partial^{f(n)/4}\mathscr{O}$ (A_n can be constructed by an open cover of balls of radius $f(n)/4$ for instance).

Define a cut-off function $\chi_n : \mathbb{R}^d \to [0,1]$ by

$$\chi_n(x) = \tilde{\chi}(4f(n)^{-1}\mathrm{dist}(x,A_n)) \qquad (x \in \mathbb{R}^d). \tag{5.29}$$

Then, $\chi_n = 0$ on an open neighbourhood of $\mathscr{O}^c$ and $\chi_n(x) = 1$ for any $x \in \mathscr{O}_n$ outside the set

$$\mathscr{U}_n := \{x \in \mathscr{O}_n : \mathrm{dist}(x, \mathscr{O}^c) \leqslant f(n)/2\}.$$

By the piecewise smoothness of ∂A_n, χ_n is weakly differentiable and, by an application of the chain rule,

$$\|\nabla\chi_n\|_{L^\infty} \leqslant 4f(n)^{-1}. \tag{5.30}$$

By Lemma 5.29, we have

$$\sup_{x\in\mathscr{O}^c\cap\mathscr{O}_n} \operatorname{dist}(x,\partial\mathscr{O}_n) \leqslant l(n) \leqslant \frac{f(n)}{2}. \tag{5.31}$$

We claim that $\mathscr{U}_n \subset \partial^{f(n)}\mathscr{O}_n$. To see this, let $x\in\mathscr{U}_n$. Then there exists $y\in\mathscr{O}^c$ with $|x-y|\leqslant f(n)/2$. If $y\in\mathscr{O}_n$, then inequality (5.31) implies that $\operatorname{dist}(y,\partial\mathscr{O}_n)\leqslant f(n)/2$ so $\operatorname{dist}(x,\partial\mathscr{O}_n)\leqslant f(n)$. If $y\notin\mathscr{O}_n$ on the other hand, then, since $x\in\mathscr{O}_n$, $\operatorname{dist}(x,\partial\mathscr{O}_n)\leqslant |x-y|\leqslant f(n)/2$ proving the claim.

Furthermore, for any $x\in\mathscr{U}_n$, we have

$$\operatorname{dist}(x,\partial\mathscr{O}) \leqslant l(n)+\operatorname{dist}(x,\partial\mathscr{O}_n) \leqslant l(n)+f(n)$$

so by hypothesis (c) and continuity of measures from above,

$$\mu_{\text{leb}}(\mathscr{U}_n) \leqslant \mu_{\text{leb}}(\operatorname{dil}_{l(n)+f(n)}(\partial\mathscr{O})) \to \mu_{\text{leb}}(\partial\mathscr{O}) = 0.$$

Let $w_n := \chi_n u_n$. Then, since $\chi_n = 0$ on an open neighbourhood of $\mathscr{O}^c$, we have $w_n\in H_0^1(\mathscr{O})$ and it suffices to show that $w_n = \chi_n u_n \rightharpoonup u$ in H^1. Let $\phi\in H^1$ be an arbitrary test function. Firstly, we have,

$$|\langle\chi_n u_n - u,\phi\rangle_{H^1}| \leqslant \underbrace{|\langle\chi_n u_n - u,\phi\rangle_{L^2}|}_{(A1)} + \underbrace{|\langle\nabla(\chi_n u_n)-\nabla u,\nabla\phi\rangle_{L^2}|}_{(A2)}.$$

Focusing on the term (A1),

$$\begin{aligned}|\langle\chi_n u_n - u,\phi\rangle_{L^2}| &\leqslant |\langle\chi_n u_n - u_n,\phi\rangle_{L^2}| + |\langle u_n - u,\phi\rangle_{L^2}|\\ &\leqslant \|u_n\|_{L^2(\mathscr{U}_n)}\|\phi\|_{L^2(\mathscr{U}_n)} + |\langle u_n - u,\phi\rangle_{L^2}| \to 0.\end{aligned}$$

Here, the second inequality holds since $u_n = 0$ almost everywhere outside $\mathscr{O}_n$ and so $\chi_n u_n = u_n$ almost everywhere outside $\mathscr{U}_n$. The limit holds by the weak convergence of (u_n) (so also (u_n) is bounded in H^1) as well as the fact that $\mu_{\text{leb}}(\mathscr{U}_n)\to 0$.

Focusing on the term (A2),

$$|\langle\nabla(\chi_n u_n)-\nabla u,\nabla\phi\rangle_{L^2}| \leqslant \underbrace{|\langle\nabla(\chi_n u_n)-\nabla u_n,\nabla\phi\rangle_{L^2}|}_{(B1)} + \underbrace{|\langle\nabla u_n-\nabla u,\nabla\phi\rangle_{L^2}|}_{(B2)}.$$

The term (B2) tends to zero by the weak convergence of (u_n). Focusing on the term (B1),

$$\begin{aligned}|\langle\nabla(\chi_n u_n)-\nabla u_n,\nabla\phi\rangle_{L^2}| &\leqslant |\langle\chi_n\nabla u_n-\nabla u_n,\nabla\phi\rangle_{L^2}|+|\langle\nabla(\chi_n)u_n,\nabla\phi\rangle_{L^2}|\\ &\leqslant \underbrace{\|\nabla u_n\|_{L^2(\mathscr{U}_n)}\|\nabla\phi\|_{L^2(\mathscr{U}_n)}}_{(C1)}+\underbrace{\|\nabla\chi_n\|_{L^\infty}\|u_n\|_{L^2(\mathscr{U}_n)}\|\nabla\phi\|_{L^2(\mathscr{U}_n)}}_{(C2)}\end{aligned}$$

where in the second inequality we used the fact that $\chi_n\nabla u_n=\nabla u_n$ almost everywhere outside $\mathscr{U}_n$ and the fact that $\mathrm{supp}(\nabla(\chi_n))\cap\mathscr{O}_n\subseteq\mathscr{U}_n$. The term (C1) tends to zero since (u_n) is bounded in H^1 and $\mu_{\mathrm{leb}}(\mathscr{U}_n)\to 0$. Focusing on the term (C2), notice first that, by the assumed Poincaré-type inequality (5.27),

$$\|u_n\|_{L^2(\mathscr{U}_n)}\leqslant\|u_n\|_{L^2(\partial^{f(n)}\mathscr{O}_n)}\leqslant Cf(n)\|\nabla u_n\|_{L^2(\partial\mathscr{O}_n^{\alpha f(n)})},$$

and so, using (5.30),

$$\|\nabla\chi_n\|_{L^\infty}\|u_n\|_{L^2(\mathscr{U}_n)}\|\nabla\phi\|_{L^2(\mathscr{U}_n)}\leqslant 4C\|\nabla u_n\|_{L^2(\partial^{\alpha f(n)}\mathscr{O}_n)}\|\nabla\phi\|_{L^2(\mathscr{U}_n)}\to 0.$$

It follows that the term (A2) tends to zero, that $w_n\rightharpoonup u$ in H^1 and hence that $u\in H^1_0(\mathscr{O})$.
Step 2 (Mosco convergence condition (2)). Let $u\in H^1_0(\mathscr{O})$ - we aim to show that there exists $u_n\in H^1_0(\mathscr{O}_n)$ such that $u_n\to u$ in H^1. Note that in this part of the proof, we shall redefine A_n, χ_n and $\mathscr{U}_n$.

For each $n\in\mathbb{N}$, let $A_n\subset\mathbb{R}^d$ be an open neighbourhood of $\mathscr{O}_n^c$ with piecewise smooth boundary such that $A_n\cap\mathscr{O}_n\subseteq\partial^{f(n)/4}\mathscr{O}_n$. Define a cut-off function $\chi_n:\mathbb{R}^d\to[0,1]$ by

$$\chi_n(x)=\tilde{\chi}(4f(n)^{-1}\mathrm{dist}(x,A_n))\qquad(x\in\mathbb{R}^d).\tag{5.32}$$

Then, $\chi_n=0$ on an open neighbourhood of $\mathscr{O}_n^c$ and $\chi_n(x)=1$ for any $x\in\mathscr{O}$ outside the set

$$\mathscr{U}_n:=\{x\in\mathscr{O}:\mathrm{dist}(x,\mathscr{O}_n^c)\leqslant f(n)/2\}.$$

χ_n is weakly differentiable and, by an application of the chain rule,

$$\|\nabla\chi_n\|_{L^\infty}\leqslant 4f(n)^{-1}.\tag{5.33}$$

By Lemma 5.29,

$$\sup_{x\in\mathscr{O}_n^c\cap\mathscr{O}}\mathrm{dist}(x,\partial\mathscr{O})\leqslant l(n)\leqslant\frac{f(n)}{2}$$

so, by a similar reasoning as in Step 1, we have $\mathscr{U}_n\subseteq\partial^{f(n)}\mathscr{O}$. By hypothesis (c) and continuity of measures from above, $\mu_{\mathrm{leb}}(\mathscr{U}_n)\to 0$.

Let $u_n := \chi_n u$. Then $u_n \in H^1_0(\mathscr{O}_n)$ since χ_n vanishes on an open neighbourhood of $\mathscr{O}_n^c$. Firstly,

$$\|u_n - u\|_{H^1} \leqslant \underbrace{\|\chi_n u - u\|_{L^2}}_{(D1)} + \underbrace{\|\nabla(\chi_n u) - \nabla u\|_{L^2}}_{(D2)}.$$

Focusing on the term (D1) and using the fact that $\chi_n u = u$ almost everywhere outside $\mathscr{U}_n$,

$$\|\chi_n u - u\|_{L^2} = \|\chi_n u - u\|_{L^2(\mathscr{U}_n)} \leqslant \|u\|_{L^2(\mathscr{U}_n)} \to 0.$$

Focusing on the term (D2), we have

$$\|\nabla(\chi_n u) - \nabla u\|_{L^2} \leqslant \underbrace{\|\chi_n \nabla u - \nabla u\|_{L^2}}_{(E1)} + \underbrace{\|\nabla(\chi_n) u\|_{L^2}}_{(E2)}.$$

The term (E1) tends to zero by the same reasoning that was applied to (D1). Focusing on the term (E2), notice first that, by the assumed Poincaré-type inequality (5.27),

$$\|u\|_{L^2(\mathscr{U}_n)} \leqslant \|u\|_{L^2(\partial^{f(n)}\mathscr{O})} \leqslant Cf(n)\|\nabla u\|_{L^2(\partial^{\alpha f(n)}\mathscr{O})},$$

and so, by (5.33),

$$\|\nabla(\chi_n)u\|_{L^2} = \|\nabla(\chi_n)u\|_{L^2(\mathscr{U}_n)} \leqslant 4f(n)^{-1}\|u\|_{L^2(\mathscr{U}_n)} \leqslant 4C\|\nabla u\|_{L^2(\partial^{\alpha f(n)}\mathscr{O})} \to 0.$$

It follows that the term (D2) tends to zero hence $u_n \to u$ strongly in H^1 as required. □

5.4.2 Characterisation of $\partial\mathscr{O}_n$ for large n

In order to verify the uniform Poincaré-type inequality needed to apply Proposition 5.30, we shall require additional hypotheses, such as regularity of the limit domain $\mathscr{O}$ and $\#_c\mathrm{int}(\mathscr{O}^c) = \#_c(\mathscr{O}^c) < \infty$. With these hypotheses at hand, we shall provide in Proposition 5.38 a characterisation of some geometric properties of the boundaries of sequences of domains $\mathscr{O}_n$, for large n. Roughly speaking, we shall prove that for each connected component ∂D_j of $\partial\mathscr{O}$, there exists a "large" path-connected subset $\gamma_n^{(j)}$ of $\partial\mathscr{O}_n$ such that $\gamma_n^{(j)}$ has comparable diameter to ∂D_j, and every other point in $\partial\mathscr{O}_n$ is close to one of the large subsets $\gamma_n^{(j)}$. Then, in Section 5.4.3, this characterisation is used in conjunction with the explicit Poincaré-type inequality of Theorem 5.6 to obtain the general Mosco result Theorem 5.3 .

Let us collect some geometric and topological lemmas in preparation for the proof of Proposition 5.38. Firstly, we shall require the following basic fact:

An open set $A \subset \mathbb{R}^d$ is regular if and only if $A^c \subset \mathbb{R}^d$ is the closure of an open set.

