

Spectral Theory of Partial Differential Equations

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Preface

A *textbook* presents far more material than any professor can cover in class. These *lecture notes* present only somewhat more than I covered during two iterations of the half-semester course Spectral Theory of Partial Differential Equations (Math 595) at the University of Illinois, Urbana–Champaign, in Fall 2011 and Spring 2017.

I claim no originality for the material presented other than some originality of emphasis: I present computable examples before developing the general theory. This approach leads to occasional redundancy, and sometimes we use ideas before they are properly defined, but I think students gain a better understanding of the purpose of a theory after they are first well grounded in specific examples.

Please email me with corrections, and suggested improvements.

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Chapter 0

Introduction, prerequisites and notation

Spectral methods permeate the theory of partial differential equations. One solves linear PDEs by separation of variables, getting eigenvalues when the spectrum is discrete and continuous spectrum when it is not. Linearized stability of a steady state or traveling wave of a nonlinear PDE depends on the sign of the first eigenvalue, or on the location of the continuous spectrum in the complex plane.

This book presents highlights of spectral theory for **selfadjoint** partial differential operators, emphasizing problems with **discrete spectrum**.

Style of the course. Research differs from course work. Research often starts with questions motivated by analogy, or by trying to generalize special cases. We find answers in a nonlinear fashion, slowly developing a coherent theory by linking up and extending our scraps of known information. We cannot predict what we will need to know in order to succeed, and we certainly do not have enough time to study all relevant background material. To succeed in research, we must develop a rough mental map of the surrounding mathematical landscape, so that we know the key concepts and canonical examples even if we do not learn the proofs. Then when we need to learn more about a topic, we know where to begin.

We will emphasize computable examples, and will be neither complete in our coverage nor always rigorous in our approach. Yet you will end up possessing a trustworthy mental map of the spectral theory of partial differential equations.

6 CHAPTER 0. INTRODUCTION, PREREQUISITES AND NOTATION

Future directions. If the course were longer, then we could treat topics such as nodal patterns, geometric bounds for the first eigenvalue and the spectral gap, majorization techniques (passing from eigenvalue sums to spectral zeta functions and heat traces), and inverse spectral problems. And we could investigate more deeply the spectral and scattering theory of operators with continuous spectrum, giving applications to stability of traveling waves and similarity solutions. These fascinating topics must await another course.

Prerequisites We assume familiarity with elementary Hilbert space theory: inner product, norm, Cauchy–Schwarz, orthogonal complement, Riesz Representation Theorem, orthonormal basis (ONB), bounded operators, and compact operators. Our treatment of discrete spectra builds on the spectral theorem for compact, selfadjoint operators.

Acronyms

LHP: left half-plane, RHP: right half-plane

BC: boundary condition, IC: initial condition

Function spaces All functions are assumed to be measurable. We use the function spaces

L^1 = integrable functions,

L^2 = square integrable functions,

L^∞ = bounded functions,

but we have no need of general L^p spaces.

We use the language of Sobolev spaces throughout. Readers unfamiliar with this language can proceed unharmed; we just need that

$$H^1 = W^{1,2} = \{L^2\text{-functions with 1 derivative in } L^2\},$$

$$H^2 = W^{2,2} = \{L^2\text{-functions with 2 derivatives in } L^2\},$$

and

$$H_0^1 = W_0^{1,2} = \{H^1\text{-functions that equal zero on the boundary}\},$$

$$H_0^2 = W_0^{2,2} = \{H^2\text{-functions that equal zero on the boundary and have first derivatives zero on the boundary}\}.$$

These characterizations are not mathematically precise, but they are good enough for our purposes. Later we will recall the standard inner products that make these Sobolev spaces into Hilbert spaces.

For more on Sobolev space theory, and related concepts of weak solutions and elliptic regularity, see [Evans].

Fourier transform Sometimes we employ the L^2 -theory of the Fourier transform,

$$\widehat{f}(\xi) = (\mathcal{F}f)(\xi) = \int_{\mathbb{R}^d} f(\mathbf{x}) e^{-2\pi i \xi \cdot \mathbf{x}} \, d\mathbf{x}.$$

Only the basic facts are needed, such as that the Fourier transform preserves the L^2 -norm, and maps derivatives in the spatial domain to multipliers in the frequency domain.

Divergence theorem Given a domain Ω with smooth enough boundary, and a vector field F on the closure of the domain, one has

$$\int_{\Omega} \nabla \cdot F \, d\mathbf{x} = \int_{\partial\Omega} F \cdot \mathbf{n} \, dS$$

where \mathbf{n} denotes the outward unit normal vector on $\partial\Omega$. In 1-dimension, the Divergence Theorem is simply the Fundamental Theorem of Calculus:

$$\int_{(a,b)} F'(x) \, dx = -F(a) + F(b)$$

where the negative sign indicates the leftward orientation of \mathbf{n} at $x = a$.

Integration by parts

$$\int_{\Omega} \frac{\partial u}{\partial x_j} v \, d\mathbf{x} = - \int_{\Omega} u \frac{\partial v}{\partial x_j} \, d\mathbf{x} + \int_{\partial\Omega} uv \, \mathbf{n}_j \, dS$$

where \mathbf{n}_j is the j th component of the normal vector.

Proof. Apply the Divergence Theorem to $F = (0, \dots, 0, uv, 0, \dots, 0)$.

Green's formulas

$$\int_{\Omega} (\nabla \mathbf{u} \cdot \nabla v + v \Delta \mathbf{u}) \, dx = \int_{\partial \Omega} v \frac{\partial \mathbf{u}}{\partial \mathbf{n}} \, dS \quad (0.1)$$

$$\int_{\Omega} (\mathbf{u} \Delta v - v \Delta \mathbf{u}) \, dx = \int_{\partial \Omega} \left(\mathbf{u} \frac{\partial v}{\partial \mathbf{n}} - v \frac{\partial \mathbf{u}}{\partial \mathbf{n}} \right) \, dS \quad (0.2)$$

where the normal derivative is defined as the normal component of the gradient vector:

$$\frac{\partial \mathbf{u}}{\partial \mathbf{n}} = \nabla \mathbf{u} \cdot \mathbf{n}.$$

Proof of Green's formulas. Apply the Divergence theorem to $\mathbf{F} = v \nabla \mathbf{u}$. Interchange \mathbf{u} and v and subtract.

Part I
Discrete Spectrum

Chapter 1

ODE overture

Goal

To review the role of eigenvalues and eigenvectors in solving 1st and 2nd order systems of linear ODEs; to interpret eigenvalues as decay rates, frequencies, and stability indices; and to observe formal analogies with PDEs.

Notational convention

Eigenvalues are written with multiplicity, and are listed in increasing order (when real valued):

$$\lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \dots$$

Spectrum of a real symmetric matrix

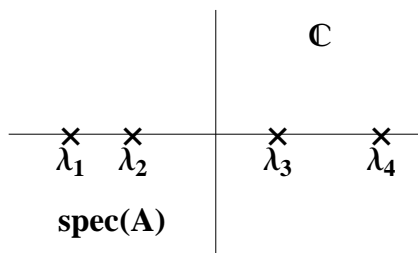
If A is a real symmetric $d \times d$ matrix (*e.g.* $A = \begin{bmatrix} a & b \\ b & c \end{bmatrix}$ when $d = 2$) then its *spectrum* is the collection of eigenvalues:

$$\text{spec}(A) = \{\lambda_1, \dots, \lambda_d\} \subset \mathbb{R}$$

(see the figure). Recall that

$$Av_j = \lambda_j v_j$$

where the eigenvectors $\{v_1, \dots, v_d\}$ can be chosen to form an ONB for \mathbb{R}^d .



Observe $A : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is diagonal with respect to the eigenbasis:

$$A\left(\sum c_j v_j\right) = \sum \lambda_j c_j v_j$$

$$\begin{bmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_d \end{bmatrix} \begin{bmatrix} c_1 \\ \vdots \\ c_d \end{bmatrix} = \begin{bmatrix} \lambda_1 c_1 \\ \vdots \\ \lambda_d c_d \end{bmatrix}$$

Corresponding statements hold for a complex Hermitian matrix acting on \mathbb{C}^d .

What does the spectrum tell us about linear ODEs? Decay rates and frequencies...

Example 1.1 (1st order).

$$\begin{aligned} \frac{dv}{dt} &= -Av && \text{ODE} \\ v(0) &= \sum c_j v_j && \text{IC} \end{aligned}$$

has solution

$$v(t) = e^{-At}v(0) \stackrel{\text{def}}{=} \sum e^{-\lambda_j t} c_j v_j.$$

Notice

$$\lambda_j = \begin{cases} \text{decay rate of the solution in direction } v_j, & \text{if } \lambda_j > 0, \\ \text{growth rate of the solution in direction } v_j, & \text{if } \lambda_j < 0. \end{cases}$$

Long-time behavior: the solution is dominated by the first mode, with

$$v(t) \simeq e^{-\lambda_1 t} c_1 v_1 \quad \text{for large } t$$

assuming $\lambda_1 < \lambda_2$ (so that the second mode decays faster than the first). The rate of collapse onto the first mode is governed by the **spectral gap** $\lambda_2 - \lambda_1$ since

$$\begin{aligned} \mathbf{v}(t) &= e^{-\lambda_1 t} \left(\mathbf{c}_1 \mathbf{v}_1 + \sum_{j=2}^d e^{-(\lambda_j - \lambda_1)t} \mathbf{c}_j \mathbf{v}_j \right) \\ &= e^{-\lambda_1 t} \left(\mathbf{c}_1 \mathbf{v}_1 + \mathcal{O}(e^{-(\lambda_2 - \lambda_1)t}) \right). \end{aligned}$$

Example 1.2 (2nd order). Assume $\lambda_1 > 0$, so that all the eigenvalues are positive. Then the system

$$\begin{aligned} \frac{d^2 \mathbf{v}}{dt^2} &= -A \mathbf{v} && \text{ODE} \\ \mathbf{v}(0) &= \sum \mathbf{c}_j \mathbf{v}_j && \text{IC displacement} \\ \mathbf{v}'(0) &= \sum \mathbf{d}_j \mathbf{v}_j && \text{IC velocity} \end{aligned}$$

has solution

$$\begin{aligned} \mathbf{v}(t) &= \cos(\sqrt{A}t) \mathbf{v}(0) + \frac{1}{\sqrt{A}} \sin(\sqrt{A}t) \mathbf{v}'(0) \\ &\stackrel{\text{def}}{=} \sum \cos(\sqrt{\lambda_j}t) \mathbf{c}_j \mathbf{v}_j + \sum \frac{1}{\sqrt{\lambda_j}} \sin(\sqrt{\lambda_j}t) \mathbf{d}_j \mathbf{v}_j. \end{aligned}$$

Notice $\sqrt{\lambda_j}$ = **frequency** of the solution in direction \mathbf{v}_j .

Example 1.3 (1st order complex). The system

$$\begin{aligned} i \frac{d\mathbf{v}}{dt} &= A \mathbf{v} && \text{ODE} \\ \mathbf{v}(0) &= \sum \mathbf{c}_j \mathbf{v}_j && \text{IC} \end{aligned}$$

has complex valued solution

$$\mathbf{v}(t) = e^{-iAt} \mathbf{v}(0) \stackrel{\text{def}}{=} \sum e^{-i\lambda_j t} \mathbf{c}_j \mathbf{v}_j.$$

Here λ_j = **frequency** of the solution in direction \mathbf{v}_j .

What does the spectrum tell us about nonlinear ODEs? In/stability...

Example 1.4 (1st order nonlinear). Suppose

$$\frac{dv}{dt} = F(v)$$

where the vector field F satisfies $F(0) = 0$, with first order Taylor expansion

$$F(v) = Bv + O(|v|^2)$$

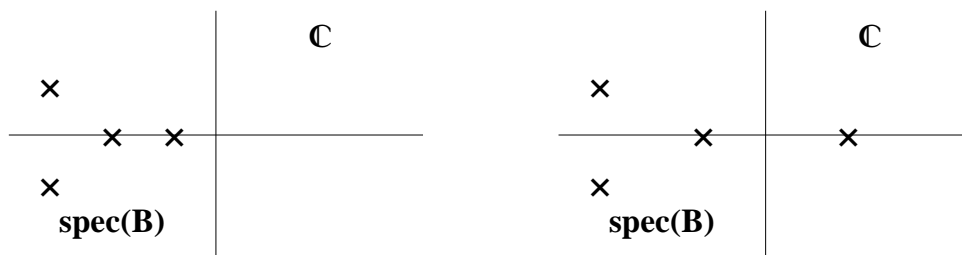
for some matrix B having d linearly independent eigenvectors v_1, \dots, v_d and corresponding eigenvalues $\lambda_1, \dots, \lambda_d \in \mathbb{C}$. (Any non-real eigenvalues come in complex conjugate pairs, since B is real.)

Clearly $v(t) \equiv 0$ is an equilibrium solution, since $F(0) = 0$. Is the equilibrium stable? To investigate, we linearize the ODE around the equilibrium to get $\frac{dv}{dt} = Bv$, which has solution

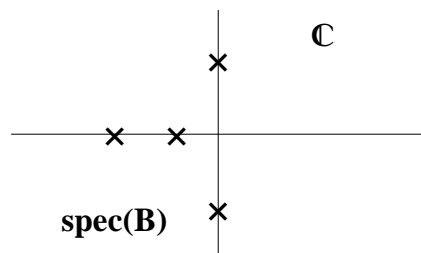
$$v(t) = e^{Bt}v(0) = \sum e^{\lambda_j t} c_j v_j.$$

Notice $v(t) \rightarrow 0$ as $t \rightarrow \infty$ if $\operatorname{Re}(\lambda_j) < 0$ for all j , whereas $|v(t)| \rightarrow \infty$ if $\operatorname{Re}(\lambda_j) > 0$ for some j (provided the corresponding coefficient c_j is nonzero, and so on). We conclude the equilibrium solution $v(t) \equiv 0$ is:

- *linearly asymptotically stable* if $\operatorname{spec}(B) \subset \text{LHP}$ (first figure below),
- *linearly unstable* if $\operatorname{spec}(B) \cap \text{RHP} \neq \emptyset$ (second figure below).



The *Linearization Theorem* of Hartman and Grobman guarantees that the nonlinear ODE indeed behaves like the linearized ODE near the equilibrium solution, in the stable and unstable cases.



The nonlinear ODE's behavior requires further investigation in the neutrally stable case where the spectrum lies in the closed left half plane and intersects the imaginary axis.

For example, if $\mathbf{B} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$ (which has eigenvalues $\pm i$), then the phase portrait for $\frac{d\mathbf{v}}{dt} = \mathbf{B}\mathbf{v}$ consists of circles centered at the origin, but the phase portrait for the nonlinear system $\frac{d\mathbf{v}}{dt} = \mathbf{F}(\mathbf{v})$ might spiral in towards the origin (stability) or out towards infinity (instability), or could display even more complicated behavior.

Looking ahead to PDEs

The negative Laplacian $\mathbf{A} = -\Delta$ on a domain $\Omega \subset \mathbb{R}^d$ with Dirichlet boundary conditions is a linear operator that behaves in some ways like a self-adjoint matrix. As we will learn in Chapter 5, its eigenvalues λ_j and eigenfunctions $\mathbf{v}_j(\mathbf{x})$ satisfy

$$\begin{aligned} -\Delta \mathbf{v}_j &= \lambda_j \mathbf{v}_j && \text{in } \Omega, \\ \mathbf{v}_j &= 0 && \text{on } \partial\Omega, \end{aligned}$$

and the spectrum is real and increases to infinity:

$$\lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \dots \rightarrow \infty.$$

The eigenfunctions form an ONB for $L^2(\Omega)$.

Formally substituting $\mathbf{A} = -\Delta$ into ODE Examples 1.1–1.3 transforms them into famous PDEs for the function $\mathbf{v}(\mathbf{x}, t)$, and transforms the formulas for \mathbf{v} into “separation of variables” solutions:

- Example 1.1 — diffusion equation $\mathbf{v}_t = \Delta \mathbf{v}$, where $\mathbf{v}(\mathbf{x}, t)$ represents chemical concentration or temperature. Solution:

$$\mathbf{v} = e^{\Delta t} \mathbf{v}(\cdot, 0) \stackrel{\text{def}}{=} \sum e^{-\lambda_j t} \mathbf{c}_j \mathbf{v}_j(\mathbf{x})$$

where the initial value is $\mathbf{v}(\cdot, 0) = \sum \mathbf{c}_j \mathbf{v}_j$. Here $\lambda_j = \text{decay rate}$.

- Example 1.2 — wave equation $\mathbf{v}_{tt} = \Delta \mathbf{v}$, where $\mathbf{v}(\mathbf{x}, t)$ represents the vertical displacement at time t of a horizontal membrane, or the oscillation of an electromagnetic signal. Solution:

$$\begin{aligned} \mathbf{v} &= \cos(\sqrt{-\Delta}t)\mathbf{v}(\cdot, 0) + \frac{1}{\sqrt{-\Delta}} \sin(\sqrt{-\Delta}t)\mathbf{v}_t(\cdot, 0) \\ &\stackrel{\text{def}}{=} \sum \cos(\sqrt{\lambda_j}t)\mathbf{c}_j \mathbf{v}_j(\mathbf{x}) + \sum \frac{1}{\sqrt{\lambda_j}} \sin(\sqrt{\lambda_j}t)\mathbf{d}_j \mathbf{v}_j(\mathbf{x}). \end{aligned}$$

In this case $\sqrt{\lambda_j} = \text{frequency}$ and $\mathbf{v}_j = \text{mode of vibration}$.

- Example 1.3 — Schrödinger equation $i\mathbf{v}_t = -\Delta \mathbf{v}$, where $|\mathbf{v}(\mathbf{x}, t)|^2$ represents the probability density at time t for the location of a quantum particle. Solution:

$$\mathbf{v} = e^{i\Delta t}\mathbf{v}(\cdot, 0) \stackrel{\text{def}}{=} \sum e^{-i\lambda_j t}\mathbf{c}_j \mathbf{v}_j(\mathbf{x}).$$

Here $\lambda_j = \text{frequency or energy level}$, and $\mathbf{v}_j = \text{quantum state}$.

Remark. The methods that will be covered in this book can handle not only the Laplacian, but a whole family of related operators including:

| | |
|----------------------------------|-----------------------|
| $A = -\Delta$ | Laplacian, |
| $A = -\Delta + V(\mathbf{x})$ | Schrödinger operator, |
| $A = (i\nabla + \vec{V})^2$ | magnetic Laplacian, |
| $A = (-\Delta)^2 = \Delta\Delta$ | biLaplacian. |

The spectral theory of these operators helps to solve the corresponding evolution equations, and explain the stability or instability of different types of equilibrium solutions, namely: steady states, standing waves, traveling waves, and similarity solutions.

Notes and comments

The Hartman–Grobman Linearization Theorem for nonlinear ODEs can be found, for example, in [Coddington and Levinson].

Chapter 2

Computable spectra and qualitative properties — Laplacian

Goal

To develop a library of explicitly computable spectra (which will motivate the later general theory) and to extract from these examples some qualitative properties such as scaling and asymptotic growth rates.

These computable spectra are classical, and so proofs are left to the reader or omitted, though the Weyl asymptotic law is proved in detail for rectangles. Completeness of the eigenfunction bases will be addressed later in the book.

Notation

Let Ω be a domain in \mathbb{R}^d , $d \geq 1$. Fix $L > 0$.

- *Dirichlet* BC means $u = 0$ on $\partial\Omega$,
- *Robin* BC means $\frac{\partial u}{\partial n} + \sigma u = 0$ on $\partial\Omega$ (where $\sigma \in \mathbb{R}$ is the Robin constant),
- *Neumann* BC means $\frac{\partial u}{\partial n} = 0$ on $\partial\Omega$.

For a vibrating drum, Dirichlet BCs mean the drum is fixed at the boundary, while Neumann BCs mean the drum is free (attached to a frictionless vertical

support). For the diffusion or heat equation, Dirichlet BCs mean the boundary is refrigerated to maintain the temperature at zero, while Neumann BCs mean the boundary is perfectly insulated and so has heat flux zero.

Spectra of the Laplacian under these BCs

Recall the Laplacian is

$$\Delta = \nabla \cdot \nabla = \left(\frac{\partial}{\partial x_1}\right)^2 + \cdots + \left(\frac{\partial}{\partial x_d}\right)^2.$$

Its eigenfunctions satisfy $-\Delta u = \lambda u$, and we put the eigenvalues in increasing order as

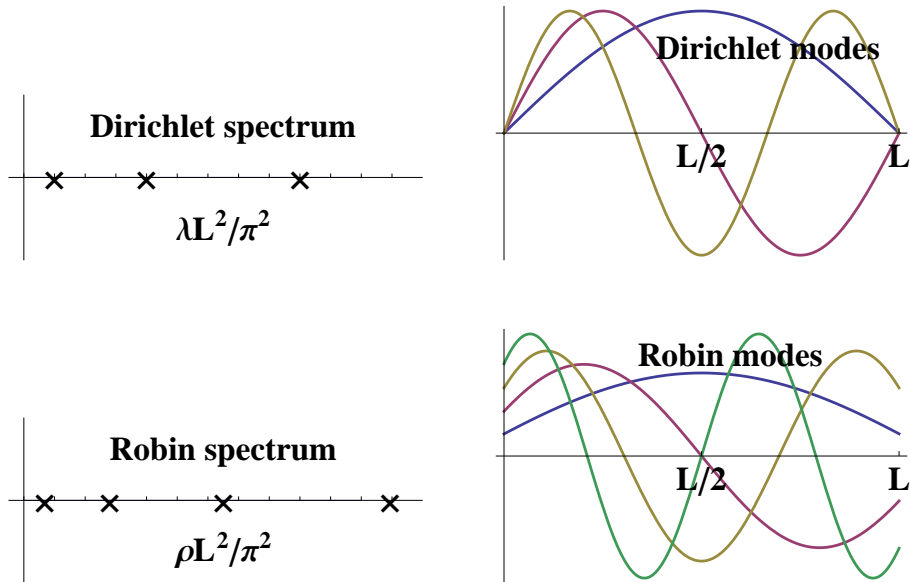
$$\lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \cdots \rightarrow \infty.$$

Chapter 5 proves existence of the spectrum under various BCs. Explicit formulas for these eigenvalues can be computed on just a handful of special domains. This chapter summarizes the most important computable cases.

Note. One usually normalizes the eigenfunctions in L^2 , in order to get an ONB, but for simplicity we do not normalize the following examples.

One dimension $-u'' = \lambda u$

1. *Circle* $\mathbb{T} = \mathbb{R}/2\pi\mathbb{Z}$, periodic BC: $u(-\pi) = u(\pi)$, $u'(-\pi) = u'(\pi)$.
 Eigenfunctions e^{ijx} for $j \in \mathbb{Z}$, or equivalently $1, \cos(jx), \sin(jx)$ for $j \geq 1$.
 Eigenvalues $\lambda_j = j^2$ for $j \in \mathbb{Z}$, or $\lambda = 0^2, 1^2, 1^2, 2^2, 2^2, \dots$
2. *Interval* $(0, L)$
 - (a) Dirichlet BC: $u(0) = u(L) = 0$.
 Eigenfunctions $u_j(x) = \sin(j\pi x/L)$ for $j \geq 1$.
 Eigenvalues $\lambda_j = (j\pi/L)^2$ for $j \geq 1$, *e.g.* $L = \pi \Rightarrow \lambda = 1^2, 2^2, 3^2, \dots$
 - (b) Robin BC: $-u'(0) + \sigma u(0) = u'(L) + \sigma u(L) = 0$. Assume $\sigma > 0$.
 Eigenfunctions $u_j(x) = \sqrt{\rho_j} \cos(\sqrt{\rho_j}x) + \sigma \sin(\sqrt{\rho_j}x)$.
 Eigenvalues $\rho_j = j$ th positive root of $\tan(\sqrt{\rho}L) = \frac{2\sigma\sqrt{\rho}}{\rho - \sigma^2}$ for $j \geq 1$.
 - (c) Neumann BC: $u'(0) = u'(L) = 0$.
 Eigenfunctions $u_j(x) = \cos((j-1)\pi x/L)$ for $j \geq 1$ (note $u_1 \equiv 1$).
 Eigenvalues $\mu_j = ((j-1)\pi/L)^2$ for $j \geq 1$, *e.g.* $L = \pi \Rightarrow \mu = 0^2, 1^2, 2^2, 3^2, \dots$



Spectral features in 1 dim: $-u'' = \lambda u$

i. Spatial frequency increases as j increases. Thus the temporal and spatial frequencies increase together.

ii. Symmetry: eigenfunctions are either even or odd with respect to the midpoint of the interval, that is, under the substitution $x \mapsto L - x$.

