XX ESCUELA VENEZOLANA DE MATEMÁTICAS

TRENDS AND TRICKS IN SPECTRAL THEORY

Lyonell Boulton
Michael Levitin

MÉRIDA, VENEZUELA, 2 AL 7 DE SEPTIEMBRE DE 2007

XX ESCUELA VENEZOLANA DE MATEMÁTICAS

Trends and Tricks in Spectral Theory

Lyonell Boulton[1]
Michael Levitin[1,2]
[1]Heriot-Watt University, [2]Cardiff University
L.Boulton@ma.hw.ac.uk, M.Levitin@ma.hw.ac.uk

MÉRIDA, VENEZUELA, 2 AL 7 DE SEPTIEMBRE DE 2007

XX ESCUELA VENEZOLANA DE MATEMÁTICAS

La Escuela Venezolana de Matemáticas es una actividad de los postgrados en matemáticas de las siguientes instituciones: Centro de Estudios Avanzados del Instituto Venezolano de Investigaciones Científicas, Facultad de Ciencias de la Universidad Central de Venezuela, Facultad de Ciencias de la Universidad de Los Andes, Universidad Simón Bolívar, Universidad Centro Occidental Lisandro Alvarado y Universidad de Oriente, y se realiza bajo el auspicio de la Asociación Matemática Venezolana.

La XX ESCUELA VENEZOLANA DE MATEMÁTICAS recibió financiamiento de la Academia de Ciencias Físicas, Matemáticas y Naturales, la Corporación Andina de Fomento (CAF), el Fondo Nacional de Ciencia, Tecnología e Innovación (FONACIT), la Fundación TALVEN, el Instituto Venezolano de Investigaciones Científicas (Departamento de Matemáticas y Ediciones IVIC), la Universidad de los Andes (CEP, CDCHT, Facultad de Ciencias y Departamento de Matemáticas) y el Rectorado de la Universidad Centroccidental Lisandro Alvarado.

2000 Mathematics Subject Classification: 35P05, (35P15, 65N25).

Trends and Tricks in Spectral Theory
Lyonell Boulton y Michael Levitin

Diseño y edición: Escuela Venezolana de Matemáticas
Preprensa e impresión: Editorial Texto
Depósito legal lf66020076002490
ISBN 978-980-261-086-0
Caracas, Venezuela
2007

Preface

The spectra of operators, under different names, manifest themselves almost everywhere in our everyday life. The colour of light we see is related to the spectra of atoms and molecules. The tones and overtones of musical instruments we hear are determined by the spectra of strings and drums. The resonances produced by cars running over a bridge —such as in the recently collapsed viaduct number 1 of the Caracas-La Guaira highway, are predicted by the spectral analysis of beams and suspension cables.

The spectral analysis of differential operators is an area of research that has been active for over one hundred years. In these lecture notes we have deliberately picked only some particular "trends" in this theory. Many good surveys are available, and it makes no sense even to attempt to compete against them. As *modus operandi* we only provide a rough overview of the theoretical aspects, and focus mostly on describing techniques and "tricks" that have been successfully used to solve some long standing problems, several of which are among the most important ones in mathematical analysis in the last century.

The book is organised in two main parts. The first part comprises Chapters 1 and 2. They serve as an overview of the basics of spectral theory and the theory of differential operators. We strongly recommend that even the readers familiar with this material attempt all the problems appearing along the text. Although they are not usually difficult, they are often non-standard and form an integral part of these notes.

Chapters 3-6 may be read independently from each other, with occasional cross-references. However, Chapters 3-5 discuss in detail various aspects involving the spectrum of Laplace operators, so they are closely connected. Chapter 6 may be read immediately after Chapter 2.

The list of references is not supposed to be complete; the readers are advised to consult these books and papers for further literature sources.

We acknowledge with thanks the financial support of the Fundación TALVEN and the several organisations which provided funding for the Escuela. Part of the research presented in this book was carried out under the grant of the Leverhulme Trust, we acknowledge their support. Michael Levitin is grateful for the hospitality of Isaac Newton Institute, Cambridge, where a large part of these notes was written.

Finally, we would like to thank Stella Brassesco, Carlos Di Prisco, and the other organisers of the XX Escuela Venezolana de Matemáticas, for their involvement in the preparation of this event.

Contents

Chapter 1

Elements of spectral theory

In this first chapter, we:

- Describe briefly the elements of spectral theory.
- Fix the notation which will be used in this course.
- Introduce various canonical operators which will be the centre of interest of later chapters.

1.1 Operators

Operators and their spectral properties are the main objects to be studied in this course. The audience is assumed to be familiar with the elements of linear algebra, functional analysis and operator theory. For the benefit of those who need further reading on the topics discussed here, we include some details on standard references.

1.1.1 Hilbert spaces

Throughout this course, the calligraphic letters, such as $\mathcal{H}$ and $\mathcal{L}$, refer to generic separable *Hilbert spaces* over the field of complex numbers, $\mathbb{C}$. The *inner product* on $\mathcal{H}$ will be denoted by $\langle \cdot, \cdot \rangle : \mathcal{H} \times \mathcal{H} \longrightarrow \mathbb{C}$ and the *norm* by $\|u\| := \langle u, u \rangle^{1/2}$, for any $u \in \mathcal{H}$.

Recall that $\langle \cdot, \cdot \rangle$ is a *sesquilinear form*:

$$\langle \alpha u + \beta v, w \rangle = \alpha \langle u, w \rangle + \beta \langle v, w \rangle \quad \text{and} \quad \langle u, v \rangle = \overline{\langle v, u \rangle},$$

for all $u, v, w \in \mathcal{H}$. The norm satisfies the *triangle inequality*

$$\|u+v\| \leq \|u\| + \|v\|, \qquad u, v \in \mathcal{H}. \tag{1.1}$$

It also satisfies the *Cauchy-Schwarz* inequality,

$$|\langle u, v\rangle| \leq \|u\|\|v\|, \qquad u, v \in \mathcal{H}. \tag{1.2}$$

An example of a Hilbert space is the *Euclidean space*, $\mathbb{C}^n$ for $n \in \mathbb{N}$. In this case elements $u \in \mathbb{C}^n$ are column vectors with entries u_j, $j = 1, \ldots, n$. We denote the inner product by $\langle u, v\rangle_{\mathbb{C}^n} = u \cdot v = \sum_{j=1}^n u_j \overline{v_j}$, so $\|u\|_{\mathbb{C}^n}^2 = \sum_{j=1}^n |u_j|^2$.

The Euclidean spaces are examples of finite-dimensional spaces. The Lebesgue L^2 spaces is an infinite-dimensional example.

Definition 1.1.1 (the Lebesgue L^2 space). Let $\Omega \subset \mathbb{R}^d$ and let $\mathrm{d}x$ be the Lebesgue measure on Ω. We denote by $L^2(\Omega)$ the Hilbert space of measurable functions $f : \Omega \longrightarrow \mathbb{C}$ such that $\int_\Omega |f(x)|^2 \,\mathrm{d}x < \infty$. The inner product is

$$\langle f, g\rangle = \langle f, g\rangle_{L^2(\Omega)} := \int_\Omega f(x)\overline{g(x)}\,\mathrm{d}x.$$

In this definition, the Lebesgue measure could be substituted by any other Borel measure. This includes the mass measure on a discrete set.

Definition 1.1.2 (the ℓ^2 space). Let $\mathcal{S}$ be a countable set, finite or infinite. We denote by $\ell^2(\mathcal{S})$ the Hilbert space of functions $f : \mathcal{S} \longrightarrow \mathbb{C}$ such that $\sum_{\omega\in\mathcal{S}} |f(\omega)|^2 < \infty$. The inner product is

$$\langle f, g\rangle = \langle f, g\rangle_{\ell^2} := \sum_{\omega\in\mathcal{S}} f(\omega)\overline{g(\omega)}.$$

Note that if $\mathcal{S}$ is finite and it has n elements, then $\ell^2(\mathcal{S}) = \mathbb{C}^n$.

Further examples of Hilbert spaces will be encounter in Section 1.3.

Problem 1.1.3. Let $\ell^1(\mathbb{N})$ be the linear space of functions $f : \mathbb{N} \longrightarrow \mathbb{C}$ such that $\|f\|_1 := \sum_{j=1}^{\infty} |f(j)| < \infty$. Then $(\ell^1(\mathbb{N}), \|\cdot\|_1)$ is a Banach space. Since $\|\cdot\|_1$ does not satisfy the parallelogram identity,

$$\|f+g\|_1^2 + \|f-g\|_1^2 \neq 2\|f\|_1^2 + 2\|g\|_1^2 \tag{1.3}$$

in general for $f, g \in \ell^1(\mathbb{N})$, then $(\ell^1(\mathbb{N}), \|\cdot\|_1)$ is not a Hilbert space. Confirm the existence of functions f, g such that (1.3) holds. Is it possible to construct a different norm $\|\cdot\|_H$ on $\ell^1(\mathbb{N})$ such that $(\ell^1(\mathbb{N}), \|\cdot\|_H)$ becomes a Hilbert space?

Throughout this book, $\mathrm{Span}(S)$ denotes the linear span of S, $S^\perp$ is the orthogonal complement of the set S and $u \perp S$ means that u is orthogonal to the set S.

1.1.2 Linear operators

We will typically denote operators acting on $\mathcal{H}$ by capital letters. Recall that a linear operator $L : \mathcal{H} \longrightarrow \mathcal{H}$ is *bounded* if its norm

$$\|L\| := \sup_{u \in \mathcal{H}} \frac{\|Lu\|}{\|u\|}$$

is finite.

Matrices acting in the obvious way on vectors in an Euclidean space are examples of bounded operators. In fact, when referring to linear operators acting on these spaces, we will not distinguish between their representation as a linear map or as a matrix.

Problem 1.1.4. Put $\mathcal{H} = L^2(\Omega)$ or $\ell^2(\Omega)$. Let $m : \Omega \longrightarrow \mathbb{C}$ be a bounded function. Show that the linear *operator of multiplication* $Mf(x) = m(x)f(x)$, $f \in \mathcal{H}$, is bounded and compute $\|M\|$.

A further class of bounded operators are the integral operators. The following is a canonical representative of this class.

Example 1.1.5. The Volterra operator. Let

$$Vf(x) = \int_0^x f(y)\,\mathrm{d}y, \qquad\qquad f \in L^2(0,1).$$

Then V is bounded and $\|V\| = 1/2$.

Problem 1.1.6. Prove the claim made in the previous example. *Hint:* use the Cauchy-Schwartz inequality.

We recall that $L : \mathrm{Dom}(L) \longrightarrow \mathcal{H}$ is *closed*, if for any sequence $u_j \in \mathrm{Dom}(L)$ such that $u_j \to u$ and $Lu_j \to v$, $u \in \mathrm{Dom}(L)$ and $Lu = v$. Alternatively, L is closed if $\mathrm{Dom}(L)$ is closed in the norm $\|f\|_L^2 = \|f\|^2 + \|Lf\|^2$. See [RSv1, Chapter VIII].

When we refer to *unbounded* operators $L : \mathrm{Dom}(L) \longrightarrow \mathcal{H}$, we will always mean that they are closed even though we might not describe their domain, $\mathrm{Dom}(L)$, explicitly. Everywhere below the domain of an operator is a dense subspace of the corresponding Hilbert space where it acts.

By the Closed Graph Theorem [RSv1, Theorem III.12], if L is closed and $\mathrm{Dom}(L) = \mathcal{H}$, then L is bounded.

Example 1.1.7. The operator $Mf(n) = n^{1/2}f(n)$ acting on $\ell^2(\mathbb{N})$ with domain

$$\mathrm{Dom}(M) = \{f \in \ell^2(\mathbb{N}) : \sum_{n=1}^{\infty} n|f(n)|^2 < \infty\}$$

is unbounded and closed.

Example 1.1.8. Let $\sigma(\xi)$ be a polynomial of d variables $\xi = (\xi_1, \dots, \xi_d)$. The operator of multiplication $Mf(\xi) = \sigma(\xi)f(\xi)$ acting on $L^2(\mathbb{R}^d)$ with domain

$$\mathrm{Dom}(M) = \{f \in L^2(\mathbb{R}^d) : \int_{\mathbb{R}^d} |\sigma(\xi)|^2 |f(\xi)|^2 < \infty\}$$

is unbounded and closed. In this example, σ can be replaced by any other unbounded function.

In this text we will use the following notation:

$$\mathrm{Ker}(L) = \{u \in \mathrm{Dom}(L) : Lu = 0\},$$
$$\mathrm{Ran}(L) = \{Lu : u \in \mathrm{Dom}(L)\}.$$

1.1.3 Self-adjointness

If $L : \mathrm{Dom}(L) \longrightarrow \mathcal{H}$ is a closed linear operator, the *adjoint* of L is defined to be the unique closed linear operator L^* acting on $\mathcal{H}$ defined as follows. A vector v lies in $\mathrm{Dom}(L^*)$ if there exists $w \in \mathcal{H}$ such that

$$\langle Lu, v\rangle = \langle u, w\rangle \qquad \text{for all } u \in \mathrm{Dom}(L),$$

and whenever $v \in \mathrm{Dom}(L^*)$ we put $L^*v = w$.

Obviously the adjoint of a matrix is its transpose conjugate.

The adjoint of a bounded operator is also bounded. In fact $\|L\| = \|L^*\| = \|L^*L\|^{1/2}$, see [RSv1, Theorem VI.3].

We say that L is *self-adjoint* if $L^* = L$.

Example 1.1.9. The adjoint of $Mf(x) = m(x)f(x)$ bounded or unbounded is $M^*f(x) = \overline{m(x)}f(x)$. In fact M is self-adjoint if and only if $m(x)$ is real-valued.

Problem 1.1.10. What is the adjoint of the Volterra operator introduced in Problem 1.1.6?

1.1.4 Symmetric quadratic forms

Self-adjoint operators are completely characterised in terms of quadratic forms. In this course we will be referring back to this theory which is described thoroughly in the monograph [K].

Here we just recall that any self-adjoint operator L acting on a Hilbert space $\mathcal{H}$ has an associated closed quadratic form

$$q_L : \mathrm{Dom}(q_L) \times \mathrm{Dom}(q_L) \longrightarrow \mathbb{C}$$

where $\mathrm{Dom}(L) \subseteq \mathrm{Dom}(q_L) \subseteq \mathcal{H}$, such that

$$q_L(u, v) = \langle Lu, v\rangle \qquad \text{for all } u, v \in \mathrm{Dom}(L).$$

Properties of q_L are in one-one correspondence with properties of L. For instance, in Chapter 2 we will demonstrate that part of the discrete spectrum of L is completely characterised by q_L.

1.2 Spectral problems

The main mathematical object to be studied in this course is the spectrum of a linear operator and its various properties.

1.2.1 The spectrum

Recall that a linear transformation $T : \mathrm{Dom}(T) \longrightarrow \mathcal{H}$ is said to be *invertible*, if there exists a bounded linear operator $T^{-1} : \mathcal{H} \longrightarrow \mathrm{Dom}(T)$ such that $TT^{-1}u = u$ for all $u \in \mathcal{H}$ and $T^{-1}Tv = v$ for all $v \in \mathrm{Dom}(T)$. The *spectrum* of the operator L, denoted by $\mathrm{Spec}(L)$, is the set of $\lambda \in \mathbb{C}$ such that $(\lambda - L)$ is not invertible.

The spectrum of an operator is always closed and the *resolvent operator*, $(z - L)^{-1}$, is a Banach space holomorphic function of the *resolvent set*, $\mathbb{C} \setminus \mathrm{Spec}(L)$, see [K, Theorem III-6.7].

If $z \notin \mathrm{Spec}(L)$, then the resolvent is bounded. The norm of the resolvent plays a fundamental role in spectral theory. In particular note that if $L = L^*$, then

$$\|(z - L)^{-1}\| = \frac{1}{\mathrm{dist}(z, \mathrm{Spec}(L))}, \qquad z \notin \mathrm{Spec}(L).$$

Here and elsewhere the *distance* from $z \in \mathbb{C}$ and a set $\mathcal{S} \subset \mathbb{C}$ is

$$\mathrm{dist}(z, \mathcal{S}) = \inf_{\omega \in \mathcal{S}} |z - \omega|.$$

In order to verify that a closed linear operator is invertible, a useful trick is to realise that it is sufficient to check only the following two properties:

(a) $\mathrm{Ran}(T)^{\perp} = \{0\}$,

(b) there exists $c > 0$ such that $\|Tu\| \geq c\|u\|$ for all $u \in \mathrm{Dom}(T)$.

Condition (a) ensures that the range of the operator is dense. Condition (b) then implies that the range is actually equal to $\mathcal{H}$, and also that the operator is one-to-one and its algebraic inverse is bounded.

Problem 1.2.1. Set $\mathcal{H} = L^2(\Omega)$ or $\ell^2(\Omega)$ and let $Mf(x) = m(x)f(x)$ be a multiplication operator. Compute $\mathrm{Spec}(M)$.

Problem 1.2.2. Compute the spectrum of the Volterra operator in Example 1.1.5. *Hint:* Use the Fundamental Theorem of Calculus to deduce and expression for $(z-V)^{-1}g$ when g is differentiable.

In this course we will mainly consider the spectrum of self-adjoint operators, hence the relevance of the following result. However some non-self-adjoint spectral problems will appear in Chapters 6.

Theorem 1.2.3. *The spectrum of a self-adjoint operator is always real.*

Proof. Let $L = L^*$ and put $z = x + iy$ where $x, y \in \mathbb{R}$. For $u \in \mathrm{Dom}(L)$ we get

$$\|(z-L)u\|^2 = \|(x-L)u\|^2 + |y|^2\|u\|^2 = \|(\overline{z}-L)u\|^2.$$

If $y \neq 0$, then

$$\|(z-L)u\|^2 \geq |y|^2\|u\|^2 \quad \text{and} \quad \|(z-L)^*u\|^2 \geq |y|^2\|u\|^2.$$

The first inequality implies (b) for $T = (z-L)$ and, since $\mathrm{Ran}(T)^\perp = \mathrm{Ker}(T^*)$, the second one implies (a). □

1.2.2 Discrete and essential spectrum

A spectral point $\lambda \in \mathrm{Spec}(L)$ is an *eigenvalue*, if it is possible to find an *eigenfunction* $u \neq 0$ such that the equation $Lu = \lambda u$ holds true. The *(geometric) multiplicity* of an eigenvalue λ is the dimension of $\mathrm{Ker}(z-L)$.

Definition 1.2.4. The *discrete spectrum* of L, $\mathrm{Spec}_{\mathrm{disc}}(L)$, is the set of eigenvalues of finite multiplicity. The *essential spectrum* of L is the remaining part of $\mathrm{Spec}(L)$,

$$\mathrm{Spec}_{\mathrm{ess}}(L) = \mathrm{Spec}(L) \setminus \mathrm{Spec}_{\mathrm{disc}}(L).$$

Example 1.2.5. The problem of finding the vibrating modes of a string fixed at both ends of an interval, say $\Omega = (-\pi, \pi)$, leads to the following spectral problem:

$$u''(x) + \lambda u(x) = 0, \qquad u(-\pi) = u(\pi) = 0. \tag{1.4}$$

Here $u(x)$ is the profile of the string at a fixed time. It is easy to verify that a complete set of eigensolutions of (1.4) is given by $\lambda_k = k^2$ and $u_k(x) =$

$\sin(kx)$. The corresponding operator $Lu(x) = -u''(x)$ acting on $L^2(\Omega)$ subject to Dirichlet boundary conditions has $\mathrm{Spec}(L) = \mathrm{Spec}_{\mathrm{disc}}(L) = \{k^2 : k \in \mathbb{N}\}$.

Problem 1.2.6. Prove that $\mathrm{Spec}_{\mathrm{disc}}(M)$ is always empty when $\mathcal{H} = L^2(\Omega)$ and M is the operator of multiplication by $m(x)$. Give an example of a function $m(x)$ with isolated eigenvalues (they should necessarily be of infinite multiplicity).

Problem 1.2.7. What is the nature of the spectral point of the Volterra operator of Problem 1.1.6?

The essential spectrum of a self-adjoint operator can also be characterised in terms of algebraic properties of $(z - L)$. As far as applications concerns, this characterisation is usually much more valuable.

Definition 1.2.8. We say that the closed operator L is *Fredholm*, if $\mathrm{Ran}(L)$ is closed, and both $\mathrm{Ker}(L)$ and $\mathrm{coKer}(L) = \mathcal{H}/\mathrm{Ran}(L)$ are finite dimensional.

The following trick is widely used to determine the spectrum of self-adjoint operators.

Theorem 1.2.9. *Let L be a self-adjoint operator.*

(a) $\lambda \in \mathrm{Spec}(L)$, *if and only if there exists a sequence* $u_j \in \mathrm{Dom}(L)$ *such that* $\|\lambda u_j - Lu_j\|/\|u_j\| \to 0$ *as* $j \to \infty$. *Such a sequence is called a Weyl sequence.*

(b) $\lambda \in \mathrm{Spec}_{\mathrm{ess}}(L)$, *if and only if* $(\lambda - L)$ *is not Fredholm.*

We leave the proof of this result as an exercise. See [D1, Problem 4.3.16].

1.3 Differential operators

1.3.1 Ellipticity

Let Ω be an open subset of $\mathbb{R}^d$, let u be a distribution in Ω and let $\alpha = (\alpha_1, \ldots, \alpha_d) \in \mathbb{N}^d$. We denote by $D^\alpha u$ the distribution obtained by differentiating u α_j times with respect to x_j for all $j = 1, \dots, d$. Let $|\alpha| = \sum_{j=1}^{d} \alpha_j$. The *order* of D^α is $|\alpha|$.

A formal *differential operator* of order n is an expression

$$Lu(x) = \sum_{|\alpha| \le n} a_\alpha(x) D^\alpha u(x)$$

where $u(x)$ and the *coefficients* $a_\alpha(x)$ are functions sufficiently regular in Ω. In this course we will be primarily interested in differential operators of order 2.

The *symbol* of a formal differential operator of order 2 is defined as

$$\sigma(x, \xi) = \sum_{r,s=1}^{d} a_{rs}(x)\xi_r\xi_s + \sum_{b=1}^{d} i a_r(x)\xi_r + a(x).$$

We will call it *(uniformly) elliptic*, if the matrix $[a_{rs}(x)]_{r,s=1}^{d}$ is real symmetric, and all the eigenvalues of this matrix are positive for $x \in \Omega$ and uniformly bounded by positive constants. Note that if $\Omega = \mathbb{R}^d$,

$$Lu(x) = (2\pi)^{-N/2} \int_{\mathbb{R}^d} e^{ix\xi} \sigma(x, \xi) \widehat{u}(\xi) \, \mathrm{d}\xi$$

where

$$\widehat{u}(\xi) = (2\pi)^{-N/2} \int_{\mathbb{R}^d} e^{ix\xi} u(x) \, \mathrm{d}x \tag{1.5}$$

is the *Fourier transform* of u.

Definition 1.3.1. Let $\Omega \subseteq \mathbb{R}^d$. The Laplace (or Laplacian) operator on Ω is given by the expression

$$\Delta u(x) = \sum_{j=1}^{d} \frac{\partial^2}{\partial x_j^2} u(x) \qquad x \in \Omega.$$

Example 1.3.2. The symbol of Δ is $-|\xi|^2$. As

$$[a_{rs}(x)]_{r,s=1}^{d} = \mathrm{diag}[-1, \dots, -1],$$

$-\Delta$ is an elliptic operator.