Next, let us solidify a notion of an outer boundary for a domain. In particular, this notion shall be crucial in defining boundary subsets $\gamma_n^{(j)}$.

Definition 5.31. The *outer boundary* $\partial^{\text{out}}A$ of a bounded, connected set $A \subset \mathbb{R}^d$ is defined as the boundary $\partial\Gamma$ of the unique unbounded connected component Γ of A^c.

The next lemma is required to ensure that the large boundary subsets $\gamma_n^{(j)}$ are path-connected.

Lemma 5.32. *Suppose that $A \subset \mathbb{R}^2$ is bounded, connected and either open or closed. If ∂A locally connected, then $\partial^{\text{out}}A$ is path-connected.*

Proof. It is a consequence of the Carathéodory theorem [56, Theorem 2.1] that if $K \subset \mathbb{R}^2$ is a connected, compact set with $\mathbb{R}^2\backslash K$ connected and there exists a locally connected, compact set L such that $\partial K \subseteq L \subseteq K$, then there exists a continuous, surjective map $\Psi : \mathbb{R}^2\backslash B_1(0) \to \mathbb{R}^2\backslash\text{int}(K)$. Restricting the map Ψ yields a continuous, surjective map $\gamma : \partial B_1(0) \to \partial K$ (the so-called *Carathéodory loop*), showing that ∂K is path-connected.

Let $A \subset \mathbb{R}^2$ be bounded and connected with ∂A locally connected. Let Γ denote the unique unbounded connected component of A^c and let $E := A^c\backslash\Gamma$.

Consider first the case that A is closed. Let $K := A \cup E$. Then K is compact, connected and $K^c = \Gamma$ is connected. Let $L := \partial A$. Then, L is compact, locally connected and satisfied $\partial^{\text{out}}A = \partial K \subseteq L \subseteq K$ so $\partial^{\text{out}}A$ is path-connected.

Now suppose that A is open. $\partial^{\text{out}}A = \partial\Gamma$ is connected since Γ and $\Gamma^c = A \cup E$ are connected [45]. Furthermore, in this case, $\partial^{\text{out}}A$ is a connected component of ∂A since $\partial\Gamma \subset \Gamma$ and Γ is separated from any other connected component of A^c. It follows that $\partial^{\text{out}}A$ is a connected, locally connected and compact metric space hence path-connected [105, Lemma 16.4]. □

The next lemma gives a property of the outer boundary of a dilation of set. It shall be utilised in Proposition 5.38 to help show that every point in the boundary $\partial\mathscr{O}_n$ of the approximating domains is close to a large subset $\gamma_n^{(j)}$ for large n.

Lemma 5.33. *If $A \subset \mathbb{R}^d$ is a bounded, connected, regular open set such that* $\text{int}(A^c)$ *is connected, then*

$$\sup_{x\in\partial A} \text{dist}(x, \partial^{\text{out}}\,\text{dil}_\varepsilon(A)) \to 0 \quad \textit{as} \quad \varepsilon \to 0.$$

Proof. Let $x \in \partial A$. By regularity, A^c is the closure of $\text{int}(A^c)$ so there exists a sequence $(x_n) \subset \text{int}(A^c)$ with $x_n \to x$. We claim that for each n, there exists $\varepsilon_n > 0$ such that x_n lies in the unbounded connected component of $\text{dil}_\varepsilon(A)^c$ for all $\varepsilon \in (0, \varepsilon_n]$. To see this first note that, since $\text{int}(A^c)$ is connected and A is bounded, there exists an unbounded, connected open set V_n such that $\overline{V}_n \subset \mathrm{int}(A^c)$ and $x_n \in V_n$. The claim follows from the fact that V_n is a subset of $\mathrm{dil}_\varepsilon(A)^c$ for small enough ε.

Without loss of generality, assume that $\varepsilon_{n+1} < \varepsilon_n$ for all n. For each $\varepsilon \in (\varepsilon_{n-1}, \varepsilon_n]$, x lies in $\mathrm{dil}_\varepsilon(A)$ and x_n lies in the unbounded connected component of $\mathrm{int}(\mathrm{dil}_\varepsilon(A)^c)$, so,

$$\delta_x(\varepsilon) := \mathrm{dist}(x, \partial^{\mathrm{out}} \mathrm{dil}_\varepsilon(A)) \leqslant |x - x_n|.$$

Since $\varepsilon_n \to 0$ monotonically as $n \to \infty$ and $|x - x_n| \to 0$ as $n \to \infty$, we have $\delta_x(\varepsilon) \to 0$ as $\varepsilon \to 0$. $\delta_x(\varepsilon)$ is equal to the distance from x to the unbounded component of $\mathrm{dil}_\varepsilon(A)^c$. Since the latter set is nested for decreasing $\varepsilon > 0$, $\delta_x(\varepsilon)$ in fact tends to zero monotonically as $\varepsilon \to 0$. Finally, ∂A is compact and $\delta_x(\varepsilon)$ is continuous in x so an application of Dini's theorem yields

$$\delta(\varepsilon) := \sup_{x \in \partial A} \delta_x(\varepsilon) \to 0 \quad \text{as} \quad \varepsilon \to 0.$$

□

Next, we prove a couple of useful elementary topological facts.

Lemma 5.34. *If $A, B \subset \mathbb{R}^d$ are such that B is open and connected, $A \cap B \neq \emptyset$ and $\partial A \subset B^c$, then $B \subset A$.*

Proof. Suppose for contradiction that $A^c \cap B \neq \emptyset$. B is path-connected so there exists a path in B from any point in $A \cap B$ to any point in $A^c \cap B$. Such a path must intersect ∂A which is the desired contradiction. □

Lemma 5.35. *If $A \subset \mathbb{R}^d$ is a connected open set such that $\#_c(A^c) < \infty$, then the union of A with any connected component of A^c is open and connected.*

Proof. Let D be any connected component of A^c. Since $\#_c(A^c) < \infty$, there exists an open neighbourhood U of D such that U does not intersect any other connected component of A^c. Consequently, $U \backslash D \subset A$ and so $A \cup D = A \cup U$. The lemma follows from the fact that the union of two open, connected sets with nonempty intersection is open and connected. □

In Proposition 5.38, we shall assume that the limit domain $\mathscr{O}$ is bounded, regular and satisfies $\#_c\mathrm{int}(\mathscr{O}^c) = \#_c(\mathscr{O}^c) < \infty$. The next lemma collects some properties of domains satisfying these hypotheses. Intuitively, such a domain has a finite number of holes $D_1, \dots, D_N$ which do not touch each other and which do not touch the unbounded exterior of the domain. The set D_{N+1} below is essentially the domain $\mathscr{O}$ with all the holes filled in.

Lemma 5.36. *Suppose that $\mathscr{O} \subset \mathbb{R}^d$ is a bounded, connected, regular open set such that $\#_c \mathrm{int}(\mathscr{O}^c) = \#_c(\mathscr{O}^c) < \infty$. Let $D_1, \ldots, D_N \subset \mathbb{R}^d$ denote the bounded connected components of* $\mathrm{int}(\mathscr{O}^c)$. *Let $D_{N+1} \subset \mathbb{R}^d$ denote the complement of the unbounded connected component of $\mathscr{O}^c$. Then,*

(a) *the collection of closed sets $\overline{D}_1, \ldots, \overline{D}_N, D^c_{N+1}$ is pairwise disjoint,*

(b) $\mathrm{int}(D^c_j)$ *is connected for each $j \in \{1, \ldots, N+1\}$,*

(c) *D_j is regular for each $j \in \{1, \ldots, N+1\}$ and*

(d) *$\partial D_1, \ldots, \partial D_{N+1}$ are the connected components of $\partial \mathscr{O}$.*

Proof. Let $E_{N+1} \subset \mathbb{R}^d$ denote the unbounded connected component of $\mathrm{int}(\mathscr{O}^c)$, so that

$$\mathrm{int}(\mathscr{O}^c) = D_1 \cup \cdots \cup D_N \cup E_{N+1}. \tag{5.34}$$

By the regularity of $\mathscr{O}$ and the fact the closure of the union of two sets is the union of the closure,

$$\mathscr{O}^c = \overline{\mathrm{int}(\mathscr{O}^c)} = \overline{D}_1 \cup \cdots \cup \overline{D}_N \cup \overline{E}_{N+1}. \tag{5.35}$$

By construction, we have that $\#_c \mathrm{int}(\mathscr{O}^c) = N+1$. By the hypothesis $\#_c \mathrm{int}(\mathscr{O}^c) = \#_c(\mathscr{O}^c)$, we must in fact have $\#_c(\mathscr{O}^c) = N+1$ and this can only hold if the collection of closed sets $\overline{D}_1, \ldots, \overline{D}_N, \overline{E}_{N+1}$ is exactly the collection of connected components of $\mathscr{O}^c$ and hence must be pairwise disjoint. In particular, since $\overline{E}_{N+1}$ is the unique unbounded connected component of $\mathscr{O}^c$, we must have $D_{N+1} = (\overline{E}_{N+1})^c$, proving (a).

Moving on to the proof of (b), first note that we have the disjoint union

$$\mathbb{R}^d = \mathscr{O} \cup \overline{D}_1 \cup \cdots \cup \overline{D}_N \cup D^c_{N+1}$$

and so, for any $j \in \{1, \ldots, N\}$,

$$\mathrm{int}(D^c_j) = (\overline{D}_j)^c = \mathscr{O} \cup \left(\bigcup_{\substack{k=1 \\ k \neq j}}^{N} \overline{D}_k \right) \cup D^c_{N+1}. \tag{5.36}$$

By N successive applications of Lemma 5.35, we see that the right hand side of (5.36) is connected, proving (b) for $j \in \{1, \ldots, N\}$. The proof of (b) for $j = N+1$ is immediate since $\mathrm{int}(D^c_{N+1}) = E_{N+1}$.

Next, focus on the regularity of D_j. Since the interior of the union of two disjoint closed sets is the union of the interior of those sets, we have

$$\mathrm{int}(\mathscr{O}^c) = \mathrm{int}(\overline{D}_1) \cup \cdots \cup \mathrm{int}(\overline{D}_N) \cup \mathrm{int}(\overline{E}_{N+1}). \tag{5.37}$$

Combined with (5.34) and disjointedness, (5.37) implies that, for any $j \in \{1,...,N\}$,

$$\begin{aligned}\operatorname{int}(\overline{D}_j) &= \overline{D}_j \cap \big(\operatorname{int}(\overline{D}_1) \cup \cdots \cup \operatorname{int}(\overline{D}_N) \cup \operatorname{int}(\overline{E}_{N+1})\big) \\ &= \overline{D}_j \cap (D_1 \cup \cdots \cup D_N \cup E_{N+1}) = D_j,\end{aligned}$$

that is, D_j is regular. D_{N+1} is also regular because $D_{N+1}^c = \overline{E}_{N+1}$ and E_{N+1} is open.

The fact that D_j is an open, connected subset of $\mathbb{R}^d$ and D_j^c is connected ensures that ∂D_j is connected for each $j \in \{1,...,N+1\}$ [45]. Then (d) follows from (5.35) and the fact that the collection of closed connected sets $\partial D_1,...,\partial D_{N+1}$ is pairwise disjoint. □

The following lemma, concerning Hausdorff convergence for the boundaries of approximations of an open set from below, follows immediately from Lemma 5.41 below.