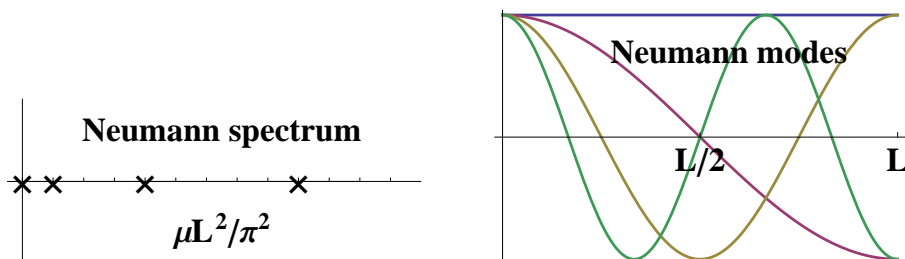
iii. Concavity: eigenfunctions are concave up wherever u is negative ($u < 0$ implies $u'' > 0$), and concave down wherever u is positive ($u > 0$ implies $u'' < 0$). Physically, this occurs because the tension in the vibrating string wants to pull it back toward the rest state.

iv. Scaling: the eigenvalue λ must balance d^2/dx^2 in the eigenvalue equation, and so $\lambda \sim (\text{length scale})^{-2}$. Intuitively, long strings produce low tones. More precisely, Dirichlet and Neumann eigenvalues scale like the reciprocal square of the length of the interval:

$$\lambda_j((0, L)) = \frac{\lambda_j((0, 1))}{L^2}$$

and similarly for the Neumann eigenvalue μ_j . Matters are slightly more complicated for Robin eigenvalues, as the Robin parameter must also be rescaled.

v. Growth rate: eigenvalues grow at a regular rate, $\lambda_j \sim (\text{const.})j^2$



vi. Robin spectrum lies between Neumann and Dirichlet, and approaches them in suitable limiting cases:

$$\text{Neumann} \xleftarrow{\sigma \rightarrow 0} \text{Robin} \xrightarrow{\sigma \rightarrow \infty} \text{Dirichlet}$$

as one sees formally letting σ approach 0 or ∞ in the Robin BC $\frac{\partial u}{\partial n} + \sigma u = 0$.

Two dimensions $-\Delta u = \lambda u$

Write $\Delta = \partial^2/\partial x^2 + \partial^2/\partial y^2$.

1. *Rectangle* $\Omega = (0, L) \times (0, M)$ (product of intervals).

We may assume the sides of the rectangle are parallel to the coordinate axes because the Laplacian, and hence its spectrum, is rotationally and translationally invariant; see the Exercises.

One finds eigenvalues by separating variables in rectangular coordinates x, y . See the formulas below and the figures at the end of the chapter.

(a) Dirichlet BC: $u = 0$

Eigenfunctions $u(x) = \sin(j\pi x/L) \sin(k\pi y/M)$ for $j, k \geq 1$.

Eigenvalues $\lambda = (j\pi/L)^2 + (k\pi/M)^2$ for $j, k \geq 1$.

e.g. $L = M = \pi \Rightarrow \lambda = j^2 + k^2$ for $j, k \geq 1$; that is, $\lambda = 2, 5, 5, 8, 10, 10, \dots$

These eigenvalues are the squares of distances from the origin to the positive integer lattice points.

(b) Neumann BC: $\frac{\partial u}{\partial n} = 0$

Eigenfunctions $u(x) = \cos((j-1)\pi x/L) \cos((k-1)\pi y/M)$ for $j, k \geq 1$.

Eigenvalues $\mu = ((j-1)\pi/L)^2 + ((k-1)\pi/M)^2$ for $j, k \geq 1$.

e.g. $L = M = \pi \Rightarrow \mu = 0, 1, 1, 2, 4, 4, \dots$

2. *Disk* $\Omega = \{x \in \mathbb{R}^2 : |x| < R\}$.

Separate variables using polar coordinates r, θ .

- (a) Dirichlet BC: $u = 0$
Eigenfunctions

$$J_0(rj_{0,m}/R) \text{ for } m \geq 1,$$

$$J_n(rj_{n,m}/R) \cos(n\theta) \text{ and } J_n(rj_{n,m}/R) \sin(n\theta) \text{ for } n \geq 1, m \geq 1.$$

Eigenvalues $\lambda = (j_{n,m}/R)^2$ for $n \geq 0, m \geq 1$, where

$$\begin{aligned} J_n &= \text{Bessel function of order } n, \\ j_{n,m} &= m\text{-th positive root of } J_n(r) = 0. \end{aligned}$$

When $n = 0$, the modes are purely radial. When $n \geq 1$, the modes have angular dependence (both cosine and sine modes), and $\lambda_{n,m}$ has multiplicity 2. The Bessel functions satisfy

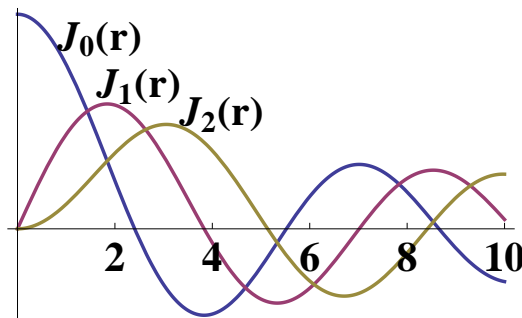
$$r^2 J_n''(r) + r J_n'(r) + (r^2 - n^2) J_n(r) = 0$$

and behave like r^n near the origin: $J_n(r) \simeq (\text{const.})r^n$ when $r \simeq 0$.

From the graphs of the Bessel functions J_0, J_1, J_2 we can read off the first four roots:

$$j_{0,1} \simeq 2.40, \quad j_{1,1} \simeq 3.83, \quad j_{2,1} \simeq 5.13, \quad j_{0,2} \simeq 5.52.$$

These roots generate the first six eigenvalues (remembering eigenvalues are double when $n \geq 1$).



- (b) Neumann BC: $\frac{\partial u}{\partial n} = 0$

Use roots of $J'_n(r) = 0$. See [Bandle, Chapter III].

3. *Equilateral triangle* of sidelength L .

Separation of variables fails, but one may reflect repeatedly to a hexagonal lattice whose eigenfunctions are trigonometric. See [Mathews and Walker, McCartin].

Dirichlet eigenvalues:

$$\lambda = \frac{16\pi^2}{9L^2}(j^2 + jk + k^2) \quad \text{for } j, k \geq 1.$$

Neumann eigenvalues:

$$\mu = \frac{16\pi^2}{9L^2}(j^2 + jk + k^2) \quad \text{for } j, k \geq 0.$$

Spectral features in 2 dim: $-\Delta u = \lambda u$

i. Scaling: the eigenvalue λ must balance Δ , and so $\lambda \sim (\text{length scale})^{-2}$. Intuitively, big drums produce low tones. More precisely, Dirichlet and Neumann eigenvalues scale like the reciprocal square of the scale of the domain:

$$\lambda_n(t\Omega) = \frac{\lambda_n(\Omega)}{t^2}$$

and similarly for the Neumann eigenvalue μ_n . This scaling relation can be verified explicitly in the examples above, and holds also for general domains as explained in the exercises.

ii. Sub/superharmonicity: eigenfunctions are subharmonic wherever u is negative (since $u < 0$ implies $\Delta u > 0$), and superharmonic wherever u is positive (since $u > 0$ implies $\Delta u < 0$). Physically, the tension in the membrane wants to pull it back toward the rest state.

iii. Degenerate domains: Dirichlet and Neumann spectra behave quite differently when the domain degenerates. Consider the rectangle, for example. Fix one side length L , and let the other side length M tend to 0. Then the first positive Dirichlet eigenvalue blows up, since taking $j = k = 1$ gives eigenvalue $(\pi/L)^2 + (\pi/M)^2 \rightarrow \infty$. Meanwhile the first positive Neumann eigenvalue is constant (independent of M) because taking $j = 1, k = 0$, gives eigenvalue $(\pi/L)^2$.

iv. Growth rate: eigenvalues of the rectangle grow at a regular rate:

Proposition 2.1. (*Weyl's law for rectangles*) The rectangle $(0, L) \times (0, M)$ satisfies

$$\lambda_n \sim \mu_n \sim \frac{4\pi n}{\text{Area}} \quad \text{as } n \rightarrow \infty,$$

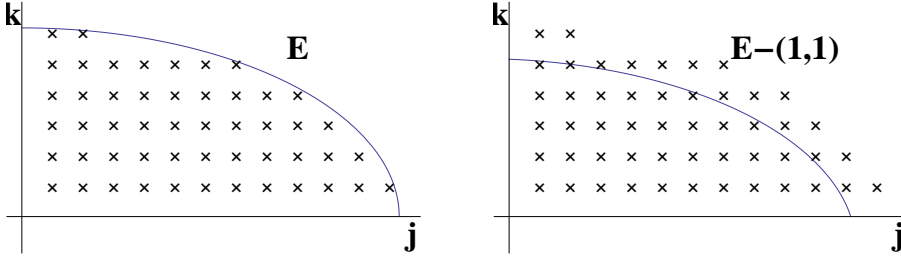
where $\text{Area} = LM$ is the area of the rectangle and $\lambda_1, \lambda_2, \lambda_3, \dots$ and $\mu_1, \mu_2, \mu_3, \dots$ are the Dirichlet and Neumann eigenvalues respectively, in increasing order.

Proof. We give a proof for Dirichlet eigenvalues; the Neumann case is similar.

Define for $\alpha > 0$ the eigenvalue counting function

$$\begin{aligned} N(\alpha) &= \#\{\text{eigenvalues} \leq \alpha\} \\ &= \#\{(j, k) \in \mathbb{N} \times \mathbb{N} : \frac{j^2}{\alpha L^2/\pi^2} + \frac{k^2}{\alpha M^2/\pi^2} \leq 1\} \\ &= \#\{(j, k) \in \mathbb{N} \times \mathbb{N} : (j, k) \in E\} \end{aligned}$$

where E is the ellipse $(x/a)^2 + (y/b)^2 \leq 1$ and $a = \sqrt{\alpha}L/\pi$, $b = \sqrt{\alpha}M/\pi$.



We associate each lattice point $(j, k) \in E$ with the square

$$S(j, k) = [j - 1, j] \times [k - 1, k]$$

whose upper right corner lies at (j, k) . These squares all lie within E , and so by comparing areas we find

$$N(\alpha) \leq (\text{area of } E \text{ in first quadrant}) = \frac{1}{4}\pi ab = \frac{\text{Area}}{4\pi}\alpha.$$

In the reverse direction, the union of the squares having $(j, k) \in E$ covers a copy of E shifted down and left by one unit, as a little thought shows:

$$\cup S(j, k) \supset (E - (1, 1)) \cap (\text{first quadrant}).$$

Comparing areas implies

$$\begin{aligned} N(\alpha) &\geq \frac{1}{4}\pi ab - a - b \\ &= \frac{LM}{4\pi}\alpha - \frac{L+M}{\pi}\sqrt{\alpha} \\ &= \frac{\text{Area}}{4\pi}\alpha - \frac{\text{Perimeter}}{2\pi}\sqrt{\alpha}. \end{aligned}$$

Combining our upper and lower estimates shows that

$$N(\alpha) \sim \frac{\text{Area}}{4\pi}\alpha$$

as $\alpha \rightarrow \infty$. To complete the proof we simply invert this last asymptotic, with the help of the lemma below. \square

Lemma 2.2. (*Inversion of asymptotics*) Fix $c > 0$. Then:

$$N(\alpha) \sim \frac{\alpha}{c} \quad \text{as } \alpha \rightarrow \infty \quad \implies \quad \lambda_n \sim cn \quad \text{as } n \rightarrow \infty.$$

Proof. Formally substituting $\alpha = \lambda_n$ and $N(\alpha) = n$ takes us from the first asymptotic to the second. The difficulty with making this substitution rigorous is that if λ_n is a multiple eigenvalue, then $N(\lambda_n)$ can exceed n . In other words, $N(\lambda_n) \geq n$ but equality need not hold.

To circumvent the problem, we argue as follows. Given $\varepsilon > 0$ we know from $N(\alpha) \sim \alpha/c$ that

$$(1 - \varepsilon)\frac{\alpha}{c} < N(\alpha) < (1 + \varepsilon)\frac{\alpha}{c}$$

for all large α . Substituting $\alpha = \lambda_n$ into the right hand inequality and recalling $N(\lambda_n) \geq n$ implies that

$$n < (1 + \varepsilon)\frac{\lambda_n}{c}$$

for all large n . Letting $0 < \delta < 1$ and substituting $\alpha = \lambda_n - \delta$ into the left hand inequality implies, since $N(\lambda_n - \delta) < n$, that

$$(1 - \varepsilon)\frac{\lambda_n - \delta}{c} < n$$

for each large n . Hence by letting $\delta \rightarrow 0$,

$$(1 - \varepsilon) \frac{\lambda_n}{c} \leq n.$$

We deduce that

$$\frac{1}{1 + \varepsilon} < \frac{\lambda_n}{cn} \leq \frac{1}{1 - \varepsilon}$$

for all sufficiently large n (depending on ε), and since ε is arbitrary we conclude

$$\lim_{n \rightarrow \infty} \frac{\lambda_n}{cn} = 1$$

as desired. □

Later, in Chapter 12, we will prove **Weyl's Asymptotic Law** that

$$\lambda_n \sim 4\pi n / \text{Area}$$

for all bounded domains in 2 dimensions, regardless of shape or boundary conditions. This Law was conjectured by Hilbert, who was Weyl's thesis advisor.

Question. What does a “typical” eigenfunction look like, in each of the examples above? See the figures below...

Exercises

Max/min problems for eigenvalues of rectangles and domains in the plane

2.1 — Find the shape of rectangle that minimizes $\lambda_1 A$ among all rectangles, where A denotes the area.

Note. The eigenvalue is multiplied by area in this problem in order to obtain a scale-invariant quantity: notice $\lambda_1 A$ does not change value when the side lengths of the rectangle are multiplied by a constant factor (replacing L and M with tL and tM , for example).

2.2 — Guess the shape of domain that minimizes $\lambda_1 A$ among all planar domains. (Faber–Krahn theorem.)

2.3 — Find the shape of rectangle that maximizes $\mu_2 A$ among all rectangles.

2.4 — Guess the shape of domain that maximizes $\mu_2 A$ among all planar domains. (Szegő–Weinberger theorem.)

The moral is the same for each of the preceding problems — namely that nature prefers symmetric optimizers.

Inverse spectral problems

2.5 — Show that a square is determined by its fundamental tone, that is, by its first Dirichlet eigenvalue. (In other words, given a square domain and its first eigenvalue, one can determine the sidelength of the square.)

2.6 — How many Dirichlet eigenvalues are needed to determine a rectangle?

2.7 — How many Dirichlet eigenvalues do you expect would determine a triangle? (Open problem! [Antunes and Freitas] investigated numerically. More about eigenvalues on triangles can be found in [Henrot *et al.*])

2.8 — How many Neumann eigenvalues are needed to determine a rectangle?

Eigenfunctions of a right isosceles triangle

2.9 — Consider the 45–45–90 degree triangle $\{(x, y) : 0 < x < y < \pi\}$, which is the region of the square $(0, \pi) \times (0, \pi)$ lying above the diagonal line $x = y$.

(i) Find an eigenfunction of the Laplacian on this triangle that satisfies the Dirichlet boundary condition on the left and top sides, and the Neumann condition on the diagonal side.

(ii) Find an eigenfunction of the Laplacian on this triangle that satisfies the Dirichlet boundary condition on all three sides.

(iii) Find infinitely many Dirichlet eigenfunctions on the triangle.

Invariance under reflections, translations and rotations in the plane

2.10 — Show the Laplacian is invariant under reflections across the y -axis:

$$\Delta(\mathbf{u}(-x, y)) = (\Delta\mathbf{u})(-x, y)$$

whenever \mathbf{u} is a smooth function of two variables. One may write the result more formally as

$$\Delta(\mathbf{u} \circ F) = (\Delta\mathbf{u}) \circ F$$

where

$$F \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} -x \\ y \end{pmatrix}$$

is the reflection of \mathbb{R}^2 across the y -axis.

2.11 — Show the Laplacian is invariant under translations:

$$\Delta(\mathbf{u} \circ T) = (\Delta\mathbf{u}) \circ T$$

where \mathbf{u} is a smooth function of two variables and

$$\mathbf{T} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x + \mathbf{a} \\ y + \mathbf{b} \end{pmatrix}$$

is a translation of \mathbb{R}^2 by the constant vector $\begin{pmatrix} \mathbf{a} \\ \mathbf{b} \end{pmatrix}$.

2.12 — Show the Laplacian is invariant under rotations:

$$\Delta(\mathbf{u} \circ \mathbf{R}) = (\Delta\mathbf{u}) \circ \mathbf{R}$$

where \mathbf{u} is a smooth function of two variables and

$$\mathbf{R} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

is a rotation of \mathbb{R}^2 by angle α .

Remark. Rotational invariance of the Laplacian might seem surprising, since the Laplacian is defined in terms of rectangular coordinates.

2.13 — Show the Dirichlet eigenvalues of a domain remain unchanged if the domain is reflected, translated or rotated. The same holds true for Neumann eigenvalues. (Physically, this invariance means vibrating membranes are unaffected by the coordinate systems we place upon them.)

These invariance properties of the spectrum hold in higher dimensions also.

Scaling invariance

2.14 — Show the Laplacian is invariant under dilations:

$$\Delta(\mathbf{u}(t\mathbf{x}, t\mathbf{y})) = t^2(\Delta\mathbf{u})(t\mathbf{x}, t\mathbf{y})$$

whenever \mathbf{u} is a smooth function of two variables and $t > 0$. That is,

$$\Delta(\mathbf{u} \circ \mathbf{D}) = t^2(\Delta\mathbf{u}) \circ \mathbf{D}$$

where

$$\mathbf{D} \begin{pmatrix} x \\ y \end{pmatrix} = t \begin{pmatrix} x \\ y \end{pmatrix}$$

is the dilation or scaling of \mathbb{R}^2 by the factor t .

2.15 — Show the Dirichlet eigenvalues of a domain Ω rescale as follows:

$$\lambda_n(t\Omega) = \frac{\lambda_n(\Omega)}{t^2}$$

whenever $t > 0$, and similarly for the Neumann eigenvalues μ_n . (Physically, this scaling formula means large drums produce low tones.) Robin eigenvalues rescale the same way under dilation, provided the Robin parameter is rescaled to σ/t on the domain $t\Omega$.

These rescaling formulas hold in higher dimensions also.

Weyl asymptotic and higher eigenvalues

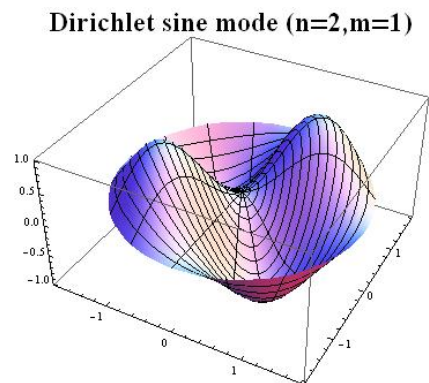
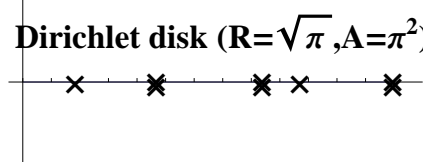
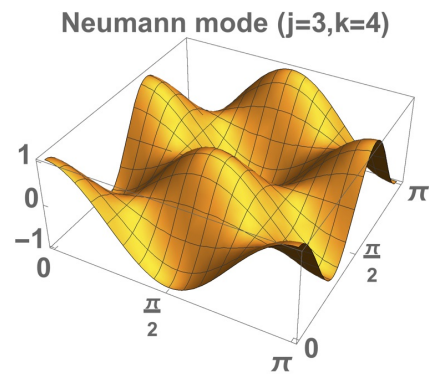
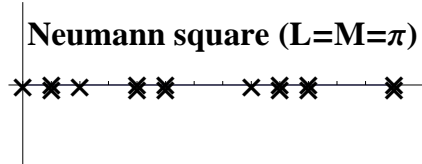
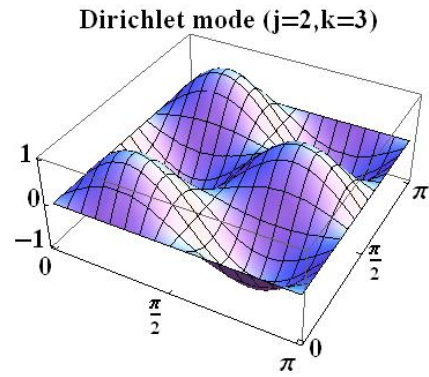
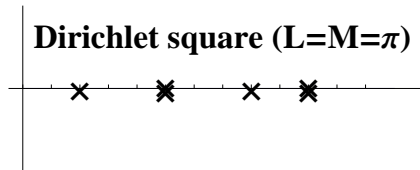
2.16 — Prove that for rectangles, the Weyl asymptotic expression provides a lower bound on each Dirichlet eigenvalue:

$$\lambda_n A \geq 4\pi n, \quad n = 1, 2, 3, \dots$$

Pólya's Conjecture claims that this inequality holds on every (bounded) domain in 2-dimensions. (Open problem! Known for tiling domains, but for general domains the conjecture remains open for all $n \geq 3$. See Chapter 13.)

Notes and comments

For the computable spectra stated in this chapter, see [Strauss] Chapters 4 and 10, and [Farlow] Lesson 30, among many other good sources.



Chapter 3

Computable spectra — Schrödinger

Goal

To present the classic examples of the harmonic oscillator (1 dim) and hydrogen atom (3 dim).

Harmonic oscillator in 1 dimension $-u'' + x^2u = Eu$

We will state first and ask questions later.

Boundary condition: $u(x) \rightarrow 0$ as $x \rightarrow \pm\infty$. (A deeper perspective on this boundary condition at infinity, in terms of a weighted L^2 -space, is examined in Chapter 7.)

Eigenfunctions $u_k(x) = H_k(x)e^{-x^2/2}$ for $k \geq 0$, where

$$H_k(x) = (-1)^k e^{x^2} \left(\frac{d}{dx}\right)^k e^{-x^2} = k\text{-th Hermite polynomial.}$$

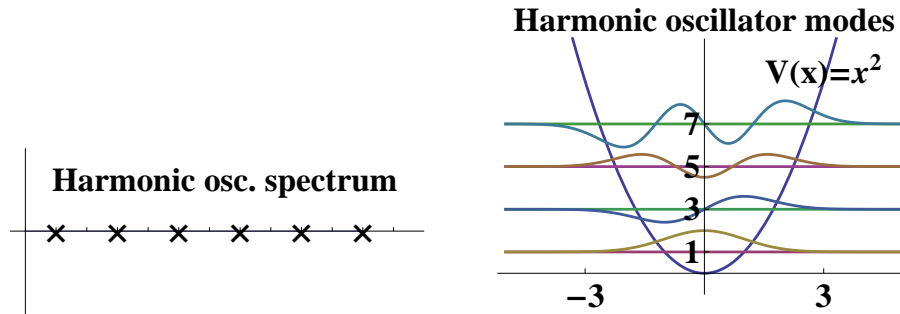
Eigenvalues $E_k = 2k + 1$ for $k \geq 0$, so that $E = 1, 3, 5, 7, \dots$

Examples. $H_0(x) = 1$, $H_1(x) = 2x$, $H_2(x) = 4x^2 - 2$.

Ground state: $u_0(x) = e^{-x^2/2} = \text{Gaussian}$. Check: $-u_0'' + x^2u_0 = u_0$.