1.3.2 Sobolev spaces

Let $l \in \mathbb{N}$. The l-th derivative *Sobolev space* is the Hilbert space of $L^2(\Omega)$ functions whose l-th derivative is also an $L^2(\Omega)$ function:

$$H^l(\Omega) = \left\{ u \in L^2(\Omega) : \int_\Omega \sum_{|\alpha|=l} |D^\alpha u(x)|^2 \, \mathrm{d}x < \infty \right\}$$

with scalar product given by

$$\langle u, v \rangle_{H^l} := \int_\Omega u(x)\overline{v(x)} + \sum_{|\alpha|=l} D^\alpha u(x) \overline{D^\alpha v(x)} \, \mathrm{d}x.$$

See [M, Chapter 1].

Note that, $u \in H^l(\Omega)$, if and only if $D^\alpha u$ are absolutely continuous on almost all straight lines which are parallel to the coordinate axes for $|\alpha| = l - 1$, [M, Theorem 1.1.3.1]. Thus

$$C^\infty(\Omega) \subset H^l(\Omega) \subset H^k(\Omega) \subset L^2(\Omega)$$

for $l > k$.

Example 1.3.3. Let $d = 1$ and $\Omega = [a, b]$. Let p and q be real valued continuous functions of Ω with $p(x) > 0$ for all $x \in \Omega$. A family of self-adjoint operators associated to the formal differential expression

$$Lu(x) = -(p(x)u'(x))' + q(x)u(x)$$

are determined by the *separated boundary conditions*. We say that $u \in \mathcal{D}_{\alpha,\beta}$, if $u \in H^2[a, b]$ and

$$\cos(\alpha)u(a) + p(a)\sin(\alpha)u'(a) = 0,$$
$$\cos(\beta)u(b) + p(b)\sin(\beta)u'(b) = 0.$$

The operators L with domain $\mathcal{D}_{\alpha,\beta}$ are all elliptic and self-adjoint in $L^2(a, b)$.

If $\alpha = \beta = 0$, L is said to be subject to *Dirichlet boundary conditions.* If $\alpha = \beta = \pi/2$, L is said to be subject to *Neumann boundary conditions*.

Problem 1.3.4. Compute $\mathrm{Spec}(-\Delta)$ in $L^2(0, 1)$ for different domains $\mathcal{D}_{\alpha,\beta}$. Study the dynamics of $\mathrm{Spec}(-\Delta)$ for the domain $\mathcal{D}_{\alpha,\alpha}$ and $0 \le \alpha \le \pi/2$.

The linear subspace $C^\infty(\Omega) \cap H^l(\Omega)$ is dense in $H^l(\Omega)$, [M, Theorem 1.1.5.2]. That is $H^l(\Omega)$ can also be defined as the completion of the smooth functions in Ω which have finite norm $\|\cdot\|_{H^l}$. Another important subspace of $H^l(\Omega)$ is $H^l_0(\Omega)$, defined to be the completion of $C^\infty_0(\Omega)$, the smooth functions with support contained in the interior of Ω. If $\Omega = \mathbb{R}^d$, then $H^l(\Omega) = H^l_0(\Omega)$, however if Ω is bounded, $H^l(\Omega) \neq H^l_0(\Omega)$.

1.3.3 Dirichlet and Neumann boundary conditions

When we consider a differential expression L as an operator, it is usually necessary to specify boundary conditions. The next theorem describes the *Dirichlet boundary conditions* for elliptic differential expressions on a region Ω. These are usually the easiest to describe and are directly related to a number of physical problems. These include the vibration of a membrane discussed in Chapters 2-5.

Theorem 1.3.5. *Let L be a second order uniformly elliptic differential expression and let*

$$\mathcal{D}_{\mathrm{D}} := \{u \in H^1_0(\Omega) : Lu \in L^2(\Omega)\}.$$

Then L with domain $\mathcal{D}_{\mathrm{D}}$ define a self-adjoint operator in $L^2(\Omega)$.

See [D2, Chapter 6]. Note that the closed quadratic form associated to L in this theorem has domain $H^1_0(\Omega)$.

Neumann boundary conditions are usually more difficult to describe. This is due, in part, to the fact that in general they lack monotonicity of the spectrum as the region Ω expands or contracts. We will discuss in detail this latter property for Dirichlet boundary conditions in Section 3.1.1.

For simplicity, here we only focus on the Laplace operator. The modifications needed for the theorem below to be satisfies by an elliptic operator with smooth coefficients are minor. However serious difficulties arise for irregular $\partial\Omega$ and/or non-smooth coefficients.

Let the quadratic form

$$q_{\mathrm{N}}(u,v) := \int_\Omega \nabla u(x)\overline{\nabla v(x)}\,\mathrm{d}x$$

defined for all $u, v \in \mathrm{Dom}(q_{\mathrm{N}}) := H^1(\Omega)$.

Theorem 1.3.6. *Let Ω be a region with smooth boundary. Let $\tilde{\mathcal{D}}$ be the space of all smooth functions $u \in C^\infty(\overline{\Omega})$, such that*

$$\left.\frac{\partial u(x)}{\partial n}\right|_{\partial\Omega} := n(x) \cdot \nabla u(x)|_{\partial\Omega} = 0$$

where $n(x)$ is the unit normal vector on $\partial\Omega$. Then the closure of q_{N} in the domain $\tilde{\mathcal{D}}$ is $(q_N, H^1(\Omega))$. Let $-\Delta_{\mathrm{N}}$ be the self-adjoint operator associated to $(q_N, H^1(\Omega))$. This operator is the unique self-adjoint extension of $(-\Delta, \tilde{\mathcal{D}})$.

For the proof of this result and further extensions see [D2, Section 7.2]. We call the operator Δ_{N}, the *Neumann Laplacian*. What is remarkable about this theorem is the fact that, in the closure, the quadratic form q_{N} does not "feel" the boundary conditions.

1.4 Further spectral results

1.4.1 The spectral theorem

Let $\mathcal{F} : L^2(\mathbb{R}^d) \longrightarrow L^2(\mathbb{R}^d)$ be the linear operator that assigns to a function its Fourier transform (1.5), $\mathcal{F}u(\xi) = \widehat{u}(\xi)$. By Parseval's Theorem, $\mathcal{F}^* = \mathcal{F}^{-1}$.

If L is an elliptic operator with constant coefficients, then its symbol is a polynomial of order 2 in ξ, constant in x and bounded below. Let this symbol be denoted by $\sigma(\xi) = \sigma(x, \xi)$. If $u \in L^2(\mathbb{R}^d)$ is such that $\sigma(\cdot)u(\cdot) \in L^2(\mathbb{R}^d)$, then $L\mathcal{F}u \in L^2(\mathbb{R}^d)$ and

$$\mathcal{F}^* L \mathcal{F} u(\xi) = \sigma(\xi) u(\xi).$$

This ensures the validity of the following result.

Lemma 1.4.1. *Let L be a constant coefficients elliptic differential expression with domain $\mathrm{Dom}(L) = H^2(\mathbb{R}^d)$. Then L defines a self-adjoint operator in $L^2(\mathbb{R}^d)$. Moreover L is unitarily equivalent to the operator of multiplication by its symbol.*

Problem 1.4.2. Compute $\mathrm{Spec}(-\Delta)$ in $L^2(\mathbb{R}^d)$.

This lemma is an infinite-dimensional version of the result establishing that any Hermitean matrix is diagonalisable.

Problem 1.4.3. We say that a matrix M is *diagonalisable*, if $M = V^{-1}DV$ where D is a diagonal matrix and $\det V \neq 0$. In general diagonalisable matrices are not self-adjoint, even when all their eigenvalues are real. For that we need V unitary, $V^*V = VV^* = I$. Nonetheless, M is diagonalisable and it has real eigenvalues, if and only if there exists an inner product on $\mathbb{C}^n$ such that M is self-adjoint in this new inner product. Prove the this assertion.

The following result generalises Lemma 1.4.1.

Theorem 1.4.4. *Let L be a self-adjoint operator acting on $\mathcal{H}$. There exists a measure μ in $\mathcal{S} = \mathbb{N} \times \operatorname{Spec}(L)$ and an operator*

$$U : \mathcal{H} \longrightarrow L^2 := L^2(\mathcal{S},\, \mathrm{d}\mu)$$

satisfying the following properties. Let $h : \mathcal{S} \longrightarrow \mathbb{R}$ be the function $h(n, s) = s$.

(a) $UU^* = U^*U$, that is U is unitary.

(b) $u \in \operatorname{Dom}(L)$ if and only if $hUu \in L^2$.

(c) $ULU^*v = hv$ for all $v \in U(\operatorname{Dom}(L))$.

See [D2, Theorem 2.5.1].

If the essential spectrum is empty, each point in $\operatorname{Spec}(L)$ is isolated and of finite multiplicity. In this case the measure μ of Theorem 1.4.4 can be chosen to be

$$\mu(\{(n, \lambda)\}) = \begin{cases} 1, & n = 1, \ldots, \operatorname{mult}(\lambda), \\ 0, & \text{otherwise.} \end{cases}$$

In this case an orthonormal basis of eigenfunctions is obtained from the corresponding orthonormal basis of $L^2(\mathcal{S},\, \mathrm{d}\mu) = \ell^2(\mathcal{S})$.

Theorem 1.4.5. *Let L be a self-adjoint operator acting on $\mathcal{H}$, such that* $\mathrm{Spec}_{\mathrm{ess}}(L) = \varnothing$. *Let* $\mathrm{Spec}(L) = \{\lambda_n\}_{n=-\infty}^{\infty}$. *There exists an orthonormal basis of $\mathcal{H}$, $\{\phi_n\}_{n=-\infty}^{\infty}$, such that:*

(a) $u \in \mathrm{Dom}(L)$ *if and only if* $\sum_{-\infty}^{\infty} \lambda_n^2 |\langle u, \phi_n\rangle|^2 < \infty$.

(b) $Lu = \sum_{-\infty}^{\infty} \lambda_n \langle u, \phi_n\rangle \phi_n$ *for all* $u \in \mathrm{Dom}(L)$.

1.4.2 Separation of variables

Let $\Omega = [0, a]^d \subset \mathbb{R}^d$ be a rectangle $(d = 2)$, a cube $(d = 3)$ or an hyper cube $(d > 3)$ of side $a > 0$. Let $L = -\Delta + V$ acting on $L^2(\Omega)$ subject to Dirichlet boundary conditions, where $V(x) = \sum_{j=1}^{d} V_j(x_j)$. Suppose we start with the eigenvalue problem

$$Lu = \lambda u \quad \text{in } \Omega, \qquad u|_{\partial\Omega} = 0. \tag{1.6}$$

If we consider solutions of the form $u(x_1, \ldots, x_d) = \prod_{j=1}^{d} u_j(x_j)$, where $u_j(x)$ are the solutions of

$$\begin{aligned} -u_j''(x) + V_j(x) u_j(x) = \mu_j u_j(x), \qquad & 0 \le x \le a, \\ u_j(0) = u_j(a) = 0, \qquad & \end{aligned} \tag{1.7}$$

then (1.6) is satisfied for $\lambda = \sum_{j=1}^{d} \mu_j$. If $\mu_j(k)$ for $k \in \mathbb{N}$ are all the eigenvalues of the Sturm-Liouville problem (1.7), then the corresponding eigenvectors form a basis of $L^2(0, a)$. Consequently the corresponding functions $u_\alpha(x_1, \ldots, x_d)$ for $\alpha \in \mathbb{N}^d$ form a basis of $L^2(\mathbb{R}^d)$. This ensures that

$$\mathrm{Spec}(L) = \{\mu_1(\alpha_1) + \ldots + \mu_d(\alpha_d) : \alpha \in \mathbb{N}\}.$$

Example 1.4.6. Let $\Omega = [0, a]^2$ and $L = -\Delta_{\mathrm{D}}$ be the Dirichlet Laplacian. Then

$$\mathrm{Spec}(L) = \left\{ \frac{\pi^2}{a^2}(k^2 + m^2) : (k, m) \in \mathbb{Z}_+^2 \right\}.$$

Here and elsewhere we denote $\mathbb{Z}_+ = \mathbb{N} \cup \{0\}$.

Problem 1.4.7. Find the spectrum of $-\Delta_{\mathrm{N}}$, the Neumann Laplacian, on $\Omega = [0, a]^d$.

The eigenvalues of the Laplace operator on the unit disc $B := \{|z| \le 1\}$ can also be found explicitly. For that we should first decompose

$$L^2(B) = \bigoplus_{n=-\infty}^{\infty} \mathcal{L}_n,$$

where

$$\mathcal{L}_n := \{u(r\cos(\theta), r\sin(\theta)) = f(r)e^{in\theta}\}.$$

Note that each $u \in \mathcal{L}_n$ is completely characterised by its corresponding *radial component* $f(r)$. Since $-\Delta$ commutes with rotations, then

$$-\Delta = \bigoplus_{n=-\infty}^{\infty} -\Delta \restriction \mathcal{L}_n.$$

The operators $-\Delta \restriction \mathcal{L}_n$ act also only on the radial component and are unitarily equivalent to the singular Sturm-Liouville operator

$$L_n f(r) := -\frac{1}{r}(rf'(r))' + \frac{n^2}{r^2} f(r), \qquad 0 < r \le 1 \tag{1.8}$$

acting on a suitable Hilbert space.

The eigenfunctions of $-\Delta_{\mathrm{D}}$ in D are found from the eigenfunctions $f : [0,1] \longrightarrow \mathbb{C}$ of (1.8), such that

$$\int_0^1 r|f(r)|^2 \,\mathrm{d}r < \infty,$$

$L_n f(r) = \lambda f(r)$ and $f(1) = 0$. The eigenvalue problem associated to L_n is known as the Bessel equation. It is a classical result in analysis that these eigenfunctions are of the form

$$f_{n,s}(r) = J_n(j_{n,s} r), \qquad s \in \mathbb{N},$$

where $j_{n,s}$ is the sth zeros of the Bessel function,

$$J_n(r) = \frac{1}{2\pi}\int_0^{2\pi} \cos(n\theta - r\sin(\theta))\,\mathrm{d}\theta,$$

see [I, Section VII.7.32]. The eigenvalues of $-\Delta_{\mathrm{D}}$ in B are $\{j_{n,s}^2\}_{(n,s)\in\mathbb{Z}\times\mathbb{N}}$. The Bessel zeros $j_{n,s}$ can be found with high accuracy on a computer. The first six eigenvalues are approximately equal to:

$$5.784,\ 14.684 \text{ (double)},\ 26.378 \text{ (double)},\ \text{and } 30.470.$$

Chapter 2

Variational techniques

If L is an elliptic differential operator with constant coefficients and Ω is a bounded region with certain symmetries, the spectrum of L can be found explicitly. However this is not possible in general. In this chapter we address the following questions:

- How can we find the spectrum of L, when Ω does not have a regular shape or when the coefficients of L are not constant?
- How can we approximate parts of the discrete spectrum of a self-adjoint operator on a computer?

2.1 The Rayleigh-Ritz principle

How do we estimate the eigenvalues of a self-adjoint operator? The techniques described in this section were discovered by Lord Rayleigh and Walter Ritz over one hundred years ago. Yet they are still the basic principle behind most procedures for approximating spectra in a wide variety of applications.

2.1.1 The Rayleigh quotient

Let A be a self-adjoint operator. The *Rayleigh quotient* of $u \in \mathrm{Dom}(q_A)$ is defined to be

$$R(u) = \frac{q_A(u,u)}{\langle u,u\rangle} \qquad \left(= \frac{\langle Au,u\rangle}{\langle u,u\rangle} \quad \text{if } u \in \mathrm{Dom}(A) \right). \tag{2.1}$$

The role of the Rayleigh quotient in eigenvalue computation may be illustrated on simple operators.

Let A be a 3×3 Hermitean matrix with eigenvalues $\lambda_1 \leq \lambda_2 \leq \lambda_3$ and normalised eigenvectors $u_1, u_2, u_3 \in \mathbb{C}^3$. The eigenvalues of A may be characterised as extremal problems involving $R(u)$. If $u = \sum \alpha_j u_j$, then

$$R(u) = \frac{\sum \lambda_j |\alpha_j|^2}{\sum |\alpha_j|^2}.$$

Thus

$$\begin{aligned} \lambda_1 &= \min\{R(u) : u \in \mathbb{C}^3\}, \\ \lambda_2 &= \min\{R(u) : u \perp \operatorname{Span}(u_1)\}, \\ \lambda_3 &= \min\{R(u) : u \perp \operatorname{Span}(u_1, u_2)\}. \end{aligned}$$

Moreover,

$$\frac{\partial R}{\partial |\alpha_k|} = \frac{2|\alpha_k| \sum |\alpha_j|^2 (\lambda_k - \lambda_j)}{(\sum |\alpha_j|^2)^2}.$$

That is, λ_j are stationary points of the map $R : \mathbb{C}^3 \longrightarrow \mathbb{R}$.

2.1.2 The min-max principle

Note that no prior knowledge of u_1, u_2 or u_3 is required in the above formula for λ_1. Can we characterise λ_2 also without information about the eigenvectors? If $\mathcal{S} \subset \mathbb{C}^3$ is an arbitrary two-dimensional space, there always exists a non-zero vector $\tilde{u} \in \mathcal{S}$ such that $\tilde{u} \perp u_1$. Since $R(\tilde{u}) \geq \lambda_2$, we gather that $\max_{u \in \mathcal{S}} R(u) \geq \lambda_2$ and

$$\lambda_2 = \min_{\dim \mathcal{S} = 2} \max_{u \in \mathcal{S}} R(u).$$

A similar argument shows that

$$\lambda_3 = \min_{\dim \mathcal{S} = 3} \max_{u \in \mathcal{S}} R(u).$$

Therefore the characterisation of the eigenvalues in terms of $R(u)$ does not require the eigenvectors.

The above procedure can be extended to matrices of any size without much difficulty, and in fact to infinite-dimensional operators. The following result is of fundamental importance and it is known as the min-max principle. Its current form is due to Courant and Fischer. Complete proofs may be found in [RSv4, Theorem XIII.1] or [D2, Theorem 4.5.2], but they do not differ in essence from the above argument.

Theorem 2.1.1. *Let A be a self-adjoint operator such that $R(u) \geq -c$ for all $u \in \mathrm{Dom}(A)$, where $c \geq 0$ is a constant. Let $\mathcal{D}$ be either $\mathrm{Dom}(A)$ or $\mathrm{Dom}(q_A)$. Let $-c \leq \mu_1 \leq \mu_2 \leq \dots$ be given by*

$$\mu_k = \min_{\substack{\dim(\mathcal{S}) = k \\ \mathcal{S} \subset \mathcal{D}}} \max_{u \in \mathcal{S}} R(u). \tag{2.2}$$

(a) If $\dim(\mathcal{H}) < \infty$, then $\mathrm{Spec}(A) = \{\mu_k\}$ counting multiplicities.

(b) If $\dim(\mathcal{H}) = \infty$, put $E = \lim_{k\to\infty} \mu_k$. Then $E = \min(\mathrm{Spec}_{\mathrm{ess}}(A))$ and $\mathrm{Spec}_{\mathrm{disc}}(A) \cap (-\infty, E) = \{\mu_k\}$ counting multiplicities.

In other words, the eigenvalues of a self-adjoint operator that are outside the extrema of the essential spectrum are completely characterised by the Rayleigh quotient.

As an immediate consequence of this theorem, note that any bounded self-adjoint operator acting on an infinite dimensional Hilbert space has non-empty essential spectrum. This is not true, however, for unbounded operators. We will say that $A = A^*$ is *semi-bounded* if it satisfies the hypothesis of the theorem above.

Corollary 2.1.2. *Let A be a semi-bounded self-adjoint operator. If $\mathrm{Spec}_{\mathrm{ess}}(A)$ is empty, then $\mathrm{Spec}(A) = \{\mu_k\}$ where the μ_k are given by* (2.2).

Problem 2.1.3. Show that any elliptic differential operator is semi-bounded.

Corollary 2.1.4. *Let $\Omega \subseteq \mathbb{R}^d$ be an open bounded region.*

(a) Let $-\Delta_{\mathrm{D}}$ be the Laplace operator on Ω subject to Dirichlet boundary conditions. Then $\mathrm{Spec}(-\Delta_{\mathrm{D}}) = \{\lambda_k\}$, where

$$\lambda_k = \min_{\substack{\dim(\mathcal{S}) = k \\ \mathcal{S} \subset H_0^1(\Omega)}} \max_{u \in \mathcal{S}} \frac{\int_\Omega |\nabla u|^2}{\int_\Omega |u|^2}.$$

(b) *Suppose that $\partial\Omega$ is smooth and let $-\Delta_{\mathrm{N}}$ be the Laplace operator on Ω subject to Neumann boundary conditions. Then* $\operatorname{Spec}(-\Delta_{\mathrm{N}}) = \{\mu_k\}$, *where*

$$\mu_k = \min_{\substack{\dim(\mathcal{S})=k \\ \mathcal{S}\subset H^1(\Omega)}} \max_{u\in\mathcal{S}} \frac{\int_\Omega |\nabla u|^2}{\int_\Omega |u|^2}.$$

Let $\Omega \subset \mathbb{R}^N$ be an open bounded set and let $V : \Omega \longrightarrow \mathbb{R}$ be a continuous function. Let

$$Lu(x) = -\Delta u(x) + V(x)u(x)$$

be the self-adjoint operator acting on $L^2(\Omega)$ subject to Dirichlet boundary conditions. The operator L is called the *Schrödinger operator* with potential V in the region Ω. Corollary 2.1.4 ensures that $\operatorname{Spec}_{\mathrm{ess}}(L) = \varnothing$. In order to see this we compare with the Schrödinger operator with constant potential for a large rectangle containing Ω.

2.1.3 The Rayleigh-Ritz principle

Let A be a semi-bounded self-adjoint operator and suppose we would like to approximate the first n eigenvalues of A which are below $\min(\operatorname{Spec}_{\mathrm{ess}}(A))$. A general technique is described next and it is usually known as the *Rayleigh-Ritz* or *variational* principle.

Pick $\mathcal{L} \subset \operatorname{Dom}(q_A)$ to be a finite-dimensional subspace of dimension much larger than n. Define the number

$$\nu_k(\mathcal{L}) = \min_{\substack{\dim(\mathcal{S})=k \\ \mathcal{S}\subseteq\mathcal{L}}} \max_{u\in\mathcal{S}} R(u) \tag{2.3}$$

for $k = 1, \dots, n$. By virtue of Theorem 2.1.1, $\nu_k(\mathcal{L}) \geq \lambda_k$, so we have an approximation from above for λ_k.