Lemma 5.37. *If $A \subset \mathbb{R}^d$ and $A_n \subset \mathbb{R}^d$, $n \in \mathbb{N}$, are bounded open sets such that $A_n \subseteq A_{n+1} \subseteq A$ for all $n \in \mathbb{N}$ and $A = \cup_{n=1}^{\infty} A_n$, then $\mathrm{d}_H(\partial A_n, \partial A) \to 0 \quad as \quad n \to \infty$.*

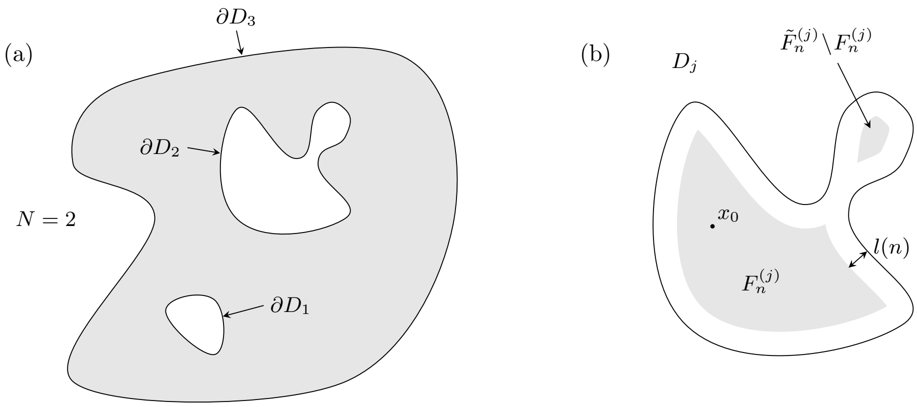

Figure 5.7 Illustration for the proof of Proposition 5.38

Proposition 5.38. *Suppose that $\mathscr{O} \subset \mathbb{R}^2$ is a bounded, connected, regular open set such that $\mu_{\mathrm{leb}}(\partial\mathscr{O}) = 0$ and $\#_c\operatorname{int}(\mathscr{O}^c) = \#_c(\mathscr{O}^c) < \infty$. Suppose that $\mathscr{O}_n \subset \mathbb{R}^2$, $n \in \mathbb{N}$, is a collection of bounded open sets such that $\partial\mathscr{O}_n$ is locally connected for all $n \in \mathbb{N}$ and*

$$l(n) = \mathrm{d}_H(\mathscr{O}_n, \mathscr{O}) + \mathrm{d}_H(\partial\mathscr{O}_n, \partial\mathscr{O}) \to 0 \quad as \quad n \to \infty.$$

Let $D_j \subset \mathbb{R}^2$, $j \in \{1,...,N+1\}$, denote the sets in Lemma 5.36. Then, there exists:

- *$n_0 \in \mathbb{N}$,*
- *a sequence $\varepsilon(n) > 0$, $n \geqslant n_0$, with $\varepsilon(n) \to 0$ as $n \to \infty$ and $\varepsilon(n) \geqslant 2l(n)$*

- *path-connected subsets* $\gamma_n^{(j)} \subseteq \partial \mathscr{O}_n$, $j \in \{1,\dots,N+1\}$, $n \geqslant n_0$,

such that for all $n \geqslant n_0$ *we have*

$$\operatorname{diam}(\gamma_n^{(j)}) \geqslant \operatorname{diam}(\partial D_j) - \varepsilon(n) \qquad (j \in \{1,\dots,N+1\}) \tag{5.38}$$

and

$$\sup_{x\in\partial\mathscr{O}_n} \operatorname{dist}(x, \gamma_n^{(1)} \cup \dots \cup \gamma_n^{(N+1)}) \leqslant \varepsilon(n). \tag{5.39}$$

Proof. Step 1 (Construction of $\gamma_n^{(j)}$*).*

Let

$$\tilde{F}_n^{(j)} := \operatorname{int}(D_j \backslash \partial^{l(n)} D_j) \qquad (j \in \{1,\dots,N+1\}, n \in \mathbb{N}).$$

Choose any point $x_0 \in D_j$. Then there exists $n_0 \in \mathbb{N}$ large enough such that $x_0 \in \tilde{F}_n^{(j)}$ for all $n \geqslant n_0$. For every $j \in \{1,\dots N+1\}$ and $n \geqslant n_0$, define $F_n^{(j)}$ as the unique path-connected component of the open set $\tilde{F}_n^{(j)}$ containing the point x_0.

$F_n^{(j)}$ is open, bounded, connected and satisfies

$$F_n^{(j)} \subset F_{n+1}^{(j)} \subset D_j$$

for all n. Furthermore, since any path in D_j from x_0 to any point $x \in D_j$ lies in $\tilde{F}_n^{(j)}$ for all large enough n, we have $x \in F_n^{(j)}$ for all large enough n and so

$$\bigcup_{n=1}^{\infty} F_n^{(j)} = D_j.$$

By Lemma 5.37, we have

$$\varepsilon_1^{(j)}(n) := \mathrm{d}_H(\partial F_n^{(j)}, \partial D_j) \to 0 \quad \text{as} \quad n \to \infty \qquad (j \in \{1,\dots,N+1\}, n \geqslant n_0). \tag{5.40}$$

Let us now focus on the case $j \in \{1,\dots,N\}$. The definitions of $F_n^{(j)}$ and $l(n)$ ensure that $\partial \mathscr{O}_n$ does not intersect $F_n^{(j)}$ and $F_n^{(j)} \cap \mathscr{O}_n^c \neq \emptyset$ hence $F_n^{(j)} \subset \mathscr{O}_n^c$ by Lemma 5.34. Define $(\mathscr{O}_n^c)_j$ as the unique connected component of $\mathscr{O}_n^c$ such that the connected set $F_n^{(j)}$ is contained in $(\mathscr{O}_n^c)_j$.

By Lemma 5.36 (a), we can ensure that n_0 is large enough so that the collection of open sets

$$\operatorname{dil}_{2l(n)}(D_1), \dots, \operatorname{dil}_{2l(n)}(D_N), \operatorname{dil}_{2l(n)}(D_{N+1}^c)$$

is pairwise disjoint for $n \geqslant n_0$. Then, for $n \geqslant n_0$, every point in $\partial \operatorname{dil}_{2l(n)}(D_j)$ lies in $\mathscr{O}$ at a distance $\geqslant 2l(n)$ from $\partial \mathscr{O}$ so

$$\partial \operatorname{dil}_{2l(n)}(D_j) \subset \mathscr{O}_n \subset (\mathscr{O}_n^c)_j^c.$$

Since also $(\mathscr{O}_n^c)_j \cap \mathrm{dil}_{2l(n)}(D_j) \neq \emptyset$, an application of Lemma 5.34 yields

$$(\mathscr{O}_n^c)_j \subset \mathrm{dil}_{2l(n)}(D_j). \tag{5.41}$$

for all $n \geqslant n_0$.

Consequently, $(\mathscr{O}_n^c)_j$ is bounded for $n \geqslant n_0$ and we can use the notion of outer boundary (cf. Definition 5.31) to make the definition

$$\gamma_n^{(j)} := \partial^{\mathrm{out}}(\mathscr{O}_n^c)_j \qquad (j \in \{1,...,N\}, n \geqslant n_0). \tag{5.42}$$

By Lemma 5.32, $\gamma_n^{(j)}$ is path-connected. Since $F_n^{(j)} \subset (\mathscr{O}_n^c)_j$ for all $n \geqslant n_0$, we have

$$\mathrm{diam}(\gamma_n^{(j)}) \geqslant \mathrm{diam}(\partial F_n^{(j)}) \geqslant \mathrm{diam}(\partial D_j) - 2\varepsilon_1^{(j)}(n) \tag{5.43}$$

where the final inequality holds by (5.40).

The construction of $\gamma_n^{(N+1)}$ is very similar. In this case, for every $n \geqslant n_0$, $F_n^{(N+1)}$ is contained inside $\mathscr{O}_n$ and we define $\mathscr{O}_{n,0} \subset \mathbb{R}^d$ as the unique connected component of $\mathscr{O}_n$ containing $F_n^{(N+1)}$. $\mathscr{O}_{n,0}$ is bounded because $\mathscr{O}_n$ is bounded hence we can make the definition

$$\gamma_n^{(N+1)} := \partial^{\mathrm{out}}\mathscr{O}_{n,0} \qquad (n \geqslant n_0). \tag{5.44}$$

By Lemma 5.32, $\gamma_n^{(N+1)}$ is path-connected. We have $F_n^{(N+1)} \subset \mathscr{O}_{n,0}$ so (5.43) holds for $j = N+1$ and $n \geqslant n_0$.

Step 2 (Properties of $\gamma_n^{(j)}$).

Let

$$\varepsilon_2^{(j)}(n) := \sup_{x \in \partial D_j} \mathrm{dist}(x, \partial^{\mathrm{out}}\,\mathrm{dil}_{2l(n)}(D_j)) \qquad (j \in \{1,...,N+1\}, n \in \mathbb{N}). \tag{5.45}$$

For each $j \in \{1,...,N+1\}$, D_j satisfies the hypotheses of Lemma 5.33 by Lemma 5.36, hence $\varepsilon_2^{(j)}(n) \to 0$ as $n \to \infty$.

We claim that

$$\sup_{x \in \partial D_j} \mathrm{dist}(x, \gamma_n^{(j)}) \leqslant \max\{\varepsilon_1^{(j)}(n), \varepsilon_2^{(j)}(n)\} \tag{5.46}$$

for each $j \in \{1,...,N+1\}$ and large enough n. Fix $x \in \partial D_j$. By the definition of $\varepsilon_1^{(j)}(n)$, there exists $y_1 \in \partial F_n^{(j)}$ such that $|y_1 - x| \leqslant \varepsilon_1^{(j)}(n)$. By the definition of $\varepsilon_2^{(j)}(n)$, there exists $y_2 \in \partial^{\mathrm{out}}\,\mathrm{dil}_{2l(n)}(D_j)$ such that $|y_2 - x| \leqslant \varepsilon_2^{(j)}(n)$.

Focus first on the case $j \in \{1,...,N\}$. By (5.41) and the fact that y_2 lies in the unbounded connected component of $\mathrm{dil}_{2l(n)}(D_j)^c$, y_2 lies in the unbounded connected component of the complement of $(\mathscr{O}_n^c)_j$ for all $n \geqslant n_0$. In addition, we have that $y_1 \in (\mathscr{O}_n^c)_j$. Consequently, the path γ consisting the union of a straight line from y_1 to x and a straight line from x to y_2 must intersect $\gamma_n^{(j)} = \partial^{\text{out}}(\mathscr{O}_n^c)_j$. Inequality (5.46) for $j \in \{1,...,N\}$ follows from the fact that every point y in the path γ satisfies $|y-x| \leqslant \max\{\varepsilon_1^{(j)}(n), \varepsilon_2^{(j)}(n)\}$.

The proof of (5.46) for $j = N+1$ is very similar. y_1 lies in $\mathscr{O}_{n,0}$ and y_2 lies in the unbounded connected component of $(\mathscr{O}_{n,0})^c$ so the path consisting of the union of a straight from y_1 to x and a straight line from x to y_2 intersects $\gamma_n^{(N+1)} = \partial^{\text{out}}\mathscr{O}_{n,0}$.

Let

$$\varepsilon(n) := 2\max\{\varepsilon_1^{(1)}(n), ..., \varepsilon_1^{(N+1)}(n), \varepsilon_2^{(1)}(n), ..., \varepsilon_2^{(N+1)}(n), l(n)\} \qquad (n \geqslant n_0). \tag{5.47}$$

Then (5.38) is satisfied since (5.43) holds for all $j \in \{1,...,N+1\}$ so it remains to prove (5.39). But (5.39) follows from (5.46) by the observation that, for large enough n,

$$\sup_{x\in\partial\mathscr{O}_n} \text{dist}(x, \gamma_n^{(1)} \cup \cdots \cup \gamma_n^{(N+1)}) \leqslant l(n) + \sup_{x\in\partial\mathscr{O}} \text{dist}(x, \gamma_n^{(1)} \cup \cdots \cup \gamma_n^{(N+1)})$$

and, using Lemma 5.36 (d),

$$\begin{aligned}
\sup_{x\in\partial\mathscr{O}} \text{dist}(x, \gamma_n^{(1)} \cup \cdots \cup \gamma_n^{(N+1)}) &\leqslant \max\{\sup_{x\in\partial D_1} \text{dist}(x, \gamma_n^{(1)}), ..., \sup_{x\in\partial D_{N+1}} \text{dist}(x, \gamma_n^{(N+1)})\} \\
&\leqslant \max\{\varepsilon_1^{(1)}(n), ..., \varepsilon_1^{(N+1)}(n), \varepsilon_2^{(1)}(n), ..., \varepsilon_2^{(N+1)}(n)\} \\
&\leqslant \varepsilon(n).
\end{aligned}$$

□

5.4.3 Proof of Theorem 5.3

Firstly, $\mathscr{O}$ and $\mathscr{O}_n$, $n \in \mathbb{N}$, satisfy the hypotheses of Proposition 5.38. Let $\varepsilon(n), D_j, N$ and $\gamma_n^{(j)}$ be as in that proposition. $\varepsilon(n)$ satisfies $\varepsilon(n) \geqslant 2l(n)$ and $\varepsilon(n) \to 0$ as $n \to \infty$ so by Proposition 5.30 it suffices to show that there exist numerical constants $C, \alpha > 0$ such that for large enough n,

$$\forall u \in H_0^1(\mathscr{O}): \quad \|u\|_{L^2(\partial^{\varepsilon(n)}\mathscr{O})} \leqslant C\varepsilon(n)\|\nabla u\|_{L^2(\partial^{\alpha\varepsilon(n)}\mathscr{O})} \tag{5.48}$$

and

$$\forall u \in H_0^1(\mathscr{O}_n): \quad \|u\|_{L^2(\partial^{\varepsilon(n)}\mathscr{O}_n)} \leqslant C\varepsilon(n)\|\nabla u\|_{L^2(\partial^{\alpha\varepsilon(n)}\mathscr{O}_n)}. \tag{5.49}$$

(5.48) follows immediately from Theorem 5.6 (with $C = 5$ and $\alpha = 2\sqrt{2}$) so it remains to show (5.49).