Spectral features

- i. Spatial frequency increases as k increases. Thus the temporal and spatial frequencies increase together.
- ii. Symmetry: eigenfunctions are either even or odd.



- iii. Scaling: the rescaled potential c^2x^2 has eigenvalues cE_k , whenever $c > 0$. Explicitly, $-v_k'' + c^2x^2v_k = cE_kv_k$ for eigenfunctions $v_k(x) = u_k(\sqrt{c}x)$.
- iv. Growth rate: eigenvalues grow at a regular rate, $E_k \sim (\text{const.})k$

Quantum mechanical interpretation

If $u(x, t)$ solves the time-dependent Schrödinger equation

$$iu_t = -u'' + x^2u$$

with potential $V(x) = x^2$ and u has L^2 -norm equal to 1, then $|u|^2$ represents the probability density for the location of a particle in a quadratic potential well.

The k -th eigenfunction $u_k(x)$ is called the k -th excited state, because it gives a “standing wave” solution

$$u(x, t) = e^{-iE_k t} u_k(x)$$

to the time-dependent equation. The higher the frequency or “energy” E_k of the excited state, the farther the wavefunction can spread out in the potential well, as the solution plots show.

Justifying the harmonic oscillator formulas

Method 1: ODEs. Since $u_0(x) = e^{-x^2/2}$ is an eigenfunction, we guess that all eigenfunctions decay like $e^{-x^2/2}$. So we try the change of variable $u = we^{-x^2/2}$. The eigenfunction equation becomes

$$w'' - 2xw' + (E - 1)w = 0,$$

which we recognize as the **Hermite equation**. The only valid power series solutions turn out to be terminating power series, namely the **Hermite polynomials**. All other solutions grow like e^{x^2} at infinity, violating the boundary condition on \mathbf{u} . Detailed calculations are in [Strauss].

Method 2: Raising and lowering energy levels. Define

$$\begin{aligned} \mathbf{h}^+ &= -\frac{d}{dx} + x && \text{(raising or creation operator),} \\ \mathbf{h}^- &= \frac{d}{dx} + x && \text{(lowering or annihilation operator).} \end{aligned}$$

Write $H = -\frac{d^2}{dx^2} + x^2$ for the harmonic oscillator operator. Then one computes

$$\begin{aligned} H &= \mathbf{h}^+ \mathbf{h}^- + 1 \\ &= \mathbf{h}^- \mathbf{h}^+ - 1. \end{aligned}$$

Claim. If \mathbf{u} is an eigenfunction with eigenvalue E then $\mathbf{h}^\pm \mathbf{u}$ is an eigenfunction with eigenvalue $E \pm 2$. (In other words, \mathbf{h}^+ “raises” the energy, and \mathbf{h}^- “lowers” the energy.)

Proof.

$$\begin{aligned} H(\mathbf{h}^+ \mathbf{u}) &= (\mathbf{h}^+ \mathbf{h}^- + 1)(\mathbf{h}^+ \mathbf{u}) \\ &= \mathbf{h}^+(\mathbf{h}^- \mathbf{h}^+ + 1)\mathbf{u} \\ &= \mathbf{h}^+(H + 2)\mathbf{u} \\ &= \mathbf{h}^+(E + 2)\mathbf{u} \\ &= (E + 2)\mathbf{h}^+ \mathbf{u} \end{aligned}$$

and similarly $H(\mathbf{h}^- \mathbf{u}) = (E - 2)\mathbf{h}^- \mathbf{u}$ (exercise).

The only exception to the Claim is that $\mathbf{h}^- \mathbf{u}$ will not be an eigenfunction if $\mathbf{h}^- \mathbf{u} \equiv 0$, which occurs precisely when $\mathbf{u} = \mathbf{u}_0 = e^{-x^2/2}$. Thus the lowering operator annihilates the ground state.

Applying the raising operator \mathbf{h}^+ to the groundstate \mathbf{u}_0 with energy 1 yields the first excited state \mathbf{u}_1 with energy 3. Applying the raising operator repeatedly yields the excited states $\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3, \dots$, with energies 3, 5, 7, ... (verification left to the reader).

It is reasonable to ask whether any other eigenfunctions exist in addition to the \mathbf{u}_k . They do not, as can be seen using the tools of either Method 1 or Method 2.

Relation to classical harmonic oscillator

Consider a classical oscillator with mass $m = 2$, spring constant $k = 2$, and displacement $x(t)$, so that $2\ddot{x} = -2x$. The total energy (kinetic plus potential) is

$$\dot{x}^2 + x^2 = \text{const.} = E.$$

To describe a quantum oscillator, one formally replaces momentum \dot{x} with the “momentum operator” $-i\frac{d}{dx}$ and lets the equation act on a function u :

$$\left[\left(-i\frac{d}{dx} \right)^2 + x^2 \right] u = Eu.$$

This is exactly the eigenfunction equation $-u'' + x^2u = Eu$ for the quantum harmonic oscillator.

Harmonic oscillator in higher dimensions $-\Delta u + |x|^2 u = Eu$

Here $|x|^2 = x_1^2 + \dots + x_d^2$. The operator separates into a sum of 1 dimensional operators, and hence has product type eigenfunctions

$$u = u_{k_1}(x_1) \cdots u_{k_d}(x_d), \quad E = (2k_1 + 1) + \dots + (2k_d + 1),$$

where $k_1, \dots, k_d \geq 0$.

Hydrogen atom in 3 dimensions $-\Delta u - \frac{2}{|x|} u = Eu$

For our second computable example, let $V(x) = -2/|x|$ be the attractive electrostatic “Coulomb” potential created by the proton in the hydrogen nucleus. Notice the gradient of this potential gives the correct $|x|^{-2}$ inverse square law for electrostatic force.

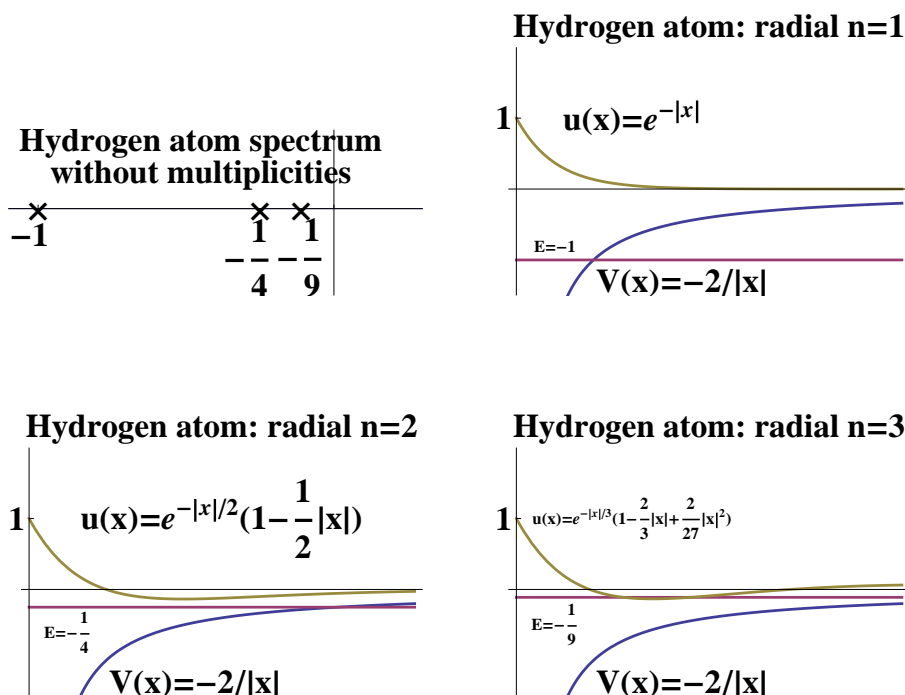
Boundary conditions: $u(x) \rightarrow 0$ as $|x| \rightarrow \infty$.

Eigenvalues: $E = -1, -\frac{1}{4}, -\frac{1}{9}, \dots$ with multiplicities $1, 4, 9, \dots$. That is, the eigenvalue $E = -1/n^2$ has multiplicity n^2 .

Eigenfunctions: $e^{-r/n} L_n^\ell(r) Y_\ell^m(\theta, \phi)$ for $0 \leq |m| \leq n - 1$, where Y_ℓ^m is a spherical harmonic and L_n^ℓ equals r^ℓ times a Laguerre polynomial.

(Recall the spherical harmonics are eigenfunctions of the spherical Laplacian in 3 dimensions, with $-\Delta_{\text{sphere}} Y_\ell^m = \ell(\ell + 1) Y_\ell^m$. In 2 dimensions the spherical harmonics have the form $Y = \cos(k\theta)$ and $Y = \sin(k\theta)$, which satisfy $-\frac{d^2}{d\theta^2} Y = k^2 Y$.)

Examples. The first three purely radial eigenfunctions ($\ell = m = 0, n = 1, 2, 3$) are e^{-r} , $e^{-r/2}(1 - \frac{r}{2})$, $e^{-r/3}(1 - \frac{2}{3}r + \frac{2}{27}r^2)$.



The corner (nonzero slope) in the graph of the eigenfunction at $r = 0$ is due to the singularity of the Coulomb potential at the origin.

Continuous spectrum Eigenfunctions with positive energy $E > 0$ do exist, but they oscillate as $|x| \rightarrow \infty$, and thus do not satisfy our boundary conditions. They represent “free electrons” that are not bound to the nucleus. See our later discussion of continuous spectrum, in Chapter 21.

Exercises

3.1 — Find the energies (eigenvalues) of the rescaled harmonic oscillator

$$-\Delta u + (c_1^2 x_1^2 + c_2^2 x_2^2)u = Eu$$

in 2-dimensions, where $c_1, c_2 > 0$ are constants and $u(x) \rightarrow 0$ as $|x| \rightarrow \infty$.

3.2 — Write E_0 for the lowest energy of the oscillator in Exercise 3.1, and let

$$\text{Area} = \int_{\{c_1^2 x_1^2 + c_2^2 x_2^2 < 1\}} dx_1 dx_2 = \frac{\pi}{c_1 c_2}$$

be the area enclosed by the level set at height 1 of the potential function. Assume the Area is fixed, say $\text{Area} = \alpha$, and minimize E_0 with respect to the allowable choices of c_1 and c_2 . Then describe your result intuitively.

3.3 — Find the energies of the more general 2-dimensional harmonic oscillator

$$-\Delta \mathbf{u} + (\mathbf{x}^\top \mathbf{A} \mathbf{x}) \mathbf{u} = E \mathbf{u},$$

where \mathbf{A} is a positive definite real symmetric 2×2 matrix, $\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$ and $\mathbf{u}(\mathbf{x}) \rightarrow 0$ as $|\mathbf{x}| \rightarrow \infty$. *Hint:* diagonalize \mathbf{A} .

3.4 — Find a Weyl-type asymptotic formula for the n -th energy of the rescaled harmonic oscillator appearing in Exercise 3.1, and similarly for Exercise 3.3.

Notes and comments

For more information on the harmonic oscillator and hydrogen atom, see [Strauss] Sections 9.4, 9.5, 10.7, and [Gustafson and Sigal] Section 7.5, 7.7.

Chapter 4

Discrete spectral theorem for sesquilinear forms

Goal

To state the spectral theorem for a coercive sesquilinear form on a dense, compactly imbedded Hilbert space, and to prove it using the spectral theorem for compact selfadjoint operators.

Later chapters will apply this spectral theorem to unify and extend the explicit examples of Chapters 2 and 3.

Preview 1 — weak eigenvectors of matrices

Consider a Hermitian matrix A (so that $A^T = \overline{A}$) and suppose \mathbf{u} is an eigenvector with eigenvalue γ , meaning $A\mathbf{u} = \gamma\mathbf{u}$. Take the dot product with an arbitrary vector \mathbf{v} to obtain

$$A\mathbf{u} \cdot \overline{\mathbf{v}} = \gamma\mathbf{u} \cdot \overline{\mathbf{v}}, \quad \forall \mathbf{v} \in \mathbb{C}^d.$$

Call this condition the “weak form” of the eigenvector equation. Clearly it implies the original “strong” form, because $(A\mathbf{u} - \gamma\mathbf{u}) \cdot \overline{\mathbf{v}} = 0$ for all \mathbf{v} implies $A\mathbf{u} - \gamma\mathbf{u} = \mathbf{0}$.

Notice the Hermitian property of the matrix guarantees the left side of the weak equation is conjugate-symmetric: $A\mathbf{u} \cdot \overline{\mathbf{v}} = \overline{A\mathbf{v} \cdot \overline{\mathbf{u}}}$. Symmetry ensures that all eigenvalues are real ($\overline{\gamma} = \gamma$), by choosing $\mathbf{v} = \mathbf{u}$ in the weak form.

The weak form of the eigenvector equation indicates the correct approach for generalizing from the matrix case to Hilbert spaces, in this chapter.

Preview 2 — weak eigenfunctions of the Laplacian

Consider an eigenfunction of the Laplacian in a domain Ω , satisfying $-\Delta \mathbf{u} = \lambda \mathbf{u}$. Multiply by a function $\mathbf{v} \in H_0^1(\Omega)$ and integrate to obtain

$$-\int_{\Omega} \mathbf{v} \Delta \mathbf{u} \, dx = \lambda \int_{\Omega} \mathbf{u} \mathbf{v} \, dx.$$

Assume \mathbf{u} and \mathbf{v} are real valued for simplicity. Green's formula (0.1) and the assumption that $\mathbf{v} = 0$ on $\partial\Omega$ imply that

$$\int_{\Omega} \nabla \mathbf{u} \cdot \nabla \mathbf{v} \, dx = \lambda \langle \mathbf{u}, \mathbf{v} \rangle_{L^2(\Omega)}, \quad \forall \mathbf{v} \in H_0^1(\Omega).$$

We take this condition as the definition of the “weak form” of the eigenfunction equation. Notice that \mathbf{u} needs only first order derivatives in order for this definition to make sense. Thus in principle, the weak eigenfunction equation is less restrictive than the original “classical” eigenfunction equation involving the Laplacian, which requires \mathbf{u} to possess second order derivatives.

Our plan is to construct an ONB of weak eigenfunctions using the Hilbert space methods of this chapter, and later invoke PDE regularity theory to conclude that weak eigenfunctions are in fact smooth functions satisfying the equation $-\Delta \mathbf{u} = \lambda \mathbf{u}$ classically. Chapter 5 will implement this plan.

Now we develop the spectral theorem for sesquilinear forms in Hilbert space.

Hypotheses

Consider two infinite dimensional Hilbert spaces \mathcal{H} and \mathcal{K} over \mathbb{R} (or \mathbb{C}):

- \mathcal{H} : inner product $\langle \mathbf{u}, \mathbf{v} \rangle_{\mathcal{H}}$, norm $\|\mathbf{u}\|_{\mathcal{H}}$,
- \mathcal{K} : inner product $\langle \mathbf{u}, \mathbf{v} \rangle_{\mathcal{K}}$, norm $\|\mathbf{u}\|_{\mathcal{K}}$.

Assume \mathcal{H} is separable (has a countable dense subset) and:

1. \mathcal{K} is continuously and densely imbedded in \mathcal{H} , meaning a continuous linear injection

$$\iota : \mathcal{K} \rightarrow \mathcal{H}$$

exists such that $\iota(\mathcal{K})$ dense in \mathcal{H} . Thus we may regard \mathcal{K} as a subset of \mathcal{H} .

2. The imbedding $\mathcal{K} \hookrightarrow \mathcal{H}$ is **compact**, meaning if E is a bounded subset of \mathcal{K} then E is precompact when considered as a subset of \mathcal{H} . Equivalently, every bounded sequence in \mathcal{K} has a subsequence that converges in \mathcal{H} .

3. A map $\mathbf{a} : \mathcal{K} \times \mathcal{K} \rightarrow \mathbb{R}$ (or \mathbb{C}) exists that is **sesquilinear**:

$\mathbf{u} \mapsto \mathbf{a}(\mathbf{u}, \mathbf{v})$ is linear, for each fixed \mathbf{v} ,

$\mathbf{v} \mapsto \mathbf{a}(\mathbf{u}, \mathbf{v})$ is linear (or conjugate linear), for each fixed \mathbf{u} ,

and **continuous**:

$$|\mathbf{a}(\mathbf{u}, \mathbf{v})| \leq (\text{const.}) \|\mathbf{u}\|_{\mathcal{K}} \|\mathbf{v}\|_{\mathcal{K}},$$

and **symmetric**:

$$\mathbf{a}(\mathbf{v}, \mathbf{u}) = \mathbf{a}(\mathbf{u}, \mathbf{v}) \quad (\text{or } \overline{\mathbf{a}(\mathbf{u}, \mathbf{v})}).$$

4. \mathbf{a} is **coercive** on \mathcal{K} , meaning

$$\mathbf{a}(\mathbf{u}, \mathbf{u}) \geq c \|\mathbf{u}\|_{\mathcal{K}}^2 \quad \forall \mathbf{u} \in \mathcal{K},$$

for some $c > 0$. Hence $\mathbf{a}(\mathbf{u}, \mathbf{u}) \asymp \|\mathbf{u}\|_{\mathcal{K}}^2$.

Symmetry and coercivity imply that:

$\mathbf{a}(\mathbf{u}, \mathbf{v})$ defines an inner product whose norm is equivalent to the $\|\cdot\|_{\mathcal{K}}$ -norm.

Spectral theorem

Theorem 4.1. *Under the hypotheses above, there exist vectors $\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3, \dots \in \mathcal{K}$ and numbers*

$$0 < \gamma_1 \leq \gamma_2 \leq \gamma_3 \leq \dots \rightarrow \infty$$

such that:

- \mathbf{u}_j is an eigenvector of $\mathbf{a}(\cdot, \cdot)$ with eigenvalue γ_j , meaning

$$\mathbf{a}(\mathbf{u}_j, \mathbf{v}) = \gamma_j \langle \mathbf{u}_j, \mathbf{v} \rangle_{\mathcal{H}} \quad \forall \mathbf{v} \in \mathcal{K}, \quad (4.1)$$

- $\{\mathbf{u}_j\}$ is an ONB for \mathcal{H} ,
- $\{\mathbf{u}_j / \sqrt{\gamma_j}\}$ is an ONB for \mathcal{K} with respect to the \mathbf{a} -inner product.

The decomposition

$$\boxed{\mathbf{f} = \sum_j \langle \mathbf{f}, \mathbf{u}_j \rangle_{\mathcal{H}} \mathbf{u}_j} \quad (4.2)$$

holds with convergence in \mathcal{H} for each $\mathbf{f} \in \mathcal{H}$, and holds with convergence in \mathcal{K} for each $\mathbf{f} \in \mathcal{K}$.

Formula (4.1) is known as the (weak) eigenvalue equation for \mathbf{a} .

The idea of the proof is to show that a certain “inverse” operator associated with the sesquilinear form is compact and selfadjoint on \mathcal{H} , and then apply the spectral theorem for compact selfadjoint operators. In terms of differential equations, \mathbf{a} corresponds to a differential operator such as $-\Delta$, which is unbounded, and the inverse corresponds to an integral operator $(-\Delta)^{-1}$, which is bounded and in fact compact. Indeed, we will begin the proof by solving the analogue of Poisson’s equation $-\Delta \mathbf{u} = \mathbf{f}$ weakly in our Hilbert space setting, with the help of the Riesz Representation Theorem.

Proof of Theorem 4.1.

Step 1. We claim for each $\mathbf{f} \in \mathcal{H}$ there exists a unique $\mathbf{u} \in \mathcal{K}$ such that

$$\mathbf{a}(\mathbf{u}, \mathbf{v}) = \langle \mathbf{f}, \mathbf{v} \rangle_{\mathcal{H}} \quad \forall \mathbf{v} \in \mathcal{K}, \quad (4.3)$$

and that the map

$$\begin{aligned} \mathbf{B} : \mathcal{H} &\rightarrow \mathcal{K} \\ \mathbf{f} &\mapsto \mathbf{u} \end{aligned}$$

is linear and bounded. To prove this claim, fix $\mathbf{f} \in \mathcal{H}$ and define a bounded linear functional $F(\mathbf{v}) = \langle \mathbf{v}, \mathbf{f} \rangle_{\mathcal{H}}$ on \mathcal{K} , noting for the boundedness that

$$\begin{aligned} |F(\mathbf{v})| &\leq \|\mathbf{v}\|_{\mathcal{H}} \|\mathbf{f}\|_{\mathcal{H}} && \text{by Cauchy–Schwarz} \\ &\leq (\text{const.}) \|\mathbf{v}\|_{\mathcal{K}} \|\mathbf{f}\|_{\mathcal{H}} && \text{since } \mathcal{K} \text{ is imbedded in } \mathcal{H} \\ &\leq (\text{const.}) \mathbf{a}(\mathbf{v}, \mathbf{v})^{1/2} \|\mathbf{f}\|_{\mathcal{H}} \end{aligned}$$

by coercivity. Hence by the Riesz Representation Theorem on \mathcal{K} (with respect to the \mathbf{a} -inner product on \mathcal{K}), a unique $\mathbf{u} \in \mathcal{K}$ exists such that $F(\mathbf{v}) = \mathbf{a}(\mathbf{v}, \mathbf{u})$ for all $\mathbf{v} \in \mathcal{K}$. That is,

$$\langle \mathbf{v}, \mathbf{f} \rangle_{\mathcal{H}} = \mathbf{a}(\mathbf{v}, \mathbf{u}) \quad \forall \mathbf{v} \in \mathcal{K},$$

as desired for (4.3). Thus the map $\mathbf{B} : \mathbf{f} \mapsto \mathbf{u}$ is well defined. Clearly it is linear. And

$$\mathbf{a}(\mathbf{u}, \mathbf{u}) = |F(\mathbf{u})| \leq (\text{const.}) \mathbf{a}(\mathbf{u}, \mathbf{u})^{1/2} \|\mathbf{f}\|_{\mathcal{H}}$$

implies $\mathbf{a}(\mathbf{u}, \mathbf{u})^{1/2} \leq (\text{const.}) \|\mathbf{f}\|_{\mathcal{H}}$, so that \mathbf{B} is bounded from \mathcal{H} to \mathcal{K} (using the \mathbf{a} -norm on \mathcal{K}), which proves our claim in Step 1.

Step 2. $\iota \circ B : \mathcal{H} \rightarrow \mathcal{K} \rightarrow \mathcal{H}$ is compact, since ι imbeds \mathcal{K} compactly into \mathcal{H} . Thus we may regard B as a compact bounded linear operator from \mathcal{H} to itself. Observe B is selfadjoint on \mathcal{H} , since for all $f, g \in \mathcal{H}$ one has

$$\begin{aligned} \langle Bf, g \rangle_{\mathcal{H}} &= \overline{\langle g, Bf \rangle_{\mathcal{H}}} && \text{by symmetry of the inner product} \\ &= \overline{\alpha(Bg, Bf)} && \text{by definition of } B \text{ in (4.3),} \\ &= \alpha(Bf, Bg) && \text{by symmetry of } \alpha, \\ &= \langle f, Bg \rangle_{\mathcal{H}} && \text{by definition of } B \text{ in (4.3),} \end{aligned}$$

which implies $B^* = B$.

Further, B is injective, because if $Bf = 0$ then (4.3) implies $\langle f, v \rangle_{\mathcal{H}} = 0$ for all $v \in \mathcal{K}$ and hence for all $v \in \mathcal{H}$ (by density of \mathcal{K} in \mathcal{H}), from which we conclude $f = 0$. Thus the kernel of B consists of just the zero vector.

Therefore the spectral theorem for compact selfadjoint operators (Appendix A) provides an ONB for \mathcal{H} consisting of eigenvectors of B , with

$$B\mathbf{u}_j = \beta_j \mathbf{u}_j$$

for some real eigenvalues $\beta_j \rightarrow 0$. Note $\beta_j \neq 0$ because the kernel of B contains only the zero vector. The decomposition (4.2) holds for $f \in \mathcal{H}$ because $\{\mathbf{u}_j\}$ forms an ONB for \mathcal{H} .