In fact, if $\mathcal{L}$ is "sufficiently close" to $\operatorname{Dom}(A)$, then $\nu_k(\mathcal{L})$ is close to λ_k. Let us be more precise about this statement. Suppose that u is a normalised eigenfunction associated to the first eigenvalue λ_1 of A. If we can find $v \in \mathcal{L}$, such that

$$\max\{\|(v-u)\|, \|A(v-u)\|\} < \delta \tag{2.4}$$

for δ sufficiently small, then

$$\begin{aligned} |\langle Av, v\rangle - \lambda_1| &= |\langle Av, v\rangle - \langle Au, u\rangle| \\ &\leq |\langle Av - Au, v\rangle| + |\langle Au, v-u\rangle| \leq (1+\delta+|\lambda_1|)\delta \end{aligned}$$

so that

$$\lambda_1 \le \nu_1(\mathcal{L}) \le \lambda_1 + \frac{1+\delta+|\lambda_1|}{(1-\delta)^2}\delta. \tag{2.5}$$

Similar results can be established for the nth eigenvalue of A counting multiplicities, with concrete sharp estimates in particular cases.

The Rayleigh-Ritz principle provides, not only an approximation for the eigenvalues of A, but also for the eigenfunctions. Indeed, the critical vector $v_k \in \mathcal{L}$ such that $\nu_k(\mathcal{L}) = q_L(v_k, v_k)$ is close to the eigenspace of L associated to λ_k. See [SF, Theorem 6.2] for a precise estimate of this type.

We now discuss a concrete implementation of the Rayleigh-Ritz principle.

2.2 The projection method

The variational principle establishes that we should find the quantities $\nu_k(\mathcal{L})$ in (2.3), in order to approximate eigenvalues of A. This may be achieved in different ways. One possibility is to write down the problem in weak form. The idea, often attributed to B. Galerkin, is known as the *projection method*.

2.2.1 Weak eigenvalue problems

Since $\mathcal{L} \subset \mathrm{Dom}(q_A)$ is finite-dimensional, the $\{\nu_k(\mathcal{L})\}$ are the eigenvalues of the *weak spectral problem*: find $\nu \in \mathbb{R}$ and $u \in \mathcal{L}$ non-zero, such that

$$q_A(u, v) = \nu \langle u, v\rangle \qquad \text{for all } v \in \mathcal{L}. \tag{2.6}$$

Indeed, if $\{e_j\}$ is an orthonormal basis of $\mathcal{L}$, then the the solutions (ν, u) of (2.6) are the eigenvalues and eigenfunctions of the Hermitean matrix $M = [q_A(e_j, e_k)]$. By applying Theorem 2.1.1 to M, we discover that these eigenvalues are given by (2.3).

Different computational methods are obtained by choosing $\mathcal{L}$ in different ways. The projection method is widely used in applications. It can be employed to approximate the spectrum of operators acting on infinite-dimensional Hilbert spaces, but it also lies at the core of important finite-dimensional linear algebra techniques. The Arnoldi algorithm for iteratively computing eigenvalues, implemented in the function `eigs` of Matlab, is one of them.

2.2.2 Estimating the Mathieu characteristic values

In order to illustrate the projection method on a simple example, we consider the computation of the Mathieu characteristic values.

Let

$$Lu(x) = -u''(x) + \cos(x)u(x)$$

acting on $\mathcal{H} = L^2(-\pi, \pi)$ subject to periodic boundary conditions. The operator L is self-adjoint in the domain

$$\mathrm{Dom}(L) = \{u \in H^2(-\pi, \pi) : u(-\pi) = u(\pi)\}$$

and $\mathrm{Spec}(L)$ is purely discrete, bounded below and accumulating at $+\infty$. The eigenvalues of L (together with the case of anti-periodic boundary conditions) are known as the *Mathieu characteristic values*, [I, p.176]. They are important in applications ranging from solid state physics to function theory. It is known that all the eigenvalues are simple, [RSv4, Example XIII.1].

We may approximate $\mathrm{Spec}(L)$ by choosing the canonical orthonormal basis of $\mathcal{H}$, the Fourier basis $e_k = (2\pi)^{-1/2}e^{ikx}$, and putting

$$\mathcal{L} = \mathrm{Span}\{e_{-n}, \dots, e_n\}.$$

The eigenvalues of (2.6) are those of the $(2n+1) \times (2n+1)$ matrix M whose entries are given by

$$M_{jk} = q_L(e_j, e_k) = \frac{1}{2\pi} \int_{-\pi}^{\pi} Le^{ijx}e^{-ikx}\,\mathrm{d}x = \begin{cases} j^2 & j = k, \\ 1/2 & j = k+1, \\ 1/2 & j = k-1, \\ 0 & \text{otherwise,} \end{cases}$$

where $j, k = -n, \dots, n$. The eigenvalues of M converge from above to those of L as $n \to \infty$.

This model is so simple that we can find the entries of M explicitly. How accurately the eigenvalues of M approach to those of L? A convergence analysis can be carried out for the first eigenvalue $\lambda_1 = \min[\mathrm{Spec}(L)]$, using the observation made in Section 2.1.3.

The eigenfunctions of L, considered as periodic functions of $\mathbb{R}$, are smooth. Let w be such that $Lw = \lambda_1 w$. Then

$$\begin{aligned}
(2\pi)^{1/2}\widehat{w}(n) &= \int_{-\pi}^{\pi} w(x)e^{-inx}\,\mathrm{d}x \\
&= \frac{1}{-in}\int_{-\pi}^{\pi} w(x)(e^{-inx})'\,\mathrm{d}x \\
&= \frac{1}{in}\int_{-\pi}^{\pi} w'(x)e^{-inx}\,\mathrm{d}x \\
&\ \ \vdots \\
&= (2\pi)^{1/2}\frac{(-1)^{p+1}}{(in)^p}\widehat{w^{(p)}}(n)
\end{aligned}$$

for all $|n|, p \in \mathbb{N}$. If we choose $v \in \mathrm{Span}\{e_{-n}, \ldots, e_n\}$ to be $v(x) = \sum_{-n}^{n} \widehat{w}(k)e^{ikx}$, then

$$\|v - w\| \leq \|w^{(p)}\|n^{-p} \qquad \text{and}$$
$$\|v'' - w''\| \leq \|w^{(p)}\|n^{p-2}.$$

By putting $\delta = an^{-r}$ in (2.4), we achieve the following from (2.5). For all $r \in \mathbb{N}$, there exists a constant $c_r > 0$ such that

$$0 \leq \nu_1(\mathcal{L}) - \lambda_1 \leq c_r n^{-r} \qquad \text{for all } n \in \mathbb{N}.$$

In other words, the first eigenvalue of M converges super-polynomially fast to λ_1 from above as $n \to \infty$.

Problem 2.2.1. Write a Matlab program to compute the spectrum of

$$Hu(x) = -u''(x) + \sin(x)u(x)$$

acting on $L^2(0, \pi)$, subject to Neumann boundary conditions: $u'(0) = u'(\pi) = 0$.

2.3 The finite element method

The mathematical origins of the finite element method (FEM) can be traced back to the work of Courant in the 1940s. Still nowadays it is regarded as one of the most widely used techniques in the numerical analysis of partial differential equations. In the present course we describe it in the context of spectral approximation.

2.3.1 Finite element spaces

Suppose we would like to apply the projection methods to an operator L acting on $L^2(\Omega)$. In the finite element method, the subspaces $\mathcal{L}$, called *finite element spaces*, are constructed by assembling together polynomial functions defined on sub-domains of Ω. These sub-domains together with the polynomial functions are called *elements*. The most commonly used sub-domains are either simplexes or hypercubes (triangles and rectangles in the plane).

Rather than focusing on the abstract theory of interpolation, let us discuss some particular cases.

2.3.2 Piecewise linear elements in 1D

Let L be the elliptic differential operator discussed in example 1.3.3,

$$Lu(x) = -(p(x)u'(x))' + q(x)u(x), \qquad 0 \le x \le 1,$$

subject to Dirichlet boundary conditions: $u(0) = u(1) = 0$. Integration by parts and the boundary conditions yield

$$q_L(u,v) = \int_0^1 p(x)u'(x)\overline{v'(x)} + q(x)u(x)\overline{v(x)}\,\mathrm{d}x$$

for all $u, v \in H^1(0,1) = \mathrm{Dom}(q_L)$. We can verify this identity first for all $u, v \in C_0^\infty(0,1)$ and then applying a density argument in the Sobolev norm. Therefore we may consider test spaces $\mathcal{L}$ of absolutely continuous functions in $[0,1]$, satisfying the corresponding boundary conditions.

The easiest possibility is to cut the interval into n sub-intervals with endpoints at $0 = x_0 < x_1 < \ldots < x_{n-1} < x_n = 1$. Then let $\mathcal{L}$ be generated by piecewise continuous functions linear in each sub-interval vanishing at 0 and 1. A basis of $\mathcal{L}$ is given by "pyramid" functions:

$$\phi_j(x) = \begin{cases} \frac{x-x_{j-1}}{x_j-x_{j-1}} & x_{j-1} \le x \le x_j, \\ \frac{x_{j+1}-x}{x_{j+1}-x_j} & x_j \le x \le x_{j+1}, \\ 0 & \text{otherwise}, \end{cases}, \qquad j = 1, \ldots, n-1.$$

Note that $\phi_j \not\perp \phi_{j+1}$. In order to solve the Rayleigh-Ritz problem (2.3), we construct the *stiffness matrix* and the *mass matrix*,

$$K_{\mathcal{L}} = [q_L(\phi_j, \phi_k)]_{jk=1}^n \quad \text{and} \quad M_{\mathcal{L}} = [\langle \phi_j, \phi_k \rangle]_{jk=1}^n. \tag{2.7}$$

The eigenvalues of the *pencil problem*

$$K_{\mathcal{L}} v = \nu M_{\mathcal{L}} v, \qquad v \neq 0, \tag{2.8}$$

are the required approximate eigenvalues $\nu_k(\mathcal{L})$. Note that in this case $S_{\mathcal{L}}$ and $M_{\mathcal{L}}$ are tri-diagonal matrices.

Example 2.3.1. Let $p(x) = p$ and $q(x) = q$ be constants. Put $h = 1/n$ for $n \in \mathbb{N}$ and let the nodes be equally spaced $x_j = jh$. Let

$$\tilde{M} = \begin{pmatrix} 4 & 1 & & & \\ 1 & 4 & 1 & & \\ & & & & \\ & & 1 & 4 & 1 \\ & & & 1 & 4 \end{pmatrix} \quad \text{and} \quad \tilde{K} = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & & & & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}.$$

Then $M_{\mathcal{L}} = \frac{h}{6}\tilde{M}$ and $K_{\mathcal{L}} = p\frac{1}{h}\tilde{K} + qM_{\mathcal{L}}$.

Note that both the stiffness and the mass matrices have *Toeplitz structure* (they are constant along the diagonal). In this very special case we can actually compute the eigenvalues $\nu_k(\mathcal{L})$ explicitly. The eigenvalues of the Toeplitz matrix

$$T = \begin{pmatrix} 0 & 1 & & & \\ 1 & 0 & 1 & & \\ & & & & \\ & & 1 & 0 & 1 \\ & & & 1 & 0 \end{pmatrix}$$

are $\tau_k = 2\cos\left(\frac{k\pi}{n+1}\right)$, $k = 1, \ldots, n$. One can easily verify that $\tilde{M}\tilde{K} = \tilde{K}\tilde{M}$. Therefore

$$\nu_k(\mathcal{L}) = \frac{6p(2 - \tau_k)}{h^2(4 + \tau_k)} + q.$$

Obviously the exact eigenvalues of this problem are known: $\lambda_k = p(k\pi)^2 + q$ for $k \in \mathbb{N}$. By carrying out explicit calculations, we can use (2.5) to verify by hand that $0 < \nu_1(\mathcal{L}) - \lambda_1 \leq Ch$ where $C > 0$ is a constant independent of h.

2.3.3 Finite elements in 2D

Although the finite element method provides a tool for analysing 1D problems, its virtue lies on the fact that it can be applied to partial differential operators. The finite element space described next was proposed by Courant in 1943 for the solution of variational problems. It is the higher-dimensional analogue of the space discussed in section 2.3.2.

Let $\Omega \subseteq \mathbb{R}^2$. In order to construct $\mathcal{L}$, we consider a polygonal domain $\Gamma \subseteq \mathbb{R}^2$ and a *triangulation* or *mesh* on Γ. Usually one should assume that the measure of $\Omega \setminus \Gamma$ is small, for instance, one might impose that the vertexes of $\partial\Gamma$ should also be in $\partial\Omega$. The mesh is a set of triangles $T_j \subset \Gamma$ such that

$$\bigcup \overline{T_j} = \Gamma \quad \text{and} \quad \operatorname{Int}(T_j) \cap \operatorname{Int}(T_k) = \varnothing, \; j \neq k.$$

The vertexes of the T_j are called the *nodes* of the triangulation.

For the Courant element, each $u \in \mathcal{L}$ is determined by its value at the nodes. They are piecewise linear continuous functions on Ω, linear at each T_j. If a boundary condition is given, then the elements of $\mathcal{L}$ might be required to satisfy additional constraints. In particular:

(a) The form domain associated to Neumann boundary conditions is $H^1(\Omega)$. In this case no restriction is needed, so a basis of $\mathcal{L}$ is determined by piecewise linear functions whose value is 1 at a single node and 0 at any other node.

(b) For Dirichlet boundary conditions, however, the form domain is $H^1_0(\Omega)$. Thus, a basis of $\mathcal{L}$ is determined by "pyramid" functions whose value is 1 at a single inner node and 0 at any other node. See Figure 2.1.

In similar fashion as for the 1D case, the stiffness and mass matrices are defined as in (2.7). The approximate eigenvalues $\nu_k(\mathcal{L})$ are obtained by solving (2.8). There are various ways of constructing $K_{\mathcal{L}}$ and $M_{\mathcal{L}}$. For an account on how to do this efficiently see [S, Section 2.2.2] or [SF, p.90].

The present is not a course on how to program the FEM, but rather how to use it. The Internet provides over 1.500.000 entries under the search for "finite element method program". There is public domain software such as ALBERT, DEAL and UG, and also commercial packages include Matlab's PDE Toolbox and Comsol.

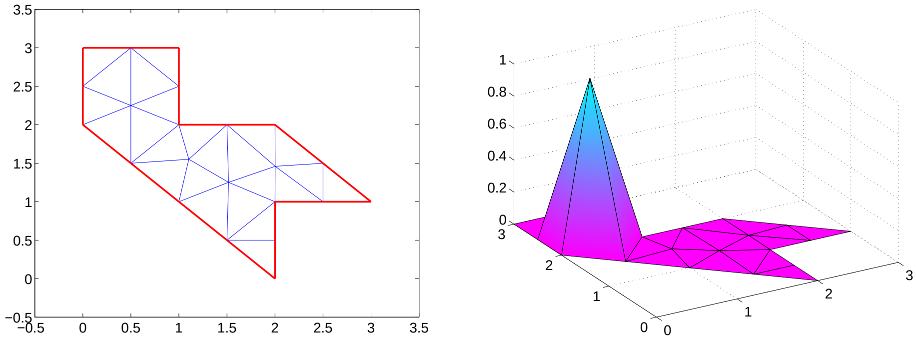

Figure 2.1: Typical mesh on a region of $\mathbb{R}^2$ along with a basis function of $\mathcal{L}$ for the Courant element.

Let us focus on the simple example of the vibration of a membrane on a domain which will be relevant in Chapter 5.

Let $\Omega \subset \mathbb{R}^2$ be the region on the left side of Figure 2.1. The vibration of a homogeneous membrane covering the region Ω fixed at $\partial\Omega$ is described by the eigenvalue problem

$$\Delta u = \lambda u \text{ in } \Omega, \qquad u|_{\partial\Omega} = 0. \tag{2.9}$$

If we disregard the material constants, the oscillation frequencies of the membrane are given by $\sqrt{\lambda}$ and the oscillation modes are the solutions u. In the language of this course, we are interested in finding the eigenvalues and eigenvectors of the Dirichlet Laplacian, $-\Delta_{\mathrm{D}}$.

For any two $u, v \in C_0^\infty(\Omega)$, we get

$$\begin{aligned} q_{\mathrm{D}}(u,v) &= \int_\Omega -\Delta u \overline{v} \,\mathrm{d}x \\ &= \int_\Omega \nabla u \cdot \overline{\nabla v} \,\mathrm{d}x - \int_{\partial\Omega} \nabla u \cdot n v \,\mathrm{d}\gamma \\ &= \int_\Omega \nabla u \cdot \overline{\nabla v} \,\mathrm{d}x. \end{aligned}$$

Therefore, by a density argument,

$$q_{\mathrm{D}}(u,v) = \int_\Omega \nabla u \cdot \overline{\nabla v} \,\mathrm{d}x \qquad u, v \in H_0^1(\Omega).$$

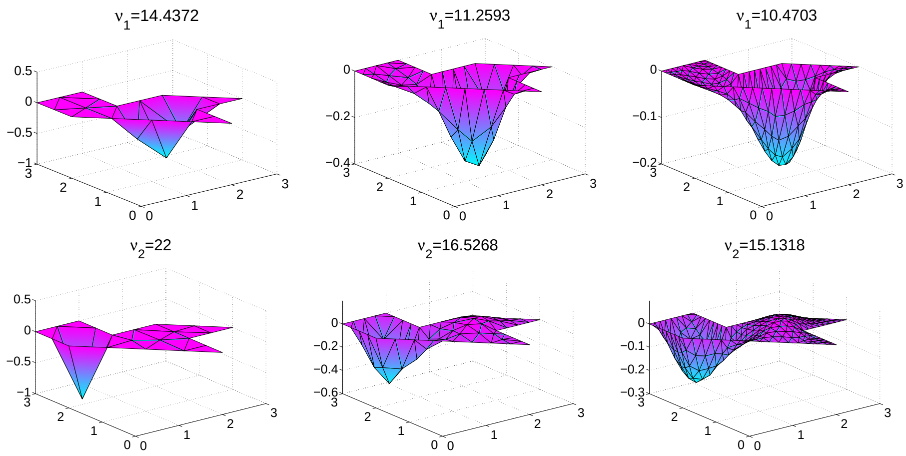

Figure 2.2: First and second eigenfrequency and eigenmode of problem (2.9).

We may compute the corresponding eigenvalues by using the Matlab PDE Toolbox. In Figure 2.2, we illustrate computations of the first and second eigenvalues along with the corresponding eigenfunction. Typically, as the size of the elements in the mesh becomes smaller, the eigenvalues will decrease converging to the exact λ_k as the Rayleigh-Ritz principle predicts.

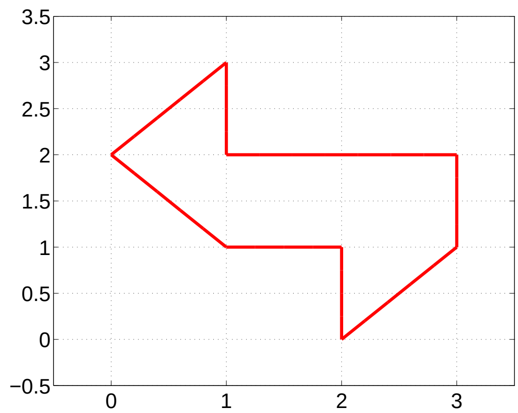

Figure 2.3: Second isospectral region of Gordon, Webb and Wolpert.

Problem 2.3.2. Let $\Omega \subset \mathbb{R}^2$ be the region of Figure 2.3. Use the Matlab PDE Toolbox to compute the frequencies and modes of the vibrating membrane problem (2.9). Compare with the results given by the region on the left of Figure 2.1.

We have not chosen ad hoc the regions of Figures 2.1 and 2.3. They are the famous example of Gordon, Webb and Wolpert, answering negatively the question posed by Marc Kac in 1966. These two regions are isospectral but not isometric. Two drums with their shape will sound exactly the same. See Chapter 5 for details.

2.3.4 Higher order elements elements

The pyramid finite elements satisfy $\mathcal{L} \subset H^1(\Omega)$. However u' or ∇u are typically discontinuous for $u \in \mathcal{L}$. If we would like to consider more regular approximate functions, one possibility is to increase the number of parameters in the interpolation of $u \in \mathcal{L}$, thus increase the degree of the polynomial at each element.

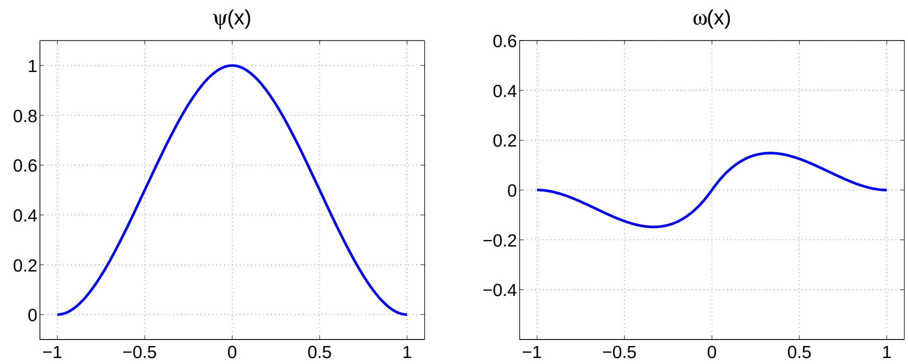

Figure 2.4: Generator functions for the basis of the 1D Hermite element of order 3.

One of the most common higher order elements is the *Hermite element of order 3*. In 1D it yields $\mathcal{L} \subset H^2(\Omega)$ and it is obtained by setting $u \in \mathcal{L}$ piecewise polynomials of order 3 with prescribed values of u and u' at the nodes. Let the functions

$$\psi(x) = (|x|-1)^2(2|x|+1) \quad \text{and} \quad \omega(x) = x(|x|-1)^2$$

defined on $-1 \leq x \leq 1$. Note that both functions have continuous derivatives if extended by 0 to $\mathbb{R}$ and that

$$\psi(0) = 1,\, \psi(\pm 1) = \psi'(0) = \psi'(\pm 1) = 0$$
$$\omega'(0) = 1,\, \omega(\pm 1) = \omega(0) = \omega'(\pm 1) = 0.$$

See Figure 2.4. A basis of $\mathcal{L}$ is obtained by translation and rescaling:

$$\phi_j(x) = \phi\left(\frac{x-x_j}{h}\right), \qquad \omega_j(x) = \omega\left(\frac{x-x_j}{h}\right).$$

For precise details of how to program on a computer the FEM using these and other higher order elements see [SF, p.57]. The convergence rate of the Hermite element of order 3 is of order h^3 as the maximum element size $h \to 0$. See [SF, Theorem 6.1].

Chapter 3

Basic estimates of eigenvalues. Counting function

The aim of this chapter is to give some answers to the following questions:

- What happens to the eigenvalues of the Dirichlet Laplacian if we extend the geometric domain in which it acts?
- What happens to the eigenvalues of the Dirichlet or Neumann Laplacian if we add extra Dirichlet/Neumann boundary conditions on some subset of co-dimension one inside the domain?
- Can one predict the asymptotic behaviour of large eigenvalues of an elliptic partial differential boundary value problem on $\Omega \subset \mathbb{R}^d$?
- What changes if the boundary of Ω is fractal?

3.1 Elementary estimates and fundamental tools

Estimates on eigenvalues of boundary value problems for the Laplacian acting in bounded domains can be obtained almost immediately from the Rayleigh-Ritz principle described in details in Chapter 2. These estimates, although simple, play a fundamental role.

Below we denote by $\nu_j(A)$, $j \in \mathbb{N}$, the eigenvalues (ordered increasingly with account of multiplicity) of a self-adjoint operator A with a purely discrete spectrum. We will write

$$\mathrm{Spec}(A) \le \mathrm{Spec}(B)$$

if $\nu_j(A) \le \nu_j(B)$ for all j.