Let

$$\mathscr{V}_n := \left(\bigcup_{j=1}^{N+1} \gamma_n^{(j)} \right)^c \qquad (n \in \mathbb{N}). \tag{5.50}$$

By inequality (5.39) in Proposition 5.38, every point in $\partial \mathscr{O}_n$ is at most a distance $\varepsilon(n)$ from $\partial \mathscr{V}_n = \cup_{j=1}^{N+1} \gamma_n^{(j)}$ so

$$\partial^{\varepsilon(n)} \mathscr{O}_n \subseteq \mathrm{dil}_{2\varepsilon(n)}(\partial \mathscr{V}_n) = \partial^{2\varepsilon(n)} \mathscr{V}_n. \tag{5.51}$$

Inequality (5.38) yields

$$Q(\partial \mathscr{V}_n) \geqslant \min\{\mathrm{diam}(\partial D_j) - \varepsilon(n) : j \in \{1, ..., N+1\}\}. \tag{5.52}$$

Since D_j are bounded open sets, we have $\mathrm{diam}(\partial D_j) > 0$ and so $4\sqrt{2}\varepsilon(n) < Q(\partial \mathscr{V}_n)$ for large enough n. Consequently, an application of Theorem 5.6 shows that

$$\|u\|_{L^2(\partial^{\varepsilon(n)} \mathscr{O}_n)} \leqslant \|u\|_{L^2(\partial^{2\varepsilon(n)} \mathscr{V}_n)} \leqslant 10\varepsilon(n) \|\nabla u\|_{L^2(\partial^{4\sqrt{2}\varepsilon(n)} \mathscr{V}_n)} \tag{5.53}$$

for all large enough n and all $u \in H_0^1(\mathscr{O}_n)$. Noting that any $u \in H_0^1(\mathscr{O}_n)$ must vanish almost everywhere on $\mathscr{O}_n^c$, we see that we have established (5.49) (with $C = 10$ and $\alpha = 4\sqrt{2}$), completing the proof.

Remark 5.39. Recall that the explicit Poincaré-type inequality of Theorem 5.6 does not require regularity of the domain. Interestingly, this is exploited in the proof of Theorem 5.3. There, Theorem 5.6 is applied to $u \in H_0^1(\mathscr{O}_n)$ as a function in $H_0^1(\mathscr{V}_n)$, and $\mathscr{V}_n$ is certainly not regular in general.

Remark 5.40. We can replace the hypothesis $Q(\partial \mathscr{O}) > 0$ with the hypothesis that the connected components of $\partial \mathscr{O}$ are path-connected. Indeed, with this replacement, the path-connected components of $\partial \mathscr{O}$ are $\partial D_1, ..., \partial D_{N+1}$, where $D_1, ..., D_{N+1}$ are the bounded, open sets of Lemma 5.36, hence

$$Q(\partial \mathscr{O}) = \min\{\mathrm{diam}(\partial D_j) : j \in \{1, ..., N+1\}\} > 0. \tag{5.54}$$

5.4.4 Hausdorff convergence for pixelated domains

We finish the section by showing that pixelation approximations (cf. Definition 5.16) satisfy the Hausdorff convergence condition of Theorem 5.3 (under suitable hypotheses). From this, we will be able to conclude that the pixelation approximations converge in the Mosco sense, which will be utilised in the study of computational spectral problems in Section 5.5.

Lemma 5.41. *If $A \subset \mathbb{R}^d$ and $A_n \subset \mathbb{R}^d$, $n \in \mathbb{N}$, are bounded open sets such that $A_n \subset A$ for all $n \in \mathbb{N}$ and any compact set $F \subset A$ is a subset of A_n for all large enough n, then*

$$\mathrm{d}_H(A, A_n) + \mathrm{d}_H(\partial A, \partial A_n) \to 0 \quad \textit{as} \quad n \to \infty.$$

Proof. We have that $\mathrm{d}_H(\partial A_n, \partial A) = \max\{D_1, D_2\}$, where

$$D_1 := \sup_{x \in \partial A} \mathrm{dist}(x, \partial A_n) \quad \text{and} \quad D_2 := \sup_{x \in \partial A_n} \mathrm{dist}(x, \partial A).$$

Focusing on D_1, let $\varepsilon > 0$ and $x \in \partial A$. By hypothesis, we can let $N(\varepsilon, x) \in \mathbb{N}$ be large enough so that $B_\varepsilon(x) \cap A_n \neq \emptyset$ for all $n \geqslant N(\varepsilon, x)$. The ball $B_\varepsilon(x)$ also intersects $A^c \subseteq A_n^c$ for all n so in fact $B_\varepsilon(x)$ intersects ∂A_n for all $n \geqslant N(\varepsilon, x)$. This shows that $\mathrm{dist}(x, \partial A_n) < \varepsilon$ for all $n \geqslant N(\varepsilon, x)$. By compactness of ∂A, we can let $N(\varepsilon) := \sup_{x \in \partial A} N(\varepsilon, x) < \infty$. Then,

$$\forall n \geqslant N(\varepsilon) : \sup_{x \in \partial A} \mathrm{dist}(x, \partial A_n) < \varepsilon$$

hence $D_1 \to 0$ as $n \to \infty$.

Focusing on D_2, suppose for contradiction that there exists a subsequence $(\partial A_{n_k})_{k \in \mathbb{N}}$ such that

$$\sup_{x \in \partial A_{n_k}} \mathrm{dist}(x, \partial A) \geqslant C$$

for some $C > 0$ independent of k. Then there exists $x_{n_k} \in \partial A_{n_k}$, $k \in \mathbb{N}$, such that $\mathrm{dist}(x_{n_k}, \partial A) \geqslant C$. $B_{C/2}(x_{n_k})$ is contained in A and intersects $A_{n_k}^c$ for all k so there exists $y_{n_k} \in B_{C/2}(x_{n_k})$, $k \in \mathbb{N}$, such that $y_{n_k} \in A_{n_k}^c \cap A$ for all k. (y_{n_k}) satisfies $\mathrm{dist}(y_{n_k}, \partial A) \geqslant C/2 > 0$ for all k. Let $y \in \overline{A}$ be an accumulation point of (y_{n_k}). y must satisfy $\mathrm{dist}(y, \partial A) \geqslant C/2$ so there exists $\delta > 0$ such that $\overline{B}_\delta(y) \subset \mathrm{int}(A) = A$. By hypothesis, $B_\delta(y) \subset A_n$ for all large enough n. But this is a contradiction to fact that y is an accumulation point of $y_{n_k} \in A_{n_k}^c$, $k \in \mathbb{N}$. It follows that $D_2 \to 0$ as $n \to \infty$ hence $\mathrm{d}_H(\partial A_n, \partial A) \to 0$ as $n \to \infty$.

Since $A_n \subseteq A$, it remains to show that $\sup_{x \in A} \mathrm{dist}(x, A_n) \to 0$. Let $\varepsilon > 0$. By hypothesis, there exists $N \in \mathbb{N}$ such that $A \backslash \partial^\varepsilon A \subset A_n$, hence $\sup_{x \in A} \mathrm{dist}(x, A_n) \leqslant \varepsilon$, for all $n \geqslant N$, completing the proof. □

In the next proposition, the hypothesis that the limit domain $\mathscr{O}$ is regular is crucial. Indeed, Proposition 5.48 features an example of a non-regular domain for which the pixelation approximations do not converge in the Hausdorff sense. The basic idea of the proof is to introduce approximations from below $\tilde{A}_n$ and E_n for the sets $\mathscr{O}$ and $\mathrm{int}(\mathscr{O}^c)$ respectively which "sandwich" the boundary $\partial\mathscr{O}_n$ of the pixelated domain.

Proposition 5.42. *If $\mathscr{O} \subseteq \mathbb{R}^d$ is a bounded, regular open set such that $\mu_{\mathrm{leb}}(\partial\mathscr{O}) = 0$, and $\mathscr{O}_n$, $n \in \mathbb{N}$, are the pixelated domains for $\mathscr{O}$, then*

$$l(n) = \mathrm{d}_H(\mathscr{O}, \mathscr{O}_n) + \mathrm{d}_H(\partial\mathscr{O}, \partial\mathscr{O}_n) \to 0 \quad as \quad n \to \infty.$$

Proof. All limits in the proof are as $n \to \infty$.

Define the following collection of open sets

$$\mathscr{B} := \bigcup_{n\in\mathbb{N}} \mathscr{B}_n \quad \text{where} \quad \mathscr{B}_n := \left\{ j + (-\tfrac{1}{n}, \tfrac{1}{n})^d : j \in \mathbb{Z}_n^d \right\}. \tag{5.55}$$

The elements of $\mathscr{B}_n$ are open boxes of side-length $2/n$ and hence overlap. Let A_n denote the union of all elements of $\mathscr{B}_n$ which are subsets $\mathscr{O}$ and let E_n denote the union of all elements of $\mathscr{B}_n$ which are subsets of $\mathrm{int}(\mathscr{O}^c)$.

We claim that for any compact set $F \subset \mathscr{O}$, we have $F \subset A_n$ for all large enough n. Let $\varepsilon > 0$ be small enough so that $\mathrm{dil}_\varepsilon(F) \subset \mathscr{O}$ and let n be any positive integer which is large enough such that $2\frac{\sqrt{d}}{n} < \varepsilon$. Let $x \in F$. There exists $j \in \mathbb{Z}_n^d$ such that $|x - j| \leqslant \frac{\sqrt{d}}{2}\frac{1}{n}$. Then,

$$j + (-\tfrac{1}{n}, \tfrac{1}{n})^d \subset \mathrm{dil}_{2\sqrt{d}/n}(F) \subset \mathrm{dil}_\varepsilon(F) \subset \mathscr{O} \tag{5.56}$$

so the box $j + (-\frac{1}{n}, \frac{1}{n})^d$ is a subset of A_n and consequently $x \in A_n$. It follows that $F \subset A_n$, proving the claim.

We also have $A_n \subset \mathscr{O}$ so A_n and $\mathscr{O}$ satisfy the hypotheses of Lemma 5.41. We similarly have $E_n \subset \mathrm{int}(\mathscr{O}^c)$ and, for any compact set $F \subset \mathrm{int}(\mathscr{O}^c)$, $F \subset E_n$ for all large enough n. Applying Lemma 5.41 to A_n and $B_X(0) \cap E_n$ for large enough $X > 0$, we obtain

$$\mathrm{d}_H(\mathscr{O}, A_n) + \mathrm{d}_H(\partial\mathscr{O}, \partial A_n) \to 0 \tag{5.57}$$

and

$$\mathrm{d}_H(B_X(0) \cap \mathrm{int}(\mathscr{O}^c), B_X(0) \cap E_n) + \mathrm{d}_H(\partial\mathscr{O}, \partial E_n) \to 0, \tag{5.58}$$

where regularity was used in the second limit to ensure that $\partial\mathrm{int}(\mathscr{O}^c) = \partial\mathscr{O}$.