Step 3. Dividing by the eigenvalue shows $\mathbf{u}_j = B(\mathbf{u}_j/\beta_j)$, which guarantees that \mathbf{u}_j belongs to the range of B and therefore $\mathbf{u}_j \in \mathcal{K}$. Next observe the eigenvalues are all positive, because

$$\beta_j \alpha(\mathbf{u}_j, \mathbf{v}) = \alpha(B\mathbf{u}_j, \mathbf{v}) = \langle \mathbf{u}_j, \mathbf{v} \rangle_{\mathcal{H}} \quad \forall \mathbf{v} \in \mathcal{K},$$

and choosing $\mathbf{v} = \mathbf{u}_j \in \mathcal{K}$ and using coercivity shows that $\beta_j > 0$. Thus the reciprocals

$$\gamma_j = \frac{1}{\beta_j}$$

are positive and tend to infinity, and satisfy

$$\alpha(\mathbf{u}_j, \mathbf{v}) = \gamma_j \langle \mathbf{u}_j, \mathbf{v} \rangle_{\mathcal{H}} \quad \forall \mathbf{v} \in \mathcal{K},$$

which is the desired eigenvalue formula (4.1). After reordering, we may further assume the γ_j are increasing: $0 < \gamma_1 \leq \gamma_2 \leq \gamma_3 \leq \cdots \rightarrow \infty$.

Step 4. Finally, the set $\{\mathbf{u}_j/\sqrt{\gamma_j}\}$ is \mathbf{a} -orthonormal because

$$\begin{aligned}\mathbf{a}(\mathbf{u}_j, \mathbf{u}_k) &= \gamma_j \langle \mathbf{u}_j, \mathbf{u}_k \rangle_{\mathcal{H}} \\ &= \gamma_j \delta_{jk} \\ &= \sqrt{\gamma_j} \sqrt{\gamma_k} \delta_{jk}.\end{aligned}$$

This orthonormal set is complete in \mathcal{K} , because if $\mathbf{a}(\mathbf{u}_j, \mathbf{v}) = 0$ for all j then $\langle \mathbf{u}_j, \mathbf{v} \rangle_{\mathcal{H}} = 0$ for all j by (4.1), so that $\mathbf{v} = 0$. Therefore each $\mathbf{f} \in \mathcal{K}$ can be decomposed as

$$\mathbf{f} = \sum_j \mathbf{a}(\mathbf{f}, \mathbf{u}_j/\sqrt{\gamma_j}) \mathbf{u}_j/\sqrt{\gamma_j}$$

with the series converging in \mathcal{K} , and this decomposition reduces to (4.2) because $\mathbf{a}(\mathbf{f}, \mathbf{u}_j) = \gamma_j \langle \mathbf{f}, \mathbf{u}_j \rangle_{\mathcal{H}}$. \square

Remark. Eigenvectors corresponding to distinct eigenvalues are automatically orthogonal, since

$$\begin{aligned}(\gamma_j - \gamma_k) \langle \mathbf{u}_j, \mathbf{u}_k \rangle_{\mathcal{H}} &= \gamma_j \langle \mathbf{u}_j, \mathbf{u}_k \rangle_{\mathcal{H}} - \overline{\gamma_k \langle \mathbf{u}_k, \mathbf{u}_j \rangle_{\mathcal{H}}} \\ &= \mathbf{a}(\mathbf{u}_j, \mathbf{u}_k) - \overline{\mathbf{a}(\mathbf{u}_k, \mathbf{u}_j)} \\ &= 0\end{aligned}$$

by symmetry of \mathbf{a} .

Notes and comments

The discrete spectral Theorem 4.1 can be found in various textbooks such as [Blanchard and Brüning] Section 6.3. It does not seem to have a standard name.

A more general spectral theorem for sesquilinear forms can be found in [Auchmuty] and certain references therein. Briefly, the eigenvectors there satisfy $\mathbf{a}(\mathbf{u}_j, \mathbf{v}) = \gamma_j \mathbf{b}(\mathbf{u}_j, \mathbf{v})$ for all $\mathbf{v} \in \mathcal{K}$, where the form \mathbf{b} is assumed to be weakly continuous on $\mathcal{K} \times \mathcal{K}$. In our situation, $\mathbf{b}(\mathbf{u}, \mathbf{v}) = \langle \mathbf{u}, \mathbf{v} \rangle_{\mathcal{H}}$ and our assumption that \mathcal{K} imbeds compactly into \mathcal{H} implies weak continuity of \mathbf{b} .

Chapter 5

Application: discrete spectrum for the Laplacian

Goal

To apply the spectral theorem from Chapter 4 to the Dirichlet, Robin and Neumann Laplacians.

Dirichlet Laplacian

We want an ONB of eigenfunctions satisfying

$$\begin{aligned} -\Delta \mathbf{u} &= \lambda \mathbf{u} && \text{in } \Omega \\ \mathbf{u} &= 0 && \text{on } \partial\Omega \end{aligned}$$

where Ω is a domain in \mathbb{R}^d having finite volume.

To verify the hypotheses of the discrete spectral Theorem 4.1 we let

$\mathcal{H} = L^2(\Omega)$, inner product $\langle \mathbf{u}, \mathbf{v} \rangle_{L^2} = \int_{\Omega} \mathbf{u} \mathbf{v} \, dx$,

$\mathcal{K} = H_0^1(\Omega) =$ Sobolev space, which is the completion of $C_0^\infty(\Omega)$ (the space of smooth functions having compact support in Ω) under the inner product

$$\langle \mathbf{u}, \mathbf{v} \rangle_{H^1} = \int_{\Omega} (\nabla \mathbf{u} \cdot \nabla \mathbf{v} + \mathbf{u} \mathbf{v}) \, dx.$$

All functions are assumed real valued, for simplicity. Note $L^2(\Omega)$ is separable [Ciarlet, Theorem 2.5-4].

Density: $C_0^\infty \subset H_0^1 \subset L^2$ and C_0^∞ is dense in L^2 , so H_0^1 is dense in L^2 .

Continuous imbedding $H_0^1 \hookrightarrow L^2$:

$$\begin{aligned} \|\mathbf{u}\|_{L^2} &= \left(\int_{\Omega} \mathbf{u}^2 \, d\mathbf{x} \right)^{1/2} \\ &\leq \left(\int_{\Omega} (|\nabla \mathbf{u}|^2 + \mathbf{u}^2) \, d\mathbf{x} \right)^{1/2} \\ &= \|\mathbf{u}\|_{H^1}. \end{aligned}$$

Compact imbedding $H_0^1 \hookrightarrow L^2$: see Rellich's Theorem B.4 in the Appendix.

Sesquilinear form: define

$$\mathbf{a}(\mathbf{u}, \mathbf{v}) = \int_{\Omega} \nabla \mathbf{u} \cdot \nabla \mathbf{v} \, d\mathbf{x} + \int_{\Omega} \mathbf{u} \mathbf{v} \, d\mathbf{x} = \langle \mathbf{u}, \mathbf{v} \rangle_{H^1}, \quad \mathbf{u}, \mathbf{v} \in H_0^1(\Omega).$$

Clearly \mathbf{a} is linear in each variable, and symmetric and continuous on $H_0^1(\Omega)$.

Coercivity: $\mathbf{a}(\mathbf{u}, \mathbf{u}) = \|\mathbf{u}\|_{H^1}^2$.

Hence the discrete spectral Theorem 4.1 gives an ONB $\{\mathbf{u}_j\}$ for $L^2(\Omega)$ (with $\mathbf{u}_j \in H_0^1(\Omega)$ also) and eigenvalues which we denote $\gamma_j = \lambda_j + 1$ satisfying

$$\langle \mathbf{u}_j, \mathbf{v} \rangle_{H^1} = (\lambda_j + 1) \langle \mathbf{u}_j, \mathbf{v} \rangle_{L^2} \quad \forall \mathbf{v} \in H_0^1(\Omega).$$

That is,

$$\int_{\Omega} \nabla \mathbf{u}_j \cdot \nabla \mathbf{v} \, d\mathbf{x} = \lambda_j \int_{\Omega} \mathbf{u}_j \mathbf{v} \, d\mathbf{x} \quad \forall \mathbf{v} \in H_0^1(\Omega), \quad (5.1)$$

which means

$$-\Delta \mathbf{u}_j = \lambda_j \mathbf{u}_j \quad \text{weakly.}$$

Thus \mathbf{u}_j is a weak eigenfunction of the Laplacian with eigenvalue λ_j .

Elliptic regularity theory says that this weak eigenfunction \mathbf{u}_j is C^∞ -smooth in Ω [Gilbarg and Trudinger, Corollary 8.11].

Next we show \mathbf{u}_j satisfies the eigenfunction equation classically. Formula (5.1) and Green's formula (0.1) imply

$$\int_{\Omega} (-\Delta \mathbf{u}_j) \mathbf{v} \, d\mathbf{x} = \int_{\Omega} (\lambda_j \mathbf{u}_j) \mathbf{v} \, d\mathbf{x} \quad \forall \mathbf{v} \in C_0^\infty(\Omega), \quad (5.2)$$

where for simplicity we work with smooth trial functions in $C_0^\infty(\Omega) \subset H_0^1(\Omega)$; note the boundary term vanishes in Green's formula because $\mathbf{v} = 0$ on $\partial\Omega$.

Thus

$$\int_{\Omega} (\Delta \mathbf{u}_j + \lambda_j \mathbf{u}_j) \mathbf{v} \, d\mathbf{x} = 0 \quad \forall \mathbf{v} \in C_0^\infty(\Omega).$$

If $\Delta \mathbf{u}_j + \lambda_j \mathbf{u}_j > 0$ on some open set then we may choose \mathbf{v} to be a nonnegative smooth function with compact support in that set such that $\int_{\Omega} (\Delta \mathbf{u}_j + \lambda_j \mathbf{u}_j) \mathbf{v} \, d\mathbf{x} > 0$, which contradicts the last displayed equation. Argue similarly if $\Delta \mathbf{u}_j + \lambda_j \mathbf{u}_j < 0$ on some open set. Hence $\Delta \mathbf{u}_j + \lambda_j \mathbf{u}_j = 0$ at every point, or

$$-\Delta \mathbf{u}_j = \lambda_j \mathbf{u}_j \quad \text{in } \Omega,$$

which means \mathbf{u}_j is an eigenfunction in the classical sense.

Dirichlet boundary condition: $\mathbf{u}_j = 0$ on $\partial\Omega$ in the sense of Sobolev spaces (the trace theorem) since H_0^1 is the closure of C_0^∞ . This boundary condition holds classically on any smooth portion of $\partial\Omega$, by elliptic regularity results.

Positivity of the Dirichlet eigenvalues: we have

$$\lambda_j = \frac{\int_{\Omega} |\nabla \mathbf{u}_j|^2 \, d\mathbf{x}}{\int_{\Omega} \mathbf{u}_j^2 \, d\mathbf{x}} \geq 0 \quad (5.3)$$

by choosing $\mathbf{v} = \mathbf{u}_j$ in the weak formulation (5.1). In fact $\lambda_j > 0$, as follows. If $\lambda_j = 0$ then $|\nabla \mathbf{u}_j| \equiv 0$ by the last formula and so \mathbf{u}_j is constant. Since $\mathbf{u}_j = 0$ on the boundary we conclude $\mathbf{u}_j \equiv 0$ in the domain. But \mathbf{u}_j cannot vanish identically because it has L^2 -norm equal to 1. Hence the Dirichlet eigenvalues are positive, with

$$0 < \lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \dots \rightarrow \infty.$$

Aside. Alternatively one may use a Sobolev inequality for H_0^1 to conclude the Dirichlet eigenvalues are positive. A suitable such inequality can be proved directly for $\mathbf{u} \in C_0^\infty(\Omega)$, when the domain is bounded:

$$\begin{aligned} \|\mathbf{u}\|_{L^2}^2 &= \int_{\Omega} \mathbf{u}^2 \, d\mathbf{x} \\ &= - \int_{\Omega} 2\mathbf{u} \frac{\partial \mathbf{u}}{\partial x_1} x_1 \, d\mathbf{x} \\ &\quad \text{by integration by parts in the } x_1\text{-direction} \\ &\leq (2 \max_{x \in \overline{\Omega}} |x_1|) \|\mathbf{u}\|_{L^2} \|\partial \mathbf{u} / \partial x_1\|_{L^2} \\ &\leq (\text{const.}) \|\mathbf{u}\|_{L^2} \|\nabla \mathbf{u}\|_{L^2}, \end{aligned}$$

so that

$$\|\mathbf{u}\|_{L^2} \leq (\text{const.}) \|\nabla \mathbf{u}\|_{L^2}$$

where the constant depends on the bounded domain Ω . This Sobolev inequality holds also for $\mathbf{u} \in H_0^1(\Omega)$, by passing to a limit. Consequently the left side of (5.3) is bounded below by a positive constant, giving $\lambda_j > 0$.

Neumann Laplacian

One seeks an ONB of eigenfunctions such that

$$\begin{aligned} -\Delta \mathbf{u} &= \mu \mathbf{u} && \text{in } \Omega \\ \frac{\partial \mathbf{u}}{\partial \mathbf{n}} &= 0 && \text{on } \partial \Omega \end{aligned}$$

where Ω is a bounded domain in \mathbb{R}^d with Lipschitz boundary.

To verify the hypotheses of the discrete spectral Theorem 4.1 we let

$$\mathcal{H} = L^2(\Omega),$$

$\mathcal{K} = H^1(\Omega) =$ Sobolev space, which is the completion of $C^\infty(\overline{\Omega})$ under the inner product $\langle \mathbf{u}, \mathbf{v} \rangle_{H^1}$; see [Gilbarg and Trudinger, p. 174].

Now argue as above for the Dirichlet Laplacian. The compact imbedding is provided by Rellich's Theorem B.6, which relies on Lipschitz smoothness of the boundary.

Writing the eigenvalues in the discrete spectral Theorem 4.1 as $\gamma_j = \mu_j + 1$, one finds

$$\int_{\Omega} \nabla \mathbf{u}_j \cdot \nabla \mathbf{v} \, dx = \mu_j \int_{\Omega} \mathbf{u}_j \mathbf{v} \, dx \quad \forall \mathbf{v} \in H^1(\Omega). \quad (5.4)$$

In particular, restricting to $\mathbf{v} \in H_0^1(\Omega)$ implies

$$-\Delta \mathbf{u}_j = \mu_j \mathbf{u}_j \quad \text{weakly.}$$

Hence \mathbf{u}_j is smooth, by elliptic regularity. Arguing as in the Dirichlet case using $\mathbf{v} \in C_0^\infty(\Omega)$, one shows \mathbf{u}_j is an eigenfunction in the classical sense, satisfying $-\Delta \mathbf{u}_j = \mu_j \mathbf{u}_j$ in Ω .

Nonnegativity of the Neumann eigenvalues: choosing $\mathbf{v} = \mathbf{u}_j$ in (5.4) proves $\mu_j \geq 0$. The first Neumann eigenvalue is zero: $\mu_1 = 0$ with a constant eigenfunction $\mathbf{u}_1 \equiv \text{const.} \neq 0$. (Note this constant function belongs to $H^1(\Omega)$, though not to $H_0^1(\Omega)$.) Hence

$$0 = \mu_1 \leq \mu_2 \leq \mu_3 \leq \cdots \rightarrow \infty.$$

Neumann “natural” boundary condition. Formula (5.4) asserts more than its Dirichlet counterpart (5.1) does, because (5.4) holds for all $\mathbf{v} \in H^1(\Omega)$ rather than just $\mathbf{v} \in H_0^1(\Omega)$. We will use this additional information to show our weak eigenfunctions in (5.4) automatically satisfy the Neumann boundary condition $\partial \mathbf{u}_j / \partial \mathbf{n} = 0$. This Neumann boundary condition holds even though it is **not** imposed in the function space \mathcal{K} .

(Functions in $H^1(\Omega)$ do not generally have vanishing normal derivative. In contrast, for the Dirichlet eigenfunctions considered earlier, the boundary condition is imposed directly by the choice of function space $H_0^1(\Omega)$: every function in that space equals zero on the boundary.)

The weak form of the eigenfunction equation (5.4) for an eigenfunction \mathbf{u} with eigenvalue μ says

$$\int_{\Omega} \nabla \mathbf{u} \cdot \nabla \mathbf{v} \, dx = \mu \int_{\Omega} \mathbf{u} \mathbf{v} \, dx \quad \forall \mathbf{v} \in H^1(\Omega). \quad (5.5)$$

Recall \mathbf{u} is smooth in Ω , by elliptic regularity theory. From (5.5) and Green's formula (0.1) we find

$$\int_{\Omega} (-\Delta \mathbf{u}) \mathbf{v} \, dx + \int_{\partial \Omega} \frac{\partial \mathbf{u}}{\partial \mathbf{n}} \mathbf{v} \, dS = \int_{\Omega} (\mu \mathbf{u}) \mathbf{v} \, dx \quad \forall \mathbf{v} \in C^\infty(\overline{\Omega}), \quad (5.6)$$

where for simplicity we work with trial functions in $C^\infty(\overline{\Omega}) \subset H^1(\Omega)$. If $\mathbf{v} \in C_0^\infty(\Omega)$ then the boundary term vanishes in (5.6), and so

$$\int_{\Omega} (\Delta \mathbf{u} + \mu \mathbf{u}) \mathbf{v} \, dx = 0 \quad \forall \mathbf{v} \in C_0^\infty(\Omega).$$

If $\Delta \mathbf{u} + \mu \mathbf{u} > 0$ on some open set then we may choose \mathbf{v} to be a nonnegative smooth function with compact support in that set such that $\int_{\Omega} (\Delta \mathbf{u} + \mu \mathbf{u}) \mathbf{v} \, dx > 0$, which is impossible. Argue similarly if $\Delta \mathbf{u} + \mu \mathbf{u} < 0$ on some open set. Hence $\Delta \mathbf{u} + \mu \mathbf{u} = 0$ at every point. Thus by using trial functions in $C_0^\infty(\Omega)$ we have obtained the eigenfunction equation

$$-\Delta \mathbf{u} = \mu \mathbf{u} \quad \text{in } \Omega.$$

Next, to get the Neumann boundary condition, we will use trial functions \mathbf{v} that do not vanish identically on the boundary. Assume for simplicity that the boundary is smooth, so that \mathbf{u} extends smoothly to $\overline{\Omega}$ by elliptic regularity. Substituting $-\Delta \mathbf{u} = \mu \mathbf{u}$ into (5.6) reduces that formula to

$$\int_{\partial \Omega} \frac{\partial \mathbf{u}}{\partial \mathbf{n}} \mathbf{v} \, dS = 0 \quad \forall \mathbf{v} \in C^\infty(\overline{\Omega}).$$

If $\partial \mathbf{u} / \partial \mathbf{n} > 0$ on some relatively open subset of the boundary (or if it is < 0 there), then we may choose a nonnegative smooth function \mathbf{v} on \mathbb{R}^d

whose restriction to $\partial\Omega$ is supported in the relatively open set and for which $\int_{\partial\Omega} (\partial\mathbf{u}/\partial\mathbf{n})\nu \, dS > 0$ (or < 0), which is a contradiction. Hence

$$\frac{\partial\mathbf{u}}{\partial\mathbf{n}} = 0 \quad \text{on } \partial\Omega,$$

which is the Neumann boundary condition.

Note. If the boundary is only piecewise smooth, then one may prove the Neumann condition on the smooth portions of the boundary, by the above reasoning.

Robin Laplacian

The task is to construct an ONB of eigenfunctions satisfying

$$\begin{aligned} -\Delta\mathbf{u} &= \rho\mathbf{u} && \text{in } \Omega \\ \frac{\partial\mathbf{u}}{\partial\mathbf{n}} + \sigma\mathbf{u} &= 0 && \text{on } \partial\Omega \end{aligned}$$

where Ω is a bounded domain in \mathbb{R}^d with Lipschitz boundary.

To verify the hypotheses of the discrete spectral Theorem 4.1 we let $\sigma > 0$ be the Robin constant and put

$$\begin{aligned} \mathcal{H} &= L^2(\Omega), \\ \mathcal{K} &= H^1(\Omega). \end{aligned}$$

The density and compact imbedding results are the same as for the Neumann case above.

Before defining the sesquilinear form, we need to make sense of the boundary values of \mathbf{u} . Sobolev functions have well defined boundary values — more precisely, there is a bounded linear operator $\mathsf{T} : H^1(\Omega) \rightarrow L^2(\partial\Omega)$ called the *trace operator* such that if $\mathbf{u} \in H^1(\Omega)$ happens to equal a continuous function on $\overline{\Omega}$ then $\mathsf{T}\mathbf{u} = \mathbf{u}$ on $\partial\Omega$. (Thus the trace operator correctly captures the boundary values of continuous functions in H^1 .) Further, if $\mathbf{u} \in H_0^1(\Omega)$ then $\mathsf{T}\mathbf{u} = 0$, so that functions in H_0^1 equal zero on the boundary in the trace sense. For these trace results, see [Evans, Section 5.5] for domains with C^1 boundary, or [Evans and Gariepy, §4.3] for the slightly rougher case of Lipschitz boundary.

Now we can define the sesquilinear form

$$\mathbf{a}(\mathbf{u}, \mathbf{v}) = \int_{\Omega} \nabla\mathbf{u} \cdot \nabla\mathbf{v} \, dx + \sigma \int_{\partial\Omega} \mathbf{u}\mathbf{v} \, dS(\mathbf{x}) + \int_{\Omega} \mathbf{u}\mathbf{v} \, dx$$

where \mathbf{u} and \mathbf{v} on the boundary should be interpreted as the trace values $\mathbb{T}\mathbf{u}$ and $\mathbb{T}\mathbf{v}$. Clearly \mathbf{a} is symmetric and continuous on $H^1(\Omega)$.

Coercivity: $\mathbf{a}(\mathbf{u}, \mathbf{u}) \geq \|\mathbf{u}\|_{H^1}^2$, since $\sigma > 0$.

Writing the eigenvalues in the discrete spectral Theorem 4.1 as $\gamma_j = \rho_j + 1$, one finds

$$\int_{\Omega} \nabla \mathbf{u}_j \cdot \nabla \mathbf{v} \, dx + \sigma \int_{\partial\Omega} \mathbf{u}_j \mathbf{v} \, dS(x) = \rho_j \int_{\Omega} \mathbf{u}_j \mathbf{v} \, dx \quad \forall \mathbf{v} \in H^1(\Omega). \quad (5.7)$$

In particular, taking $\mathbf{v} \in H_0^1(\Omega)$ implies $-\Delta \mathbf{u}_j = \rho_j \mathbf{u}_j$ weakly. Hence \mathbf{u}_j is smooth by elliptic regularity and satisfies the eigenvalue equation classically by the argument used above in the Dirichlet case with $\mathbf{v} \in C_0^\infty(\Omega)$.

Positivity of the Robin eigenvalues: choosing $\mathbf{v} = \mathbf{u}_j$ in (5.7) gives

$$\rho_j = \frac{\int_{\Omega} |\nabla \mathbf{u}_j|^2 \, dx + \sigma \int_{\partial\Omega} \mathbf{u}_j^2 \, dS(x)}{\int_{\Omega} \mathbf{u}_j^2 \, dx} \geq 0,$$

using that $\sigma > 0$. Further, $\rho_j > 0$ as follows. If $\rho_j = 0$ then $|\nabla \mathbf{u}_j| \equiv 0$ and so $\mathbf{u}_j \equiv \mathbf{c}$ is constant, which implies $\mathbb{T}\mathbf{u}_j = \mathbf{c}$ on the boundary. Since also $\int_{\partial\Omega} (\mathbb{T}\mathbf{u}_j)^2 \, dS = 0$ we conclude $\mathbf{c} = 0$ and hence $\mathbf{u}_j \equiv 0$ in the domain, which contradicts the fact that \mathbf{u}_j is an eigenfunction. Hence when the Robin constant σ is positive one has

$$0 < \rho_1 \leq \rho_2 \leq \rho_3 \leq \dots \rightarrow \infty.$$

Robin “natural” boundary condition. The Robin boundary condition is derived similarly to the Neumann case above, starting from the weak Robin eigenfunction equation (5.7), which says

$$\int_{\Omega} \nabla \mathbf{u} \cdot \nabla \mathbf{v} \, dx + \sigma \int_{\partial\Omega} \mathbf{u} \mathbf{v} \, dS = \rho \int_{\Omega} \mathbf{u} \mathbf{v} \, dx \quad \forall \mathbf{v} \in H^1(\Omega).$$

Once again, one employs trial functions $\mathbf{v} \in C_0^\infty(\Omega)$ to obtain the eigenvalue equation $-\Delta \mathbf{u} = \rho \mathbf{u}$, and then uses $\mathbf{v} \in C^\infty(\overline{\Omega})$ to deduce the Robin boundary condition

$$\frac{\partial \mathbf{u}}{\partial \mathbf{n}} + \sigma \mathbf{u} = 0 \quad \text{on } \partial\Omega$$

on smooth portions of the boundary.