From now on, we will denote by $-\Delta_{\mathrm{D}}(\Omega)$ (resp. $-\Delta_{\mathrm{N}}(\Omega)$) the Dirichlet (resp. Neumann) Laplacian on a bounded open set $\Omega \subset \mathbb{R}^d$; if the set is clear from the context we will just write $-\Delta_{\mathrm{D}}$ or $-\Delta_{\mathrm{N}}$. As a shorthand, and slightly abusing notation, we will denote the Dirichlet eigenvalues by $\lambda_j = \lambda_j(\Omega) := \nu_j(-\Delta_{\mathrm{D}}(\Omega))$ and the Neumann eigenvalues by $\mu_j = \mu_j(\Omega) := \nu_j(-\Delta_{\mathrm{N}}(\Omega))$.

3.1.1 Domain monotonicity for the Dirichlet Laplacian

Theorem 3.1.1. *Let $\Omega' \subseteq \Omega$ be two bounded open sets of $\mathbb{R}^d$. Then for any $j \ge 1$,*

$$\lambda_j(\Omega) \le \lambda_j(\Omega'). \tag{3.1}$$

Idea of the proof. We start with the min-max characterisation of eigenvalues for both problems, as in Chapter 2. Note that there is a natural embedding $H_0^1(\Omega') \subseteq H_0^1(\Omega)$: indeed, if $v \in H_0^1(\Omega')$ then the function

$$u(x) := \begin{cases} v(x)\,, & \text{for } x \in \Omega'; \\ 0\,, & \text{for } x \in \Omega \setminus \Omega' \end{cases}$$

belongs to $H_0^1(\Omega)$. The infima in the formulae for $\lambda_j(\Omega')$ are taken over a wider set than those in the formulae for $\lambda_j(\Omega)$, and the former are therefore not bigger than the latter. □

Problem 3.1.2. Let $\Omega \subset \mathbb{R}^2$. By using the domain monotonicity for the Dirichlet Laplacian, write down a two-sided estimate on the first eigenvalue $\lambda_1(\Omega)$ for a bounded open set Ω in terms of zeros of Bessel functions, the radius R_- of the biggest disk contained in Ω and the radius R_+ of the smallest disk containing Ω.

It is extremely important to note that there is no general analog of the domain monotonicity principal for the Neumann eigenvalues (even if a look on the Neumann eigenvalues of rectangles suggests otherwise!) This is one of the reasons why Dirichlet problems are often easier to treat than the Neumann ones.

Problem 3.1.3. Give an example of two open sets $\Omega' \subset \Omega \subset \mathbb{R}^2$ such that $\mu_2(\Omega') < \mu_2(\Omega)$.

3.1.2 Dirichlet-Neumann bracketing

This term is used to describe monotonicity of eigenvalues of a quadratic form with respect to the underlying functional space. We will not try to state the most general form of this principle here; rather, we illustrate the idea by two examples which are widely used in applications.

Theorem 3.1.4. *Let $\Omega \subset \mathbb{R}^d$ be an open set with sufficiently smooth boundary $\partial\Omega$. Then*

$$\mu_j(\Omega) \le \lambda_j(\Omega) \text{ for all } j.$$

Theorem 3.1.4 follows from the embedding $H_0^1(\Omega) \subset H^1(\Omega)$.

The inequality of Theorem 3.1.4 can be in fact sharpened, see next chapter. It can be also generalised to the case of boundary value problems with mixed Dirichlet and Neumann boundary conditions in the following sense. For any reasonable partition of the boundary $\partial\Omega = \Gamma_1 \cup \Gamma_2$ (one of the Γ_k may be empty), let $\lambda_j(\Omega; \Gamma_1, \Gamma_2)$ denote the eigenvalues of the Laplacian subject to Dirichlet condition on Γ_1 and Neumann condition on Γ_2; this operator will be denoted $-\Delta_{\mathrm{DN}}(\Omega; \Gamma_1, \Gamma_2)$. For any reasonable boundary partition $\partial\Omega = \partial_1\Omega \cup \partial_2\Omega \cup \partial_3\Omega$ we have

$$\lambda_j(\Omega; \partial_1\Omega, \partial_2\Omega \cup \partial_3\Omega) \le \lambda_j(\Omega; \partial_1\Omega \cup \partial_2\Omega, \partial_3\Omega)$$

for all j; in other words 'extra' Dirichlet boundary conditions imposed on the boundary increase the eigenvalues.

Another useful version of Dirichlet-Neumann bracketing involves imposing additional boundary conditions on some surface of dimension $d-1$ inside Ω. Namely, assume that $\Omega \subset \mathbb{R}^d$ is split by a surface Γ into two domains,

Ω_1 and Ω_2, with boundaries $\partial_1\Omega\cup\Gamma$ and $\partial_2\Omega\cup\Gamma$, the boundary of Ω being $\partial\Omega = \partial_1\Omega \cup \partial_2\Omega$. Note that $\Omega_1 \cup \Omega_2 \neq \Omega$.

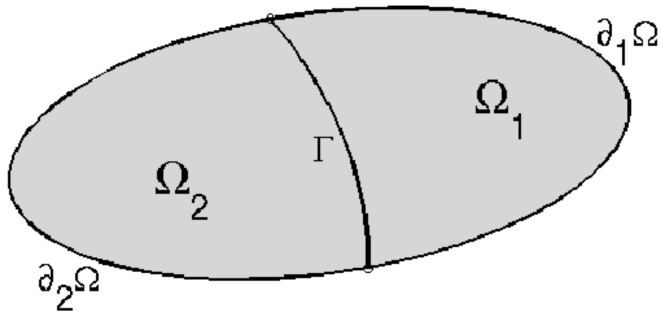

Figure 3.1: $\partial\Omega = \partial_1\Omega \cup \partial_2\Omega$.

We have

Theorem 3.1.5.

$$\begin{aligned}\operatorname{Spec}(-\Delta_{\mathrm{DN}}(\Omega_1 \cup \Omega_2; \partial_1\Omega \cup \partial_2\Omega, \Gamma)) &\le \operatorname{Spec}(-\Delta_{\mathrm{D}}(\Omega)) \\ &\le \operatorname{Spec}(-\Delta_{\mathrm{D}}(\Omega_1 \cup \Omega_2))\,.\end{aligned}$$

Thus, adding the Dirichlet (resp. Neumann) boundary condition inside the domain increases (resp. decreases) the eigenvalues. Note that the set of eigenvalues of the union of two disjoint domains is of course the union of the two sets of eigenvalues.

Problem 3.1.6. By using Dirichlet-Neumann bracketing, find two-sided estimates for the first few eigenvalues of the Dirichlet Laplacian on an L-shaped domain such as the one shown in Figure 3.2. Compute the eigenvalues using FEM and Matlab's PDE Toolbox, and compare with the estimates.

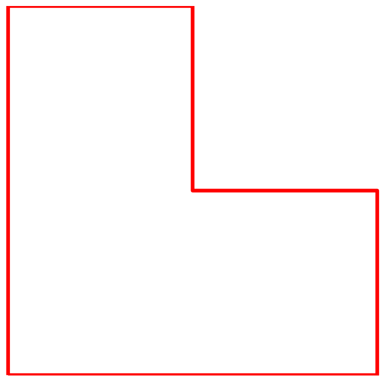

Figure 3.2: An L-shaped domain.

Finally, we make another useful remark. For $\Omega \subset \mathbb{R}^d$, consider the boundary value problem

$$-\Delta u = \lambda u \quad \text{in } \Omega\,, \qquad \left.\frac{\partial u}{\partial n} - gu\right|_{\partial\Omega} = 0\,,$$

where $g : \partial\Omega \to \mathbb{R}$ is a sufficiently smooth function. As easily seen by integration by parts, the corresponding quadratic form is

$$a_g[u] := \int_\Omega |\nabla u|^2 \,\mathrm{d}x - \int_{\partial\Omega} g|u|^2 \,\mathrm{d}\sigma$$

with the domain $H^1(\Omega)$; the corresponding operator is denoted A_g. It immediately follows from the monotonicity of form domains that $\lambda_j(A_g) \geq \lambda_j(A_h)$ for all j, whenever $g(\sigma) \leq h(\sigma)$ for all $\sigma \in \partial\Omega$.

3.2 Counting function

Definition 3.2.1. For a self-adjoint semi-bounded operator L with discrete spectrum, we denote by

$$N(\lambda; L) = \#\{\nu_j \in \operatorname{Spec}(L) : \nu_j < \lambda\} \tag{3.2}$$

the *eigenvalue counting function* of L.

Finding the asymptotes of $N(\lambda; L)$ as $\lambda \to \infty$ for differential operators L corresponding, in particular, to boundary value problems in bounded domains, has been one of the fundamental problems of analysis for more than a hundred years.

3.2.1 Weyl's one-term asymptotics

We start with the following simple calculation. Let $Q_a \subset \mathbb{R}^2$ be a square of side a, and let $-\Delta_{\mathrm{D}}(Q_a)$ be the Dirichlet Laplacian on Q_a. As we have seen before, by separation of variables the spectrum of this operator is the set

$$\left\{ \frac{\pi^2}{a^2}(k^2+m^2) : (k,m) \in \mathbb{Z}_+^2 \right\} .$$

Thus, $\lambda_{k,m} < \lambda$ implies $k^2+m^2 < a^2\pi^{-2}\lambda$ and the counting function $N(\lambda; -\Delta_{\mathrm{D}}(Q_a))$ coincides with the number of integer lattice points inside the first quadrant in the circle of radius $a\sqrt{\lambda}/\pi$.

A famous result of Gauss states that the number of integer points in the circle of radius R behaves asymptotically as

$$\#\{(k,m) \in \mathbb{Z}^2 : |(k,m)| < R\} = \pi R^2 + o(R^2) \qquad \text{as } R \to +\infty\,, \quad (3.3)$$

thus giving

$$N(\lambda; -\Delta_{\mathrm{D}}(Q_a)) = \frac{a^2}{4\pi}\lambda + o(\lambda)\,, \qquad (3.4)$$

which may be also re-written as

$$N(\lambda; -\Delta_{\mathrm{D}}(Q_a)) = \frac{1}{4\pi}|Q_a|_2\lambda + o(\lambda)\,.$$

Here and later $|\Omega|_d$ denotes the d-dimensional volume of a set Ω.

Remark 3.2.2. Finding the sharp remainder estimate for $o(R^2)$ in (3.3) is a very difficult and still open question in number theory, which may have been finally answered in 2007, see [CS].

There are similar formulae for the number of integer points in a ball of a higher dimension.

Using Gauss' formulae, in 1911–13 H. Weyl generalised this result for arbitrary domains. The history of this result is fascinating and involves a lot of famous mathematicians, see [SaVa].

Theorem 3.2.3 (Weyl's one-term asymptotic formula)**.** *Let $\Omega \subset \mathbb{R}^d$ be a bounded domain with sufficiently regular boundary. Then, with $-\Delta(\Omega)$ denoting either the Dirichlet or Neumann Laplacian on Ω,*

$$N(\lambda; -\Delta(\Omega)) = (2\pi)^{-d}\omega_d|\Omega|_d\lambda^{d/2} + o(\lambda^{d/2})\,, \tag{3.5}$$

where $\omega_d := \pi^{d/2}/\Gamma\left(1+\frac{d}{2}\right)$ is the volume of a unit ball in $\mathbb{R}^d$.

The expression $W(\lambda;\Omega) := (2\pi)^{-d}\omega_d|\Omega|_d\lambda^{d/2}$ is often referred to as the *Weyl's term*.

There are analogues of Theorem 3.2.3 for more general classes of operators. For example, if A is an uniformly elliptic operator of order m with the principal symbol $\sigma_0(x,\xi)$ acting in a domain $\Omega \subset \mathbb{R}^d$, then

$$N(\lambda; A) \sim a_0\lambda^{d/m}\,,$$

with

$$a_0 = (2\pi)^{-d}\int_\Omega |\{\xi \in \mathbb{R}^d : \sigma_0(x,\xi) < 1\}|_d\,\mathrm{d}x\,.$$

Problem 3.2.4. By using Matlab, Maple or Mathematica, and explicit formulae, plot the actual eigenvalue counting function for the Dirichlet and Neumann Laplacians on a square together with the one-term Weyl's asymptotics. Roughly estimate the error of the asymptotic formula.

3.2.2 Method of proof — counting the squares

The method of proof of Theorem 3.2.3 is quite instructive as it relies heavily on the material of Section 3.1. We briefly outline it here in a planar case $d = 2$ for the Dirichlet boundary condition without going into details.

Let $\Omega \subset \mathbb{R}^2$ be a bounded domain. Choose a sufficiently small number $a > 0$ and consider a covering of Ω by squares $Q_{a,i}$, $i \in \mathbb{N}$, of side a. There are some squares wholly inside Ω — denote the set of their indices by I, and some which intersect the boundary $\partial\Omega$ — denote the set of their indices by B. By Dirichlet domain monotonicity and Dirichlet-Neumann bracketing,

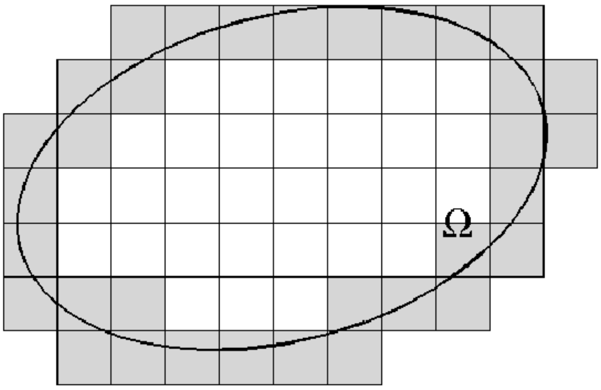

Figure 3.3: Covering of a region $\Omega \subset \mathbb{R}^2$.

we have:

$$\begin{aligned} N(\lambda; -\Delta_{\mathrm{D}}(\Omega)) &\geq N(\lambda; -\Delta_{\mathrm{D}}(\bigcup_{i\in I} Q_{a,i})) \\ &\geq \sum_{i\in I} N(\lambda; -\Delta_{\mathrm{D}}(Q_{a,i})) \\ &= \sum_{i\in I} \frac{1}{4\pi}|Q_{a,i}|_2\lambda + o(\lambda) \\ &\geq \frac{1}{4\pi}(|\Omega|_2 - \varepsilon)\lambda + o(\lambda)\,, \end{aligned} \tag{3.6}$$

where ε is small for sufficiently small a.

Similarly,

$$\begin{aligned} N(\lambda; -\Delta_{\mathrm{D}}(\Omega)) &\le N(\lambda; -\Delta_{\mathrm{D}}(\bigcup_{i\in I\cup B} Q_{a,i})) \\ &\le \sum_{i\in I\cup B} N(\lambda; -\Delta_{\mathrm{N}}(Q_{a,i})) \\ &= \sum_{i\in I\cup B} \frac{1}{4\pi}|Q_{a,i}|_2\lambda + o(\lambda) \\ &\le \frac{1}{4\pi}(|\Omega|_2 + \varepsilon)\lambda + o(\lambda)\,. \end{aligned} \tag{3.7}$$

Taking $a \to 0$ in (3.6) and (3.7), proves (3.5) in the planar case.

3.2.3 Two-term asymptotics

If you managed to do Problem 3.2.4 you have seen what mathematicians observed a long time ago — one-term Weyl's asymptotic formula is not very sharp as it does not take into account the boundary of the domain or the type of the boundary conditions. Weyl himself conjectured that a sharper asymptotics should be valid, with the next asymptotic term proportional to $|\partial\Omega|_{d-1}\lambda^{(d-1)/2}$ for elliptic second order operators on a domain $\Omega \subset \mathbb{R}^d$. It took however the better part of the century, and the introduction of some new and extremely powerful methods, to prove this conjecture and establish the correct constants. V. Ivrii and R. Melrose independently proved the following remarkable result:

Theorem 3.2.5. *Let $\Omega \subset \mathbb{R}^d$ be a bounded domain with a piecewise smooth boundary. Then, subject to the additional geometric condition on Ω ("not too many periodic billiard trajectories"),*

$$N(\lambda; -\Delta(\Omega)) = W(\lambda;\Omega) \mp \frac{1}{4}(2\pi)^{(d-1)}\omega_{d-1}|\partial\Omega|_{d-1}\lambda^{(d-1)/2} + o(\lambda^{(d-1)/2}), \tag{3.8}$$

where a '$-$' sign is taken for the Dirichlet Laplacian and the '$+$' sign for the Neumann Laplacian.

Problem 3.2.6. Modify your programme for Problem 3.2.4 to include the plots of the two-term spectral asymptotics (3.8).

It should be noted that, although it is believed that the condition on the number of periodic billiard trajectories holds for any Euclidean domain, this has not yet been proved in all generality.

Theorem 3.2.5 has been extended for a variety of other cases: higher order operators, systems, general boundary conditions, etc, see [SaVa]. There are situations, however, when the second asymptotic term behaves quite differently; we shall consider one of these cases in the next section.

3.2.4 Fractal boundary

Suppose now that the condition on the smoothness of the boundary is dropped. What happens to the asymptotics of the eigenvalue counting function, especially when the boundary is very 'rough', e.g. fractal?

Before proceeding, we need to describe some definitions and results from fractal geometry.

Definition 3.2.7. Let Ω be an arbitrary non-empty open set in $\mathbb{R}^d$ with boundary $\partial\Omega$. For a given number $\varepsilon > 0$, the set $\Omega^\varepsilon_{\mathrm{int}} := \{x \in \Omega : \mathrm{dist}(x, \partial\Omega) < \varepsilon\}$ is called the *interior Minkowski sausage* of $\partial\Omega$ of radius ε. In what follows we denote

$$\mu(\varepsilon; \Omega) := |\Omega^\varepsilon_{\mathrm{int}}|_d$$

the d-dimensional volume of the interior Minkowski sausage of $\partial\Omega$.

Definition 3.2.8. Let Ω be an arbitrary non-empty bounded open set in $\mathbb{R}^d$ with boundary $\partial\Omega$. For a given $s > 0$, denote

$$\mathcal{M}^*(s; \partial\Omega) := \limsup_{\varepsilon\to+0} \varepsilon^{-(d-s)}\mu(\varepsilon; \Omega)$$

and

$$\mathcal{M}_*(s; \partial\Omega) := \liminf_{\varepsilon\to+0} \varepsilon^{-(d-s)}\mu(\varepsilon; \Omega)\,.$$

The *interior Minkowski dimension* of $\partial\Omega$ (or, in other words, the *Minkowski dimension of $\partial\Omega$ relative to* Ω) is the number

$$\mathfrak{d} := \inf\{h \geq 0 : \mathcal{M}^*(h; \partial\Omega) = 0\} = \sup\{h \geq 0 : \mathcal{M}_*(h; \partial\Omega) = +\infty\}\ .$$

Remark 3.2.9. One can define the *exterior Minkowski dimension* and *Minkowski dimension* of $\partial\Omega$ exactly in the same manner, the only difference being that in the first case one should replace the interior Minkowski sausage by the *exterior Minkowski sausage* $\Omega^{\varepsilon}_{\text{ext}} := \{x \notin \Omega : \operatorname{dist}(x, \partial\Omega) < \varepsilon\}$ and in the second case by the *Minkowski sausage* $\Omega_{\varepsilon} := \Omega^{\varepsilon}_{\text{int}} \cup \Omega^{\varepsilon}_{\text{ext}}$. We will use only the *interior* Minkowski dimension.

Problem 3.2.10. Write down the explicit formulae for the volumes of the exterior and interior Minkowski sausages of a boundary ∂Q of the cube $Q \subset \mathbb{R}^d$ of side 1. Hence prove that the interior and exterior Minkowski dimension of ∂Q coincides with its Euclidean dimension $d-1$.

Definition 3.2.11. Let $r > 0$. A mapping $\mathcal{R}$ in $\mathbb{R}^d$ is called a *similitude with coefficient* r, if it changes the Euclidean distances by a factor of r, i.e.,

$$\operatorname{dist}(\mathcal{R}x, \mathcal{R}y) = r\operatorname{dist}(x, y) \qquad \text{for any} \quad x, y \in \mathbb{R}^d .$$

Any similitude $\mathcal{R}$ with coefficient r in $\mathbb{R}^d$ can be represented as a composition of a homothety with coefficient r, a translation and an orthonormal transformation.

Obviously, for any bounded open set $\Omega \subset \mathbb{R}^d$ and any similitude $\mathcal{R}$ with coefficient r

$$|\mathcal{R}\Omega|_d = r^d |\Omega|_d .$$

A set $A \subset \mathbb{R}^d$ is called *self-similar* if

$$A = \bigcup_{j=1}^{M} \mathcal{R}_j A ,$$

where the $\mathcal{R}_j$ are similitudes with coefficients $r_j \in (0,1)$ and all the sets $\mathcal{R}_j A$ are disjoint (or, more generally, satisfy the so-called open set condition). The Minkowski dimension of any self-similar set is equal to the unique positive real root $\mathfrak{d}$ of the equation

$$\sum_{j=1}^{M} (r_j)^{\mathfrak{d}} = 1$$

and coincides with its Hausdorff dimension.

Example 3.2.12. Let Γ be a von Koch snowflake curve; its construction is shown on the left of Figure 3.4.

Then Γ is the union of four copies of itself each scaled with coefficient $1/3$, and therefore its Minkowski dimension $\mathfrak{d}$ solves $4 \cdot 3^{-\mathfrak{d}} = 1$ giving

$$\mathfrak{d} = \frac{\ln 4}{\ln 3} \qquad \text{so} \qquad \mathfrak{d} \in (1,2)\,.$$

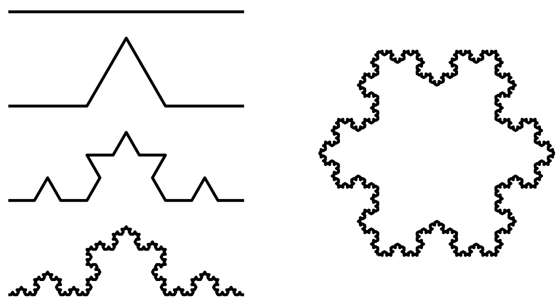

Figure 3.4: Construction of the von Koch snowflake curve (left) and the von Koch snowflake domain (right).

The general result on the asymptotics of the eigenvalue counting function for domains with fractal boundary can only give the order of the correction term:

Theorem 3.2.13 ([Lap])**.** *Let $\Omega \subset \mathbb{R}^d$ have a fractal boundary $\partial\Omega$ with Minkowski dimension $\mathfrak{d} \in (d-1,d)$. Then*

$$N(\lambda; -\Delta_{\mathrm{D}}(\Omega)) - W(\lambda;\Omega) = O\left(\lambda^{\mathfrak{d}/2}\right) \qquad \textit{as } \lambda \to \infty\,.$$

Example 3.2.14. Let $\mathfrak{S}$ be a triadic von Koch snowflake whose boundary is obtained by joining together three copies of the snowflake curve shown above, see the right-hand side of Figure 3.4.