Define also the following subset of A_n,

$$\tilde{A}_n := \mathrm{int}\left(\bigcup_{j\in A_n\cap\mathbb{Z}_n^d} (j + [-\tfrac{1}{2n}, \tfrac{1}{2n}]^d) \right) \qquad (n \in \mathbb{N}). \tag{5.59}$$

Any point in A_n is in a box $j+(-\frac{1}{n},\frac{1}{n})^d$ for some $j\in A_n\cap\mathbb{Z}_n^d$ hence at most a distance $\sqrt{d}/n$ from a point in $\tilde{A}_n$. Consequently

$$\mathrm{d}_H(A_n,\tilde{A}_n)\leqslant\frac{\sqrt{d}}{n}. \tag{5.60}$$

Firstly, we claim that

$$\tilde{A}_n\subseteq\mathscr{O}_n\subseteq E_n^c. \tag{5.61}$$

To see the first inclusion in (5.61), note that any grid point $j\in A_n\cap\mathbb{Z}_n^d$ is in $\mathscr{O}$ so the the corresponding cell $j+[-1/(2n),1/(2n)]^d$ is a subset of $\overline{\mathscr{O}}_n$. Focus now on the second inclusion. Any point in x in E_n lies in $j+(\frac{1}{n},\frac{1}{n})^d$ for some $j\in\mathbb{Z}_n^d\cap E_n$. Since the corners of the closed box $j+[-\frac{1}{n},\frac{1}{n}]^d$ lie in $\mathbb{Z}_n^d\cap\overline{E}_n$, x lies in $j'+[-\frac{1}{2n},\frac{1}{2n}]^d$ for some $j'\in\mathbb{Z}_n^d\cap\overline{E}_n$. This shows that

$$E_n\subseteq\bigcup_{j\in\overline{E}_n\cap\mathbb{Z}_n^d}\left(j+[-\tfrac{1}{2n},\tfrac{1}{2n}]^d\right).$$

The fact that any point in $\mathbb{Z}_n^d\cap\overline{E}_n$ lies in $\mathscr{O}^c$ implies that $E_n\subseteq\mathscr{O}_n^c$, proving the claim.

Secondly, we claim that

$$\mu_{\mathrm{leb}}(E_n^c\backslash A_n)\to 0. \tag{5.62}$$

Let $X>0$ be large enough so that $E_n^c\backslash A_n\subset B_X(0)$. Then,

$$\mu_{\mathrm{leb}}(E_n^c\backslash A_n)=\mu_{\mathrm{leb}}(B_X(0))-\mu_{\mathrm{leb}}(B_X(0)\cap A_n)-\mu_{\mathrm{leb}}(B_X(0)\cap E_n). \tag{5.63}$$

Using continuity of measures from below, the hypothesis that $\mu_{\mathrm{leb}}(\partial\mathscr{O})=0$ and regularity, we have

$$\mu_{\mathrm{leb}}(B_X(0)\cap A_n)\to\mu_{\mathrm{leb}}(B_X(0)\cap\mathscr{O})$$

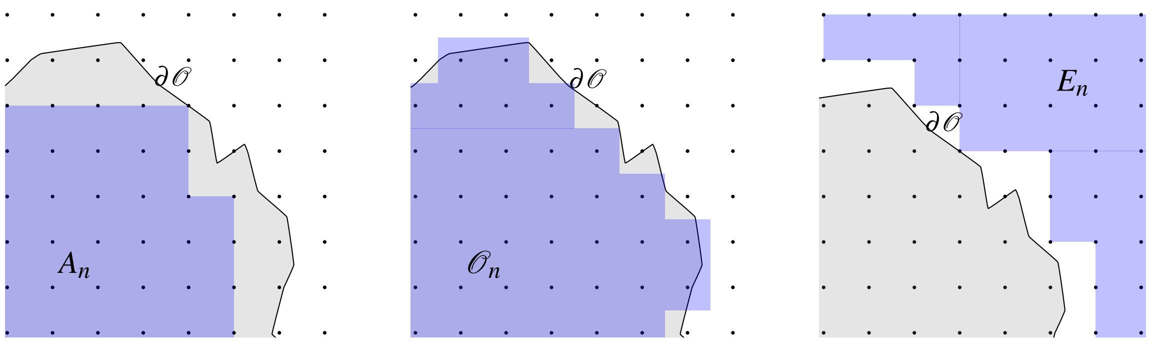

Figure 5.8 Sketch of the domains A_n (left), $\mathscr{O}_n$ (centre) and E_n (right).

and

$$\mu_{\mathrm{leb}}(B_X(0)\cap E_n)\to\mu_{\mathrm{leb}}(B_X(0)\cap\operatorname{int}(\mathscr{O}^c))=\mu_{\mathrm{leb}}(B_X(0)\cap\mathscr{O}^c).$$

It follows that the right hand side of (5.63) tends to zero, proving the claim.

Next we claim that

$$\sup_{x\in\partial\mathscr{O}_n}\operatorname{dist}(x,\partial A_n\cup\partial E_n)\to 0. \tag{5.64}$$

This can be seen by considering an expanding ball around any point in $E_n^c\backslash A_n$. More precisely, for any $x\in E_n^c\backslash A_n$, define the quantity

$$r(x):=\inf\{r>0:B_r(x)\cap(\partial A_n\cup\partial E_n)\neq\emptyset\}\in[0,\infty).$$

For all $x\in E_n^c\backslash A_n$, we have

$$\operatorname{dist}(x,\partial A_n\cup\partial E_n)=r(x)\quad\text{and}\quad B_{r(x)}(x)\subseteq E_n^c\backslash A_n.$$

Note that we consider that $B_0(x)=x$. The set $E_n^c\backslash A_n$ is compact so we can define

$$r_n:=\sup_{x\in E_n^c\backslash A_n}r(x)<\infty$$

and there exists $x_n\in E_n^c\backslash A_n$ such that $r_n=r(x_n)$. The limit (5.62), combined with the fact that $B_{r_n}(x_n)\subseteq E_n^c\backslash A_n$, yields

$$\mu_{\mathrm{leb}}(B_{r_n}(x_n))\leqslant\mu_{\mathrm{leb}}(E_n^c\backslash A_n)\to 0$$

which implies that $r_n\to 0$. (5.64) is obtained by applying the inclusions (5.61) to get

$$\begin{aligned}\sup_{x\in\partial\mathscr{O}_n}\operatorname{dist}(x,\partial A_n\cup\partial E_n)&\leqslant\sup_{x\in E_n^c\backslash\tilde{A}_n}\operatorname{dist}(x,\partial A_n\cup\partial E_n)\\&\leqslant\max\left\{\frac{\sqrt{d}}{n},\sup_{x\in E_n^c\backslash A_n}\operatorname{dist}(x,\partial A_n\cup\partial E_n)\right\}\\&=\max\left\{\frac{\sqrt{d}}{n},r_n\right\}\to 0,\end{aligned}$$

where the second inequality holds because any point in $A_n\backslash\tilde{A}_n$ is at most a distance $\sqrt{d}/n$ from ∂A_n.

Combining the limits (5.57) and (5.58) gives

$$\mathrm{d}_H(\partial\mathscr{O},\partial A_n\cup\partial E_n)\to 0 \tag{5.65}$$

and

$$\mathrm{d}_H(\partial A_n, \partial E_n) \to 0. \tag{5.66}$$

Furthermore, we claim that

$$\sup_{x\in\partial A_n\cup\partial E_n} \mathrm{dist}(x, \partial\mathscr{O}_n) \to 0. \tag{5.67}$$

This can be seen by considering length minimising lines between $\partial\tilde{A}_n$ and ∂E_n. More precisely, let $x \in \partial E_n$ and let $y = y(x) \in \partial\tilde{A}_n$ be such that $|x-y| = \mathrm{dist}(x, \partial\tilde{A}_n)$. The straight line connecting x and y must intersect $\partial\mathscr{O}_n$ since one end is in $\mathscr{O}_n$ and the other is in $\mathscr{O}_n^c$. This fact implies that

$$\begin{aligned}\sup_{x\in\partial E_n} \mathrm{dist}(x, \partial\mathscr{O}_n) &\leqslant \sup_{x\in\partial E_n} \mathrm{dist}(x, \partial\tilde{A}_n)\\ &\leqslant \sup_{x\in\partial E_n} \mathrm{dist}(x, \partial A_n) + \mathrm{d}_H(\partial A_n, \partial\tilde{A}_n) \to 0\end{aligned}$$

where the limit holds by (5.66) and (5.60). It can be similarly seen that

$$\sup_{x\in\partial A_n} \mathrm{dist}(x, \partial\mathscr{O}_n) \to 0.$$

giving us (5.67). The limits (5.64) and (5.67) prove that $\mathrm{d}_H(\partial\mathscr{O}_n, \partial A_n \cup \partial E_n) \to 0$ which, combined with (5.65), gives $\mathrm{d}_H(\partial\mathscr{O}, \partial\mathscr{O}_n) \to 0$.

By (5.57), (5.58) and regularity of $\mathscr{O}$,

$$\mathrm{d}_H(A_n, \mathscr{O}) \to 0 \quad \text{and} \quad \mathrm{d}_H(E_n^c, \mathscr{O}) \to 0 \tag{5.68}$$

so, in particular, $\mathrm{d}_H(A_n, E_n^c) \to 0$. Using this combined with the inclusions (5.61) and inequality (5.60) for $\mathrm{d}_H(A_n,\tilde{A}_n)$, we have

$$\mathrm{d}_H(E_n^c, \mathscr{O}_n) = \sup_{x\in E_n^c} \mathrm{dist}(x, \mathscr{O}_n) \leqslant \sup_{x\in E_n^c} \mathrm{dist}(x,\tilde{A}_n) \to 0.$$

Combining this with the second limit in (5.68), shows that $\mathrm{d}_H(\mathscr{O}, \mathscr{O}_n) \to 0$, completing the proof. □

5.5 Arithmetic algorithms for the spectral problem

In this section we study the computability of the Dirichlet spectrum. Subsections 5.5.1 and 5.5.2 are devoted to the proof of Theorem 5.15, whereas Section 5.5.3 provides a counterexample that proves Proposition 5.14. We begin with the study of generalised matrix eigenvalue problems which arise naturally from finite element approximations.

5.5.1 Matrix pencil eigenvalue problem

Recall that a *matrix pencil eigenvalue problem* takes the form:

$$\text{Find} \quad u \in \mathbb{C}^N \quad \text{and} \quad \lambda \in \mathbb{C} \quad \text{such that} \quad Au = \lambda Bu.$$

First, we show that there exists a family of arithmetic algorithms capable of solving such problems to arbitrary specified precision, restricting ourselves to the case where A and B are real, symmetric and B is positive definite. Let

$$\Omega_{\mathrm{mat},M} := \left\{(A,B) \in (\mathbb{R}^{M\times M})^2 : A,B \text{ symmetric, } B \text{ positive definite}\right\},$$

$$\Lambda_{\mathrm{mat},M} := \left\{(A,B) \mapsto A_{j,k} : A_{j,k} \text{ matrix element of } A\right\} \\ \cup \left\{(A,B) \mapsto B_{j,k} : B_{j,k} \text{ matrix element of } B\right\}.$$

and

$$\Lambda^{\varepsilon}_{\mathrm{mat},M} := \Lambda_{\mathrm{mat},M} \cup \{(A,B) \mapsto \varepsilon\}.$$

Applying a-posteriori bounds of Oishi [111] for the matrix eigenvalue problem gives the following family of arithmetic algorithms:

Lemma 5.43. *For each $\varepsilon > 0$ and $m \in \mathbb{N}$, there exists an arithmetic algorithm $\Gamma^{\varepsilon}_{\mathrm{mat},M} : \Omega_{\mathrm{mat},M} \to \mathbb{R}^M$ with input $\Lambda^{\varepsilon}_{\mathrm{mat},M}$, such that*

$$|\Gamma^{\varepsilon}_{\mathrm{mat},M}(A,B)_k - \lambda_k| \leqslant \varepsilon \quad \textit{for all} \quad (A,B) \in \Omega_{\mathrm{mat},M} \quad \textit{and} \quad k \in \{1,\dots,M\},$$

where λ_k denotes the k^{th} eigenvalues of the matrix pencil (A,B) and $\Gamma^{\varepsilon}_{\mathrm{mat},M}(A,B)_k$ denotes the k^{th} component of $\Gamma^{\varepsilon}_{\mathrm{mat},M}(A,B)$.

Proof. Since $\Lambda^{\varepsilon}_{\mathrm{mat},M}$ is a finite set, we can define the information available to the (arithmetic) algorithm $\Gamma^{\varepsilon}_{\mathrm{mat},M}$ as $\Lambda_{\Gamma^{\varepsilon}_{\mathrm{mat},M}}(A,B) = \Lambda^{\varepsilon}_{\mathrm{mat},M}$. By Gaussian elimination, the matrix elements of B^{-1} can be computed with a finite number of arithmetic operations. Then the eigenvalues of the matrix pencil (A,B) are exactly the eigenvalues $(\lambda_k)_{k=1}^M$ of $E := B^{-1}A$ and the matrix elements of E are accessible to the algorithm.