Negative Robin constant, $\sigma < 0$

Coercivity is more difficult to prove when $\sigma < 0$. We start by controlling the boundary values in terms of the gradient and L^2 -norm. We have

$$\int_{\partial\Omega} \mathbf{u}^2 \, d\mathcal{S}(\mathbf{x}) \leq (\text{const.}) \int_{\Omega} |\nabla \mathbf{u}| |\mathbf{u}| \, d\mathbf{x} + (\text{const.}) \int_{\Omega} \mathbf{u}^2 \, d\mathbf{x},$$

as one sees by inspecting the proof of the trace theorem ([Evans, §5.5] or [Evans and Gariepy, §4.3]). An application of Cauchy-with- ε gives

$$\int_{\partial\Omega} \mathbf{u}^2 \, d\mathcal{S}(\mathbf{x}) \leq \varepsilon \|\nabla \mathbf{u}\|_{L^2}^2 + C \|\mathbf{u}\|_{L^2}^2$$

for some constant $C = C(\varepsilon) > 0$. Choose $\varepsilon = 1/2|\sigma|$, so that

$$\frac{1}{2} \|\mathbf{u}\|_{H^1}^2 \geq |\sigma| \int_{\partial\Omega} \mathbf{u}^2 \, d\mathcal{S}(\mathbf{x}) - C|\sigma| \|\mathbf{u}\|_{L^2}^2$$

and hence

$$\mathbf{a}(\mathbf{u}, \mathbf{u}) \geq \frac{1}{2} \|\mathbf{u}\|_{H^1}^2 - C|\sigma| \|\mathbf{u}\|_{L^2}^2.$$

Hence the new sesquilinear form $\tilde{\mathbf{a}}(\mathbf{u}, \mathbf{v}) = \mathbf{a}(\mathbf{u}, \mathbf{v}) + C|\sigma| \langle \mathbf{u}, \mathbf{v} \rangle_{L^2}$ is coercive. We apply the discrete spectral theorem to this new form, and then obtain the eigenvalues of \mathbf{a} by subtracting $C|\sigma|$ (with the same ONB of eigenfunctions).

Negativity of some Robin eigenvalues: $\rho_1 < 0$ when $\sigma < 0$, as one sees by substituting the trial function $\mathbf{u} \equiv 1$ into the variational characterization for ρ_1 in Chapter 11, later in the book.

Eigenfunction expansions in the L^2 and H^1 norms

The L^2 -ONB of eigenfunctions $\{\mathbf{u}_j\}$ of the Laplacian gives the decomposition

$$\mathbf{f} = \sum_j \langle \mathbf{f}, \mathbf{u}_j \rangle_{L^2} \mathbf{u}_j \tag{5.8}$$

with convergence in the L^2 and H^1 norms, whenever \mathbf{f} belongs to the following spaces:

$$\mathbf{f} \in \begin{cases} H_0^1(\Omega) & \text{for Dirichlet,} \\ H^1(\Omega) & \text{for Neumann,} \\ H^1(\Omega) & \text{for Robin.} \end{cases}$$

These claims follow immediately from the discrete spectral Theorem 4.1, in view of our work above.

Exercises

Regular Sturm–Liouville problem

5.1 — Consider the eigenvalue problem

$$\begin{aligned} -(\mathbf{p}u')' + \mathbf{q}u &= \lambda wu && \text{on the interval } (0, L), \\ u(0) = 0, \quad u(L) &= 0, \end{aligned}$$

where the coefficient functions $\mathbf{p}, \mathbf{q}, w$ are smooth and real valued on $[0, L]$, and \mathbf{p} and w are positive on $[0, L]$.

(i) Formulate this regular Sturm–Liouville eigenvalue problem in terms of appropriate Hilbert spaces \mathcal{H} and \mathcal{K} and a sesquilinear form $\mathbf{a}(u, v)$.

(ii) Verify the hypotheses of the discrete spectral Theorem 4.1.

(iii) Find a lower bound on the first eigenvalue λ_1 in terms of the coefficient functions. For simplicity, assume in this part that \mathbf{q} is nonnegative.

Elliptic operator

5.2 — Consider the second order elliptic eigenvalue problem

$$-\nabla \cdot (A(x)\nabla u) = \lambda u$$

on a bounded domain $\Omega \subset \mathbb{R}^d$, where the real symmetric $\mathbf{d} \times \mathbf{d}$ matrix $A(x)$ depends smoothly on $x \in \overline{\Omega}$ and is uniformly elliptic, meaning

$$\mathbf{y}^T A(x)\mathbf{y} \geq c|\mathbf{y}|^2, \quad x, \mathbf{y} \in \mathbb{R}^d,$$

for some constant $c > 0$. (In other words, the lowest eigenvalue of the matrix is bounded below away from 0.)

Formulate the Dirichlet eigenvalue problem for this elliptic operator in terms of the function spaces H_0^1 and L^2 , for a suitable sesquilinear form $\mathbf{a}(u, v)$, and verify the hypotheses of the discrete spectral Theorem 4.1.

Laplacian on manifolds

Consider a compact, connected, smooth, \mathbf{d} -dimensional Riemannian manifold (M, \mathbf{g}) . Note M has no boundary, since it is compact. The gradient and divergence operators are defined in terms of the metric (see [Chavel, §I.1]) and the Laplacian is then

$$\Delta u = \operatorname{div}(\operatorname{grad} u).$$

(Geometers usually include a negative sign on the right side of this definition, but we follow the analyst's convention like in Euclidean space.) Green's formulas hold as usual ([Chavel, §I.2]).

The space $L^2(\mathcal{M})$ of square integrable functions is defined using integration against the volume form dV [Chavel, §I.3]. The space $H^1(\mathcal{M})$ of square integrable functions with one weak derivative in L^2 is defined analogously to the Euclidean case ([Chavel, §I.5]), with inner product

$$\langle u, v \rangle_{H^1} = \int_{\mathcal{M}} (g(\text{grad } u, \text{grad } v) + uv) dV.$$

Then H^1 imbeds compactly into L^2 , as one sees by localizing to coordinate charts with a partition of unity and invoking Rellich's Theorem B.6 in Euclidean space. Further, elliptic regularity theory holds on \mathcal{M} , again by working locally.

5.3 — Prove an ONB $\{u_j\}$ for $L^2(\mathcal{M})$ exists with each u_j being smooth on \mathcal{M} and satisfying

$$-\Delta u_j = \lambda_j u_j$$

for some eigenvalues

$$0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \dots \rightarrow \infty.$$

(It is standard on compact manifolds to begin indexing the eigenvalues with $j = 0$.) Also, show the zero-th eigenfunction u_0 is a constant, and every other eigenfunction has integral zero:

$$\int_{\mathcal{M}} u_j dV = 0, \quad j = 1, 2, 3, \dots$$

Remark. The spectrum of a compact manifold behaves like the spectrum of a domain with Neumann boundary conditions, where the lowest eigenvalue is again zero and the corresponding eigenfunction is a constant.

5.4 — Suppose \mathcal{M} is the circle ($d = 1$) with the standard metric induced from the Euclidean metric on the plane. Show the Laplacian is $\Delta = \partial_{\theta\theta}$ and the eigenfunctions are

$$u(\theta) = 1, \cos \theta, \sin \theta, \cos 2\theta, \sin 2\theta, \cos 3\theta, \sin 3\theta, \dots;$$

with corresponding eigenvalues

$$\lambda = 0^2, 1^2, 1^2, 2^2, 2^2, 3^2, 3^2, \dots$$

Here the eigenfunctions have not been normalized in L^2 . More efficiently, the eigenfunctions in complex form are $u(\theta) = e^{in\theta}$, $n \in \mathbb{Z}$, with corresponding eigenvalues n^2 .

5.5 — Take M to be the sphere ($d = 2$) with the standard metric induced from Euclidean 3-space. Show the eigenfunctions are the spherical harmonics, and hence that the first four eigenfunctions are

$$u = 1, x, y, z$$

where x, y, z are the coordinate functions on \mathbb{R}^3 .

Chapter 6

Application: discrete spectrum for the Laplacian with magnetic field

Goal

To apply the spectral theorem from Chapter 4 to the magnetic Laplacian, which is the Schrödinger operator describing a quantum particle in a classical magnetic field.

Magnetic Laplacian

Take a domain Ω with finite volume in \mathbb{R}^d , where $d = 2$ or $d = 3$. We seek an ONB of eigenfunctions for the *magnetic Laplacian*

$$\begin{aligned} (i\nabla + \vec{A})^2 \mathbf{u} &= \beta \mathbf{u} && \text{in } \Omega, \\ \mathbf{u} &= 0 && \text{on } \partial\Omega, \end{aligned}$$

where $\mathbf{u}(\mathbf{x})$ is complex valued and

$$\vec{A} : \mathbb{R}^d \rightarrow \mathbb{R}^d$$

is a given vector field, assumed to be bounded.

Physically, \vec{A} represents the *vector potential*, whose curl (assuming \vec{A} is differentiable) represents equals the magnetic field: $\nabla \times \vec{A} = \vec{B}$. In 2 dimensions, one extends $\vec{A} = (A_1, A_2)$ to a 3-vector $(A_1, A_2, 0)$ before taking

the curl. Then the field $\vec{B} = (0, 0, \frac{\partial A_2}{\partial x_1} - \frac{\partial A_1}{\partial x_2})$ cuts vertically through the planar domain.

Now we choose the Hilbert spaces and sesquilinear form, and verify the hypotheses of Theorem 4.1. Consider only the Dirichlet boundary condition, for simplicity. Let:

$\mathcal{H} = L^2(\Omega; \mathbb{C})$ (complex valued functions), with inner product

$$\langle \mathbf{u}, \mathbf{v} \rangle_{L^2} = \int_{\Omega} \mathbf{u} \bar{\mathbf{v}} \, dx;$$

$\mathcal{K} = H_0^1(\Omega; \mathbb{C})$, with inner product

$$\langle \mathbf{u}, \mathbf{v} \rangle_{H^1} = \int_{\Omega} (\nabla \mathbf{u} \cdot \bar{\nabla} \mathbf{v} + \mathbf{u} \bar{\mathbf{v}}) \, dx.$$

Density: \mathcal{K} contains C_0^∞ , which is dense in L^2 .

Continuous imbedding: $H_0^1 \hookrightarrow L^2$ since $\|\mathbf{u}\|_{L^2} \leq \|\mathbf{u}\|_{H^1}$. The imbedding is compact by Rellich's Theorem B.4.

Sesquilinear form: define

$$\mathbf{a}(\mathbf{u}, \mathbf{v}) = \int_{\Omega} (i\nabla + \vec{A})\mathbf{u} \cdot \overline{(i\nabla + \vec{A})\mathbf{v}} \, dx + C \int_{\Omega} \mathbf{u} \bar{\mathbf{v}} \, dx, \quad \mathbf{u}, \mathbf{v} \in H_0^1(\Omega; \mathbb{C}),$$

with $C = \|\vec{A}\|_{L^\infty}^2 + \frac{1}{2}$. Clearly \mathbf{a} is symmetric ($\mathbf{a}(\mathbf{v}, \mathbf{u}) = \overline{\mathbf{a}(\mathbf{u}, \mathbf{v})}$) and is continuous on H_0^1 .

Coercivity:

$$\begin{aligned} & \mathbf{a}(\mathbf{u}, \mathbf{u}) \\ &= \int_{\Omega} (|\nabla \mathbf{u}|^2 + 2 \operatorname{Re}(i\nabla \mathbf{u} \cdot \vec{A} \bar{\mathbf{u}}) + |\vec{A}|^2 |\mathbf{u}|^2 + C |\mathbf{u}|^2) \, dx \\ &\geq \int_{\Omega} (|\nabla \mathbf{u}|^2 - 2|\nabla \mathbf{u}| |\vec{A}| |\mathbf{u}| + 2|\vec{A}|^2 |\mathbf{u}|^2 + \frac{1}{2} |\mathbf{u}|^2) \, dx \quad \text{by definition of } C \\ &\geq \int_{\Omega} \left(\frac{1}{2} |\nabla \mathbf{u}|^2 + \frac{1}{2} |\mathbf{u}|^2 \right) \, dx \quad \text{since } \frac{1}{2} p^2 - 2pq + 2q^2 \geq 0 \\ &= \frac{1}{2} \|\mathbf{u}\|_{H^1}^2. \end{aligned}$$

The discrete spectral Theorem 4.1 gives an ONB $\{\mathbf{u}_j\}$ for $L^2(\Omega; \mathbb{C})$. Write the corresponding eigenvalues as $\gamma_j = \beta_j + C$, so that

$$\int_{\Omega} (i\nabla + \vec{A})\mathbf{u}_j \cdot \overline{(i\nabla + \vec{A})\mathbf{v}} \, dx = \beta_j \int_{\Omega} \mathbf{u}_j \bar{\mathbf{v}} \, dx \quad \forall \mathbf{v} \in H_0^1(\Omega; \mathbb{C}). \quad (6.1)$$

That is,

$$(i\nabla + \vec{A})^2 \mathbf{u}_j = \beta_j \mathbf{u}_j \quad \text{weakly,}$$

and hence classically, where we assume from here on that the vector potential \vec{A} is smooth. The eigenvalues satisfy

$$\beta_j = \frac{\int_{\Omega} |(i\nabla + \vec{A})\mathbf{u}_j|^2 \, dx}{\int_{\Omega} |\mathbf{u}_j|^2 \, dx} \geq 0, \quad (6.2)$$

as we see by choosing $\mathbf{v} = \mathbf{u}_j$ in the weak formulation (6.1), and so

$$0 \leq \beta_1 \leq \beta_2 \leq \beta_3 \leq \cdots \rightarrow \infty.$$

We claim $\beta_1 > 0$ if there is no open set on which the magnetic field vanishes identically. For if $\beta_1 = 0$ then $(i\nabla + \vec{A})\mathbf{u}_1 \equiv 0$, which implies $\vec{A} = -i\nabla \log |\mathbf{u}_1|$ on the open set where \mathbf{u}_1 is nonzero, and $\vec{B} = \nabla \times \vec{A} = 0$ on that open set since the curl of a gradient vanishes identically. Note this argument does not rely on the Dirichlet boundary condition.

A similar argument (in the Exercises) shows that if $\beta_1 = 0$ then $|\mathbf{u}_1|$ is constant. Then the Dirichlet boundary condition forces \mathbf{u}_1 to vanish everywhere, a contradiction. Thus in the Dirichlet case one knows the ground state energy is positive, $\beta_1 > 0$.

Gauge invariance

Many different vector potentials can generate the same magnetic field. For example, in 2 dimensions the potentials

$$\vec{A} = (0, x_1), \quad \vec{A} = (-x_2, 0), \quad \vec{A} = \frac{1}{2}(-x_2, x_1),$$

all generate the magnetic field $\nabla \times \vec{A} = (0, 0, 1)$. Indeed, adding any gradient vector ∇f to the potential leaves the magnetic field unchanged, since the curl of a gradient equals zero. This phenomenon goes by the name of **gauge invariance**.

How is the spectral theory of the magnetic Laplacian affected by gauge invariance? The sesquilinear form definitely changes when we replace \vec{A} with $\vec{A} + \nabla f$. Fortunately, the new eigenfunctions are related to the old by a unitary transformation, as follows. Suppose f is smooth on the closure of the domain. For any trial function $\mathbf{u} \in H_0^1(\Omega; \mathbb{C})$, the modulated function $e^{if}\mathbf{u}$ also belongs to $H_0^1(\Omega; \mathbb{C})$ and

$$(i\nabla + \vec{A})\mathbf{u} = e^{-if}(i\nabla + \vec{A} + \nabla f)(e^{if}\mathbf{u}).$$

Thus if we write \mathbf{a} for the original sesquilinear form and $\tilde{\mathbf{a}}$ for the analogous form coming from the vector potential $\vec{A} + \nabla f$, we have

$$\mathbf{a}(\mathbf{u}, \mathbf{v}) = \tilde{\mathbf{a}}(e^{if}\mathbf{u}, e^{if}\mathbf{v})$$

for all trial functions \mathbf{u}, \mathbf{v} . Since also $\langle \mathbf{u}, \mathbf{v} \rangle_{L^2} = \langle e^{if}\mathbf{u}, e^{if}\mathbf{v} \rangle_{L^2}$, the ONB of eigenfunctions \mathbf{u}_j associated with \mathbf{a} transforms to an ONB of eigenfunctions $e^{if}\mathbf{u}_j$ associated with $\tilde{\mathbf{a}}$. The eigenvalues (energy levels) β_j are unchanged by this transformation.

Exercises

6.1 — Use formula (6.2) to show that if $\beta_1 = 0$ then $|\mathbf{u}_1|^2$ is constant.

Notes and comments

For a brief explanation of how the magnetic Laplacian arises from the correspondence between classical energy functions and quantum mechanical Hamiltonians, see [Reed and Simon 2, p. 173].

For invariance of the magnetic Laplacian spectrum with respect to rotations, reflections and translations, and for a discussion of the Neumann and Robin situations, see [Laugesen, Liang and Roy, Appendix A].

In higher dimensions one identifies the vector potential $\vec{A} : \mathbb{R}^d \rightarrow \mathbb{R}^d$ with a 1-form

$$\mathbf{A} = A_1 dx_1 + \cdots + A_d dx_d$$

and obtains the magnetic field from the exterior derivative:

$$\mathbf{B} = d\mathbf{A}.$$

Otherwise, the spectral theory proceeds as in dimensions 2 and 3.

Chapter 7

Application: discrete spectrum for Schrödinger in a potential well

Goal

To apply the spectral theorem from Chapter 4 to the harmonic oscillator and more general potential wells in higher dimensions.

Schrödinger with finite-volume sublevel potential

Consider a real valued, measurable potential V that is locally bounded above and globally bounded below, with

$$V(x) \geq -C, \quad x \in \mathbb{R}^d,$$

for some constant $C > 0$. Assume the sublevel set

$$B(t) = \{x : V(x) < t\}$$

has finite volume for each $t \in \mathbb{R}$. For example, the sublevel sets have finite volume if the potential grows to infinity at ∞ , that is, if

$$V(x) \rightarrow \infty \quad \text{as } |x| \rightarrow \infty.$$

The harmonic oscillator potential $V(x) = |x|^2$ satisfies this last condition.

We aim to prove existence of an ONB of eigenfunctions for

$$\begin{aligned} (-\Delta + V)u &= Eu && \text{in } \mathbb{R}^d, \\ u &\rightarrow 0 && \text{as } |x| \rightarrow \infty. \end{aligned}$$

Let:

$$\Omega = \mathbb{R}^d,$$

$$\mathcal{H} = L^2(\mathbb{R}^d), \text{ inner product } \langle u, v \rangle_{L^2} = \int_{\mathbb{R}^d} uv \, dx.$$

$$\mathcal{K} = H^1(\mathbb{R}^d) \cap L^2(|V| \, dx) \text{ with inner product}$$

$$\begin{aligned} \langle u, v \rangle_{\mathcal{K}} &= \langle u, v \rangle_{H^1} + \langle u, v \rangle_{L^2(|V| \, dx)} \\ &= \int_{\mathbb{R}^d} (\nabla u \cdot \nabla v + (1 + |V|)uv) \, dx. \end{aligned}$$

Density: \mathcal{K} contains C_0^∞ , which is dense in L^2 .

Continuous imbedding: $\mathcal{K} \hookrightarrow L^2$ since $\|u\|_{L^2} \leq \|u\|_{\mathcal{K}}$.

Compact imbedding: $\mathcal{K} \hookrightarrow L^2$ compactly, as we now show. Suppose $\{f_k\}$ is a bounded sequence in \mathcal{K} , say with $\|f_k\|_{\mathcal{K}} \leq M$ for all k , so that in particular $\{f_k\}$ is bounded in $H^1(\mathbb{R}^d)$. We must prove the existence of a subsequence converging in $L^2(\mathbb{R}^d)$.

Each sublevel set $B(t)$ has finite volume, by hypothesis. Take $t = 1$. The Restriction Theorem B.5 provides a subsequence that converges in $L^2(B(1))$. Repeat with $t = 2$ to get a sub-subsequence converging in $L^2(B(2))$. Continue in this fashion and then consider the diagonal subsequence, to obtain a subsequence that converges in $L^2(B(t))$ for each $t > 0$.

Relabel and call this subsequence $\{f_\ell\}$. We show it converges in $L^2(\mathbb{R}^d)$. For $t > 0$,

$$\begin{aligned} t \int_{\mathbb{R}^d \setminus B(t)} f_\ell^2 \, dx &\leq \int_{\mathbb{R}^d \setminus B(t)} f_\ell^2 V \, dx \\ &\leq \|f_\ell\|_{\mathcal{K}}^2 \\ &\leq M^2 \end{aligned}$$

for all ℓ . Since $\{f_\ell\}$ converges in $L^2(B(t))$, we have from above that

$$\limsup_{\ell, m \rightarrow \infty} \|f_\ell - f_m\|_{L^2(\mathbb{R}^d)} = \limsup_{\ell, m \rightarrow \infty} \|f_\ell - f_m\|_{L^2(\mathbb{R}^d \setminus B(t))} \leq 2M/\sqrt{t}.$$

Letting $t \rightarrow \infty$ shows that $\|f_\ell - f_m\|_{L^2(\mathbb{R}^d)} \rightarrow 0$ as $\ell, m \rightarrow \infty$, and so $\{f_\ell\}$ is Cauchy in $L^2(\mathbb{R}^d)$ and hence converges, as we wanted to show for compactness of the imbedding.

Incidentally, if the potential grows to infinity at ∞ ($V(x) \rightarrow \infty$ as $|x| \rightarrow \infty$) then one may instead take $B(t)$ to be the open ball of radius t and use that $\inf_{\mathbb{R}^d \setminus B(t)} V \rightarrow \infty$ as $t \rightarrow \infty$.

Sesquilinear form: define

$$a(u, v) = \int_{\mathbb{R}^d} (\nabla u \cdot \nabla v + Vuv) \, dx + (2C + 1) \int_{\mathbb{R}^d} uv \, dx, \quad u, v \in \mathcal{K}.$$

Clearly a is symmetric and continuous on \mathcal{K} .

Coercivity: $a(u, u) \geq \|u\|_{\mathcal{K}}^2$, since $V + 2C + 1 \geq 1 + |V|$.

The discrete spectral Theorem 4.1 gives an ONB $\{u_j\}$ for $L^2(\mathbb{R}^d)$ and corresponding eigenvalues which we denote $\gamma_j = E_j + 2C + 1$ satisfying

$$\int_{\mathbb{R}^d} (\nabla u_j \cdot \nabla v + Vu_j v) \, dx = E_j \int_{\mathbb{R}^d} u_j v \, dx \quad \forall v \in \mathcal{K}.$$

In particular, this last formula holds for all $v \in H^1(\mathbb{R}^d)$ with compact support, and so

$$-\Delta u_j + Vu_j = E_j u_j \quad \text{weakly.}$$

Hence u_j is smooth (assuming smoothness of V), and the eigenfunction equation holds classically by arguing as we did in the Dirichlet case in Chapter 5. Thus u_j is an eigenfunction of the Schrödinger operator $-\Delta + V$, with eigenvalue E_j , where

$$E_1 \leq E_2 \leq E_3 \leq \dots \rightarrow \infty.$$

Boundary condition at infinity: the boundary condition $u_j \rightarrow 0$ at infinity is interpreted as meaning u_j belongs to the space $H^1(\mathbb{R}^d) \cap L^2(|V| \, dx)$. In 1 dimension, belonging to $H^1(\mathbb{R})$ already insures that $u(x) \rightarrow 0$ as $|x| \rightarrow \infty$, by Exercise 7.1.