Then

$$N(\lambda; -\Delta_{\mathrm{D}}(\mathfrak{S})) - W(\lambda; \mathfrak{S}) = O\left(\lambda^{\ln 2/\ln 3}\right) \qquad \text{as } \lambda \to \infty\,.$$

In general, finding the explicit form of the second term is difficult. This is however possible if we consider some specially chosen unions of disjoint sets. The following construction is a partial case of [LeVa].

We construct an open set $\mathfrak{G}$ with fractal boundary as follows.

Fix some bounded open set $G_0 \subset \mathbb{R}^d$ with smooth boundary ∂G_0 and fix a set of similitudes $\{\mathcal{R}_1, \ldots, \mathcal{R}_M\}$ all with the same coefficient $r \in (0,1)$. We begin by constructing M sets of the first generation $G_1^1, \ldots, G_1^M$ as the images $\mathcal{R}_k G_0$, $k = 1, \ldots, M$. Repeat the procedure for all the sets of the first generation, obtaining M^2 sets of the second generation, and continue this process in order to build subsequent generations. We include in $\mathfrak{G}$ all the sets of all the generations (starting from G_0 and up to infinity):

$$\mathfrak{G} := \left(\bigcup_{n=1}^{+\infty} \bigcup_{\{i_1, \ldots, i_n\}} \mathcal{R}_{i_1 \ldots i_n} G_0 \right) \cup G_0\,.$$

Here n is the number of the generation, each of the indices i_k takes the values from 1 to M, and $\mathcal{R}_{i_1 \ldots i_n} := \mathcal{R}_{i_1} \circ \cdots \circ \mathcal{R}_{i_n}$. Note that the indices $i_1, \ldots, i_n$ are not necessarily different. We assume that all the sets $\mathcal{R}_{i_1 \ldots i_n} G_0$ are disjoint from each other and from G_0.

Remark 3.2.15. The relative position of the "components" of $\mathfrak{G}$ is irrelevant as long as they are disjoint. We may use different similitudes $\mathcal{R}_k$ (with the same index k) on different steps, requiring only that all of them belong to the class of similitudes with the same coefficient r_k. Despite the fact that these $\mathcal{R}_k$ may differ by a translation or orthonormal transformation, for the sake of simplicity we shall denote them by the same symbol $\mathcal{R}_k$.

We shall always impose the condition

$$Mr^d < 1 < Mr^{d-1}$$

on the coefficient of the similitudes. The left inequality guarantees that we can place all the sets $\mathcal{R}_{i_1 \ldots i_n} G_0$ in $\mathbb{R}^d$ in such a way that they are disjoint from each other and from G_0, and that $\mathfrak{G}$ is bounded. The right inequality guarantees that the Minkowski dimension $\mathfrak{d} = -\ln M/\ln r$ lies between $d-1$ and d.

We denote $\rho = -\ln r$.

Theorem 3.2.16. *The counting function of the Dirichlet Laplacian on $\mathfrak{G}$ has the asymptotic expansion*

$$N(\lambda; -\Delta_{\mathrm{D}}(\mathfrak{G})) = W(\lambda; \mathfrak{G}) - q(\ln\lambda)\,\lambda^{\mathfrak{d}/2} + o\left(\lambda^{\mathfrak{d}/2}\right), \qquad \textit{as } \lambda \to +\infty$$

where

$$q(z) := -\sum_{k=-\infty}^{+\infty} \left(N\left(e^{z-2k\rho}; -\Delta_{\mathrm{D}}(G_0)\right) - W\left(e^{z-2k\rho}; G_0\right)\right) e^{-\mathfrak{d}(z-2k\rho)/2}$$

is a bounded left-continuous 2ρ-periodic function. The set of points of discontinuity of the function q is dense in $\mathbb{R}$.

3.3 An inequality between Dirichlet and Neumann eigenvalues

3.3.1 Statement and proof

We have already seen that for any $\Omega \subset \mathbb{R}^d$, and any $k \in \mathbb{N}$, $\mu_k(\Omega) \le \lambda_k(\Omega)$. In 1992, L. Friedlander [Fri] proved a much stronger result:

Theorem 3.3.1 (Friedlander; conjectured by Pólya and Weinberger)**.** *For any $\Omega \subset \mathbb{R}^d$, and any $k \in \mathbb{N}$,*

$$\mu_{k+1}(\Omega) \le \lambda_k(\Omega)\,.$$

Friedlander's proof assumes additionally the smoothness of $\partial\Omega$; we discuss it briefly below, but present here and alternative proof due to N. Filonov [Fil].

Proof. Let $\Phi := \mathrm{Span}\{\phi_1, \dots \phi_{k+1}\} \subset H^1(\Omega)$ be a subspace formed in $H^1(\Omega)$ by any $(k+1)$ linearly independent functions ϕ_j. Then, as $H^1(\Omega)$ is the form domain for the Neumann Laplacian, by Rayleigh-Ritz principle

$$\mu_{k+1}(\Omega) \le \sup_{\phi\in\Phi} \frac{\int_\Omega |\nabla\phi|^2}{\int_\Omega |\phi|^2}\,. \tag{3.9}$$

Let us choose

$$\phi_j = u_j\,, \quad j = 1, \dots, k\,, \qquad \phi_{k+1} = \mathrm{e}^{ix\cdot\xi}\,,$$

where u_j are the orthonormalised eigenfunctions of the Dirichlet Laplacian corresponding to the eigenvalues λ_j and $\xi \in \mathbb{R}^d$ is such that $|\xi|^2 = \lambda_k$. Choose some constants $c_1, \dots, c_{k+1} \in \mathbb{C}$ and set $\phi := \sum_{j=1}^{k+1} c_j \phi_j$. By (3.9) we have $\mu_{k+1} \le \frac{\int_\Omega |\nabla\phi|^2}{\int_\Omega |\phi|^2}$.

By the orthonormality of the eigenfunctions of the Dirichlet Laplacian, mutual orthogonality of their gradients, and the fact that $\int_\Omega |\mathrm{e}^{ix\cdot\xi}|^2 = |\Omega|_d$ and $\int_\Omega |\nabla \mathrm{e}^{ix\cdot\xi}|^2 = |\xi|^2 |\Omega|_d$, we have

$$I_1 := \int_\Omega |\phi|^2 = |\Omega|_d + \sum_{j=1}^k |c_j|^2 + 2\sum_{j=1}^k \mathrm{Re}\left(c_j \int_\Omega e^{ix\cdot\xi}\overline{u_j}\right)$$

and

$$I_2 := \int_\Omega |\nabla\phi|^2 = |\xi|^2|\Omega|_d + \sum_{j=1}^k \lambda_j |c_j|^2 + 2\sum_{j=1}^k \mathrm{Re}\left(c_j \int_\Omega \nabla e^{ix\cdot\xi}\cdot\overline{\nabla u_j}\right).$$

Integrating by parts in the last integral in I_2 gives

$$\mathrm{Re}\left(c_j \int_\Omega \nabla e^{ix\cdot\xi}\cdot\overline{\nabla u_k}\right) = |\xi|^2 \,\mathrm{Re}\left(c_j \int_\Omega e^{ix\cdot\xi}\overline{u_k}\right).$$

As $|\xi|^2 = \lambda_k$ and $\lambda_j \le \lambda_k$, we immediately conclude that $I_2 \le \lambda_k I_1$, and so $\mu_{k+1} \le I_2/I_1 \le \lambda_k$. □

3.3.2 Dirichlet-to-Neumann map

As we said, an original proof of Theorem 3.3.1 is due to Friedlander and uses a different approach. Namely, it assumes that $d > 1$, that $\partial\Omega$ is smooth and that $\lambda \notin \mathrm{Spec}(-\Delta_{\mathrm{D}}(\Omega))$, and considers a non-homogenious boundary value problem

$$-\Delta u = \lambda u \quad \text{in } \Omega\,, \qquad u|_{\partial\Omega} = f,$$

for a given function $f \in H^{1/2}(\partial\Omega)$. This problem has a unique solution $u \in H^1(\Omega)$ and we can define the map

$$\mathcal{R}_\lambda : f \mapsto \left.\frac{\partial u}{\partial n}\right|_{\partial\Omega}, \tag{3.10}$$

which depends on λ as a parameter. This map is usually called the *Dirichlet-to-Neumann map* and can be identified with an operator acting in $L^2(\partial\Omega)$

It can be shown (see e.g. [Fri]) that the Dirichlet-to-Neumann map possesses a lot of remarkable properties:

(a) $\mathcal{R}_\lambda$ is a pseudodifferential operator of order one acting on the boundary, with the principal symbol $|\xi|$.

(b) For real λ, $\mathcal{R}_\lambda$ is a self-adjoint operator in $L^2(\partial\Omega)$.

(c) $\mathcal{R}_\lambda$ has a discrete spectrum with a finite number of negative eigenvalues.

(d) Eigenvalues of $\mathcal{R}_\lambda$ are monotone decreasing functions of λ in each interval not containing points of $\mathrm{Spec}(-\Delta_{\mathrm{D}}(\Omega))$.

(e) $0 \in \mathrm{Spec}(\mathcal{R}_\lambda)$ if and only if $\lambda \in \mathrm{Spec}(-\Delta_{\mathrm{N}}(\Omega))$.

(f) Most crucially, the following relation holds between the counting functions of the Dirichlet-to-Neumann map and Dirichlet and Neumann Laplacians: $N(0, \mathcal{R}_\lambda) = N(\lambda; -\Delta_{\mathrm{N}}(\Omega)) - N(\lambda; -\Delta_{\mathrm{D}}(\Omega))$.

Friedlander actually showed that one always has $N(0, \mathcal{R}_\lambda) \geq 1$, thus, in view of (f), proving Theorem 3.3.1.

Problem 3.3.2. Construct explicitly the Dirichlet-to-Neumann map for the interval $[0, \pi]$. (Hint: some properties in the one-dimensional case are different from those listed above.) Find a transcendental equation for the eigenvalues of $\mathcal{R}_\lambda$, solve it numerically, and plot the results.

Problem 3.3.3. Repeat the previous problem for the Dirichlet-to-Neumann map for the unit disk in $\mathbb{R}^2$; plot only the lowest eigenvalue of $\mathcal{R}_\lambda$.

Chapter 4

Isoperimetric and universal estimates of eigenvalues

The aim of this chapter is to describe some more complicated estimates for the eigenvalues of the Laplacian, including:

- Isoperimetric estimates — that is, estimates for low eigenvalues which are optimal when the geometry changes.
- Universal estimates — valid for all eigenvalues irrespectively of the geometry.

4.1 Isoperimetric estimates of eigenvalues

The term "isoperimetric inequality" originated in geometry. A classical Isoperimetric inequality, for example, is the fact that of all the domains with a given perimeter, the disk has the largest area; or, equivalently, that of all the domains with given area the disk has the smallest perimeter. In spectral theory, "isoperimetric" refers to similar type of questions, e.g. of all domains of a given volume, which one has the lowest first Dirichlet eigenvalue.

The contents of this section mostly follow [Ash].

4.1.1 Symmetrisation. Faber-Krahn inequality

We start with a couple of useful concepts from real analysis.

Definition 4.1.1. For a bounded measurable set $\Omega \subset \mathbb{R}^d$, we define its *spherical rearrangement* Ω^* as the ball centred at the origin with the same volume as Ω.

Definition 4.1.2. For a bounded measurable function $f : \Omega \to \mathbb{R}$ on a bounded measurable set $\Omega \subset \mathbb{R}^d$, we define its *level sets* as

$$\Omega_t[f] := \{x \in \Omega : |f(x)| > t\}.$$

Definition 4.1.3. For a bounded measurable function $f : \Omega \to \mathbb{R}$ on a bounded measurable set $\Omega \subset \mathbb{R}^d$, we define its *spherical rearrangement* as the function $f^* : \Omega^* \to \mathbb{R}$ given by

$$f^*(x) = \inf\{t \geq 0 : |\Omega_t[f]|_d < \omega_d |x|^d\}.$$

In other words, f^* is the spherically symmetric radially non-increasing function on the ball Ω^* whose level sets are the concentric balls of the same measure as the corresponding level sets of f.

Problem 4.1.4. For the function $f(x_1, x_2) := x_1 + x_2$ on a square $Q = \{(x_1, x_2) : 0 \leq x_1, x_2 \leq \sqrt{\pi}\}$, construct explicitly the spherical rearrangement f^* on Q^*.

There are two crucial facts about spherical rearrangement which we will use later (for proofs and further discussion on the subject see e.g. [Kaw]).

Lemma 4.1.5.

(a) For any function $f \in L^2(\Omega)$ we have $f^* \in L^2(\Omega^*)$ and moreover

$$\|f\|_{L^2(\Omega)} = \|f^*\|_{L^2(\Omega^*)}.$$

(b) For any function $f \in H_0^1(\Omega)$ we have $f^* \in H_0^1(\Omega^*)$ and moreover

$$\int_{\Omega^*} |\nabla f^*|^2 \leq \int_{\Omega} |\nabla f|^2.$$

Lemma 4.1.5 plays a central role in the proof of what was historically the first isoperimetric inequality for the eigenvalues of the Dirichlet Laplacian established independently by G. Faber and E. Krahn in the early 1920s.

Theorem 4.1.6 (Faber-Krahn). *For any bounded measurable set in $\Omega \subset \mathbb{R}^d$,*

$$\lambda_1(\Omega) \geq \lambda_1(\Omega^*)\,,$$

with equality if and only if Ω is a ball. Thus the ball has the smallest possible first Dirichlet eigenvalue among all the sets of the same measure.

Proof. Let u_1 be the first eigenfunction of $-\Delta_{\mathrm{D}}(\Omega)$, corresponding to the eigenvalue $\lambda_1(\Omega)$. Then by Lemma 4.1.5(b), $u_1^* \in H_0^1(\Omega^*)$, and is therefore a valid test-function for $\lambda_1(\Omega^*)$. By the variational principle and Lemma 4.1.5, we have

$$\lambda_1(\Omega^*) \leq \frac{\|\nabla u_1^*\|_{L^2(\Omega^*)}}{\|u_1^*\|_{L^2(\Omega^*)}} \leq \frac{\|\nabla u_1\|_{L^2(\Omega)}}{\|u_1\|_{L^2(\Omega)}} = \lambda_1(\Omega)\,.$$

□

Problem 4.1.7. For a measurable $\Omega \subset \mathbb{R}^2$, write down an explicit lower bound on $\lambda_1(\Omega)$ in terms of $|\Omega|_2$ and the zeros of the Bessel functions.

4.1.2 Other isoperimetric inequalities. Ratios of eigenvalues, numerics

There is a number of other isoperimetric inequalities; the proofs of many of them also use rearrangement tricks among other methods but would be too complicated to present here. We list a few of these results below.

Theorem 4.1.8 (Szőgo-Weinberger). *The second (i.e. the first non-zero) Neumann eigenvalue $\mu_2(\Omega)$ satisfies*

$$\mu_2(\Omega) \leq \mu_2(\Omega^*)\,,$$

with equality if and only if Ω is a ball.

Theorem 4.1.9 (Ashbauch-Benguria). *The ratio of the first two Dirichlet eigenvalues for a measurable set $\Omega \subset \mathbb{R}^d$ satisfies*

$$\frac{\lambda_2(\Omega)}{\lambda_1(\Omega)} \leq \frac{\lambda_2(B)}{\lambda_1(B)}\,,$$

where B is a d-dimensional ball, with equality if and only if Ω is a d-dimensional ball.

These two theorems, as well as the one of Faber-Krahn, present optimal inequalities — i.e. these are the estimates where the equality can be attained. The situation becomes more difficult as one progresses "upwards" in the spectrum. For example, a lot of attention has been paid to trying to find an admissible range of values $(\lambda_2(\Omega)/\lambda_1(\Omega), \lambda_3(\Omega)/\lambda_1(\Omega))$ for planar domains Ω. The results of numerous theoretical efforts were combined by Ashbauch and Benguria in the following graphical form:

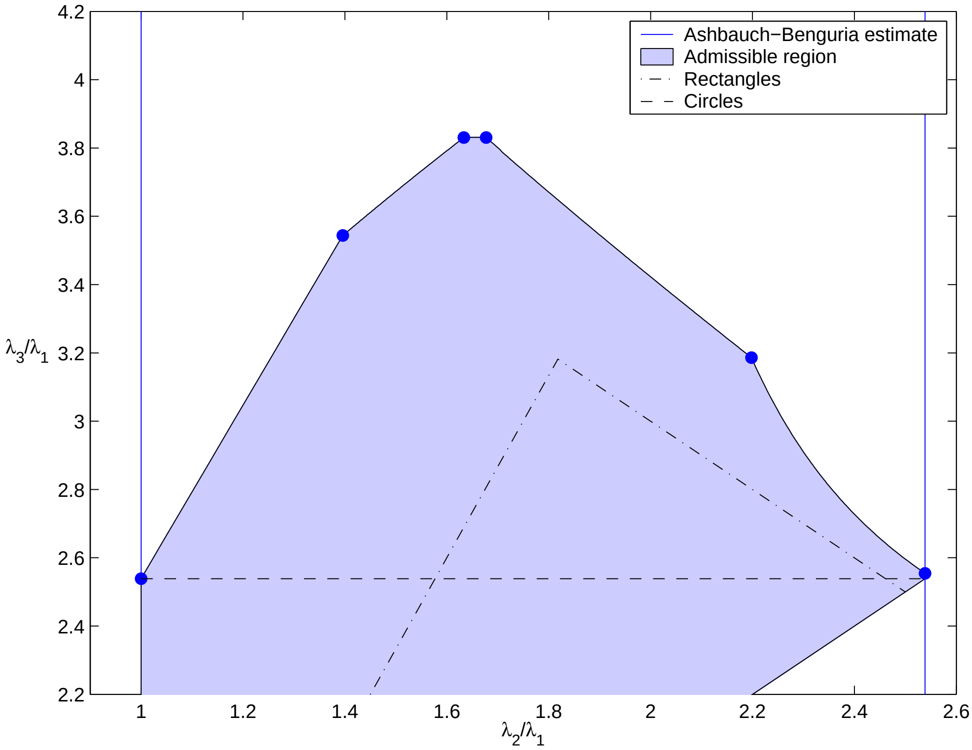

Figure 4.1: Estimates of the admissible range (shaded) of $(\lambda_2(\Omega)/\lambda_1(\Omega), \lambda_3(\Omega)/\lambda_1(\Omega))$ according to Ashbauch and Benguria. Shown for comparison are the maximum values of λ_3/λ_1 as functions of λ_2/λ_1 for rectangles and disjoint unions of circles.

On the other hand, extensive numerical experiments of Levitin and Yagudin (see [LeYa] and references therein) have demonstrated that the actual admissible range is in fact much smaller.

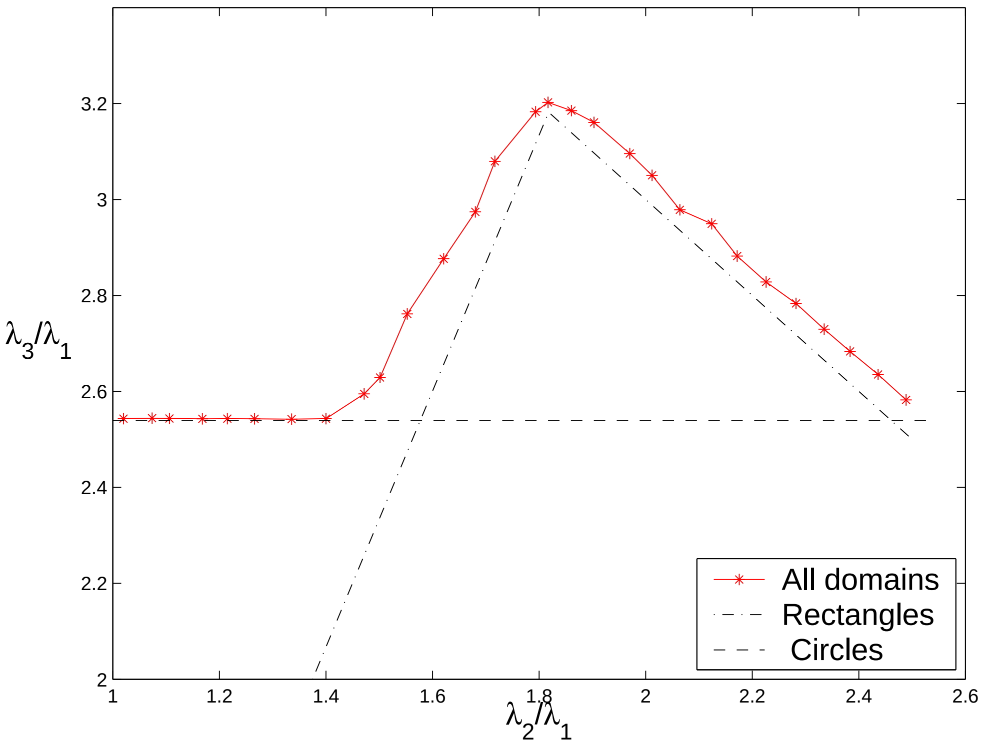

Figure 4.2: Numerically computed admissible range is below the curve for all domains.

4.2 Universal estimates of eigenvalues

4.2.1 Payne-Pólya-Weinberger and Yang's inequalities for the Dirichlet Laplacian

In 1956, Payne, Pólya and Weinberger showed that the Dirichlet eigenvalues of the Laplacian $\lambda_m = \lambda_m(\Omega)$, $\Omega \subset \mathbb{R}^d$, always satisfy

$$\lambda_{m+1} - \lambda_m \leq \frac{4}{md} \sum_{j=1}^{m} \lambda_j \tag{PPW}$$

for each $m \in \mathbb{N}$. This inequality was improved to

$$\sum_{j=1}^{m} \frac{\lambda_j}{\lambda_{m+1} - \lambda_j} \geq \frac{md}{4} \tag{HP}$$

by Hile and Protter. This is indeed stronger than (PPW), which is obtained from (HP) by replacing all λ_j in the denominators in the left-hand side by λ_m.

Later, Hongcang Yang proved an even stronger inequality

$$\sum_{j=1}^{m} (\lambda_{m+1} - \lambda_j) \left(\lambda_{m+1} - \left(1 + \frac{4}{d}\right) \lambda_j \right) \leq 0\,, \tag{HCY-1}$$

which after some modifications implies an explicit estimate

$$\lambda_{m+1} \leq \left(1 + \frac{4}{d}\right) \frac{1}{m} \sum_{j=1}^{m} \lambda_j. \tag{HCY-2}$$

These two inequalities are known as Yang's first and second inequalities, respectively. We note that the sharpest so far known explicit upper bound on λ_{m+1} is also derived from (HCY-1), see [Ash, formula (3.33)].

Payne-Pólya-Weinberger, Hile-Protter and Yang's inequalities are commonly referred to as *universal estimates* for the eigenvalues of the Dirichlet Laplacian. These estimates are valid uniformly over all bounded domains in $\mathbb{R}^d$. The derivation of all four results is similar and uses the variational principle with ingenious choices of test functions, as well as the Cauchy-Schwarz inequality. We refer the reader to the extensive survey [Ash] which provides the detailed proofs as well as the proof of the implication

$$\text{(HCY-1)} \Longrightarrow \text{(HCY-2)} \Longrightarrow \text{(HP)} \Longrightarrow \text{(PPW)}\,.$$

In 1997, Harrell and Stubbe showed that all of these results are consequences of a certain abstract operator identity and that this identity has several other applications.