By the Jacobi eigenvalue algorithm (cf. [125]) there exists a family of approximations $(\tilde{\lambda}^m_k, \tilde{x}^m_k) \in \mathbb{R} \times \mathbb{R}^M$, $k \in \{1,\dots,M\}$, $m \in \mathbb{N}$, such that $(\tilde{\lambda}^m_k, \tilde{x}^m_k)$ can be computed with finitely many arithmetic operations and

$$\|P_m^T D_m P_m - E\|_F + \|P_m^T P_m - I\|_F \to 0 \quad \text{as} \quad m \to \infty \tag{5.69}$$

where

$$D_m := \operatorname{diag}(\tilde{\lambda}_1^m, ..., \tilde{\lambda}_M^m) \quad \text{and} \quad P_m := (\tilde{x}_1^m, ..., \tilde{x}_M^m).$$

Here, $\|\cdot\|_F$ denotes the Frobenius matrix norm. By [111, Theorem 2],

$$|\lambda_k - \tilde{\lambda}_k^m| \leqslant |\tilde{\lambda}_k^m| \|P_m^T P_m - I\|_F + \|P_m^T D_m P_m - E\|_F =: \mathscr{E}_k(m)$$

for all $k \in \{1, ..., M\}$. Let $m(\varepsilon)$ denote the smallest positive integer such that $\mathscr{E}_k(m(\varepsilon)) \leqslant \varepsilon$ for all $k \in \{1, ..., M\}$. $m(\varepsilon)$ can be determined by the algorithm since, for each m, $\mathscr{E}_k(m)$ can be computed in finitely many arithmetic operations. The proof is completed by letting

$$\Gamma^{\varepsilon}_{\mathrm{mat},M}(A,B) := (\tilde{\lambda}_k^{m(\varepsilon)})_{k=1}^M.$$

□

5.5.2 Algorithm for computing Laplacian eigenvalues

Next, we show that there exists a family of arithmetic algorithms capable of computing, to arbitrary specified precision, the spectrum of the Dirichlet Laplacian on domains of the form

$$\mathscr{U} = \operatorname{int}\left(\bigcup_{j=1}^{N} \left(x_j + \left[-\tfrac{1}{2n}, \tfrac{1}{2n}\right]^2\right)\right) \tag{5.70}$$

with $n, N \in \mathbb{N}$ and $(x_1, ..., x_N) \in (\mathbb{Z}_n^2)^N$. Let

$$\Omega_{\mathrm{pix},n} := \left\{\mathscr{U} \subset \mathbb{R}^2 : \exists N \in \mathbb{N} \text{ and } (x_1, ..., x_N) \in (\mathbb{Z}_n^2)^N \text{ such that (5.70) holds}\right\},$$

$$\Lambda_{\mathrm{pix},n} := \left\{\mathscr{U} \mapsto \chi_{\mathscr{U}}(x) : x \in \mathbb{Z}_n^2\right\}.$$

and

$$\Lambda^{\varepsilon}_{\mathrm{pix},n} := \Lambda_{\mathrm{pix},n} \cup \{\mathscr{U} \mapsto N(\mathscr{U})\} \cup \{\mathscr{U} \mapsto \varepsilon\}, \tag{5.71}$$

where $N(\mathscr{U}) := |\mathscr{U} \cap \mathbb{Z}_n^2|$ denotes the number of "pixels" that make up $\mathscr{U}$. The results of Liu and Oishi [100] combined with Lemma 5.43 yield the following:

Lemma 5.44. *Let $n \in \mathbb{N}$ be fixed. For each $\varepsilon > 0$, there exists an arithmetic algorithm $\Gamma^{\varepsilon}_{\mathrm{pix},n} : \Omega_{\mathrm{pix},n} \to \mathrm{cl}(\mathbb{C})$ with input $\Lambda^{\varepsilon}_{\mathrm{pix},n}$, such that*

$$\mathrm{d_{AW}}\left(\Gamma^{\varepsilon}_{\mathrm{pix},n}(\mathscr{U}), \sigma(\mathscr{U})\right) \leqslant \varepsilon \quad \textit{for all} \quad \mathscr{U} \in \Omega_{\mathrm{pix},n}.$$

$\mathcal{T}_0$: $\mathcal{T}_1$:

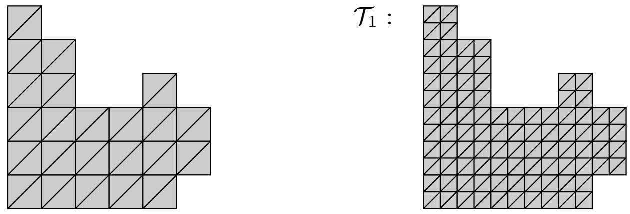

Figure 5.9 Sketch of the triangulation $\mathscr{T}_m$ and refinement for $m \in \{0,1\}$ and fixed $n \in \mathbb{N}$.

Proof. First, we fix a finite subset $\Lambda_{\Gamma^{\varepsilon}_{\mathrm{pix},n}}(\mathscr{U}) \subset \Lambda^{\varepsilon}_{\mathrm{pix},n}$ which defines the information available to the (arithmetic) algorithm $\Gamma^{\varepsilon}_{\mathrm{pix},n}$, which we aim to construct. Choose

$$\Lambda_{\Gamma^{\varepsilon}_{\mathrm{pix},n}}(\mathscr{U}) := \{\mathscr{U} \mapsto \chi_{\mathscr{U}}(x) : x \in \mathbb{Z}^2_n \cap \overline{B}_{\kappa(\mathscr{U})}(0)\} \cup \{\mathscr{U} \mapsto N(\mathscr{U})\} \cup \{\mathscr{U} \mapsto \varepsilon\},$$

where $\kappa(\mathscr{U})$ is defined as the smallest positive integer such that $|\overline{B}_{\kappa(\mathscr{U})}(0) \cap \mathscr{U} \cap \mathbb{Z}^2_n| = N(\mathscr{U})$. The consistency hypothesis (cf. Definition 5.9) holds because $\kappa(\mathscr{U})$ can be computed with a finite number of arithmetic computations from subsets of $\{f(\mathscr{U}) : f \in \Lambda_{\Gamma^{\varepsilon}_{\mathrm{pix},n}}(\mathscr{U})\}$. With this choice, the algorithm has access to the list $(x_1, \ldots, x_N) \in (\mathbb{R}^2)^N$ for which (5.70) holds.

Using this list, we can construct, for each $m \in \mathbb{N}$, a uniform triangulation $\mathscr{T}^m$ of $\mathscr{U}$ such that the elements of $\mathscr{T}^m$ have diameter $\sqrt{2}/(n2^m) =: \sqrt{2}h$ (cf. Figure 5.9). Let $V^m \subset H^1_0(\mathscr{U})$ denote the piecewise-linear continuous finite element space for the triangulation $\mathscr{T}^m$. Let $\{\phi^m_k\}_{m=1}^{M_0}$ denote the basis of 'hat' functions for V^m, where $M_0 := \dim(V^m)$. Let $\{\lambda_k\}_{k=1}^{\infty}$ denote the Dirichlet eigenvalues of the domain $\mathscr{U}$, ordered such that $\lambda_k \leqslant \lambda_{k+1}$ for all $k \in \mathbb{N}$.

The Ritz-Galerkin finite element approximations for $\{\lambda_k\}_{k=1}^{\infty}$ are the eigenvalues $\{\lambda^m_k\}_{k=1}^{M_0}$, $m \in \mathbb{N}$, of the matrix pencil (A^m, B^m), where the matrix elements of the matrices A^m and B^m read

$$A^m_{j,k} := \langle \nabla\phi^m_j, \nabla\phi^m_k \rangle_{L^2(\mathscr{U})} \quad \text{and} \quad B^m_{j,k} := \langle \phi^m_j,\ \phi^m_k \rangle_{L^2(\mathscr{U})} \qquad (j,k \in \{1, \ldots, M_0\})$$

respectively. These matrix elements can be computed from the information $(x_1, \ldots, x_N)$, n and m with a finite number of arithmetic computations. Note that A and B are symmetric and B is positive definite.

In [100], the authors introduce a quantity

$$q^m := l^m + (C_0/n2^m)^2,$$

where,

- $C_0 > 0$ can be bounded above by an explicit expression [100, Section 2] and,
- l^m is the maximum eigenvalue of a matrix pencil (D^m, E^m) [100, eq. (3.22)]. Here, the matrix elements of D^m and E^m are explicitly constructed from inner products between overlapping basis functions of piecewise-linear finite element spaces on $\mathscr{T}^m$ and hence can be computed with a finite number of arithmetic computations on $(x_1, ..., x_N)$, n and m. Also, E^m is diagonal and positive definite.

By [100, Remark 3.3], it holds that $q^m \to 0 \quad \text{as} \quad m \to \infty$. [100, Theorem 4.3] states that, for each $m \in \mathbb{N}$ and each $k \in \{1, ..., M_0\}$, if $q^m \lambda_k^m < 1$, then

$$\lambda_k^m / (1 + \lambda_k^m q^m) \leqslant \lambda_k \leqslant \lambda_k^m. \tag{5.72}$$

Since the matrix elements of A^m, B^m, D^m and E^m are available to the algorithm $\Gamma^{\varepsilon}_{\text{pix},n}$, by Lemma 5.43, the approximations

$$\lambda_k^{m,\delta} := \Gamma^{\delta}_{\text{mat},M_0}(A^m, B^m)_k \qquad \text{and} \qquad q^{m,\delta} := \Gamma^{\delta}_{\text{mat},M_0}(D^m, E^m)_{M_0}$$

are also available to $\Gamma^{\varepsilon}_{\text{pix},n}$, for any $\delta > 0$. These approximations provide upper and lower bounds for λ_k^m and q^m

$$\lambda_k^m \in [\lambda_k^{m,\delta} - \delta, \lambda_k^{m,\delta} + \delta], \qquad q^m \in [q^{m,\delta} - \delta, q^{m,\delta} + \delta]. \tag{5.73}$$

We claim that if $(M, m, \delta) \in \mathbb{N} \times \mathbb{N} \times \mathbb{R}_+$ is such that $(\lambda_M^{m,\delta} + \delta)(q^{m,\delta} + \delta) < 1$, then

$$\mathrm{d_{AW}}\left(\{\lambda_k^{m,\delta}\}_{k=1}^M, \sigma(\mathscr{U})\right) \leqslant \delta + \mathscr{E}_1(M,m,\delta) + \mathscr{E}_2(M,m,\delta) \tag{5.74}$$

where

$$\mathscr{E}_1(M,m,\delta) := \max\left\{(q^{m,\delta} + \delta)(\lambda_k^{m,\delta} + \delta)^2 / (1 + (q^{m,\delta} - \delta)_+ (\lambda_k^{m,\delta} - \delta)_+) : k \in \{1, ..., M\}\right\}$$

and

$$\mathscr{E}_2(M,m,\delta) := 2^{-(\lambda_M^{m,\delta} - \delta)/2 + 1}.$$

To see this,first note that, using the formula

$$\mathrm{d_{AW}}(A,B) \leqslant \mathrm{d}_H(A,B) \qquad (A, B \subset \mathbb{C} \text{ bounded}),$$

we have

$$\begin{aligned}\mathrm{d_{AW}}\big(\{\lambda_k^{m,\delta}\}_{k=1}^M,\sigma(\mathscr{U})\big) &\leqslant \mathrm{d}_H(\{\lambda_k^{m,\delta}\}_{k=1}^M,\{\lambda_k^m\}_{k=1}^M)+\mathrm{d_{AW}}\left(\{\lambda_k^m\}_{k=1}^M,\sigma(\mathscr{U})\right)\\ &\leqslant \delta+\sum_{j=1}^{\lfloor\lambda_M\rfloor}2^{-j}\min\left\{1,\sup_{|x|\leqslant j}\left|\mathrm{dist}\big(x,\{\lambda_k^m\}_{k=1}^M\big)-\mathrm{dist}(x,\{\lambda_k\}_{k=1}^\infty)\right|\right\}+\sum_{j=\lceil\lambda_M\rceil}^\infty 2^{-j}.\end{aligned} \tag{5.75}$$

Since $\mathrm{dist}(x,\{\lambda_k\}_{k=1}^\infty)=\mathrm{dist}(x,\{\lambda_k\}_{k=1}^M)$ for $|x|\leqslant\lfloor\lambda_M\rfloor$, the second term on the right hand side of (5.75) is bounded by

$$\begin{aligned}\mathrm{d_{AW}}\left(\{\lambda_k^m\}_{k=1}^M,\{\lambda_k\}_{k=1}^M\right) &\leqslant \mathrm{d}_H(\{\lambda_k^m\}_{k=1}^M,\{\lambda_k\}_{k=1}^M)\\ &\leqslant \max\{|\lambda_k-\lambda_k^m| : k\in\{1,\dots,M\}\}\leqslant\mathscr{E}_1(\delta,M,m)\end{aligned}$$

where the final inequality follows from (5.72) and (5.73). Applying (5.72) and (5.73) again and noting that the condition $(\lambda_M^{m,\delta}+\delta)(q^{m,\delta}+\delta)<1$ ensures that $\lambda_M^m q^m\leqslant 1$, we have

$$\sum_{j=\lceil\lambda_M\rceil}^\infty 2^{-j}\leqslant 2^{-\lambda_M+1}\leqslant 2^{-\lambda_M^m/2+1}\leqslant\mathscr{E}_2(M,\delta,m),$$

bounding the third term on the right hand side of (5.75) and proving (5.74).