The eigenvalues satisfy

$$E_j = \frac{\int_{\mathbb{R}^d} (|\nabla u_j|^2 + Vu_j^2) \, dx}{\int_{\mathbb{R}^d} u_j^2 \, dx},$$

as we see by choosing $v = u_j$ in the weak formulation. Hence if $V \geq 0$ then the eigenvalues are all positive.

Exercises

7.1 — Suppose $\mathbf{u} \in H^1(\mathbb{R})$, so that \mathbf{u} is absolutely continuous and the fundamental theorem of calculus holds for it.

(a) Show \mathbf{u} is Hölder continuous with exponent $1/2$:

$$|\mathbf{u}(\mathbf{x}) - \mathbf{u}(\mathbf{y})| \leq \|\mathbf{u}'\|_{L^2} |\mathbf{x} - \mathbf{y}|^{1/2}, \quad \mathbf{x}, \mathbf{y} \in \mathbb{R}.$$

(b) Prove $\mathbf{u}(\mathbf{x}) \rightarrow 0$ as $\mathbf{x} \rightarrow \pm\infty$.

7.2 — *f-Laplacian*. Given a positive smooth function f on \mathbb{R}^d , define the f -Laplacian to be the operator

$$\Delta_f \mathbf{u} = \frac{1}{f} \nabla \cdot (f \nabla \mathbf{u}).$$

(a) Show the f -Laplacian conjugates to a Schrödinger operator, with

$$-e^{-g/2} \Delta_f e^{g/2} = -\Delta + V$$

where

$$f = e^{-g}$$

and the potential is

$$V = \frac{1}{4} |\nabla g|^2 - \frac{1}{2} \Delta g.$$

(b) Conclude formally that if

$$V(\mathbf{x}) \rightarrow \infty \quad \text{as } |\mathbf{x}| \rightarrow \infty, \quad (7.1)$$

or more generally if

$$V \text{ is bounded below and its sublevel sets have finite volume,} \quad (7.2)$$

then the f -Laplacian has discrete spectrum. State a formula expressing eigenfunctions of Δ_f in terms of eigenfunctions of $-\Delta + V$.

(c) Let $f = e^{-x^2}$ be the Gaussian in 1-dimension. Verify condition (7.1), compute the potential V , and show the spectrum is $\lambda = 0, 2, 4, 6, \dots$

(d) To justify rigorously that the f -Laplacian has discrete spectrum, under assumption (7.1) or (7.2), let

$$\begin{aligned} \tilde{\mathcal{H}} &= L^2(\mathbb{R}^d, f \, d\mathbf{x}), & \langle \mathbf{u}, \mathbf{v} \rangle_{\tilde{\mathcal{H}}} &= \int \mathbf{u} \mathbf{v} e^{-g} \, d\mathbf{x}, \\ \tilde{\mathcal{K}} &= H^1(\mathbb{R}^d, f \, d\mathbf{x}), & \langle \mathbf{u}, \mathbf{v} \rangle_{\tilde{\mathcal{K}}} &= \int (\nabla \mathbf{u} \cdot \nabla \mathbf{v} + \mathbf{u} \mathbf{v}) e^{-g} \, d\mathbf{x}, \end{aligned}$$

and verify the hypotheses of the discrete spectral Theorem 4.1.

Hint. Consider the spaces \mathcal{H} and \mathcal{K} that we used earlier for the Schrödinger operator with potential well. Show that $\mathbf{u} \in \mathcal{H}$ if and only if $\mathbf{u}e^{g/2} \in \tilde{\mathcal{H}}$, and $\mathbf{u} \in \mathcal{K}$ if and only if $\mathbf{u}e^{g/2} \in \tilde{\mathcal{K}}$, with comparable norms.

Chapter 8

Application: discrete spectrum for Sturm–Liouville operators

Goal

To apply the spectral theorem from Chapter 4 to regular and singular Sturm–Liouville operators, obtaining discreteness criteria for the spectrum.

Consider the Sturm–Liouville eigenvalue equation

$$-(pu')' + qu = \lambda wu \quad \text{on the interval } (0, L), \quad (8.1)$$

where the coefficient functions p, q, w are smooth and real valued on $(0, L)$, with p and w positive at every point.

Assumptions on coefficient functions

Near the left endpoint assume either

$$q/w \rightarrow \infty \quad \text{as } x \rightarrow 0, \text{ or} \quad (8.2)$$

$$q/w \text{ is bounded below and } w \text{ and } Pw \text{ are integrable on } (0, L/2), \quad (8.3)$$

where P is an antiderivative of $1/p$. Near the right endpoint assume either

$$q/w \rightarrow \infty \quad \text{as } x \rightarrow L, \text{ or} \quad (8.4)$$

$$q/w \text{ is bounded below and } w \text{ and } Pw \text{ are integrable on } (L/2, L). \quad (8.5)$$

There is nothing special about the number $L/2$. Any point in the interval could be used.

Boundary conditions

In order to formulate a Dirichlet boundary condition at $x = L$, in the function space \mathcal{K} below, we assume

$$\int_{L/2}^L \frac{1}{p(x)} dx < \infty. \quad (8.6)$$

We will not impose a boundary condition at $x = 0$. Later we discuss the natural BC that arises at that left endpoint.

Remarks

Conditions (8.2)–(8.5) can handle various singular Sturm–Liouville problems. An application to Bessel functions and the vibrating circular drum will be given later in the chapter, while the exercises cover other famous examples.

The example $p = 1$, $q = x^{-2}$, $w = x^{-1}$ satisfies (8.2) but not (8.3), since w is not integrable. In the other direction, the example $p = q = w = 1$ satisfies (8.3) but not (8.2), since q/w is bounded.

The regular Sturm–Liouville eigenvalue problem (see exercise in Chapter 5) is covered by the results in this chapter, since conditions (8.3), (8.5) and (8.6) hold if p, q, w are continuous on the closed interval $[0, L]$ and p and w are positive there.

Hilbert spaces and sesquilinear form

Let us proceed to verify the hypotheses of the discrete spectral theorem. Write $\mathcal{I} = (0, L)$ for the interval and put

$$m = \inf_{\mathcal{I}} \frac{q}{w}.$$

Then $-\infty < m < \infty$ by assumptions (8.2)–(8.5), and so

$$q - mw \geq 0.$$

Define Hilbert spaces

$$\mathcal{H} = L^2(\mathcal{I}, w dx),$$

$$\mathcal{K} = \{u \in H_{loc}^1(\mathcal{I}) : u' \in L^2(\mathcal{I}, p dx), u \in L^2(\mathcal{I}, (q - mw + w) dx), u(L) = 0\},$$

with inner products

$$\begin{aligned}\langle \mathbf{u}, \mathbf{v} \rangle_{\mathcal{H}} &= \int_0^L \mathbf{u} \mathbf{v} \mathbf{w} \, dx, \\ \langle \mathbf{u}, \mathbf{v} \rangle_{\mathcal{K}} &= \int_0^L (\mathbf{u}' \mathbf{v}' \mathbf{p} + \mathbf{u} \mathbf{v} (\mathbf{q} - m\mathbf{w} + \mathbf{w})) \, dx.\end{aligned}$$

The boundary value $\mathbf{u}(L)$ in the definition of \mathcal{K} is well defined: it equals

$$\mathbf{u}(L) = \int_{L/2}^L \mathbf{u}'(x) \, dx + \mathbf{u}(L/2),$$

where the integral is finite since

$$\int_{L/2}^L |\mathbf{u}'| \, dx \leq \left(\int_{L/2}^L (\mathbf{u}')^2 \mathbf{p} \, dx \right)^{1/2} \left(\int_{L/2}^L \frac{1}{\mathbf{p}} \, dx \right)^{1/2} < \infty$$

by Cauchy–Schwarz and hypothesis (8.6).

Separability: \mathcal{H} is separable by a short argument relying on separability of the unweighted L^2 -space.

Density: \mathcal{K} contains $C_0^\infty(\mathcal{I})$, which is already dense in \mathcal{H} .

Continuous imbedding: $\mathcal{K} \hookrightarrow \mathcal{H}$ because

$$\begin{aligned}\|\mathbf{u}\|_{\mathcal{H}}^2 &= \int_0^L \mathbf{u}^2 \mathbf{w} \, dx \\ &\leq \int_0^L \mathbf{u}^2 (\mathbf{q} - m\mathbf{w} + \mathbf{w}) \, dx \\ &\leq \|\mathbf{u}\|_{\mathcal{K}}^2.\end{aligned}$$

Compact imbedding: $\mathcal{K} \hookrightarrow \mathcal{H}$: suppose $\{f_k\}$ is a bounded sequence in \mathcal{K} , say with $\|f_k\|_{\mathcal{K}} \leq M$ for all k . The goal is to prove the existence of a subsequence converging in $\mathcal{H} = L^2(\mathcal{I}, \mathbf{w} \, dx)$. First we find a subsequence converging on the left half of the interval. Analogous arguments yield a subsequence that converges on the right half of the interval, completing the proof.

Construction for compact imbedding on $(0, L/2)$, assuming (8.2).

Let $\delta_3 = L/3$. Then \mathbf{p} and $\mathbf{q} - m\mathbf{w} + \mathbf{w}$ are positive on the closed interval

$[\delta_3, L/2]$, and so the sequence $\{f_k\}$ is bounded in $W^{1,2}((\delta_3, L/2))$. Rellich's Theorem B.6 provides a subsequence of $\{f_k\}$ that converges in $L^2((\delta_3, L/2))$ and hence in $L^2((\delta_3, L/2), w \, dx)$. Repeating with $\delta_4 = L/4$ provides a sub-subsequence converging in $L^2((\delta_4, L/2), w \, dx)$. Continue in this fashion, and then consider the diagonal subsequence, which converges in $L^2((\delta, L/2), w \, dx)$ for each $\delta < L/2$. After relabelling, we denote this diagonal subsequence by $\{f_\ell\}$.

In fact, this sequence converges in $L^2((0, L/2), w \, dx)$, as we now show. Let $\varepsilon > 0$. Since q/w grows to infinity as $x \rightarrow 0$ by (8.2), we may choose $\delta < L/2$ small enough that

$$\frac{q(x)}{w(x)} \geq \frac{1}{\varepsilon} \quad \text{whenever } x \in (0, \delta).$$

Consider now two cases. If $m \leq 1$ then $mw \leq w$ and so

$$w \leq \varepsilon q \leq \varepsilon(q - mw + w).$$

On the other hand, if $m > 1$ then $(m-1)mw \leq (m-1)q$ and so

$$w \leq \varepsilon q \leq \varepsilon m(q - mw + w).$$

In both cases $w \leq \varepsilon(1 + |m|)(q - mw + w)$, and so

$$\int_0^\delta f_\ell^2 w \, dx \leq \varepsilon(1 + |m|) \|f_\ell\|_{\mathcal{K}}^2 \leq \varepsilon(1 + |m|) M^2$$

for all ℓ . Since $\{f_\ell\}$ converges in $L^2((\delta, L/2), w \, dx)$, we may restrict attention to the interval $(0, \delta)$ and deduce

$$\begin{aligned} \limsup_{\ell, n \rightarrow \infty} \|f_\ell - f_n\|_{L^2((0, L/2), w \, dx)} &= \limsup_{\ell, n \rightarrow \infty} \|f_\ell - f_n\|_{L^2((0, \delta), w \, dx)} \\ &\leq 2\sqrt{\varepsilon(1 + |m|)} M. \end{aligned}$$

Letting $\varepsilon \rightarrow 0$ shows $\{f_\ell\}$ is Cauchy in $L^2((0, L/2), w \, dx)$, and hence converges.

Construction for compact imbedding on $(0, L/2)$, assuming (8.3). The proof goes like above, except we need a different argument to control

$\int_0^\delta f_\ell^2 w \, dx$. Write $P(x) = \int_{L/2}^x p(y)^{-1} \, dy$, so that P is an antiderivative of $1/p$. Let $\varepsilon > 0$ and choose $\delta \in (0, L/2)$ such that

$$\int_0^\delta w(x) \, dx \leq \varepsilon \quad \text{and} \quad \int_0^\delta |P(x)| w(x) \, dx \leq \varepsilon,$$

which is possible since w and Pw are integrable by assumption (8.3). Then for $x < L/2$ we have

$$\begin{aligned} f_\ell(x) &= f_\ell(L/2) - \int_x^{L/2} f'_\ell(y) \, dy \\ &\leq C \|f_\ell\|_{H^1(L/4, 3L/4)} + \left(\int_x^{L/2} f'_\ell(y)^2 p(y) \, dy \right)^{1/2} \left(\int_x^{L/2} p(y)^{-1} \, dy \right)^{1/2} \\ &\quad \text{by Lemma 8.1 below and Cauchy-Schwarz} \\ &\leq C \|f_\ell\|_{\mathcal{K}} + \|f_\ell\|_{\mathcal{K}} |P(x)|^{1/2} \end{aligned}$$

where the constant C in the last line depends on the behavior of the coefficient functions on the interval $[L/4, 3L/4]$. Hence

$$\begin{aligned} \left(\int_0^\delta f_\ell^2 w \, dx \right)^{1/2} &\leq C \|f_\ell\|_{\mathcal{K}} \left(\int_0^\delta w \, dx \right)^{1/2} + \|f_\ell\|_{\mathcal{K}} \left(\int_0^\delta |P(x)| w(x) \, dx \right)^{1/2} \\ &\leq (C + 1) M \sqrt{\varepsilon} \end{aligned}$$

by our choice of δ . Now the proof can be concluded like in the previous case.

Sesquilinear form: define $\mathbf{a} : \mathcal{K} \times \mathcal{K} \rightarrow \mathbb{R}$ by

$$\mathbf{a}(\mathbf{u}, \mathbf{v}) = \int_0^L (\mathbf{u}'\mathbf{v}'p + \mathbf{u}\mathbf{v}(q - m\mathbf{w} + \mathbf{w})) \, dx = \langle \mathbf{u}, \mathbf{v} \rangle_{\mathcal{K}}$$

so that \mathbf{a} is linear, continuous, and symmetric.

Coercivity: $\mathbf{a}(\mathbf{u}, \mathbf{u}) = \|\mathbf{u}\|_{\mathcal{K}}^2$.

Conclusions. We have verified the assumptions of the discrete spectral Theorem 4.1, and so we obtain from it an ONB of weak eigenfunctions satisfying

$$\mathbf{a}(\mathbf{u}_j, \mathbf{v}) = \gamma_j \langle \mathbf{u}_j, \mathbf{v} \rangle_{\mathcal{H}} \quad \forall \mathbf{v} \in \mathcal{K},$$

which simplifies to

$$\int_0^L (u_j' v' p + u_j v q) \, dx = \lambda_j \int_0^L u_j v w \, dx \quad \forall v \in \mathcal{K},$$

where

$$\lambda_j = \gamma_j + m - 1.$$

The preceding formula holds in particular whenever $v \in H^1(\mathcal{I})$ has compact support in the interval, and so

$$-(p u_j')' + q u_j = \lambda w u_j \quad \text{weakly on } (0, L).$$

It follows by regularity theory that u_j is smooth.

Dirichlet boundary condition at $x = L$: the condition $u(L) = 0$ was imposed in the definition of the space \mathcal{K} .

Neumann boundary condition at $x = 0$: by the natural boundary condition argument in Chapter ??, one obtains formally the Neumann BC

$$p u'|_{x=0^+} = 0.$$

To make this derivation rigorous, one requires the space \mathcal{K} to contain a function v that equals 1 near $x = 0$, which is true if $\int_0^{L/2} q \, dx < \infty$ and $\int_0^{L/2} w \, dx < \infty$. Weaker conditions might suffice to obtain the natural boundary condition, of course, in particular cases.

It remains to establish a lemma used in the proof above.

Lemma 8.1 (Boundedness of Sobolev functions in 1 dimension). *Fix $s < t$. If $f \in H^1(s, t)$ then*

$$\|f\|_{L^\infty} \leq C \|f\|_{H^1}$$

where the constant C depends on the length $t - s$.

Proof. f is Hölder continuous with exponent $1/2$, since

$$|f(x) - f(y)| = \left| \int_x^y f'(z) \, dz \right| \leq \|f'\|_{L^2} |x - y|^{1/2}, \quad x, y \in (s, t).$$

Hence

$$|f(x)| \leq |f(y)| + \|f'\|_{L^2} (t - s)^{1/2}.$$

Integrating with respect to \mathbf{y} gives

$$\begin{aligned} |f(\mathbf{x})| &\leq \frac{1}{\mathbf{t} - \mathbf{s}} \int_{\mathbf{s}}^{\mathbf{t}} |f(\mathbf{y})| \, d\mathbf{y} + \|f'\|_{L^2}(\mathbf{t} - \mathbf{s})^{1/2} \\ &\leq \frac{1}{(\mathbf{t} - \mathbf{s})^{1/2}} \|f\|_{L^2} + \|f'\|_{L^2}(\mathbf{t} - \mathbf{s})^{1/2} \end{aligned}$$

and so $|f(\mathbf{x})| \leq C\|f\|_{H^1}$. □

Example — Bessel eigenfunctions

The Bessel eigenvalue problem with parameter $\mathbf{n} \geq 0$ is

$$-u''(r) - \frac{1}{r}u'(r) + \frac{\mathbf{n}^2}{r^2}u(r) = \lambda u(r), \quad 0 < r < 1, \quad (8.7)$$

which can be rewritten in standard form as

$$-(ru')' + \mathbf{n}^2 r^{-1}u = \lambda ru, \quad 0 < r < 1.$$

The coefficient functions

$$p(r) = r, \quad q(r) = \mathbf{n}^2 r^{-1}, \quad w(r) = r,$$

satisfy assumptions (8.2), (8.3) and (8.5).

We may impose a Dirichlet condition $u(1) = 0$ at the right endpoint, since p satisfies assumption (8.6).

This Bessel eigenvalue problem satisfies the hypotheses of this Chapter, and so one gets an ONB of eigenfunctions in the weighted space $L^2((0, 1), r \, dr)$. One may compute the eigenfunctions explicitly by solving the ODE and applying the boundary condition at $r = 1$. The solutions, before normalizing in L^2 , are $J_{\mathbf{n}}(j_{\mathbf{n},k}r)$ for $k = 1, 2, 3, \dots$, where $j_{\mathbf{n},k}$ is the k -th root of the Bessel function $J_{\mathbf{n}}$.

The Bessel eigenvalue problem arises from separating variables to find eigenvalues of the Laplacian on the disk. Indeed, by substituting either $f = u(r) \cos n\theta$ or $f = u(r) \sin n\theta$ into the Laplacian eigenvalue equation

$$-\Delta f = \lambda f$$

and recalling that the Laplacian in polar coordinates has the form $\Delta = \partial_{rr} + r^{-1}\partial_r + r^{-2}\partial_{\theta\theta}$, we arrive immediately at (8.7). The restriction $\nabla f \in L^2(\mathbb{D})$ means in polar coordinates that $u' \in L^2((0, 1), r \, dr)$ and $u \in L^2((0, 1), r^{-1} \, dr)$. The Dirichlet condition $u(1) = 0$ for the Bessel problem corresponds to a Dirichlet condition for f on the boundary of the disk.

Exercises

Show the following eigenvalue problems are covered by the results in this chapter, after a translation and multiplying through by an integrating factor if necessary. Ignore boundary conditions, and do not impose (8.6) for a Dirichlet boundary condition at $x = L$.

8.1 — Legendre problem

$$-((1 - x^2)u')' = \lambda u, \quad -1 < x < 1.$$

8.2 — Chebyshev problem

$$-(1 - x^2)u'' + xu' = \lambda u, \quad -1 < x < 1.$$

8.3 — Harmonic oscillator in disguise

$$-\frac{d}{d\theta} \left(\cos^2 \theta \frac{du}{d\theta} \right) + (\sec^2 \theta \tan^2 \theta)u = \lambda(\sec^2 \theta)u, \quad -\frac{\pi}{2} < \theta < \frac{\pi}{2}.$$

8.4 — Laguerre problem

$$-xu'' + (x - 1)u' = \lambda u, \quad 0 < x < \infty.$$

The semi-infinite interval in this last exercise requires a modification of the proof, using a diagonal argument on a sequence of intervals of the form $(1, n)$.

Notes and comments

The methods of this chapter are similar to the treatment of the Schrödinger operator with a potential well, in Chapter 7.

The literature on Sturm–Liouville problems is vast. Two particularly interesting sources are an old paper by [Friedrichs] and a more recent book by [Zettl].

Chapter 9

Application: discrete spectrum for the biLaplacian

Goal

To apply the spectral theorem from Chapter 4 to the biLaplacian, which is a fourth order operator.

BiLaplacian — vibrating plates

The fourth order wave equation

$$\phi_{tt} = -\Delta\Delta\phi$$

describes the transverse vibrations of a rigid plate, which in one dimension simplifies to the *beam equation*

$$\phi_{tt} = -\phi''''.$$

After separating out the time variable with $\phi = \sin(\sqrt{\Lambda}t)\mathbf{u}(\mathbf{x})$, one arrives at the eigenvalue problem for the biLaplacian:

$$\Delta\Delta\mathbf{u} = \Lambda\mathbf{u} \quad \text{in } \Omega.$$

We will prove existence of an orthonormal basis of eigenfunctions. For simplicity we start with the Dirichlet case, which has boundary conditions

$$\mathbf{u} = |\nabla\mathbf{u}| = 0 \quad \text{on } \partial\Omega.$$

Let:

Ω = domain of finite volume in \mathbb{R}^d ,

$\mathcal{H} = L^2(\Omega)$,

$\mathcal{K} = H_0^2(\Omega) =$ completion of $C_0^\infty(\Omega)$ under the inner product

$$\begin{aligned} \langle \mathbf{u}, \mathbf{v} \rangle_{H^2} &= \int_{\Omega} \left(\sum_{m,n=1}^d u_{x_m x_n} v_{x_m x_n} + \sum_{m=1}^d u_{x_m} v_{x_m} + uv \right) dx \\ &= \int_{\Omega} (D^2 \mathbf{u} \cdot D^2 \mathbf{v} + \nabla \mathbf{u} \cdot \nabla \mathbf{v} + uv) dx \end{aligned}$$

where $D^2 \mathbf{u}$ denotes the Hessian matrix of \mathbf{u} (the matrix of second derivatives) and the dot products act component-wise.

Intuitively, H_0^2 consists of functions in L^2 whose first and second derivatives belong to L^2 and for which the function and its first derivatives vanish on the boundary.

Recall $L^2(\Omega)$ is separable [Ciarlet, Theorem 2.5-4].

Density: $C_0^\infty \subset H_0^2 \subset L^2$ and C_0^∞ is dense in L^2 , so H_0^2 is dense in L^2 .

Compact imbedding: $H_0^2 \hookrightarrow H_0^1 \hookrightarrow L^2$. The second imbedding is compact by Rellich's Theorem B.4, and so the composition of imbeddings is compact also.

Sesquilinear form: define

$$\mathbf{a}(\mathbf{u}, \mathbf{v}) = \int_{\Omega} (D^2 \mathbf{u} \cdot D^2 \mathbf{v} + uv) dx, \quad \mathbf{u}, \mathbf{v} \in H_0^2(\Omega).$$

Clearly \mathbf{a} is linear, and symmetric and continuous on $H_0^2(\Omega)$.