Similar universal estimates were also obtained in spectral problems for operators other than the Euclidean Dirichlet Laplacian (or Schrödinger operator), e.g. higher order differential operators in $\mathbb{R}^d$, operators on manifolds, the Lamé system of elasticity etc., see the already mentioned survey paper [Ash].

4.2.2 General commutator method

In 2002, Levitin and Parnovski [LePa] generalised the Harrell-Stubbe results and produced an abstract scheme of constructing universal eigenvalue estimates in a very general setting.

The first main result of [LePa] is a general abstract operator identity which holds under minimal restrictions:

Theorem 4.2.1. *Let H and G be self-adjoint operators acting on a Hilbert space with domains such that $G(\operatorname{Dom} H) \subseteq \operatorname{Dom} H$. Assume additionally that H has a purely discrete spectrum, and let λ_j and ϕ_j be eigenvalues and normalised eigenvectors of H. Then for each j*

$$\begin{aligned} \sum_k \frac{|\langle [H,G]\phi_j, \phi_k\rangle|^2}{\lambda_k - \lambda_j} &= -\frac{1}{2}\langle [[H,G],G]\phi_j, \phi_j\rangle \\ &= \sum_k (\lambda_k - \lambda_j)|\langle G\phi_j, \phi_k\rangle|^2. \end{aligned} \tag{4.1}$$

Here the standard commutator notation $[H,G] := HG - GH$ is used.

This theorem has a lot of applications, notably the estimates of the eigenvalue gaps of various operators. In particular, we shall show later that the results of Payne, Pólya and Weinberger for the Dirichlet Laplacian follow from (4.1), if we set G to be an operator of multiplication by the coordinate x_l. In this case (4.1) takes a particularly simple and elegant form:

$$4\sum_k \frac{\left|\int_\Omega \dfrac{\partial \phi_j}{\partial x_l}\,\phi_k\right|^2}{\lambda_k - \lambda_j} = \sum_k (\lambda_k - \lambda_j)\left|\int_\Omega \phi_j\,\phi_k\right|^2 = 1\,. \tag{4.2}$$

Estimate (PPW) follows from (4.2) if we sum these equalities over l and use some simple bounds, see below. There are other applications of Theorem 4.2.1 – in each particular case one should work out what is the optimal choice of G.

Problem 4.2.2. Compute explicitly the commutators $[-\Delta, x_l]$ and $[[-\Delta, x_l], x_l]$ and thus deduce (4.2) from (4.1).

Problem 4.2.3. Explain why $H = -\Delta_{\mathrm{N}}$ and G, $Gu = x_l \cdot u$ do not satisfy the conditions of Theorem 4.2.1.

Remark 4.2.4. In the context of a Schrödinger operator acting in $\mathbb{R}^d$, the second equation in (4.2) is known as the *Thomas–Reiche–Kuhn sum rule* in the physics literature. It was derived by W. Heisenberg in 1925. The name attached to the sum rule comes from the fact that W. Thomas, F. Reiche, and W. Kuhn derived some semiclassical analogues of this formula in their study of the width of the lines of the atomic spectra.

Similarly, taking G to be the operator of multiplication by $e^{i\xi\cdot x}$ (with a real vector ξ), one arrives at the *Bethe sum rule*,

$$\sum_k (\lambda_k - \lambda_j) \left| \int_{\mathbb{R}^d} e^{i\xi\cdot x} \phi_j \, \phi_k \right|^2 = |\xi|^2 .$$

Both the Thomas–Reiche–Kuhn and Bethe sum rules are discussed in standard text books on quantum mechanics.

We shall now demonstrate how to deduce (PPW) from (4.2). First of all, drop all the negative terms, i.e. those with $k < j$, in the sum on the left of (4.2). The sum will increase. Then replace all the denominators by the smallest one, $\lambda_{j-1} - \lambda_j$. The sum will increase further. Now extend the summation again to k from 1 to ∞, giving

$$\frac{4}{\lambda_{j+1} - \lambda_j} \sum_k \left| \int_\Omega \frac{\partial \phi_j}{\partial x_l} \, \phi_k \right|^2 \geq 1 \tag{4.3}$$

By Parseval's equality,

$$\sum_k \left| \int_\Omega \frac{\partial \phi_j}{\partial x_l} \, \phi_k \right|^2 = \sum_k \langle \frac{\partial \phi_j}{\partial x_l}, \phi_k \rangle^2 = \left\| \frac{\partial \phi_j}{\partial x_l} \right\|^2_{L^2(\Omega)} .$$

Substituting this expression into (4.3), summing the resulting inequalities over l from 1 to d and using the fact that

$$\sum_{l=1}^{d} \left\| \frac{\partial \phi_j}{\partial x_l} \right\|_{L^2(\Omega)}^2 = \|\nabla \phi_j\|_{L^2(\Omega)}^2 = \lambda_j$$

we obtain (PPW).

Roughly the same procedure is applicable in the general case, giving for an abstract self-adjoint operator a PPW-type bound.

Theorem 4.2.5. *Under the conditions of Theorem 4.2.1,*

$$-(\lambda_{m+1} - \lambda_m) \sum_{j=1}^{m} ([[H, G], G]\phi_j, \phi_j) \leq 2 \sum_{j=1}^{m} \|[H, G]\phi_j\|^2 . \tag{4.4}$$

A somewhat more complicated analysis of [LePa] also produces abstract versions of (HP) and (HCY-1).

4.2.3 Polya's conjecture

Let us return once more to the one-term Weyl's asymptotic formula (3.5). Solving the approximate equation

$$k \approx (2\pi)^{-d} \omega_d |\Omega|_d \nu_k^{d/2} ,$$

we obtain, for large indices k, the asymptotic formula

$$\nu_k \approx 4\pi \left(\frac{\Gamma(1 + d/2)}{|\Omega|_d} \right)^{2/d} k^{2/d} \tag{4.5}$$

valid both for eigenvalues $\nu_k = \lambda_k(\Omega)$ of the Dirichlet Laplacian and eigenvalues $\nu_k = \mu_k(\Omega)$ of the Neumann Laplacian.

The celebrated conjecture of Pólya states that there are inequalities between the left- and right-hand sides of (4.5) valid for all k, and not only the large ones. We have

Conjecture 4.2.6 (Pólya)**.** *For any $k \in \mathbb{N}$ and a measurable set $\Omega \in \mathbb{R}^d$,*

$$\mu_k(\Omega) \leq 4\pi \left(\frac{\Gamma(1 + d/2)}{|\Omega|_d} \right)^{2/d} k^{2/d} \leq \lambda_k(\Omega).$$

Despite its apparent simplicity, this conjecture has only been proved for domains $\Omega \subset \mathbb{R}^d$ which tile the space (i.e. when one can cover $\mathbb{R}^d$ without gaps by shifted and rotated copies of Ω). Even more surprisingly, it is not even known whether the conjecture holds for a ball! There are various partial results, the best estimates so far are due to Laptev [Lap].

Chapter 5

Isospectrality and symmetry tricks

The aim of this chapter is to give examples of the use of obvious or hidden symmetries in spectral problems associated to the Laplacian, and also to discuss the following questions:

- Can one determine the domain uniquely from its Dirichlet spectrum?
- Can one determine the boundary conditions in a mixed problem from the spectrum?

5.1 Can one hear the shape of a drum?

Throughout this section we shall, for simplicity, deal mostly with Laplacians in a bounded planar domain $\Omega \subset \mathbb{R}^2$, although the majority of the results also apply not only to multidimensional cases, but, with suitable modifications, to Laplacians on manifolds with and without boundary.

5.1.1 Heat trace asymptotics, heat invariants, Kac's question

Recall that in Chapter 3 we have discussed the asymptotics of the spectral counting function $N(\lambda; -\Delta_{\mathrm{D}}(\Omega))$. Often it is more convenient to consider instead the function

$$Z(t) = Z(t;\Omega) := \operatorname{Tr} e^{-\Delta_{\mathrm{D}} t} = \sum_{j=1}^{\infty} e^{-t\lambda_j(\Omega)} = \int e^{-t\lambda}\, \mathrm{d}N(\lambda; -\Delta_{\mathrm{D}}(\Omega))\,. \tag{5.1}$$

The function $Z(t)$ is called the *trace of the heat semigroup* or the *partition function* of the Dirichlet Laplacian.

In some sense, the partition function is a "smoothened version" of the counting function. By (5.1) and Abel's Theorem, one can easily construct the one- or two-term asymptotic expansion of $Z(t)$ as $t \to +0$ just by taking the Laplace transform of the corresponding expansion for $N(\lambda)$. Unfortunately, the converse is not possible.

The partition function $Z(t)$ can be effectively treated by heat equation methods. It turns out that it admits a *full* asymptotic expansion.

Theorem 5.1.1 (Pleijel-Minakshisundaram)**.** *For $\Omega \subset \mathbb{R}^d$, the function $Z(t;\Omega)$ has the asymptotic expansion*

$$Z(t;\Omega) = (2\pi)^{-d} t^{-d/2} \sum_{k=0}^{\infty} a_k t^{k/2}\,, \qquad \text{as } t \to +0\,.$$

The coefficients a_k depend on geometric characteristics of Ω; in particular a_0 is proportional to $|\Omega|_d$ and a_1 is proportional to $|\partial\Omega|_{d-1}$.

Thus, if one knows the spectrum of $-\Delta_{\mathrm{D}}(\Omega)$, one also knows the function $Z(t;\Omega)$ and its asymptotic expansion. From this, one can deduce some geometric characteristics of Ω, e.g. its area and the length of its boundary. A natural question arises: is it possible to recover the domain Ω completely from the spectrum of the Laplacian on Ω? This is the question asked in 1966 by Mark Kac in his famous paper "Can one hear the shape of a drum?", [Kac].

5.1.2 Negative answer to Kac's question — example of two isospectral domains by Gordon, Webb and Wolpert

Mark Kac's question was in fact quite difficult. Only in the early 1990s, Gordon, Webb and Wolpert [GWW] gave a negative question to the answer by producing two domains in $\mathbb{R}^2$ which are *isospectral* (i.e. whose Dirichlet spectra coincide) but not isometric, see Figure 5.1.

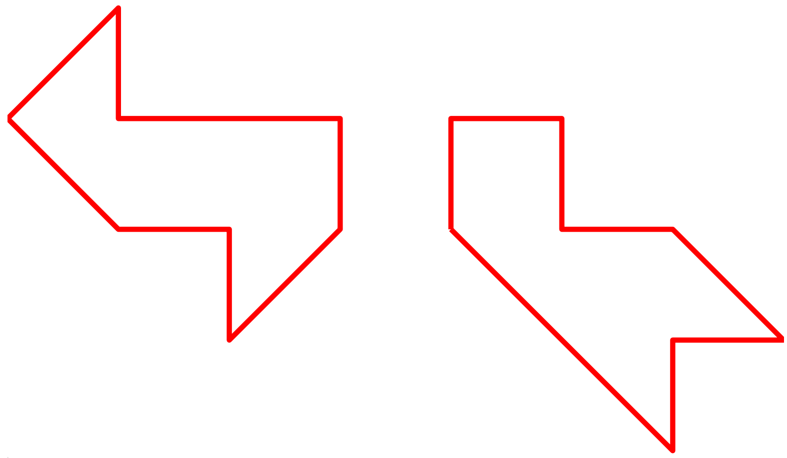

Figure 5.1: Two isospectral domain of Gordon, Webb and Wolpert.

There were further interesting extensions e.g. by Berard, Brooks and Buser. However, to the best of our knowledge there are still no known examples of sets of more than two non-isometric isospectral domains, as well as of non-simply connected domains. Also, Kac's question still remains open for smooth (as well as for convex) domains.

The proof of the Gordon, Webb and Wolpert isospectrality result is a bit involved. We therefore choose to consider a slightly more general problem which, on the other hand, admits an easier explanation.

5.2 Can one hear boundary conditions?

5.2.1 Zaremba problem, mixed Dirichlet-Neumann isospectrality and transplantation tricks

We consider a modification of the isospectrality question for the case of mixed Dirichlet-Neumann boundary conditions (the so called Zaremba problem) which illustrates the approach suggested in [LPP], see also the references there.

Let $\Omega_j \subset \mathbb{R}^2$, $j = 1, 2$, be two bounded domains, their piecewise smooth boundaries being decomposed as $\partial\Omega_j = \overline{\partial_{\mathrm{D}}\Omega_j \cup \partial_{\mathrm{N}}\Omega_j}$, where $\partial_{\mathrm{D}}\Omega_j$, $\partial_{\mathrm{N}}\Omega_j$ are finite unions of open segments of $\partial\Omega_j$ and $\partial_{\mathrm{D}}\Omega_j \cap \partial_{\mathrm{N}}\Omega_j = \varnothing$. Suppose that there are no isometries of $\mathbb{R}^2$ mapping Ω_1 onto Ω_2 in such a way that $\partial_{\rm D}\Omega_1$ maps onto $\partial_{\rm D}\Omega_2$. (We shall call such pairs of domains *nontrivial*.)

Consider on each Ω_j a mixed boundary value problem for the Laplacian, with a Dirichlet condition imposed on $\partial_{\rm D}\Omega_j$, and thee Neumann conditions on $\partial_{\rm N}\Omega_j$. In the notation of Section 3.1.2, the corresponding operators are denoted $-\Delta_{\rm DN}(\Omega_j;\partial_{\rm D}\Omega_j,\partial_{\rm N}\Omega_j)$. For brevity, we write

$$\mathrm{Spec}_{\rm DN}(\Omega_j) := \mathrm{Spec}(-\Delta_{\rm DN}(\Omega_j;\partial_{\rm D}\Omega_j,\partial_{\rm N}\Omega_j))\,,$$

Our aim is to study nontrivial isospectral pairs Ω_1, Ω_2 (i.e. such that $\mathrm{Spec}_{\rm DN}(\Omega_1)=\mathrm{Spec}_{\rm DN}(\Omega_2)$).

We start with the following trivial example, see Figure 5.2.

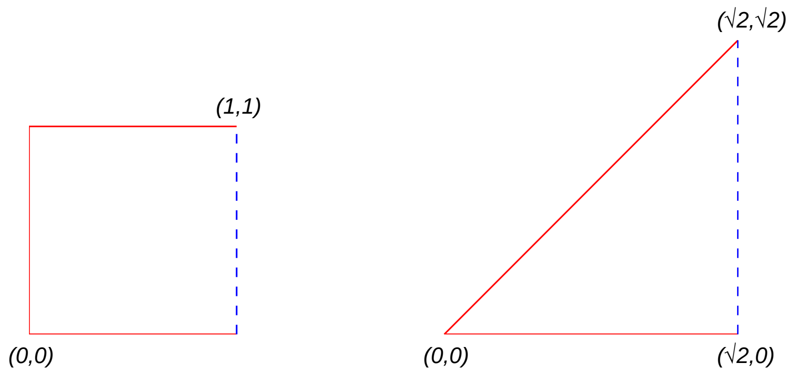

Figure 5.2: The unit square Ω_1 and the isosceles triangle Ω_2. Here and further on, solid lines denote the Dirichlet boundary conditions and dashed lines denote the Neumann ones.

The spectra $\mathrm{Spec}_{\rm DN}(\Omega_j)$ are easily calculated by separation of variables. The eigenfunctions for Ω_1 are

$$\sin((1/2+m)\pi x)\sin(n\pi y)\,,\qquad \text{for } n,m\in\mathbb{N},$$

and the eigenfunctions for Ω_2 are

$$\sin\left(\frac{(1/2+k)\pi x}{\sqrt{2}}\right)\sin\left(\frac{(1/2+l)\pi y}{\sqrt{2}}\right)\\ -\sin\left(\frac{(1/2+l)\pi x}{\sqrt{2}}\right)\sin\left(\frac{(1/2+k)\pi y}{\sqrt{2}}\right)\,,\quad \text{for } k,l\in\mathbb{N},\ k>l.$$

Problem 5.2.1. Using the above expressions, prove the following formulae for eigenvalues $\lambda_{m,n} \in \mathrm{Spec}_{\mathrm{DN}}(\Omega_1)$ and $\mu_{k,l} \in \mathrm{Spec}_{\mathrm{DN}}(\Omega_1)$:

$$\lambda_{m,n} = \frac{\pi^2}{4}\left((2m+1)^2 + 4n^2\right), \qquad \mu_{k,l} = \frac{\pi^2}{4}\,\frac{(2k+1)^2 + (2l+1)^2}{2}.$$

It turns out that

$$\mathrm{Spec}_{\mathrm{DN}}(\Omega_1) = \mathrm{Spec}_{\mathrm{DN}}(\Omega_2). \tag{5.2}$$

Problem 5.2.2. Using your solution of Problem 5.2.1, prove (5.2).

The example above shows that isospectral domains with mixed boundary conditions can be quite simple (compared to classical Dirichlet isospectral pairs). Indeed, dependence of the spectra on boundary decomposition brings more flexibility to the problem.

We note that this example is somewhat reminiscent of Chapman's example of two disconnected Dirichlet isospectral domains: in his case the first disconnected domain is a disjoint union of a square of side one and an isosceles right triangle of side two, and the second one is a disjoint union of a rectangle with sides one and two, and an isosceles right triangle of side $\sqrt{2}$.

We can now describe a rather general way of constructing isospectral pairs, see [LPP]. The above example is in fact the easiest implementation of an algorithm for the construction of isospectral domains which we outline below.

We start by describing a suitable class of *construction blocks* which we shall later use to build pairs of planar isospectral domains. Let a, b be two lines on the plane (which may be parallel), and let K be a bounded open set lying in a sector formed by a and b (or between them if they are parallel). The set K need not be connected, but we assume that ∂K has non-empty intersections with a and b which we denote by $\partial_a K$ and $\partial_b K$, respectively. Denote by $\partial_0 K := \partial K \setminus (\partial_a K \cup \partial_b K)$ the remaining part of the boundary ∂K.

Let T_a, T_b denote the reflections with respect to the lines a and b. We first construct the domains Ω_1 and Ω_2 just by adding to K its image under the reflections T_a, T_b, respectively:

$$\Omega_1 := \mathrm{Int}(\overline{K \cup T_a(K)})\,, \qquad \Omega_2 := \mathrm{Int}(\overline{K \cup T_b(K)})\,.$$

We now need to impose mixed boundary conditions on Ω_1 and Ω_2. To do so, let us first decompose $\partial_0 K$ into the union of two non-intersecting sets $\partial_{0,\mathrm{D}} K$ and $\partial_{0,\mathrm{N}} K$ (one of which may be empty). Then we set

$$\partial_{\mathrm{D}}\Omega_1 := \partial_{0,\mathrm{D}} K \cup T_a(\partial_{0,\mathrm{D}} K) \cup T_a(\partial_b K)\,;$$

$$\partial_{\mathrm{N}}\Omega_1 := \partial_{0,\mathrm{N}} K \cup T_a(\partial_{0,\mathrm{N}} K) \cup \partial_b K\,;$$

$$\partial_{\mathrm{D}}\Omega_2 := \partial_{0,\mathrm{D}} K \cup T_b(\partial_{0,\mathrm{D}} K) \cup \partial_a K\,;$$

$$\partial_{\mathrm{N}}\Omega_2 := \partial_{0,\mathrm{N}} K \cup T_b(\partial_{0,\mathrm{N}} K) \cup T_b(\partial_a K)\,;$$

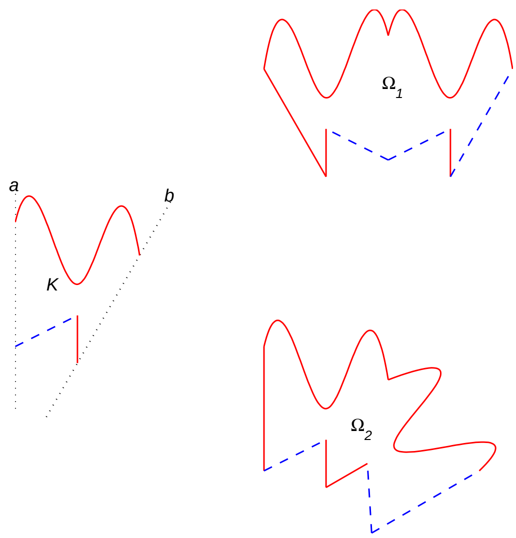

Figure 5.3: A generic construction block and resulting domains Ω_1 and Ω_2.

Theorem 5.2.3. *For any choice of lines a, b, of a construction block K, and of its boundary decomposition $\partial_{0,\mathrm{D}} K$ and $\partial_{0,\mathrm{N}} K$, we have*

$$\mathrm{Spec}_{\mathrm{DN}}(\Omega_1) = \mathrm{Spec}_{\mathrm{DN}}(\Omega_2)$$

with the account of multiplicities.

Proof. The theorem is proved using the transplantation technique developed by Berard and Buser. We show that there is a one-to-one correspondence between the eigenfunctions on Ω_1 and Ω_2. Let $u_1(x)$ be an eigenfunction of the mixed Dirichlet-Neumann boundary problem on Ω_1. We represent $u_1(x)$ as follows:

$$u_1(x) = \begin{cases} u_{11}(x), & x \in K, \\ u_{12}(T_a x), & x \in T_a K, \end{cases} \tag{5.3}$$

where $u_{11}(x)$, $u_{12}(x)$ are functions on K satisfying

$$u_{11}(x) = u_{12}(x),\ (\partial/\partial n)u_{11}(x) = -(\partial/\partial n)u_{12}(x),$$

for $x \in \partial_a K$. Let

$$u_{21}(x) = u_{11}(x) - u_{12}(x), \quad u_{22}(x) = u_{11}(x) + u_{12}(x). \tag{5.4}$$

One can check by inspection that the function

$$u_2(x) = \begin{cases} u_{21}(x), & x \in K, \\ u_{22}(T_b x), & x \in T_b K, \end{cases} \tag{5.5}$$

is an eigenfunction of the corresponding mixed Dirichlet-Neumann boundary value problem on Ω_2. It is easy to see that, by inverting this procedure, one obtains an eigenfunction of the problem on Ω_1 from an eigenfunction of the corresponding problem on Ω_2. Note also that since (5.4) is a linear transformation, we get $\mathrm{Spec}_{\mathrm{DN}}(\Omega_1) = \mathrm{Spec}_{\mathrm{DN}}(\Omega_2)$ with the account of multiplicities. This completes the proof of the theorem. □

The construction of this section also gives us the basic example shown earlier if we take the construction block K to be an isosceles right-angled triangle with leg size one, a being the hypotenuse of K, b being one of the legs, and $\partial_{0,\mathrm{N}} K$ chosen to be empty.

We illustrate the general construction described above by a number of particular examples taken from [LPP], see Figures 5.4–5.6.

Problem 5.2.4. Describe a construction block used in Figure 5.6.

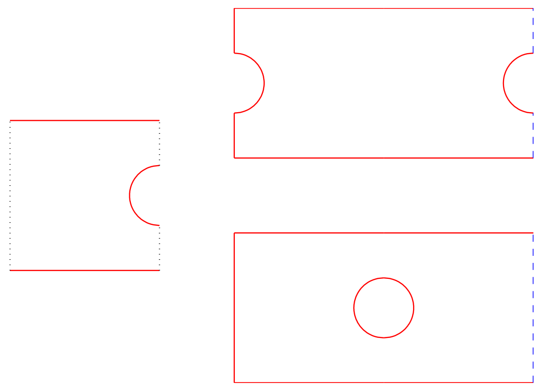

Figure 5.4: Isospectral simply connected and a non-simply connected domains, and their construction block.