Let $\delta(M):=1/M$. Define $m(M)$ as the smallest $m\in\mathbb{N}$ such that

$$(q^{m,\delta(M)}+\delta(M))(\lambda_M^{m,\delta(M)}+\delta(M))^2\leqslant 1/M.$$

Then, $\mathscr{E}_1(M,m(M),\delta(M))\leqslant 1/M$. For each $M\in\mathbb{N}$, $m(M)$ can be determined by the algorithm since it can compute the quantities $q^{m,\delta(M)}$ and $\lambda_M^{m,\delta(M)}$. Define $M(\varepsilon)$ as the smallest positive integer such that

$$\delta\circ M(\varepsilon)+\mathscr{E}_1(M(\varepsilon),m\circ M(\varepsilon),\delta\circ M(\varepsilon))+\mathscr{E}_2(M(\varepsilon),m\circ M(\varepsilon),\delta\circ M(\varepsilon))\leqslant\varepsilon,$$

where $m\circ M(\varepsilon)=m(M(\varepsilon))$ and $\delta\circ M(\varepsilon)=\delta(M(\varepsilon))$. For each $\varepsilon>0$, $M(\varepsilon)$ can be determined by the algorithm since $\mathscr{E}_1$ and $\mathscr{E}_2$ can be computed. The proof of the lemma is completed by letting

$$\Gamma_{\mathrm{pix},n}^\varepsilon(\mathscr{U}):=\left\{\lambda_k^{m\circ M(\varepsilon),\delta\circ M(\varepsilon)}\right\}_{k=1}^{M(\varepsilon)}. \tag{5.76}$$

□

Remark 5.45. The results of [100] are formulated for connected domains only. While this assumption is not necessarily satisfied for domains in $\Omega_{\mathrm{pix},n}$, the results from [100] can be applied to every connected component of a set $\mathscr{U}\in\Omega_{\mathrm{pix},n}$ separately. This is justified, because the Dirichlet spectrum of $\mathscr{U}$ is simply the union of the Dirichlet spectra of all connected components of $\mathscr{U}$. Moreover, any $\mathscr{U} \in \Omega_{\mathrm{pix},n}$ consists of only finitely many connected components, which can be determined in a finite number of steps from the information given in $\Lambda_{\mathrm{pix},n}$.

We have shown that the Dirichlet spectrum of an arbitrary (but fixed) pixelated domain from $\Omega_{\mathrm{pix},n}$ is computable via an arithmetic algorithm. It remains to pass from pixelated domains to arbitrary domains in Ω_1 (recall (5.16)). To this end, we combine the Mosco convergence results from Section 5.4.2 with the following proposition.

Proposition 5.46. *Let*

$$\Omega_M := \left\{ \mathscr{O} \subset \mathbb{R}^2 : \mathscr{O} \text{ open, bounded and } \mathscr{O}_n \xrightarrow{\mathrm{M}} \mathscr{O} \text{ where } \mathscr{O}_n \text{ pixelated domains for } \mathscr{O} \right\}.$$

Then there exists a sequence of arithmetic algorithms $\Gamma_n : \Omega_M \to \mathrm{cl}(\mathbb{C})$*,* $n \in \mathbb{N}$*, with input* Λ_0 *such that*

$$\mathrm{d_{AW}}\left(\Gamma_n(\mathscr{O}), \sigma(\mathscr{O})\right) \to 0 \quad \textit{as} \quad n \to \infty \qquad \textit{for all} \qquad \mathscr{O} \in \Omega_M.$$

Proof. Let $\mathscr{O} \in \Omega_M$. Let $\mathscr{O}_n \subset \mathbb{R}^2$, $n \in \mathbb{N}$, denote the corresponding pixelated domains (cf. Definition 5.16).

We shall construct a family of (arithmetic) algorithms $\Gamma_n : \Omega_1 \to \mathrm{cl}(\mathbb{C})$ with input Λ_0. First, we define the information available to each algorithm Γ_n, by fixing a finite subset $\Lambda_{\Gamma_n} \subset \Lambda_0$. Let

$$\Lambda_{\Gamma_n} := \left\{ \mathscr{O} \mapsto \chi_{\mathscr{O}}(x) : x \in \mathbb{Z}_n^2 \text{ with } |x| \leqslant n \right\},$$

so that the algorithm Γ_n has access to the set $\{x_1, \ldots, x_N\} := \mathscr{O} \cap B_n(0) \cap \mathbb{Z}_n^2$.

Let

$$\tilde{\mathscr{O}}_n := \mathrm{int}\left(\bigcup_{j=1}^{N} \left(x_j + \left[-\tfrac{1}{2n}, \tfrac{1}{2n}\right]^2 \right) \right).$$

It holds that $\tilde{\mathscr{O}}_n \in \Omega_{\mathrm{pix},n}$ for each n and, since $\mathscr{O}$ is bounded, $\tilde{O}_n = \mathscr{O}_n$ for all sufficiently large n. Hence using the hypothesis that $\mathscr{O}_n \xrightarrow{\mathrm{M}} \mathscr{O}$, $\tilde{\mathscr{O}}_n$ converges to $\mathscr{O}$ in the Mosco sense as $n \to \infty$. By Lemma 5.2,

$$\mathrm{d_{AW}}\left(\sigma(\tilde{\mathscr{O}}_n), \sigma(\mathscr{O})\right) \to 0 \quad \text{as} \quad n \to \infty.$$

Since $\tilde{O}_n$ is defined entirely by Λ_{Γ_n}, we can define

$$\Gamma_n(\mathscr{O}) = \Gamma_{\mathrm{pix},n}^{1/n}(\tilde{O}_n)$$

for each $n \in \mathbb{N}$. Note that the consistency property Definition 5.9 (ii) holds trivially since Λ_{Γ_n} does not depend on $\mathcal{O}$. The proposition is proved by the fact that

$$\begin{aligned} \mathrm{d_{AW}}\left(\Gamma^{1/n}_{\mathrm{pix},n}(\tilde{\mathcal{O}}_n), \sigma(\mathcal{O})\right) &\leqslant \mathrm{d_{AW}}\left(\Gamma^{1/n}_{\mathrm{pix},n}(\tilde{\mathcal{O}}_n), \sigma(\tilde{\mathcal{O}}_n)\right) + \mathrm{d_{AW}}\left(\sigma(\tilde{\mathcal{O}}_n), \sigma(\mathcal{O})\right) \\ &\leqslant \frac{1}{n} + o(1) \to 0 \quad \text{as} \quad n \to \infty. \end{aligned} \tag{5.77}$$

□

Theorem 5.15 now follows by combining Proposition 5.46 with Theorem 5.3 and Proposition 5.42.

Remark 5.47. From the perspective of the SCI hierarchy it is natural to ask whether any finer classification might be possible, specifically in terms of explicit error bounds. This remains an open question and it is clear that our method cannot yield any explicit error bounds for general domains in Ω_1. This is perhaps most clearly demonstrated in the final error bound (5.77). The behaviour $\mathrm{d_{AW}}(\sigma(\tilde{\mathcal{O}}_n), \sigma(\mathcal{O})) = o(1)$ on the right hand side of (5.77) was deduced from the Mosco convergence $\mathcal{O}_n \xrightarrow{\mathrm{M}} \mathcal{O}$, for which no uniform convergence rate can be expected in general.

While the question remains open, the fact that no uniform regularity assumption (such as Hölder continuity with fixed exponent) was made on $\partial\mathcal{O}$ suggests that no explicit error bound is possible.

5.5.3 Counter-example

In this section we give a counterexample showing that if the regularity assumptions on the domain are relaxed too much, computability fails to be true, i.e. the Dirichlet spectrum cannot be computed by a single sequence of algorithms anymore and at least two limits are necessary. Proposition 5.14 follows immediately from the following result.

Proposition 5.48. *Let $\Gamma_n : \Omega_0 \to \mathcal{M}$, $n \in \mathbb{N}$, be any family of arithmetic algorithms with input Λ_0. Then, for any $\mathcal{O} \in \Omega_0$ with $\mu_{\mathrm{leb}}(\partial\mathcal{O}) = 0$ and any $\varepsilon > 0$, there exists $\mathcal{O}_\varepsilon \in \Omega_0$ with $\mathcal{O}_\varepsilon \subseteq \mathcal{O}$ and $\mu_{\mathrm{leb}}(\mathcal{O}_\varepsilon) \leqslant \varepsilon$ such that $\Gamma_n(\mathcal{O}) = \Gamma_n(\mathcal{O}_\varepsilon)$ for all n and, for sufficiently small $\varepsilon > 0$, $\sigma(\mathcal{O}) \neq \sigma(\mathcal{O}_\varepsilon)$.*

Proof. Let Γ_n be as hypothesised, let $\varepsilon > 0$ and let $\mathcal{O} \in \Omega_0$. Define the geometric quantity

$$r_{\mathrm{int}}(\mathcal{O}) := \sup\{r > 0 : \exists \text{square } [s, s+r] \times [t, t+r] \subset \mathcal{O}\}.$$

Openness of $\mathscr{O}$ implies that $r_{\text{int}}(\mathscr{O}) > 0$. For any fixed n, $\Gamma_n(\mathscr{O})$ depends only on finitely many values of $\chi_{\mathscr{O}}(x)$, say $x_1^n, \dots, x_{k_n}^n$. We assume without loss of generality that the set $\{x_1^n, \dots, x_{k_n}^n\}$ is growing with n, i.e. that, for all n,

$$\{x_1^n, \dots, x_{k_n}^n\} \subset \{x_1^{n+1}, \dots, x_{k_{n+1}}^{n+1}\} \quad \text{and} \quad x_j^n = x_j^{n+1}, \quad j = 1, \dots, k_n. \tag{5.78}$$

Thus, we may drop the superscript n and merely write $\{x_1, \dots, x_{k_n}\}$. Let us denote by $\{y_1, \dots, y_{l_n}\}$ the subset of points for which $\chi_{\mathscr{O}}(y_i) = 1$. Now, define a new domain $\mathscr{O}_\varepsilon$ as follows. For $t > 0$ define the strips $S_t^k := \big(\big((y_k)_1 - \frac{t}{2}, (y_k)_1 + \frac{t}{2}\big) \times \mathbb{R}\big) \cap \mathscr{O}$. Next, let

$$\mathscr{O}_\varepsilon^n := \bigcup_{k=1}^{l_n} S_{2^{-k}\varepsilon}^k \quad \text{and} \quad \mathscr{O}_\varepsilon := \left(\bigcup_{n=1}^{\infty} \mathscr{O}_\varepsilon^n\right) \cup \partial^\varepsilon \mathscr{O} \tag{5.79}$$

where, recall that $\partial^\varepsilon \mathscr{O} = \{x \in \mathscr{O} : \operatorname{dist}(x, \partial\mathscr{O}) < \varepsilon\}$. Note that, by (5.78), we have

$$\mathscr{O}_\varepsilon^n \subset \mathscr{O}_\varepsilon^{n+1} \tag{5.80}$$

for all n. Note also that $\mathscr{O}_\varepsilon$ is bounded, open and connected for any $\varepsilon > 0$. One has $\chi_{\mathscr{O}}(x_k) = \chi_{\mathscr{O}_\varepsilon}(x_k)$ for all $k \in \{1, \dots, k_n\}$ and all $n \in \mathbb{N}$, and therefore, by consistency of algorithms (cf. Definition 5.9 (ii)), $\Gamma_n(\mathscr{O}_\varepsilon) = \Gamma_n(\mathscr{O})$ for all $n \in \mathbb{N}$.