Coercivity:

$$\begin{aligned} \|\mathbf{u}\|_{H^2}^2 &= \mathbf{a}(\mathbf{u}, \mathbf{u}) + \sum_{m=1}^d \int_{\Omega} u_{x_m}^2 dx \\ &= \mathbf{a}(\mathbf{u}, \mathbf{u}) - \sum_{m=1}^d \int_{\Omega} u_{x_m x_m} u dx \quad \text{by parts} \\ &\leq \mathbf{a}(\mathbf{u}, \mathbf{u}) + \sum_{m=1}^d \int_{\Omega} (u_{x_m x_m}^2 + u^2) dx \\ &\leq (1 + d)\mathbf{a}(\mathbf{u}, \mathbf{u}). \end{aligned}$$

Hence the discrete spectral Theorem 4.1 gives an ONB $\{\mathbf{u}_j\}$ for $L^2(\Omega)$ and corresponding eigenvalues which we denote $\gamma_j = \Lambda_j + 1$ satisfying

$$\mathbf{a}(\mathbf{u}_j, \mathbf{v}) = (\Lambda_j + 1)\langle \mathbf{u}_j, \mathbf{v} \rangle_{L^2} \quad \forall \mathbf{v} \in H_0^2(\Omega).$$

Equivalently,

$$\int_{\Omega} \sum_{m,n=1}^d (\mathbf{u}_j)_{x_m x_n} v_{x_m x_n} \, dx = \Lambda_j \int_{\Omega} \mathbf{u}_j v \, dx \quad \forall v \in H_0^2(\Omega). \quad (9.1)$$

That is,

$$\sum_{m,n=1}^d (\mathbf{u}_j)_{x_m x_m x_n x_n} = \Lambda_j \mathbf{u}_j \quad \text{weakly,}$$

or

$$\Delta \Delta \mathbf{u}_j = \Lambda_j \mathbf{u}_j \quad \text{weakly.}$$

Hence \mathbf{u}_j is a weak eigenfunction of the biLaplacian with eigenvalue Λ_j . Elliptic regularity gives that \mathbf{u}_j is C^∞ -smooth, and hence satisfies the eigenfunction equation classically.

Dirichlet boundary condition: $\mathbf{u}_j = |\nabla \mathbf{u}_j| = 0$ on $\partial\Omega$ in the sense of Sobolev spaces (since \mathbf{u}_j and each partial derivative $(\mathbf{u}_j)_{x_m}$ belong to H_0^1). The boundary condition holds classically on any smooth portion of $\partial\Omega$, by elliptic regularity results.

Positivity of the eigenvalues:

$$\Lambda_j = \frac{\int_{\Omega} |D^2 \mathbf{u}_j|^2 \, dx}{\int_{\Omega} \mathbf{u}_j^2 \, dx} \geq 0$$

by choosing $v = \mathbf{u}_j$ in the weak formulation (9.1). Further, $\Lambda_j > 0$ because if $\Lambda_j = 0$ then $(\mathbf{u}_j)_{x_m x_n} \equiv 0$ by the last formula, and so $(\mathbf{u}_j)_{x_m} \equiv (\text{const.})$; one deduces $(\mathbf{u}_j)_{x_m} \equiv 0$ since $(\mathbf{u}_j)_{x_m}$ vanishes on the boundary; hence \mathbf{u}_j itself is constant and thus identically zero because it vanishes on the boundary, which contradicts the normalization of the L^2 -norm of \mathbf{u}_j to equal 1. We conclude that

$$0 < \Lambda_1 \leq \Lambda_2 \leq \Lambda_3 \leq \cdots \rightarrow \infty.$$

BiLaplacian — natural boundary conditions

Natural boundary conditions for the biLaplacian acting on $\mathbf{u} \in H^2(\Omega)$ can be derived by a process like in Chapter ?? [Chasman, §5]. These natural conditions are much more complicated than for the Laplacian.

Chapter 10

Variational characterizations of eigenvalues

Goal

To obtain minimax and maximin characterizations of the eigenvalues of the sesquilinear form in Chapter 4.

Motivation and hypotheses. How can one estimate the eigenvalues if the spectrum cannot be computed explicitly? We will develop two complementary variational characterizations of eigenvalues. The intuition for these characterizations comes from the special case of eigenvalues of a Hermitian (or real symmetric) matrix \mathbf{A} , for which the sesquilinear form is $\mathbf{a}(\mathbf{u}, \mathbf{v}) = \mathbf{A}\mathbf{u} \cdot \bar{\mathbf{v}}$ and the first eigenvalue is

$$\gamma_1 = \min_{\mathbf{v} \neq 0} \frac{\mathbf{A}\mathbf{v} \cdot \bar{\mathbf{v}}}{\mathbf{v} \cdot \bar{\mathbf{v}}}.$$

Poincaré's minimax characterization of the eigenvalues

We work under the assumptions of the discrete spectral theorem in Chapter 4, for the sesquilinear form \mathbf{a} . Recall the ordering

$$\gamma_1 \leq \gamma_2 \leq \gamma_3 \leq \cdots \rightarrow \infty.$$

Define the *Rayleigh quotient* of \mathbf{u} to be

$$\frac{\mathbf{a}(\mathbf{u}, \mathbf{u})}{\langle \mathbf{u}, \mathbf{u} \rangle_{\mathcal{H}}}.$$

Rayleigh principle for the first eigenvalue

The first eigenvalue γ_1 equals the minimum value of the Rayleigh quotient:

$$\gamma_1 = \min_{f \in \mathcal{K} \setminus \{0\}} \frac{\mathbf{a}(f, f)}{\langle f, f \rangle_{\mathcal{H}}}. \quad (10.1)$$

The minimum is attained if and only if f is an eigenfunction with eigenvalue γ_1 .

Proof of Rayleigh principle. The arbitrary vector $f \in \mathcal{K}$ can be expanded in terms of the ONB of eigenvectors as

$$f = \sum_j c_j \mathbf{u}_j$$

where $c_j = \langle f, \mathbf{u}_j \rangle_{\mathcal{H}}$. This series converges in both \mathcal{H} and \mathcal{K} , as proved in Chapter 4. Hence we may substitute the series into the Rayleigh quotient to obtain

$$\begin{aligned} \frac{\mathbf{a}(f, f)}{\langle f, f \rangle_{\mathcal{H}}} &= \frac{\sum_{j,k} c_j \overline{c_k} \mathbf{a}(\mathbf{u}_j, \mathbf{u}_k)}{\sum_{j,k} c_j \overline{c_k} \langle \mathbf{u}_j, \mathbf{u}_k \rangle_{\mathcal{H}}} \\ &= \frac{\sum_j |c_j|^2 \gamma_j}{\sum_j |c_j|^2} \end{aligned} \quad (10.2)$$

since the eigenvectors $\{\mathbf{u}_j\}$ are orthonormal in \mathcal{H} and the collection $\{\mathbf{u}_j/\sqrt{\gamma_j}\}$ is \mathbf{a} -orthonormal in \mathcal{K} (that is, $\mathbf{a}(\mathbf{u}_j, \mathbf{u}_k) = \gamma_j \delta_{jk}$). The expression (10.2) is obviously greater than or equal to γ_1 .

Equality holds if and only if f is a first eigenfunction, that is, if and only if $f = \sum_{j=1}^J c_j \mathbf{u}_j$ where $\gamma_1 = \cdots = \gamma_J < \gamma_{J+1}$. (In most applications the first eigenvalue is simple, in which case $J = 1$ and equality holds in the Rayleigh quotient if and only if f is a multiple of \mathbf{u}_1 .)

Rayleigh principle for second eigenvalue

A variant of the Rayleigh principle is sometimes used for the second eigenvalue:

$$\gamma_2 = \min_{0 \neq f \perp \mathbf{u}_1} \frac{\mathbf{a}(f, f)}{\langle f, f \rangle_{\mathcal{H}}} \quad (10.3)$$

where the trial vector satisfies $f \in \mathcal{K}$, $f \neq 0$ and $\langle f, \mathbf{u}_1 \rangle_{\mathcal{H}} = 0$. The proof mimics that of the Rayleigh principle, except now with $c_1 = 0$ since f is orthogonal to the first eigenvector

Poincaré principle for higher eigenvalues

The j -th eigenvalue for any $j \geq 1$ is given by the following minimax formula:

$$\gamma_j = \min_S \max_{f \in S \setminus \{0\}} \frac{\mathbf{a}(f, f)}{\langle f, f \rangle_{\mathcal{H}}} \quad (10.4)$$

where S ranges over all j -dimensional subspaces of \mathcal{K} .

Remark. The Rayleigh and Poincaré principles provide *upper bounds* on eigenvalues, since they express γ_1 and γ_j as minima of computable quantities. That is, an upper bound on γ_1 follows from substituting any vector f into the Rayleigh quotient in (10.1), and an upper bound on γ_j is obtained by choosing S to be any j -dimensional subspace and evaluating the maximum over $f \in S$ of the Rayleigh quotient in (10.4).

Proof of Poincaré principle. We prove the minimax formula (10.4) for $j = 2$, and leave the case of higher j -values as an exercise.

“ \geq ” direction of the proof. Choose $S = \{c_1 \mathbf{u}_1 + c_2 \mathbf{u}_2 : c_1, c_2 \text{ scalars}\}$ to be the span of the first two eigenvectors. Then

$$\max_{f \in S \setminus \{0\}} \frac{\mathbf{a}(f, f)}{\langle f, f \rangle_{\mathcal{H}}} = \max_{(c_1, c_2) \neq (0, 0)} \frac{\sum_{j=1}^2 |c_j|^2 \gamma_j}{\sum_{j=1}^2 |c_j|^2} = \gamma_2.$$

Hence $\gamma_2 \geq$ right side of (10.4).

“ \leq ” direction of the proof. To prove the opposite inequality, consider an arbitrary 2-dimensional subspace $S \subset \mathcal{K}$. Note this subspace is arbitrary, and need not equal the span of two of the eigenvectors.

The subspace contains a nonzero vector \mathbf{g} that is orthogonal to \mathbf{u}_1 . (Proof: given a basis $\{\mathbf{v}_1, \mathbf{v}_2\}$ for the subspace, there exist scalars $\mathbf{d}_1, \mathbf{d}_2$ not both zero such that $\mathbf{d}_1 \langle \mathbf{v}_1, \mathbf{u}_1 \rangle_{\mathcal{H}} + \mathbf{d}_2 \langle \mathbf{v}_2, \mathbf{u}_1 \rangle_{\mathcal{H}} = 0$. Hence the vector $\mathbf{g} = \mathbf{d}_1 \mathbf{v}_1 + \mathbf{d}_2 \mathbf{v}_2$ satisfies $\langle \mathbf{g}, \mathbf{u}_1 \rangle_{\mathcal{H}} = 0$.) Thus $c_1 = 0$ in the orthonormal expansion for \mathbf{g} , and so by (10.2),

$$\frac{\mathbf{a}(\mathbf{g}, \mathbf{g})}{\langle \mathbf{g}, \mathbf{g} \rangle_{\mathcal{H}}} = \frac{\sum_{j=2}^{\infty} |c_j|^2 \gamma_j}{\sum_{j=2}^{\infty} |c_j|^2} \geq \gamma_2.$$

Hence

$$\max_{f \in S \setminus \{0\}} \frac{\mathbf{a}(f, f)}{\langle f, f \rangle_{\mathcal{H}}} \geq \frac{\mathbf{a}(\mathbf{g}, \mathbf{g})}{\langle \mathbf{g}, \mathbf{g} \rangle_{\mathcal{H}}} \geq \gamma_2,$$

which implies that $\gamma_2 \leq$ right side of (10.4). \square

Variational characterization of eigenvalue sums.

The sum of the first n eigenvalues has a “minimum” characterization similar to the Rayleigh principle for the first eigenvalue, but now involving pairwise orthogonal trial vectors:

$$\begin{aligned} & \gamma_1 + \cdots + \gamma_n & (10.5) \\ & = \min \left\{ \frac{\mathbf{a}(f_1, f_1)}{\langle f_1, f_1 \rangle_{\mathcal{H}}} + \cdots + \frac{\mathbf{a}(f_n, f_n)}{\langle f_n, f_n \rangle_{\mathcal{H}}} : f_j \in \mathcal{K} \setminus \{0\}, \langle f_j, f_k \rangle_{\mathcal{H}} = 0 \text{ when } j \neq k \right\}. \end{aligned}$$

See the notes at the end of the chapter.

Courant’s maximin characterization

Eigenvalues of the sesquilinear form are given also by Courant’s maximin principle:

$$\gamma_j = \max_{\mathbf{S}} \min_{0 \neq f \perp \mathbf{S}} \frac{\mathbf{a}(f, f)}{\langle f, f \rangle_{\mathcal{H}}} \quad (10.6)$$

where here \mathbf{S} ranges over all $(j - 1)$ -dimensional subspaces of \mathcal{K} .

Remark. The Courant principle provides *lower bounds* on eigenvalues, since it expresses γ_j as a maximum. The lower bounds are difficult to compute, though, because \mathbf{S}^\perp is an infinite dimensional space.

Sketch of proof of Courant principle. The Courant principle reduces to Rayleigh’s principle when $j = 1$, since in that case \mathbf{S} is the zero subspace and $\mathbf{S}^\perp = \mathcal{K}$.

Take $j = 2$. (The proof for higher j -values is left to the reader.) For the “ \leq ” direction of the proof, choose \mathbf{S} to be the 1-dimensional space spanned by the first eigenvector \mathbf{u}_1 . Then every $f \in \mathbf{S}^\perp$ has $c_1 = \langle f, \mathbf{u}_1 \rangle_{\mathcal{H}} = 0$ and so

$$\gamma_2 \leq \min_{f \in \mathbf{S}^\perp \setminus \{0\}} \frac{\mathbf{a}(f, f)}{\langle f, f \rangle_{\mathcal{H}}}$$

by expanding $f = \sum_{j=2}^{\infty} c_j \mathbf{u}_j$ and computing just as in the proof of the Poincaré principle.

For the “ \geq ” direction of the proof, consider an arbitrary 1-dimensional subspace \mathbf{S} of \mathcal{K} . Then \mathbf{S}^\perp contains some vector of the form $f = c_1 \mathbf{u}_1 + c_2 \mathbf{u}_2$ with c_1 or c_2 nonzero. Hence

$$\min_{0 \neq f \perp \mathbf{S}} \frac{\mathbf{a}(f, f)}{\langle f, f \rangle_{\mathcal{H}}} \leq \frac{\sum_{j=1}^2 |c_j|^2 \gamma_j}{\sum_{j=1}^2 |c_j|^2} \leq \gamma_2.$$

Eigenvalues as critical values of the Rayleigh quotient

Even if one did not know the existence of an ONB of eigenvectors, one could still prove the Rayleigh principle by the following direct approach. Define γ^* to equal the infimum of the Rayleigh quotient:

$$\gamma^* = \inf_{f \in \mathcal{K} \setminus \{0\}} \frac{\mathbf{a}(f, f)}{\langle f, f \rangle_{\mathcal{H}}}.$$

We will prove γ^* is an eigenvalue. It follows that γ^* is the lowest eigenvalue, $\gamma^* = \gamma_1$ (because if any eigenvector f corresponded to a smaller eigenvalue, then the Rayleigh quotient of f would be smaller than γ^* , a contradiction).

First, choose an infimizing sequence $\{f_k\}$ normalized with $\|f_k\|_{\mathcal{H}} = 1$, so that

$$\mathbf{a}(f_k, f_k) \rightarrow \gamma^*.$$

By weak sequential compactness of the closed ball in the Hilbert space \mathcal{K} , we may suppose after passing to a subsequence that f_k converges weakly in \mathcal{K} to some $\mathbf{u} \in \mathcal{K}$. Hence f_k also converges weakly in \mathcal{H} to \mathbf{u} (because if $F(\cdot)$ is any bounded linear functional on \mathcal{H} then it is also a bounded linear functional on \mathcal{K}). We may further suppose f_k converges in \mathcal{H} to some $\mathbf{v} \in \mathcal{H}$, by compactness of the imbedding $\mathcal{K} \hookrightarrow \mathcal{H}$, and then f_k converges also weakly in \mathcal{H} to \mathbf{v} , so that $\mathbf{v} = \mathbf{u}$. To summarize: $f_k \rightharpoonup \mathbf{u}$ weakly in \mathcal{K} and $f_k \rightarrow \mathbf{u}$ in \mathcal{H} . In particular, $\|\mathbf{u}\|_{\mathcal{H}} = 1$. Therefore

$$\begin{aligned} 0 &\leq \mathbf{a}(f_k - \mathbf{u}, f_k - \mathbf{u}) \\ &= \mathbf{a}(f_k, f_k) - 2 \operatorname{Re} \mathbf{a}(f_k, \mathbf{u}) + \mathbf{a}(\mathbf{u}, \mathbf{u}) \\ &\rightarrow \gamma^* - 2 \operatorname{Re} \mathbf{a}(\mathbf{u}, \mathbf{u}) + \mathbf{a}(\mathbf{u}, \mathbf{u}) \quad \text{using weak convergence } f_k \rightharpoonup \mathbf{u} \\ &= \gamma^* - \mathbf{a}(\mathbf{u}, \mathbf{u}) \\ &\leq 0 \end{aligned}$$

by definition of γ^* as an infimum. Thus equality holds throughout, and so $\gamma^* = \mathbf{a}(\mathbf{u}, \mathbf{u})$, which means the infimum defining γ^* is actually a minimum:

$$\gamma^* = \min_{f \in \mathcal{K} \setminus \{0\}} \frac{\mathbf{a}(f, f)}{\langle f, f \rangle_{\mathcal{H}}}.$$

The minimum is attained when $f = \mathbf{u}$.

Our second task is to show \mathbf{u} is an eigenvector with eigenvalue γ^* . Let $\mathbf{v} \in \mathcal{K}$ be arbitrary and use $f = \mathbf{u} + t\mathbf{v}$ as a trial vector in the Rayleigh

quotient. Since $\mathbf{t} = \mathbf{0}$ gives the minimizer $\mathbf{f} = \mathbf{u}$, the derivative of the Rayleigh quotient at $\mathbf{t} = \mathbf{0}$ must equal zero by the first derivative test from calculus:

$$0 = \left. \frac{d}{dt} \frac{\mathbf{a}(\mathbf{u} + t\mathbf{v}, \mathbf{u} + t\mathbf{v})}{\langle \mathbf{u} + t\mathbf{v}, \mathbf{u} + t\mathbf{v} \rangle_{\mathcal{H}}} \right|_{t=0} = 2 \operatorname{Re} \mathbf{a}(\mathbf{u}, \mathbf{v}) - \gamma^* 2 \operatorname{Re} \langle \mathbf{u}, \mathbf{v} \rangle_{\mathcal{H}}.$$

The same equation holds with Im instead of Re , as we see by replacing \mathbf{v} with $i\mathbf{v}$. (This last step is unnecessary when working with real Hilbert spaces, of course.) Hence

$$\mathbf{a}(\mathbf{u}, \mathbf{v}) = \gamma^* \langle \mathbf{u}, \mathbf{v} \rangle_{\mathcal{H}} \quad \forall \mathbf{v} \in \mathcal{K},$$

which means \mathbf{u} is an eigenvector for the sesquilinear form \mathbf{a} with eigenvalue γ^* .

Notes and comments

Variational principles can be developed not just for individual eigenvalues, but also for combinations such as the sum of the first n eigenvalues, and the sum of the first n reciprocal eigenvalues. See [Bandle] Section III.1.2.

Chapter 11

Monotonicity properties of eigenvalues

Goal

To establish monotonicity results for Dirichlet and Neumann eigenvalues of the Laplacian, and a diamagnetic comparison for the magnetic Laplacian.

Rayleigh quotients

The spectral problems in Chapters 5–9 have Rayleigh quotients and function spaces as follows.

$$\begin{aligned} \text{Dirichlet Laplacian: } & \frac{\int_{\Omega} |\nabla f|^2 \, dx}{\int_{\Omega} f^2 \, dx}, & f \in H_0^1(\Omega). \\ \text{Robin Laplacian: } & \frac{\int_{\Omega} |\nabla f|^2 \, dx + \sigma \int_{\partial\Omega} f^2 \, dS}{\int_{\Omega} f^2 \, dx}, & f \in H^1(\Omega). \\ \text{Neumann Laplacian: } & \frac{\int_{\Omega} |\nabla f|^2 \, dx}{\int_{\Omega} f^2 \, dx}, & f \in H^1(\Omega). \end{aligned}$$

$$\begin{aligned}
\text{magnetic Laplacian: } & \frac{\int_{\Omega} |i\nabla f + \vec{A}f|^2 \, dx}{\int_{\Omega} |f|^2 \, dx}, & f \in H_0^1(\Omega). \\
\text{Schrödinger: } & \frac{\int_{\mathbb{R}^d} (|\nabla f|^2 + Vf^2) \, dx}{\int_{\mathbb{R}^d} f^2 \, dx}, & f \in H^1(\mathbb{R}^d) \cap L^2(|V| \, dx). \\
\text{Sturm–Liouville: } & \frac{\int_0^L (|f'|^2 p + f^2 q) \, dx}{\int_0^L f^2 w \, dx}, & f \in \mathcal{K} \text{ (see below)}. \\
\text{Dirichlet biLaplacian: } & \frac{\int_{\Omega} \sum_{m,n=1}^d f_{x_m x_n}^2 \, dx}{\int_{\Omega} f^2 \, dx}, & f \in H_0^2(\Omega), \\
& = \frac{\int_{\Omega} (\Delta f)^2 \, dx}{\int_{\Omega} f^2 \, dx}.
\end{aligned}$$

The Sturm–Liouville function space used above is

$$\mathcal{K} = \{u \in H_{\text{loc}}^1(\mathcal{I}) : u' \in L^2(\mathcal{I}, p \, dx), u \in L^2(\mathcal{I}, (q - mw + w) \, dx), u(L) = 0\}$$

where $\mathcal{I} = (0, L)$ and $m = \inf_{\mathcal{I}} q/w > -\infty$.

The Poincaré principle (10.4) gives a minimax formula for the eigenvalues in terms of these Rayleigh quotients. In particular, for the Dirichlet, Robin and Neumann spectra of the Laplacian one has

$$\begin{aligned}
\lambda_j &= \min_S \max_{f \in S \setminus \{0\}} \frac{\int_{\Omega} |\nabla f|^2 \, dx}{\int_{\Omega} f^2 \, dx}, \\
\rho_j &= \min_T \max_{f \in T \setminus \{0\}} \frac{\int_{\Omega} |\nabla f|^2 \, dx + \sigma \int_{\partial\Omega} f^2 \, dS}{\int_{\Omega} f^2 \, dx}, \\
\mu_j &= \min_U \max_{f \in U \setminus \{0\}} \frac{\int_{\Omega} |\nabla f|^2 \, dx}{\int_{\Omega} f^2 \, dx},
\end{aligned}$$

where S ranges over j -dimensional subspaces of $H_0^1(\Omega)$, and T and U range over j -dimensional subspaces of $H^1(\Omega)$.

Neumann \leq Robin \leq Dirichlet

Free membranes give lower tones than partially free and fixed membranes:

Theorem 11.1 (Neumann–Robin–Dirichlet comparison). *Let Ω be a bounded domain in \mathbb{R}^d with Lipschitz boundary, and fix $\sigma > 0$.*

Then the Neumann eigenvalues of the Laplacian lie below their Robin counterparts, which in turn lie below the Dirichlet eigenvalues:

$$\mu_j \leq \rho_j \leq \lambda_j \quad \forall j \geq 1.$$

Proof. Clearly $\mu_j \leq \rho_j$, since $\sigma > 0$ in the Robin Rayleigh quotient.

Next, every subspace \mathbf{S} is also a valid \mathbf{T} , since $H_0^1 \subset H^1$ by definition. Thus the minimum for the Robin eigenvalue ρ_j is taken over a larger class of subspaces than the minimum for the Dirichlet eigenvalue λ_j . Further, the boundary term vanishes in the Robin Rayleigh quotient for each $f \in \mathbf{S} \subset H_0^1$. Hence $\rho_j \leq \lambda_j$. \square

Incidentally, remember the first Neumann eigenvalue is zero: $\mu_1 = 0$.