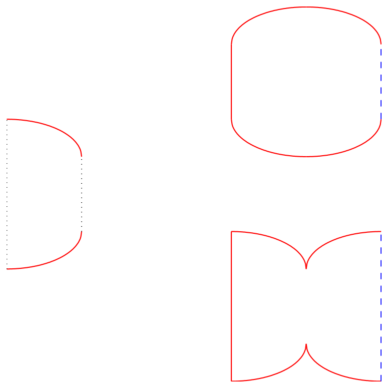

Figure 5.5: Isospectral smooth and a non-smooth domains, and their construction block.

5.2.2 Symmetry tricks

Later on we will provide an alternative proof of Theorem 5.2.3. We start though with an abstract decomposition results.

Definition 5.2.5. A mapping T is called an *involution* if $T^2 = I$.

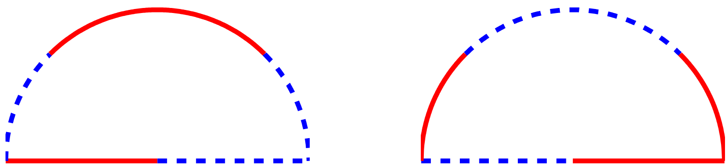

Figure 5.6: A pair of domains isospectral with respect to Dirichlet-Neumann swap.

Theorem 5.2.6. *Let A be a self-adjoint operator, and let T be an involution commuting with A (i.e. $TA = AT$). Then each eigenvector u of A can be chosen in such a way that u is either symmetric or anti-symmetric with respect to T, i.e. $Tu = \pm u$.*

Proof. For simplicity, we only consider the case when u is an eigenfunction corresponding to a *simple* eigenvalue λ, $Au = \lambda u$. A symmetrisation u_s and anti-symmetrisation u_a of u are defined by the identities

$$u_\mathrm{s} = \frac{u + Tu}{2}, \qquad u_\mathrm{a} = \frac{u - Tu}{2}.$$

Obviously, $Tu_\mathrm{s} = u_\mathrm{s}$ and $Tu_\mathrm{a} = -u_\mathrm{a}$. Also, as T commutes with A, if both u_s and u_a are non-zero, they both are eigenvectors of A corresponding to λ. As λ is simple, u_s and u_a should be linearly dependent. This immediately implies that one of them vanishes, whence the result. □

As any symmetry is an involution, Theorem 5.2.6 immediately implies the following useful result.

Let $\Omega \subset \mathbb{R}^d$ be a bounded domain symmetric with respect to a hyperplane P. Let T be an associated involution. The hyperplane P splits Ω into two bounded domains Ω_1 and $\Omega_2 = T\Omega_1$ and its boundary $\partial\Omega$ into two parts $\partial_1\Omega$ and $\partial_2\Omega = T\partial_1\Omega$. If we identify P with $P \cap \Omega$, we then have

$$\partial\Omega_k = \partial_k\Omega \cup P,$$

see Figure 5.7.

Theorem 5.2.7. *Let $-\Delta_\mathrm{D}(\Omega)$ be the Dirichlet Laplacian on a domain Ω symmetric with respect to a hyperplane P. Then its eigenfunctions can*

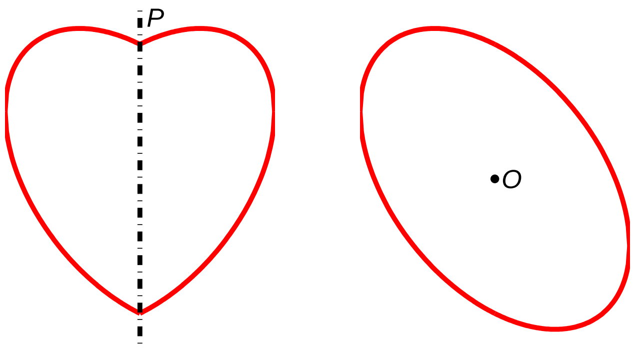

Figure 5.7: An axially symmetric domain Ω and a centrally symmetric domain $\tilde{\Omega}$.

be chosen in such a way that each one satisfies either the Dirichlet or the Neumann condition on L, and

$$\mathrm{Spec}(-\Delta_{\mathrm{D}}(\Omega)) = \mathrm{Spec}(-\Delta_{\mathrm{DN}}(\Omega_1; \partial_1\Omega, P)) \cup \mathrm{Spec}(-\Delta_{\mathrm{D}}(\Omega_1))\,.$$

A similar decomposition takes place for the Neumann Laplacian on Ω or for the operator of the Zaremba problem as long as the original boundary conditions are symmetric with respect to P.

Theorem 5.2.7 is sometimes useful, normally together with Dirichlet-Neumann bracketing, for obtaining estimates on eigenvalues. As an example of a somewhat non-trivial estimate, we state the following result, see [JLNP].

Suppose that a line of symmetry P split a domain $\Omega \subset \mathbb{R}^2$ into two subdomains Ω_1 and Ω_2. Let O be the midpoint of the interval $P \cap \Omega$. Consider also a spherically symmetric domain $\tilde{\Omega}$ which is the interior of

$\overline{\Omega_1 \cup T_O\Omega_1}$, T_O being the central symmetry with respect to O. Then

$$\lambda_1(-\Delta_{\mathrm{D}}(\Omega)) \leq \lambda_1(-\Delta_{\mathrm{D}}(\tilde{\Omega}))\,,$$

with equality if and only if Ω has an additional line of symmetry P_1 perpendicular to P and passing through O.

5.2.3 Symmetries and isospectrality

In this section we outline an alternative proof of Theorem 5.2.3 and, at the same time, relate in an indirect way the spectra $\mathrm{Spec}_{\mathrm{DN}}(\Omega_j)$ and the spectra of boundary value problems on the construction block K. For illustrative purposes all the figures in this section use a construction block K with parallel sides a, b, which is different from the construction block shown in the previous section.

To start with, consider an eight-sheet covering $\overset{\frown}{K}_8$ of the block K. It is constructed by "gluing" together four copies of K and four copies of its reflection T_aK, and identifying the outer edges, as shown in Figure 5.8.

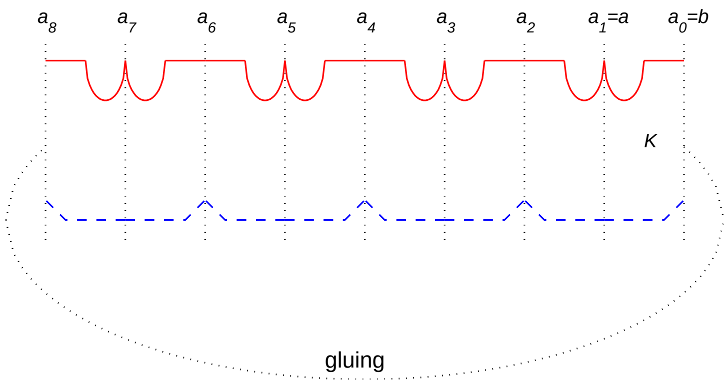

Figure 5.8: $\overset{\frown}{K}_8$, an eight-sheeted covering of K. Here the construction block K is bounded by two parallel lines a and b. The main construction described above gives an isospectral pair, with Ω_1 being bounded by a_2 (with the Dirichlet condition imposed) and a_0 (Neumann), and Ω_2 being bounded by a_3 (Dirichlet) and a_1 (Neumann).

The dotted lines show the original bounding lines and their images under reflections; we set

$$a_0 := b\,, \qquad a_1 := a\,, \qquad a_j := T_{a_{j-1}}(a_{j-2}) \quad \text{for } j = 2, \dots, 8$$

and identify a_0 and a_8.

The eight-sheet covering $\overset{\frown}{K}_8$ is a flat manifold with boundary on which we consider a mixed Dirichlet-Neumann problem with conditions imposed according to the original choice of $\partial_{0,D}K$ and $\partial_{0,N}K$, and their reflections. We denote the spectrum of the corresponding Laplacian by $\mathrm{Spec}(\overset{\frown}{K}_8)$.

Any pair of lines $a_k \cup a_{k+4}$, $k = 0, \dots, 4$ defines a symmetry on $\overset{\frown}{K}_8$ which preserves both a_k and a_{k+4} and exchanges $a_{(k-j) \mod 8}$ with $a_{(k+j) \mod 8}$ for $j = 1, 2, 3$. Consider, e.g., the case $k = 0$. Then the lines a_0, a_4 split $\overset{\frown}{K}_8$ into two identical domains; denote one of them K_4. The eigenfunctions on $\overset{\frown}{K}_8$ can be chosen in such a way that each one shall satisfy either a Dirichlet or a Neumann boundary condition on $a_0 \cup a_4$. Moreover

$$\mathrm{Spec}(\overset{\frown}{K}_8) = \mathrm{Spec}_{\mathrm{DD}}(K_4) \cup \mathrm{Spec}_{\mathrm{NN}}(K_4)\,,$$

where $\mathrm{Spec}_{\mathrm{DD,NN}}(K_4)$ stand for the spectra of the Laplacian on K_4 with corresponding boundary conditions imposed on a_0 and a_4, and the union is understood with account of multiplicities.

Consider now these two new problems on K_4. For each one of them, a_2 is the line of symmetry which divides K_4 into two copies of Ω_1. By the same argument,

$$\begin{aligned} &\mathrm{Spec}_{\mathrm{DD}}(K_4) = \mathrm{Spec}_{\mathrm{DN}}(\Omega_1) \cup \mathrm{Spec}_{\mathrm{DD}}(\Omega_1) \qquad \text{and} \\ &\mathrm{Spec}_{\mathrm{NN}}(K_4) = \mathrm{Spec}_{\mathrm{ND}}(\Omega_1) \cup \mathrm{Spec}_{\mathrm{NN}}(\Omega_1)\,; \end{aligned}$$

here once again the indices D and N, correspond to the boundary conditions imposed on the sides a_0 and a_2 of Ω_1. Obviously, $\mathrm{Spec}_{\mathrm{ND}}(\Omega_1) = \mathrm{Spec}_{\mathrm{DN}}(\Omega_1)$ by symmetry.

Repeating the argument once more for symmetric problems on Ω_1, we get

$$\begin{aligned} &\mathrm{Spec}_{\mathrm{DD}}(\Omega_1) = \mathrm{Spec}_{\mathrm{DN}}(K) \cup \mathrm{Spec}_{\mathrm{DD}}(K) \qquad \text{and} \\ &\mathrm{Spec}_{\mathrm{NN}}(\Omega_1) = \mathrm{Spec}_{\mathrm{ND}}(K) \cup \mathrm{Spec}_{\mathrm{NN}}(K)\,. \end{aligned}$$

Thus

$$\begin{aligned} &\mathrm{Spec}_{\mathrm{DN}}(\Omega_1) \cup \mathrm{Spec}_{\mathrm{DN}}(\Omega_1) = \\ &\qquad \mathrm{Spec}(\overset{\frown}{K}_8) \setminus (\mathrm{Spec}_{\mathrm{DD}}(K) \cup \mathrm{Spec}_{\mathrm{DN}}(K) \\ &\qquad\qquad \cup \mathrm{Spec}_{\mathrm{ND}}(K) \cup \mathrm{Spec}_{\mathrm{NN}}(K))\,, \end{aligned} \tag{5.6}$$

i.e. the spectrum $\mathrm{Spec}_{\mathrm{DN}}(\Omega_1)$ taken with double multiplicities is obtained by removing from the spectrum $\mathrm{Spec}(\overset{\frown}{K}_8)$ of the problem on the eight-sheeted covering, the spectra of the four boundary value problems on the "construction block" K.

We can now repeat the whole process but start by considering the symmetry with respect to $a_1 \cup a_5$. Then instead of K_4 we should consider a different set K_4' bounded by a_1 and a_5, which has a line of symmetry a_3 dividing it into two copies of Ω_2. The previous argument gives again (5.6), with Ω_1 replaced by Ω_2, thus providing an alternative proof of Theorem 5.2.3.

Chapter 6

Eigenvalue enclosures and spectral pollution

The projection method is a powerful tool for studying eigenvalues of operators outside the extrema of the essential spectrum. However, in this chapter we discuss the following questions:

- Can the projection method be trusted if we want to detect the presence of discrete spectrum in a gap on the essential spectrum?
- Is the limit of the spectrum always equal to the spectrum of the limit?
- Is there an alternative method that we can always trust?
- Can one possibly get two-sided estimates on eigenvalues?

6.1 Spectral pollution

6.1.1 Spurious eigenvalues

We begin by considering an elementary example.

Let

$$Au(x) = \operatorname{sgn}(x)u(x) \qquad u \in L^2(-\pi, \pi) \tag{6.1}$$

where $\operatorname{sgn}(x) = \frac{x}{|x|}$. The spectrum of A is purely essential and it consists of two eigenvalues ± 1, both of infinite multiplicity. Following the discussion of Section 2.2.2, let us apply the projection method to A with finite-dimensional spaces $\mathcal{L}$ generated by the Fourier basis:

$$e_j(x) = \frac{1}{\sqrt{2\pi}} e^{-ijx}, \qquad \mathcal{L} = \mathrm{Span}\{e_{-n}, \dots, e_n\}. \tag{6.2}$$

Since the e_j form an orthonormal basis, the approximate Rayleigh-Ritz values $\nu_j(\mathcal{L})$ in (2.3) are the eigenvalues of the $(2n+1)\times(2n+1)$ matrix

$$\begin{aligned} K_{jk} &= \frac{1}{2\pi} \int \mathrm{sgn}(x) e_j(x) \overline{e_k(x)}\, \mathrm{d}x = \widehat{\mathrm{sgn}}(k-j) \\ &= \begin{cases} 0, & k-j \text{ even}, \\ \frac{2i}{(k-j)\pi}, & k-j \text{ odd}. \end{cases} \end{aligned} \tag{6.3}$$

It is easy to seen that K has $n+1$ columns whose odd entries are zero and n columns whose even entries are zero. The former have only n non-zero entries, so they must be linearly dependent. Therefore $0 \in \mathrm{Spec}(K)$, for all the subspaces $\mathcal{L}$ constructed in the above manner, even though $0 \notin \mathrm{Spec}(A)$.

If we are in a situation like this, that is, where there are eigenvalues of the Rayleigh-Ritz problem (2.3) accumulating at regions of the resolvent set, we say that we are in the presence of *spectral pollution*. The points of these regions are called *spurious eigenvalues*.

In the very simple example just presented, the origin is a spurious eigenvalue, but it is by no means the only one. The important message here is that the projection method should be treated with care when applied in gaps of the essential spectrum. If we did not know $\mathrm{Spec}(A)$ beforehand, from the above analysis we might be driven to a false conclusion that 0 is (or is near to) a spectral point of A.

We can say much more about this model. From the theory of Toeplitz operators one can actually show that

$$\lim_{n\to\infty} \mathrm{Spec}(K) = [-1, 1]. \tag{6.4}$$

That is, the whole interval $(-1, 1)$ fills up with spurious eigenvalues of the projection method as n increases. This shows that, in general, the limit of the spectrum is not the spectrum of the limit. In Figure 6.1 we graph $\mathrm{Spec}(K)$ in the vertical axis, for several values of n in the horizontal axis.

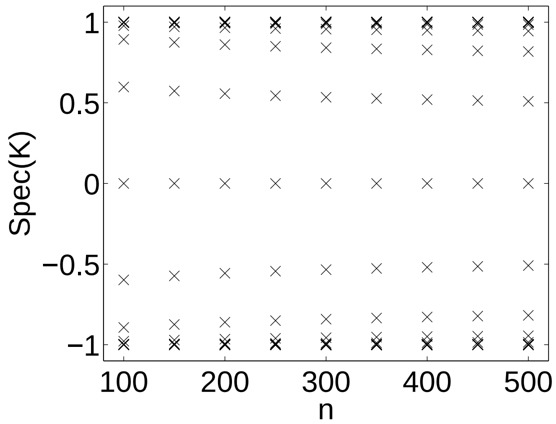

Figure 6.1: The spectrum of K for $n = 100 : 50 : 500$. This graph shows that spectral pollution arises if we apply the projection method to $Au(x) = \mathrm{sgn}(x)u(x)$ with $\mathcal{L}$ generated by the Fourier basis. Even though there is a heavy accumulation of eigenvalues near ± 1, spurious eigenvalues also appear in $(-1, 1)$ and eventually fill this interval.

Problem 6.1.1. Let $a \in \mathbb{R}$ and let

$$Bu(x) = \mathrm{sgn}(x)u(x) + a\widehat{u}(0)$$

acting on $L^2(-\pi, \pi)$. Write a Matlab program for computing the Rayleigh-Ritz values $\nu_k(\mathcal{L})$ when $\mathcal{L}$ is generated by the Fourier basis. What is the essential spectrum of B? Are there eigenvalues outside the extrema of the essential spectrum for $a \neq 0$? Are there any inside the gap?

6.1.2 Why does the projection method pollute?

Let $L = L^*$ and $\mathcal{L} \subset \mathrm{Dom}(L)$. Denote by $\Pi \equiv \Pi_{\mathcal{L}} : \mathcal{H} \longrightarrow \mathcal{L}$ the orthogonal projection onto $\mathcal{L}$. For $z \in \mathbb{C}$, let

$$\tilde{F}(z) := \min_{0 \neq v \in \mathcal{L}} \frac{\|\Pi(z - L)v\|}{\|v\|}.$$

Then $\nu \equiv \nu(\mathcal{L})$ is a solution to the Rayleigh-Ritz problem (2.3), if and only if $\tilde{F}(\nu) = 0$. Indeed, both conditions are equivalent to saying that ν is an eigenvalue of the finite-dimensional operator $K_{\mathcal{L}} = \Pi L \restriction \mathcal{L} : \mathcal{L} \longrightarrow \mathcal{L}$.

Now, if $\tilde{F}(\nu) = 0$, the only assertion that we can make in general is that there exists $\tilde{v} \in \mathcal{L}$, such that

$$(\nu - L)\tilde{v} \perp \mathcal{L}. \tag{6.5}$$

In particular, see (2.1), $R(\tilde{v}) = \nu$. If $\nu < \min \operatorname{Spec}_{\mathrm{ess}}(L)$, Theorem 2.1.1 ensures that there will be discrete eigenvalues of L below ν. Similarly if $\nu > \max \operatorname{Spec}_{\mathrm{ess}}(L)$, there will be discrete eigenvalues of L above ν. Furthermore conditions such as (2.4) yield ν close to $\operatorname{Spec}_{\mathrm{disc}}(L)$. However, in general, (6.5) does not guarantee that ν is close to $\operatorname{Spec}(L)$ as $\|(\nu - L)v\|/\|v\|$ is not necessarily small for $v = \tilde{v}$, any other $v \in \mathcal{L}$ or, for that matter, any $v \in \mathcal{H}$.

This limitation of the projection method is not caused by lack of convergence. In the example presented in Section 6.1.1, we had a sequence of subspaces $\mathcal{L} \equiv \mathcal{L}_n$ such that, putting $L = A$,

$$\lim_{n\to\infty} \|L^p(u - \Pi_{\mathcal{L}_n} u)\| = 0\,, \tag{6.6}$$

for all $p \in \mathbb{N} \cup \{0\}$ and all $u \in \mathcal{H}$.

A general result on spectral pollution can be established. The next lemma directly follows from [LeSh, Theorem 2.1].

Lemma 6.1.2. *If $\lambda \notin \operatorname{Spec}_{\mathrm{ess}}(L)$ is such that $\alpha < \lambda < \beta$ where $\alpha, \beta \in \operatorname{Spec}_{\mathrm{ess}}(L)$, there exists a sequence of subspaces $\mathcal{L}_n$ satisfying* (6.6) *for all $p \in \mathbb{N}$ and all $u \in \operatorname{Dom}(L)$, such that $\lambda \in \operatorname{Spec}(K_{\mathcal{L}_n})$ for all $n \in \mathbb{N}$.*

The standard approach to deal with spectral pollution is very much dependent on the nature of the operator L. It involves choosing "special" subspaces $\mathcal{L}$, in order to ensure the smallness of $\|(\nu - L)\tilde{v}\|/\|\tilde{v}\|$ when $\tilde{F}(\nu) = 0$. We will not pursue this direction here, but rather refer to [DoEsSe], [BoBr] and [RaSa^{2}Va], for particularly successful applications of this idea.

Problem 6.1.3. Let B be the operator of Problem 6.1.1 and

$$f_n(x) = \begin{cases} \frac{e^{in(2x+\pi)}}{\sqrt{\pi}}, & x \in [-\pi, 0), \\ 0, & x \in [0, \pi), \end{cases} \quad g_n(x) = \begin{cases} 0, & x \in [-\pi, 0), \\ \frac{e^{in(2x+\pi)}}{\sqrt{\pi}}, & x \in [0, \pi). \end{cases}$$

Write a Matlab program for computing $\nu_k(\mathcal{L})$ with

$$\mathcal{L} = \mathrm{Span}\{f_{-n}(x), g_{-n}(x), \dots, f_n(x), g_n(x)\}.$$

Compare with the results obtained in Problem 6.1.1.

6.1.3 The distance function from the spectrum and the Davies-Plum approach

We now discuss a strategy suggested by Davies and Plum, [DaPl], for computing the spectrum of self-adjoint operators.

Let $L = L^*$ and $\mathcal{L} \subset \mathrm{Dom}(L)$. For $z \in \mathbb{C}$, define the function

$$F(z) = \min_{0 \neq v \in \mathcal{L}} \frac{\|(z - L)v\|}{\|v\|}. \tag{6.7}$$

Note that we just have dropped the projection from the expression of $\tilde{F}(z)$. The following lemma is fundamental.

Lemma 6.1.4. *Let $F(z)$ be as in* (6.7)*. Then*

$$F(z) \geq \mathrm{dist}(z, \mathrm{Spec}(L)) \qquad z \in \mathbb{C}. \tag{6.8}$$

Proof. The conclusion follows from the fact that

$$\begin{aligned} F(z) &\geq \inf_{v \in \mathrm{Dom}(L)} \frac{\|(z - L)v\|}{\|v\|} \\ &= \|(z - L)^{-1}\|^{-1} = \mathrm{dist}(z, \mathrm{Spec}(L)). \end{aligned}$$

□

Therefore $|F(x)|$ is small if and only if $x \in \mathbb{R}$ is close to $\mathrm{Spec}(L)$. A plausible strategy to approximate a portion of the spectrum of L that lies on the interval $[a,b]$, is to fix a mesh $a = x_0 < \ldots < x_n = b$ and compute $F(x_j)$ for all $j = 0, \ldots, n$, then search for the local minima of $F(x_j)$.