However, it is easily seen from the min-max principle that for the lowest eigenvalue $\lambda_1(\mathscr{O})$, of $-\Delta_{\mathscr{O}}$, one has

$$\lambda_1(\mathscr{O}) \leqslant \frac{\pi^2}{r_{\text{int}}(\mathscr{O})^2},$$

Next, we use Poincaré's inequality [75, eq. (7.44)] to get

$$\begin{aligned}
\|u\|_{L^2(\mathscr{O}_\varepsilon)} &\leqslant C\mu_{\text{leb}}(\mathscr{O}_\varepsilon)^{\frac{1}{2}} \|\nabla u\|_{L^2(\mathscr{O}_\varepsilon)} \\
&\leqslant C\left(\mu_{\text{leb}}(\partial^\varepsilon \mathscr{O}) + \sum_{k=1}^{\infty} 2^{-k}\varepsilon \operatorname{diam}(\mathscr{O})\right)^{\frac{1}{2}} \|\nabla u\|_{L^2(\mathscr{O}_\varepsilon)}
\end{aligned}$$

for some constant $C > 0$ independent of ε and all $u \in H_0^1(\mathscr{O}_\varepsilon)$, where in the second inequality, we used the expression (5.79) for $\mathscr{O}_\varepsilon$. Since $\mu_{\text{leb}}(\partial^\varepsilon \mathscr{O}) \to 0$ as $\varepsilon \to 0$ by continuity of measures, we conclude using the min-max principle that $\lambda_1(\mathscr{O}_\varepsilon) \to \infty$ as $\varepsilon \to 0$ and hence $\sigma(\mathscr{O}) \neq \sigma(\mathscr{O}_\varepsilon)$ for small enough $\varepsilon > 0$. $\square$

Remark 5.49. The counterexample in the proof of Proposition 5.48 is pathological in the sense that the complement of the domain $\mathscr{O}_\varepsilon$ may have infinitely many connected components. This is not crucial. Indeed, one can easily construct a counterexample

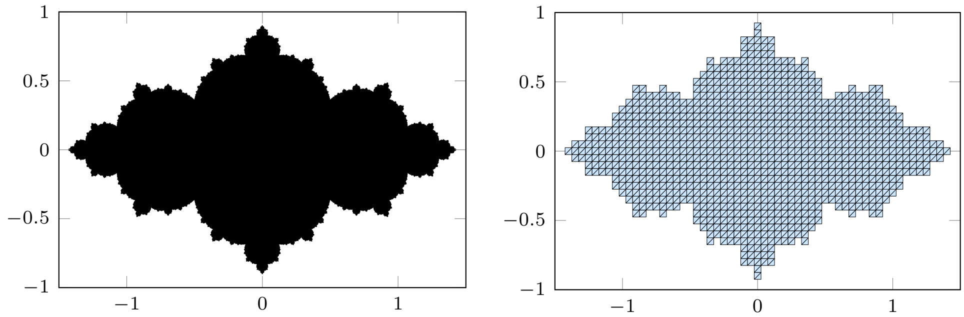

Figure 5.10 The set $\mathscr{O}$ (left) and pixelated domain $\mathscr{O}_n$ for $n = 20$ and $h = 1/n$ (right).

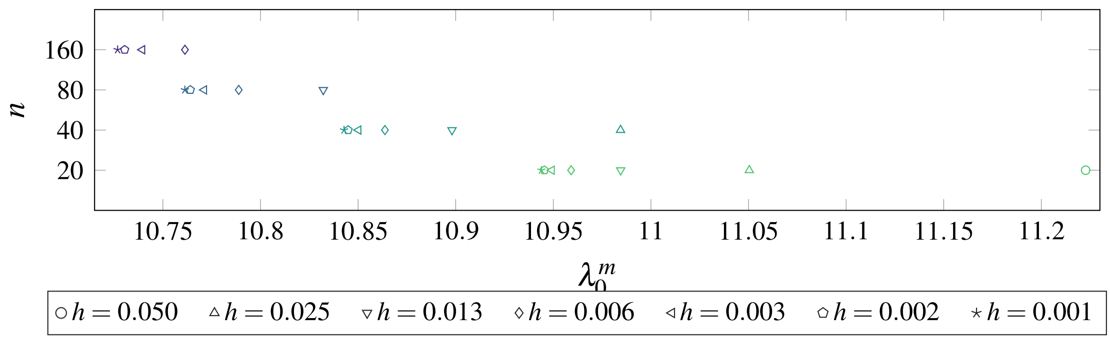

Figure 5.11 Approximations of lowest eigenvalue for different values of $h = 2^{-m}$ and n.

whose complement has only one connected component: Let $\mathscr{O} = (0,1)^2$ be the unit square and

$$\mathscr{O}_\varepsilon := \left(\bigcup_{n=1}^{\infty} \bigcup_{k=1}^{k_n} S^k_{2^{-k}\varepsilon} \right) \cup \big((0,1) \times (0,\varepsilon)\big),$$

with the notation from the previous proof. Then $\Gamma_n(\mathscr{O}_\varepsilon) = \Gamma_n(\mathscr{O})$ for all n and $\sigma((0,1)^2) \neq \sigma(\mathscr{O}_\varepsilon)$ for sufficiently small $\varepsilon > 0$ while $\mathscr{O}_\varepsilon^c$ is connected.

5.6 Numerical Results

In this section we illustrate the abstract ideas from the previous sections with a concrete numerical example. The closure of the domain we study belongs to the class of filled Julia sets described in Example 5.5 hence the pixelation approximations converge in the Mosco sense and the sequence of arithmetic algorithms constructed in Section 5.5.2 converge in the Attouch-Wets metric. Numerical experiments for the Laplacian on filled Julia sets were also recently performed in [134].

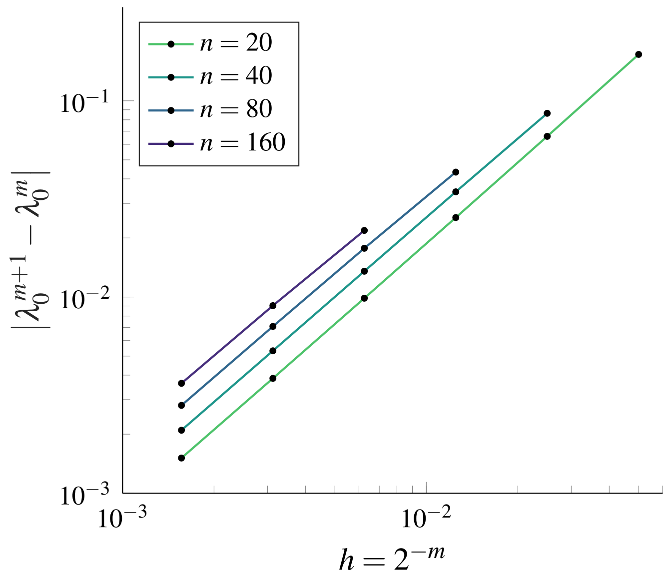

Figure 5.12 Double logarithmic plot of relative differences $|\lambda_0^{m+1} - \lambda_0^m|$ for $n \in \{20, 40, 80, 160\}$, $m \in \{0, \ldots, 160/n\}$.

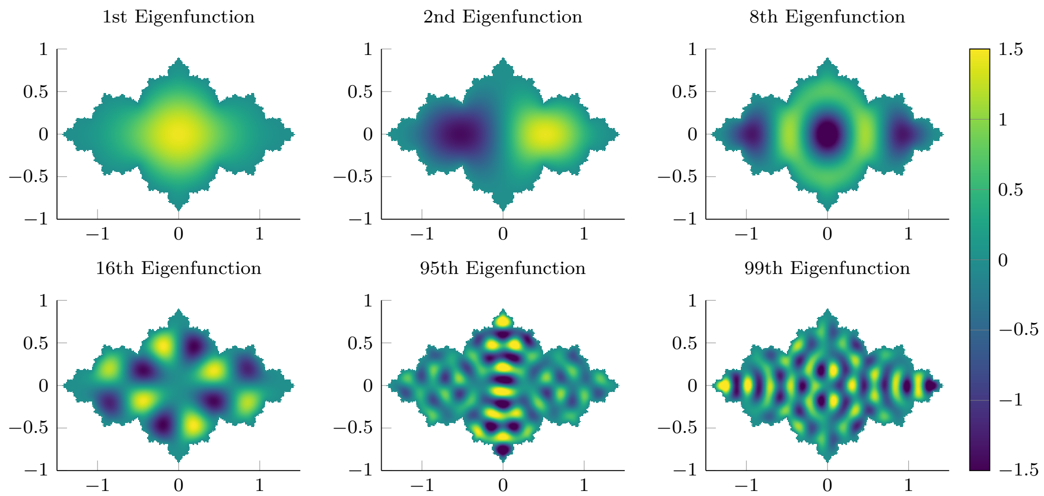

Figure 5.13 Selected approximated eigenfunctions of $\mathscr{O}$ for $n = 100$, $h = 1/n$ (normalised such that $v_i^\top B^m v_i = 1$).

We consider the filled Julia set K defined by

$$K = \{z \in \mathbb{C} : |f^{\circ n}(z)| \leqslant 2 \, \forall n \in \mathbb{N}\}, \quad \text{where} \quad f(z) = z^2 + \frac{\sqrt{5} - 1}{2}.$$

It can be shown that K has a fractal boundary (cf. [101]). Mandelbrot suggested the name “San Marco Set” for K, because it resembles the Basilica of Venice together with its reflection in a flooded piazza (see Figure 5.10).

We implemented a finite element method on subsequent pixelated domains for $\mathscr{O} = \mathrm{int}(K)$ and computed approximations to the lowest eigenvalue with increasingly fine meshes. To be more precise, for $n \in \{20, 40, 80, 160\}$ we approximated lowest eigenvalue λ_0^m of $-\Delta_{\mathscr{O}_n}$ for meshes $\mathscr{T}^m$ with $m \in \{0, 1, \dots, \frac{160}{n}\}$ (or equivalently $h \in \{2^{-m}n^{-1} : m \in \{0, \dots, \frac{160}{n}\}\}$, recall Section 5.5.2).

Because our the emphasis is theoretical, implementing the full a-posteriori error computation of [100] would be beyond the scope of the current work. Instead, the approximation to the lowest eigenvalue in each case was computed using the Rayleigh-Ritz method for the pair (A^m, B^m) of stiffness and mass matrix: the Rayleigh quotient $(v^\top A^m v)/(v^\top B^m v)$ was minimised via a straightforward gradient descent method. The gradient descent was iterated until the derivative of the Rayleigh quotient was less than 10^{-10}. The results are shown in Figures 5.11 and 5.12. The data points in Figure 5.11 suggest that for each fixed n the refinement of the mesh leads to a convergent sequence of approximations.

The decay of the successive differences between the λ_0^m in Figure 5.12 suggests a convergence rate of approximately $1.33 \approx 2 \cdot \frac{2}{3}$, which is in accordance with the regularity of the pixelated domain, which has reentrant corners of angle $\frac{3}{2}\pi$ (cf. [6]). Figure 5.12 also suggests a worsening of the convergence rate if both n and h are increased simultaneously. This is reflected in the fact that the lines in Figure 5.12 move to the left as n increases. This degradation of the convergence rate is to be expected as to the rough boundary of $\mathscr{O}$ is better and better approximated by $\mathscr{O}_n$ as n increases.

For triangulations which are not prohibitively fine, also the approximations of higher eigenvalues and eigenfunctions can be computed. Figure 5.13 shows 6 selected approximated eigenfunctions $v_1, v_2, v_8, v_{16}, v_{95}$ and v_{99} for $n = 100$, $h = n^{-1}$ (i.e. $m = 0$). The approximations are normalised such that $v_i^\top B^m v_i = 1$, where B^m is the mass matrix associated with $\mathscr{T}^m$.

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