How do we estimate $F(x)$? The following trick is useful. Suppose that $\mathcal{L} \subset \mathrm{Dom}(L^2) = \{u \in \mathrm{Dom}(L) : Lu \in \mathrm{Dom}(L)\}$. Then

$$\begin{aligned} F(x)^2 &= \min_{v \in \mathcal{L}} \frac{\langle \Pi(x-L)^2 v, v\rangle}{\|v\|^2} \\ &= \min_{v \in \mathcal{L}} \frac{\|\Pi(x-L)^2 v\|}{\|v\|} \end{aligned} \tag{6.9}$$

for all $x \in \mathbb{R}$. Let

$$Q(z) = \Pi(z-L)^2 \upharpoonright \mathcal{L}. \tag{6.10}$$

The second equality in (6.9) is consequence of the fact that $Q(x)$ is non-negative for $x \in \mathbb{R}$. Since

$$F(x)^4 = \min \mathrm{Spec}(Q(x)^* Q(x)),$$

we may compute $F(x)$ by finding the square root of the smallest *singular value* of $Q(x)$, that is the quartic root of the smallest eigenvalue of $Q(x)^* Q(x) \geq 0$.

Example 6.1.5. Let $L = A$ be the operator of multiplication by $\mathrm{sgn}(x)$ as in (6.1) and $\mathcal{L}$ be as in (6.2). In this case

$$Q(x) = x^2 + 1 - 2xK_{\mathcal{L}}. \tag{6.11}$$

Figure 6.2 shows the graph of $F(x)$ for $n = 2, 4, 6, 8$. It is remarkable that in this particular example, $F(x)$ is very close to $\mathrm{dist}(x, \mathrm{Spec}(A))$ even for small values of n. Note that $F(0) = 1$ for all $n \in \mathbb{N}$.

Problem 6.1.6. Let B and $\mathcal{L}$ be the operator and subspace of Problem 6.1.1. Write a Matlab program for computing $F(x)$ on a mesh of the interval $[-2, 2]$. Depict the profile of $F(x)$ with a suitable mesh size for small values of n. Could you draw any conclusion about the spectrum of B from your pictures?

The strategy developed in [DaPl] is actually more sophisticated than simply locating the minima of $F(x)$. It involves finding two-sided estimates of the spectral point of interest by approximating $F'(x)$ near local *maxima* of $F(x)$ instead. We will not discuss this in further detail, but consider a slightly different approach for computing spectra.

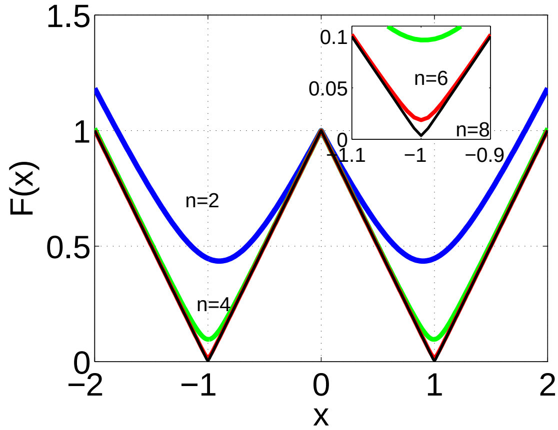

Figure 6.2: Graph of $F(x)$ for $L = A$, the operator of multiplication by $\operatorname{sgn}(x)$. Note that for small values of n we already achieve a good approximations of $\operatorname{dist}(x, \operatorname{Spec}(A))$.

6.2 The quadratic projection method

For $z \in \mathbb{C}$, let $Q(z)$ be as in (6.10) and

$$G(z) = \min_{v \in \mathcal{L}} \frac{\|Q(z)v\|}{\|v\|}. \tag{6.12}$$

Then $F(x)^2 = G(x)$ for all $x \in \mathbb{R}$, however they may differ outside the real axis. Indeed, the determinant of $Q(z)$ is a polynomial of degree $2 \dim \mathcal{L}$ (here we take a matrix representation for $Q(z)$). Hence $G(z)$ will always have zeros on the complex plane, at most $2 \dim \mathcal{L}$ of them, while $F(z)$ never vanishes outside $\mathbb{R}$ due to (6.8).

Since $G(z)^* = G(\overline{z})$, the zeros of $G(z)$ appear in conjugate pairs. If $G(\mu) = 0$ and μ is close to $\mathbb{R}$, one should expect $G(\operatorname{Re}(\mu)) = F(\operatorname{Re}(\mu))^2$ to be small, so once again due to (6.8), $\operatorname{Re}(\mu)$ must be close to the spectrum of L. The quadratic projection method, which we describe next, is a rigorous realisation of this observation.

6.2.1 Weak formulation of the method

Let $L = L^*$ and let $\mathcal{L} \subset \mathrm{Dom}(L)$ be a finite dimensional subspace. In the *quadratic projection method* we seek for the solutions $\{\mu_k(\mathcal{L})\}$ of the *weak quadratic eigenvalue problem*: find $\mu \in \mathbb{C}$ and $u \in \mathcal{L}$ non-zero, such that

$$\langle Lu, Lv\rangle - 2\mu\langle Lu, v\rangle + \mu^2\langle u, v\rangle = 0 \qquad \text{for all } v \in \mathcal{L}. \tag{6.13}$$

If $\mathcal{L} = \mathrm{Span}\{b_1, \dots, b_n\}$, where the vectors b_j are linearly independent, the solutions of (6.13) are those $\mu \in \mathbb{C}$ such that $\det Q(\mu) = 0$, where $Q(z) = Q_{\mathcal{L}}(z)$ is an $n \times n$ matrix whose entries are given by

$$Q(z)_{jk} = \langle Lb_j, Lb_k\rangle - 2z\langle Lb_j, b_k\rangle + z^2\langle b_j, b_k\rangle. \tag{6.14}$$

Note that, whenever $\mathcal{L} \subset \mathrm{Dom}(L^2)$, we can find a similarity transformation $V : \mathcal{L} \longrightarrow \mathbb{C}^n$ independent of z, such that

$$V^{-1}Q(z)V = \Pi(z - L)^2 \upharpoonright \mathcal{L},$$

so we come back to the representation (6.10).

Observe that $Q(z)$ is a quadratic polynomial in z with matrix coefficients. By analogy to the linear spectral problem discussed largely in the previous chapters, we denote

$$\mathrm{Spec}(Q) = \{\mu \in \mathbb{C} : \det Q(\mu) = 0\}. \tag{6.15}$$

If $G(z)$ is defined as in (6.12), then $G(\mu) = 0$ if and only if $\mu \in \mathrm{Spec}(Q)$. That is, $Q(z)$ characterises completely the zeros of $G(z)$.

6.2.2 The Shargorodsky theorem

Let $\mu = \alpha + i\beta$ with $\alpha, \beta \in \mathbb{R}$. For $u, v \in \mathcal{L}$, the left side of (6.13) is

$$\begin{aligned}&\langle(\mu - L)u, (\overline{\mu} - L)v\rangle = \\ &\qquad \langle(\alpha - L)u, (\alpha - L)v\rangle + 2i\beta\langle(\alpha - L)u, v\rangle - \beta^2\langle u, v\rangle.\end{aligned}$$

Let $u \in \mathcal{L}$ be such that (6.13) holds true with $\beta \neq 0$. By taking $v = u$ in the above expression, we get

$$\|(\alpha - L)u\|^2 - \beta^2\|u\|^2 + 2i\beta\langle(\alpha - L)u, u\rangle = 0.$$

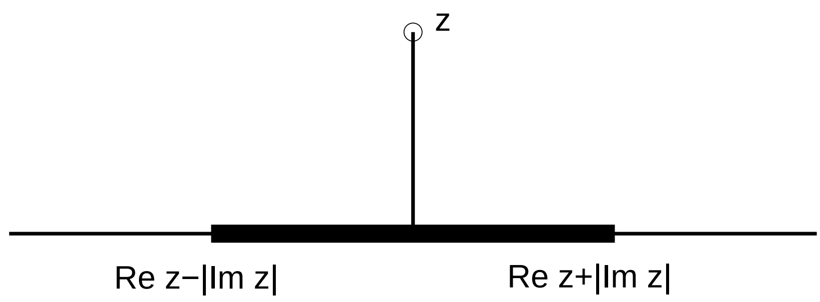

Figure 6.3: The interval intersecting the spectrum of L according to Theorem 6.2.2.

Thus

$$\beta^2 = \frac{\|(\alpha - L)u\|^2}{\|u\|^2} \quad \text{and} \quad \langle(\alpha - L)u, u\rangle = 0.$$

The first equality yields an important relation between $F(z)$ and $G(z)$.

Lemma 6.2.1. *If* $G(\mu) = 0$ *then* $F(\operatorname{Re}\mu) \le |\operatorname{Im}\mu|$.

If we combine this lemma with (6.8), we recover:

Theorem 6.2.2 (Shargorodsky)**.** *If* $G(\mu) = 0$*, then*

$$[\operatorname{Re}\mu - |\operatorname{Im}\mu|, \operatorname{Re}\mu + |\operatorname{Im}\mu|] \cap \operatorname{Spec}(L) \neq \varnothing.$$

A more refined result implying Theorem 6.2.2 may be found in [Sh] and [LeSh]. However, the current version contains the central idea behind the quadratic projection method. In order to approximate the spectrum of L we should:

(a) Fix a finite-dimensional subspace $\mathcal{L} \subset \operatorname{Dom}(L)$ and a basis of $\mathcal{L}$.

(b) Assemble the matrix polynomial $Q(z)$ according to (6.14).

(c) Find the points of $\operatorname{Spec}(Q)$, that is the zeros of $G(z)$, which are close to $\mathbb{R}$.

Those points will *necessarily* be close to $\operatorname{Spec}(L)$ with a two-sided error estimate given explicitly by Theorem 6.2.2.

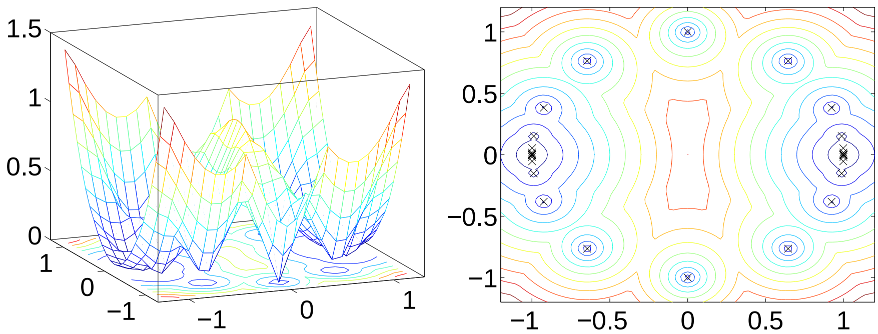

Figure 6.4: In this figure we show the graph of $G(z)$ (left) and its contours and zeros (right), for $L = A$ the operator of multiplication by $\mathrm{sgn}(x)$.

Example 6.2.3. Let $L = A$ be the operator of multiplication by $\mathrm{sgn}(x)$ as in (6.1) and let $\mathcal{L}$ be as in (6.2). According to (6.11), which holds true for all $x \in \mathbb{C}$, $\det Q(\mu) = 0$ if and only if $\frac{\mu+\mu^{-1}}{2} \in \mathrm{Spec}(K) \subset (-1, 1)$. Here K is the matrix whose entries are given by (6.3). Therefore the zeros of $G(z)$ must lie on the unit circle.

This example is so elementary, that we can find explicitly the region where the zeros of $G(z)$ accumulate as $n \to \infty$. By virtue of (6.4), $\mathrm{Spec}(Q)$ accumulates in the unit circle $\{z \in \mathbb{C} : |z| = 1\}$ for large n. In Figure 6.4 we show the graph of $G(z)$, its contours and zeros when $n = 50$. This should be compared with Figure 6.2.

Two natural questions arise:

- How to find $\mathrm{Spec}(Q)$?
- Are there ever zeros of $G(z)$ near the real line?

We now address these questions in some detail.

6.2.3 Quadratic matrix eigenvalue problems

The theory of quadratic matrix polynomials is a well developed subject in the area of linear algebra and its applications. We refer to the monograph [Go] for a thorough account on the theory of matrix polynomials of any order.

The quadratic projection method prescribes finding the spectrum, see (6.15), of the quadratic matrix polynomial

$$Q(z) = R - 2zK + z^2 M,$$

where $R, K, M \in \mathbb{C}^{n\times n}$. In applications, these matrices are expected to be sparse and real. They are always Hermitean, so $Q(z)^* = Q(\overline{z})$ and hence $\mathrm{Spec}(Q)$ is symmetric with respect to $\mathbb{R}$.

The standard way of finding $\mathrm{Spec}(Q)$ is to construct a suitable companion linear pencil eigenvalue problem,

$$Av = \mu Bv, \qquad 0 \neq v \in \mathcal{L} \oplus \mathcal{L}, \tag{6.16}$$

such that $\mu \in \mathrm{Spec}(Q)$ if and only if (6.16) holds true. The coefficients, A, B, of the companion form, $(A - zB)$, are twice the size of the coefficients of $Q(z)$. They are not unique. Two possible companion forms are:

$$A = \begin{pmatrix} 0 & I \\ -R & 2K \end{pmatrix} \qquad B = \begin{pmatrix} I & 0 \\ 0 & M \end{pmatrix} \tag{6.17}$$

and

$$A = \begin{pmatrix} -R & 0 \\ 0 & I \end{pmatrix} \qquad B = \begin{pmatrix} -2K & M \\ I & 0 \end{pmatrix}, \tag{6.18}$$

where I is the identity matrix. In fact we can generate many more if we substitute I for any non-singular matrix in the above expressions.

Problem 6.2.4. Substitute $w = zu$ in the equation $Q(z)u = 0$, $u \in \mathbb{C}^n$, and write this equation in two different ways:

$$zMw - 2Kw + Ru = 0$$
$$zMw - z2Ku + Ru = 0.$$

Use the first equation to verify that $\mu \in \mathrm{Spec}(Q)$ if and only if (6.16) holds true where A and B are given by (6.17). Use the second one to verify the same statement but where now A and B are given by (6.18).

There are infinitely many possible companion forms of a matrix polynomial problem. Different companion forms lead to different stability properties of the linear pencil problem to be solved once the matrices have been assembled. For small size matrices it does not matter which companion form one chooses. However the performance of computer algorithms is seriously dependant on the companion form for large size matrices. A recent study on the matter can be found in [Hi].

Note that computation of the spectrum of matrix polynomials is automatically implemented in the Matlab command `polyeig`.

Problem 6.2.5. Let B and $\mathcal{L}$ be the operator and subspace of Problem 6.1.1. Write a Matlab program for finding $\mathrm{Spec}(Q)$. Plot $\mathrm{Spec}(Q)$ for various values of n. Can you detect any eigenvalue in the gap of the essential spectrum? Compare with your previous results and with the graph on the left side of Figure 6.4.

6.2.4 Spectral exactness

The second question posed at the end of Section 6.2.2 is slightly more subtle. It strongly depends on non-trivial regularity properties of the function $G(z)$. Here we present the results without proof.

Lemma 6.2.6. *Let $L = L^*$, $\mathcal{L} \subset \mathrm{Dom}(L)$ and $G(z)$ be defined as in (6.12). Then $G(z)$ is C^∞ except on a union of algebraic curves. Moreover it is Lipschitz continuous and superharmonic in $\mathbb{C}$.*

A general version of this lemma may be found in [BLP]. See also [D1, Theorem 9.2.8]. The conclusion that is relevant to us in the present discussion is that $G(z)$ vanishes at its local minima. This key property implies the following.

Theorem 6.2.7. *Let $\lambda \in \mathrm{Spec}_{\mathrm{disc}}(L)$, let $\{u_j\}_{j=1}^k$ be an orthonormal set of eigenfunctions associated to λ and let $d > 0$ be such that*

$$\{z \in \mathbb{C} : |z - \lambda| \le d\} \cap \mathrm{Spec}(L) = \{\lambda\}.$$

There exist $b > 1$, only dependent on λ and d, satisfying the following properties. If $\mathcal{L} \subset \mathrm{Dom}(L^2)$ is a subspace such that

$$\max_{\substack{p\,=\,0,\,1,\,2 \\ j\,=\,1,\,\dots,\,k}} \|L^p(u_j - \Pi_{\mathcal{L}} u_j)\| < \delta \tag{6.19}$$

for $0 < \delta < \frac{d^2}{4b^2}$, then *(a) there exists* $\mu \in \mathrm{Spec}(Q)$ *such that* $|\mu - \lambda| < b\delta^{1/2}$*,*

(b) $\{z \in \mathbb{C} : b\delta^{1/2} \le |z - \lambda| \le d/2\} \cap \mathrm{Spec}(Q) = \varnothing$*.*

The proof of this result may be found in [Bo]. The condition (6.19) is comparable with (2.4).

Formally speaking this theorem establishes that if the subspace $\mathcal{L}$ approximates "fairly well" the eigenspace associated to a discrete eigenvalue λ, then it is guaranteed that "isolated" zeros of $G(z)$ will be close to λ. This theorem is applicable in multiple situations. We immediately obtain the following general statement.

Corollary 6.2.8. *Let* A *be a bounded self-adjoint operator acting on* $\mathcal{H}$*. Let* $\mathcal{L}_n \subset \mathcal{H}$ *be a sequence of subspaces such that* $\Pi_{\mathcal{L}_n} u \to u$ *for all* $u \in \mathcal{H}$*. For any* $\lambda \in \mathrm{Spec}_{\mathrm{disc}}(A)$*, there exist a sequence* $\{\mu_n\}$ *of zeros of* $G_{\mathcal{L}_n}(z)$ *such that* $\mu_n \to \lambda$*.*

Problem 6.2.9. Show that if B and $\mathcal{L}_n$ are the operator and subspace of Problem 6.1.1. Then any point in the discrete spectrum will be approximated at a speed at least as fast as $n^{-1/2}$.

Bibliography

[Ash] M. Ashbaugh, Isoperimetric and universal inequalities for eigenvalues. *Spectral theory and geometry (Edinburgh, 1998)*, 95–139, London Math. Soc. Lecture Note Ser., 273, Cambridge Univ. Press, Cambridge, 1999.

[BoBr] D. Boffi, F. Brezzi, L. Gastaldi, On the problem of spurious eigenvalues in the approximation of linear elliptic problems in mixed form. *Math. Comp.* 69 (1999) 121-140.

[Bo] L. Boulton, Non-variational approximation of discrete eigenvalues of self-adjoint operators. *IMA J. Numer. Anal.* 27 (2007) 102-121.

[BLP] L. Boulton, P. Lancaster, P. Psarrakos, On pseudospectra of matrix polynomials and their boundary. *Math. Comp.* to appear (2007).

[CS] S.E. Cappell, J.L. Shaneson, *Some Problems in Number Theory I: The Circle Problem*, preprint arXiv:math/0702613, http://arxiv.org/abs/math/0702613 (2007).

[D1] E.B. Davies, *Linear Operators and their Spectra*, Cambridge University Press, Cambridge (2007).

[D2] E.B. Davies, *Spectral Theory and Differential Operators*, Cambridge University Press, Cambridge (1996).

[DaPl] E.B. Davies, M. Plum, Spectral pollution. *IMA J. Numer. Anal.* 24 (2004) 417-438.

[DoEsSe] J. Dolbeault, M.J. Esteban, E. Séré, On the eigenvalues of operators with gaps. Application to Dirac operators. *J. Funct. Anal.* 174 (2000) 208–226.

[Fil] N. Filonov, On an inequality for the eigenvalues of the Dirichlet and Neumann problems for the Laplace operator. (Russian) *Algebra i Analiz* 16 (2004), no. 2, 172-176. Translation in *St. Petersburg Math. J.* 16 (2005), no. 2, 413-416.

[Fri] L. Friedlander, Some inequalities between Dirichlet and Neumann eigenvalues. *Arch. Rational Mech. Anal.* 116 (1991), no. 2, 153-160.

[Go] I. Gohberg, P. Lancaster, L. Rodman, *Matrix Polynomials*, Academic Press, New York (1982).

[GWW] C. Gordon, D. Webb, S. Wolpert, One cannot hear the shape of a drum. *Bull. Amer. Math. Soc.* 27 (1992), no. 1, 134–138.

[Hi] N. Higham, D.S. Mackey, F. Tisseur, The conditioning on linearizations of matrix polynomials. *SIAM J. Matrix Anal. Appl.* 28 (2006) 1005-1028.

[I] E.L. Ince, *Ordinary Differential Equations*, Dover, New York (1956).

[JLNP] D. Jakobson, M. Levitin, N. Nadirashvili, I. Polterovich, Spectral problems with mixed Dirichlet-Neumann boundary conditions: isospectrality and beyond. *J. Comput. Appl. Math.* 194 (2006), no. 1, 141-155.

[Kac] M. Kac, Can one hear the shape of a drum? *Amer. Math. Monthly* 73 1966 no. 4, part II, 1-23.

[K] T. Kato, *Perturbation Theory of Linear Operators*, Springer-Verlag, Berlin (1995).

[Kaw] B. Kawohl, *Rearrangements and convexity of level sets in PDE.* Lecture Notes in Mathematics, 1150. Springer-Verlag, Berlin, 1985.

[Lap] A. Laptev, Dirichlet and Neumann eigenvalue problems on domains in Euclidean spaces. *J. Funct. Anal.* 151 (1997), 531-545.

[LePa] M. Levitin, L. Parnovski, Commutators, spectral trace identities, and universal estimates for eigenvalues. *J. Funct. Anal.* 192 (2002), no. 2, 425-445.

[LPP] M. Levitin, L. Parnovski, I. Polterovich, Isospectral domains with mixed boundary conditions. *J. Phys. A* 39 (2006), no. 9, 2073-2082.

[LeSh] M. Levitin, E. Shargorodsky, Spectral pollution and second order relative spectra for self-adjoint operators. *IMA J. Numer. Anal.* 24 (2004) 393-416.

[LeVa] M. Levitin, D. Vassiliev, Spectral asymptotics, renewal theorem, and the Berry conjecture for a class of fractals. *Proc. London Math. Soc.* (3) 72 (1996), no. 1, 188-214.

[LeYa] M. Levitin, R. Yagudin, Range of the first three eigenvalues of the planar Dirichlet Laplacian. *LMS J. Comput. Math.* 6 (2003), 1-17 (electronic).

[M] V. Maz'ja, *Sobolev Spaces*, Springer-Verlag, Berlin (1980).

[RaSa^{2}Va] J. Rappaz, J. Sanchez Hubert, E. Sanchez Palencia, D. Vassiliev, On spectral pollution in the finite element approximation of thin elastic 'membrane' shell. *Numer. Math.* 75 (1997) 473–500.

[RSv1] M. Reed, B. Simon, *Methods of Modern Mathematical Physics: Volume I*, Academic Press, London (1980).

[RSv4] M. Reed, B. Simon, *Methods of Modern Mathematical Physics: Volume IV*, Academic Press, London (1978).

[S] H. Schwarz, *Finite Element Methods*, Academic Press, London (1988).

[SaVa] Yu. Safarov, D. Vassiliev, *The asymptotic distribution of eigenvalues of partial differential operators*, Translations of Mathematical Monographs, **155**, American Mathematical Society, Providence, RI (1997).

[Sh] E. Shargorodsky, Geometry of higher order relative spectra and projection methods. *J. Oper. Theo.* 44 (2000) 43-62.

[SF] G. Strang, G. Fix, *An analysis of the Finite Element Method*, Prentice-Hall, Englewood Clifs (1973).

La Asociación Matemática Venezolana fue fundada en 1990 como una organización civil sin fines de lucro, cuya finalidad es trabajar por el desarrollo de la matemática en Venezuela.

Asociación Matemática Venezolana
Apartado 47.898, Caracas 1041-A, Venezuela
http://amv.ivic.ve/