Domain monotonicity for Dirichlet spectrum

Making a drum smaller increases its frequencies of vibration:

Theorem 11.2. *Let Ω and $\tilde{\Omega}$ be domains of finite volume in \mathbb{R}^d with eigenvalues λ_j and $\tilde{\lambda}_j$ for the Dirichlet Laplacian, respectively. If $\Omega \supset \tilde{\Omega}$ then*

$$\lambda_j \leq \tilde{\lambda}_j \quad \forall j \geq 1.$$

Proof. Poincaré’s minimax principle gives

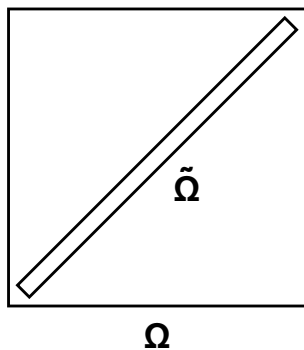
$$\lambda_j = \min_{\mathbf{S}} \max_{f \in \mathbf{S} \setminus \{0\}} \frac{\int_{\Omega} |\nabla f|^2 \, dx}{\int_{\Omega} f^2 \, dx}, \quad \tilde{\lambda}_j = \min_{\tilde{\mathbf{S}}} \max_{f \in \tilde{\mathbf{S}} \setminus \{0\}} \frac{\int_{\tilde{\Omega}} |\nabla f|^2 \, dx}{\int_{\tilde{\Omega}} f^2 \, dx},$$

where \mathbf{S} ranges over j -dimensional subspaces of $H_0^1(\Omega)$ and $\tilde{\mathbf{S}}$ ranges over j -dimensional subspaces of $H_0^1(\tilde{\Omega})$.

Every subspace $\tilde{\mathbf{S}}$ is also a valid \mathbf{S} since $H_0^1(\tilde{\Omega}) \subset H_0^1(\Omega)$, by extending $f \in H_0^1(\tilde{\Omega})$ to equal 0 outside $\tilde{\Omega}$. This extension by 0 does not change the value of the Rayleigh quotient, and hence does not change the value of the maximum over $f \in \tilde{\mathbf{S}}$. Therefore $\lambda_j \leq \tilde{\lambda}_j$. \square

Counterexample to Neumann domain monotonicity

A smaller domain can have smaller Neumann eigenvalues, as the figure below shows for a rectangle contained in a unit square. Recall from Chapter 2 that $\mu_2 = \pi^2/L^2$ for a rectangle with longer side length L . The square has both sides of length 1 and hence $\mu_2 = \pi^2$, while the rectangle has longer side length $(0.9)\sqrt{2}$ (just a little shorter than the diagonal length $\sqrt{2}$) and so $\tilde{\mu}_2 = \pi^2/(1.62)$. Thus the second Neumann eigenvalue is smaller for the rectangle even though the rectangle is smaller than the square. Thus domain monotonicity can fail for Neumann eigenvalues.



To see where the Dirichlet domain monotonicity proof breaks down for Neumann eigenvalues, note that although one can extend a function in $H^1(\tilde{\Omega})$ to belong to $H^1(\Omega)$, the extended function must generally be nonzero outside $\tilde{\Omega}$ and so the L^2 -norm of the function and its gradient will differ from those of the original function; hence the Rayleigh quotient will differ too.

Rescaling gives a kind of monotonicity that is sometimes useful for Neumann eigenvalues:

$$\mu_j(t\Omega) = \frac{\mu_j(\Omega)}{t^2},$$

as shown in the Chapter 2 exercises.

Restricted reverse monotonicity for Neumann spectrum

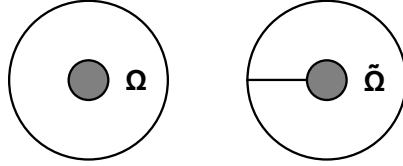
Neumann monotonicity does hold in a certain restricted situation, with the inequality reversed from the Dirichlet case — the smaller drum has smaller tones.

Theorem 11.3. *Let Ω and $\tilde{\Omega}$ be bounded Lipschitz domains in \mathbb{R}^d with eigenvalues μ_j and $\tilde{\mu}_j$ for the Neumann Laplacian, respectively.*

If $\Omega \supset \tilde{\Omega}$ and $\Omega \setminus \tilde{\Omega}$ has measure zero, then

$$\mu_j \geq \tilde{\mu}_j \quad \forall j \geq 1.$$

One might imagine the smaller domain $\tilde{\Omega}$ as being constructed by removing a hypersurface of measure zero from Ω , thus introducing an additional boundary surface that behaves like a “tear” in the fabric of the membrane. Reverse monotonicity then makes sense, because an eigenfunction can take different values on the two sides of this additional piece of boundary, enabling the eigenfunction to “relax” and the eigenvalue (frequency) to decrease.



In contrast, introducing additional boundary surfaces to a Dirichlet problem would have the opposite effect: the eigenfunction would face additional constraints, and hence the eigenvalue (frequency) would increase.

Proof of Theorem 11.3. Poincaré’s minimax principle gives

$$\mu_j = \min_S \max_{f \in S \setminus \{0\}} \frac{\int_{\tilde{\Omega}} |\nabla f|^2 \, dx}{\int_{\tilde{\Omega}} f^2 \, dx}, \quad \tilde{\mu}_j = \min_{\tilde{S}} \max_{f \in \tilde{S} \setminus \{0\}} \frac{\int_{\tilde{\Omega}} |\nabla f|^2 \, dx}{\int_{\tilde{\Omega}} f^2 \, dx},$$

where S ranges over j -dimensional subspaces of $H^1(\Omega)$ and \tilde{S} ranges over j -dimensional subspaces of $H^1(\tilde{\Omega})$. In the Rayleigh quotient for μ_j we should really integrate over Ω instead of $\tilde{\Omega}$, but it makes no difference because $\Omega \setminus \tilde{\Omega}$ has measure zero.

Every subspace S is also a valid \tilde{S} , since functions in $H^1(\Omega)$ obviously restrict to functions in $H^1(\tilde{\Omega})$. Therefore $\mu_j \geq \tilde{\mu}_j$. \square

Diamagnetic comparison

Our final monotonicity property says that the ground state energy of the Dirichlet Laplacian goes up when a magnetic field is imposed.

Theorem 11.4 (Diamagnetic comparison). *If Ω is a domain of finite volume in \mathbb{R}^2 or \mathbb{R}^3 then*

$$\beta_1 \geq \lambda_1.$$

First we prove a pointwise comparison.

Lemma 11.5 (Diamagnetic inequality).

$$|(i\nabla + \vec{A})f| \geq |\nabla|f||$$

Proof. Write f in polar form as $f = Re^{i\Theta}$. Then

$$\begin{aligned} |i\nabla f + \vec{A}f|^2 &= |ie^{i\Theta}\nabla R - Re^{i\Theta}\nabla\Theta + \vec{A}Re^{i\Theta}|^2 \\ &= |i\nabla R - R\nabla\Theta + \vec{A}R|^2 \\ &= |\nabla R|^2 + R^2|\nabla\Theta - \vec{A}|^2 \\ &\geq |\nabla R|^2 = |\nabla|f||^2. \end{aligned}$$

□

Proof of Theorem 11.4. The proof is immediate from the diamagnetic inequality in Lemma 11.5 and the following Rayleigh principles:

$$\beta_1 = \min_{f \in H_0^1(\Omega; \mathbb{C})} \frac{\int_{\Omega} |i\nabla f + \vec{A}f|^2 \, dx}{\int_{\Omega} |f|^2 \, dx}, \quad \lambda_1 = \min_{f \in H_0^1(\Omega; \mathbb{R})} \frac{\int_{\Omega} |\nabla f|^2 \, dx}{\int_{\Omega} f^2 \, dx}.$$

□

Notes and comments

Monotonicity properties for Sturm–Liouville and biLaplace spectra can be proved by the methods of this chapter too. For example, increasing the weight function w on the right side of the Sturm–Liouville equation decreases the Rayleigh quotient (provided $q \geq 0$) and hence decreases the eigenvalues.

The argument used to prove the diamagnetic inequality shows the Dirichlet Laplacian has a nonnegative groundstate, the point being that for real valued functions,

$$|\nabla f| \geq |\nabla|f||.$$

Additional arguments then show the first Dirichlet eigenvalue is simple (see [Gilbarg and Trudinger, Theorem 8.38]), which means

$$\lambda_1 < \lambda_2.$$

Chapter 12

Weyl's asymptotic for high eigenvalues

Goal

To determine the rate of growth of eigenvalues of the Laplacian.

References [Arendt *et al.*]; [Courant and Hilbert] Section VI.4

Notation

The asymptotic notation $\alpha_j \sim \beta_j$ means

$$\lim_{j \rightarrow \infty} \frac{\alpha_j}{\beta_j} = 1.$$

Write V_d for the volume of the unit ball in d -dimensions.

Growth of eigenvalues

The eigenvalues of the Laplacian grow at a rate $cj^{2/d}$ where the constant depends only on the volume of the domain, independent of the boundary conditions.

Theorem 12.1 (Weyl's law). *Let Ω be a bounded domain in \mathbb{R}^d with piecewise smooth boundary. As $j \rightarrow \infty$ the eigenvalues grow according to:*

$$\lambda_j \sim \rho_j \sim \mu_j \sim \begin{cases} (\pi j/|\Omega|)^2 & (d = 1) \\ 4\pi j/|\Omega| & (d = 2) \\ (6\pi^2 j/|\Omega|)^{2/3} & (d = 3) \end{cases}$$

and more generally,

$$\lambda_j \sim \rho_j \sim \mu_j \sim 4\pi^2 \left(\frac{j}{V_d |\Omega|} \right)^{2/d} \quad (d \geq 1).$$

Here $|\Omega|$ denotes the d -dimensional volume of the domain, in other words its length when $d = 1$ and area when $d = 2$.

In 1 dimension the theorem is proved by the explicit formulas for the eigenvalues in Chapter 2. We will prove the theorem in 2 dimensions, by a technique known as ‘‘Dirichlet–Neumann bracketing’’. The higher dimensional proof is similar.

An alternative proof using small-time heat kernel asymptotics can be found (for example) in the survey paper by Arendt *et al.* [Arendt *et al.*, §1.6].

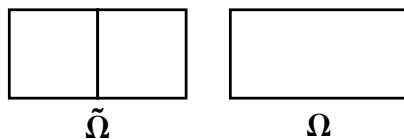
Proof of Weyl asymptotic — Step 1: rectangular domains. In view of the Neumann–Robin–Dirichlet comparison (Theorem 11.1), we need only prove Weyl's law for the Neumann and Dirichlet eigenvalues. We provided a proof in Proposition 2.1, for rectangles. \square

Proof of Weyl asymptotic — Step 2: finite union of rectangles. Next we suppose R_1, \dots, R_n are disjoint rectangular domains and put

$$\begin{aligned} \tilde{\Omega} &= \cup_{m=1}^n R_m, \\ \Omega &= \text{Int} \left(\cup_{m=1}^n \overline{R_m} \right). \end{aligned}$$

For example, if R_1 and R_2 are adjacent squares of side length 1, then $\tilde{\Omega}$ is the disjoint union of those squares whereas Ω is the 2×1 rectangular domain formed from the interior of their union.

Admittedly $\tilde{\Omega}$ is not connected, but the spectral theory of the Laplacian remains valid on a finite union of disjoint domains: the eigenfunctions are



simply the eigenfunctions of each of the component domains extended to be zero on the other components, and the spectrum equals the union of the spectra of the individual components. (On an infinite union of disjoint domains, on the other hand, one would lose compactness of the imbedding $H^1 \hookrightarrow L^2$, and the zero eigenvalue of the Neumann Laplacian would have infinite multiplicity.)

Write $\tilde{\lambda}_j$ and $\tilde{\mu}_j$ for the Dirichlet and Neumann eigenvalues of $\tilde{\Omega}$.

Then by the restricted reverse Neumann monotonicity (Theorem 11.3), Neumann–Robin–Dirichlet comparison (Theorem 11.1) and Dirichlet monotonicity (Theorem 11.2), we deduce that

$$\tilde{\mu}_j \leq \mu_j \leq \rho_j \leq \lambda_j \leq \tilde{\lambda}_j \quad \forall j \geq 1.$$

Hence if we can prove Weyl’s law

$$\tilde{\mu}_j \sim \tilde{\lambda}_j \sim \frac{4\pi j}{|\tilde{\Omega}|} \tag{12.1}$$

for the union-of-rectangles domain $\tilde{\Omega}$, then Weyl’s law will follow for the original domain Ω .

Define the eigenvalue counting functions of the rectangle R_m to be

$$\begin{aligned} N_{\text{Neu}}(\alpha; R_m) &= \#\{j \geq 1 : \mu_j(R_m) \leq \alpha\}, \\ N_{\text{Dir}}(\alpha; R_m) &= \#\{j \geq 1 : \lambda_j(R_m) \leq \alpha\}. \end{aligned}$$

We know from Weyl’s law for rectangles (Step 1 of the proof above) that

$$N_{\text{Neu}}(\alpha; R_m) \sim N_{\text{Dir}}(\alpha; R_m) \sim \frac{|R_m|}{4\pi} \alpha \tag{12.2}$$

as $\alpha \rightarrow \infty$.

The spectrum of $\tilde{\Omega}$ is the union of the spectra of the R_m , and so (here comes the key step in the proof!) the eigenvalue counting functions of $\tilde{\Omega}$

equal the sums of the corresponding counting functions of the rectangles:

$$\begin{aligned} N_{\text{Neu}}(\alpha; \tilde{\Omega}) &= \sum_{m=1}^n N_{\text{Neu}}(\alpha; R_m), \\ N_{\text{Dir}}(\alpha; \tilde{\Omega}) &= \sum_{m=1}^n N_{\text{Dir}}(\alpha; R_m). \end{aligned}$$

Combining these sums with the asymptotic (12.2) shows that

$$N_{\text{Neu}}(\alpha; \tilde{\Omega}) \sim \left(\sum_{m=1}^n \frac{|R_m|}{4\pi} \right) \alpha = \frac{|\Omega|}{4\pi} \alpha$$

and similarly

$$N_{\text{Dir}}(\alpha; \tilde{\Omega}) \sim \frac{|\Omega|}{4\pi} \alpha$$

as $\alpha \rightarrow \infty$. We can invert these last two asymptotic formulas with the help of Lemma 2.2, thus obtaining Weyl's law (12.1) for $\tilde{\Omega}$. \square

Proof of Weyl asymptotic — Step 3: approximation of arbitrary domains. Lastly we suppose Ω is an arbitrary domain with piecewise smooth boundary. The idea is to approximate Ω with a union-of-rectangles domain such as in Step 2, such that the volume of the approximating domain is within ε of the volume of Ω . We refer to the text of Courant and Hilbert for the detailed proof [Courant and Hilbert, §VI.4.4]. \square

Chapter 13

Pólya's conjecture and the Berezin–Li–Yau Theorem

Goal

To describe Pólya's conjecture about Weyl's law, and to state the “tiling domain” and “summed” versions that are known to hold.

References [AIM, Kellner, Laptev, Pólya]

Pólya's conjecture

Weyl's law (Theorem 12.1) says that

$$\lambda_j \sim \frac{4\pi j}{|\Omega|} \sim \mu_j \quad \text{as } j \rightarrow \infty,$$

for a bounded plane domain Ω with piecewise smooth boundary. (We restrict to plane domains, in this chapter, for simplicity.)

Pólya conjectured that these asymptotic formulas hold as inequalities.

Conjecture 13.1 ([Pólya], 1960).

$$\lambda_j \geq \frac{4\pi j}{|\Omega|} \geq \mu_j \quad \forall j \geq 1.$$

The conjecture remains open even for a disk.

Pólya proved the Dirichlet part of the inequality for tiling domains [Pólya], and Kellner did the same for the Neumann part [Kellner]. Recall that a

“tiling domain” covers the plane with congruent copies of itself (translations, rotations and reflections). For example, parallelograms and triangles are tiling domains, as are many variants of these domains (a fact that M. C. Escher exploited in his artistic creations).

Pólya and Kellner's proofs are remarkably simple, using a rescaling argument together with Weyl's law.

For arbitrary domains, Pólya's conjecture has been proved only for λ_1, λ_2 (see [Henrot, Th. 3.2.1 and (4.3)]) and for μ_1, μ_2, μ_3 (see [Girouard]). The conjecture remains open for $j \geq 3$ (Dirichlet) and $j \geq 4$ (Neumann).

Berezin–Li–Yau results

The major progress for arbitrary domains has been on a “summed” version of the conjecture. (Quite often in analysis, summing or integrating an expression produces a significantly more tractable quantity.) Li and Yau [Li and Yau] proved that

$$\sum_{k=1}^j \lambda_k \geq \frac{2\pi j^2}{|\Omega|},$$

which is only slightly smaller than the quantity $(2\pi/|\Omega|)j(j+1)$ that one gets by summing the left side of the Pólya conjecture. An immediate consequence is a Weyl-type inequality for Dirichlet eigenvalues:

$$\lambda_j \geq \frac{2\pi j}{|\Omega|}$$

by combining the very rough estimate $j\lambda_j \geq \sum_{k=1}^j \lambda_k$ with the Li–Yau inequality. The last formula has 2π whereas Pólya's conjecture demands 4π , and so we see the conjecture is true up to a factor of 2, at worst.

Similar results hold for Neumann eigenvalues.

A somewhat more general approach had been obtained earlier by Berezin. For more information, consult the work of Laptev [Laptev] and a list of open problems from recent conferences [AIM].

Chapter 14

Trace of the heat kernel

Goal

To extract geometric information about a domain from the spectrum of the Laplacian, via the trace of the heat kernel.

Definition

Throughout the chapter, $\Omega \subset \mathbb{R}^d$ is a bounded domain with piecewise smooth boundary, so that Weyl's Law holds. Write $\{\mathbf{u}_j\}$ for an ONB of Dirichlet eigenfunctions with corresponding eigenvalues λ_j , satisfying

$$\begin{aligned} -\Delta \mathbf{u}_j &= \lambda_j \mathbf{u}_j && \text{in } \Omega, \\ \mathbf{u}_j &= 0 && \text{on } \partial\Omega, \end{aligned}$$

and

$$0 < \lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \dots \rightarrow \infty.$$

Define the **heat kernel**

$$K(t, \mathbf{x}, \mathbf{y}) = \sum_j e^{-\lambda_j t} \mathbf{u}_j(\mathbf{x}) \mathbf{u}_j(\mathbf{y}), \quad t > 0, \quad \mathbf{x}, \mathbf{y} \in \overline{\Omega}.$$

Then the function

$$\mathbf{u}(\mathbf{x}, t) = \int_{\Omega} K(t, \mathbf{x}, \mathbf{y}) f(\mathbf{y}) \, d\mathbf{y}$$

solves the heat equation IVP

$$\begin{aligned} u_t &= \Delta u && \text{in } \Omega, \\ u &= 0 && \text{for } x \in \partial\Omega, \\ u &= f && \text{at } t = 0. \end{aligned}$$

One may verify formally that u solves the IVP. A rigorous proof (if desired) can be obtained using a weak formulation of the IVP.

The **trace of the heat kernel**, or **heat trace**, is the spectral functional

$$\text{Tr}(t) = \int_{\Omega} K(t, x, x) \, dx = \sum_j e^{-\lambda_j t}, \quad t > 0.$$

Example. The interval $\Omega = (0, \pi)$ in 1-dimension has Dirichlet eigenvalues $\lambda_j = j^2$, and so $\text{Tr}(t) = \sum_{j=1}^{\infty} e^{-j^2 t}$. This heat trace is closely related to the Jacobi theta function ϑ_3 .

Upper bound on the heat kernel and trace

The heat kernel for the whole space \mathbb{R}^d is given not by an eigenfunction expansion but instead by a simple closed form:

$$K_{\mathbb{R}^d}(t, x, y) = \frac{e^{-|x-y|^2/4t}}{(4\pi t)^{d/2}}.$$

Proposition 14.1 (Gaussian upper bound). *The heat kernel of a domain is bounded above by the heat kernel of the whole space:*

$$K(t, x, y) \leq \frac{e^{-|x-y|^2/4t}}{(4\pi t)^{d/2}}, \quad x, y \in \Omega, \quad t > 0.$$

In particular, $K(t, x, x) \leq (4\pi t)^{-d/2}$ and hence

$$\text{Tr}(t) \leq \frac{|\Omega|}{(4\pi t)^{d/2}}, \quad t > 0.$$

Proof. Fix $\mathbf{y} \in \Omega$ and let $v(\mathbf{x}, t) = K(t, \mathbf{x}, \mathbf{y}) - K_{\mathbb{R}^d}(t, \mathbf{x}, \mathbf{y})$ for $\mathbf{x} \in \Omega, t > 0$. Then v satisfies the heat equation ($v_t = \Delta v$) with initial condition

$$v(\mathbf{x}, 0) = \delta(\mathbf{x} - \mathbf{y}) - \delta(\mathbf{x} - \mathbf{y}) = 0$$

and boundary condition

$$v(\mathbf{x}, t) = 0 - K_{\mathbb{R}^d}(t, \mathbf{x}, \mathbf{y}) \leq 0 \quad \mathbf{x} \in \partial\Omega.$$

Hence $v \leq 0$ by the Maximum Principle, which proves the main inequality in the proposition. Taking $\mathbf{x} = \mathbf{y}$ shows $K(t, \mathbf{x}, \mathbf{x}) \leq (4\pi t)^{-d/2}$, and then integrating over $\mathbf{x} \in \Omega$ gives the trace estimate.

Note. If one wishes to avoid delta measures in the initial condition, then let $f \in C_0^\infty(\Omega)$ be a nonnegative bump function supported around \mathbf{y} and repeat the above argument for the function

$$v(\mathbf{x}, t) = \int_{\Omega} K(t, \mathbf{x}, \mathbf{y}) f(\mathbf{y}) \, d\mathbf{y} - \int_{\mathbb{R}^d} K_{\mathbb{R}^d}(t, \mathbf{x}, \mathbf{y}) f(\mathbf{y}) \, d\mathbf{y}.$$

Clearly v satisfies the heat equation in Ω and has initial condition $f - f = 0$ and boundary condition ≤ 0 . The Maximum Principle implies $v(\mathbf{x}) \leq 0$ for all $\mathbf{x} \in \Omega$. Since this inequality holds for all such f , one concludes that $K(t, \mathbf{x}, \mathbf{y}) \leq K_{\mathbb{R}^d}(t, \mathbf{x}, \mathbf{y})$ for all \mathbf{x}, \mathbf{y} and t . \square

First order asymptotics

For small time the heat equation does not “feel the boundary”. Thus we expect the heat kernel $K(t, \mathbf{x}, \mathbf{y})$ on Ω to be well approximated by the heat kernel for the whole space \mathbb{R}^d . In particular, putting $\mathbf{x} = \mathbf{y}$ one expects $K(t, \mathbf{x}, \mathbf{x}) \sim 1/(4\pi t)^{d/2}$ and hence $\text{Tr}(t) \sim |\Omega|/(4\pi t)^{d/2}$ for small t . That is, one expects the upper bound in Proposition 14.1 to be asymptotically exact.

Proposition 14.2.

$$\text{Tr}(t) \sim \frac{|\Omega|}{(4\pi t)^{d/2}} \quad \text{as } t \rightarrow 0 \quad \text{and} \quad \text{Tr}(t) \sim e^{-\lambda_1 t} \quad \text{as } t \rightarrow \infty.$$

Proof. For the long-time asymptotic, note that $\lambda_1 < \lambda_2$ (see Notes and Comments for Chapter 11), and so

$$\frac{\text{Tr}(t)}{e^{-\lambda_1 t}} = 1 + \sum_{j=2}^{\infty} e^{(\lambda_1 - \lambda_j)t} \rightarrow 1$$

as $t \rightarrow \infty$.

For the short-time asymptotic in 2-dimensions we argue using Weyl's Law (Theorem 12.1), which says

$$\lambda_j \sim \frac{4\pi j}{A} \quad \text{as } j \rightarrow \infty$$

where $A = \text{area of } \Omega$. Let $C > 1$, and choose J large enough that

$$C^{-1} \frac{4\pi j}{A} \leq \lambda_j \leq C \frac{4\pi j}{A} \quad \forall j > J.$$

The lower bound on λ_j implies

$$\begin{aligned} \text{Tr}(t) &\leq \sum_{j=1}^J e^{-\lambda_j t} + \sum_{j=J+1}^{\infty} e^{-4\pi j t / AC} \\ &\leq J + \sum_{j=J+1}^{\infty} e^{-j\delta} \quad \text{where } \delta = 4\pi t / AC \\ &\leq J + \delta^{-1} \int_{J\delta}^{\infty} e^{-z} dz \end{aligned}$$

by estimating the integral from below with right Riemann sums having step size δ . Hence

$$\limsup_{t \rightarrow 0} \frac{4\pi t}{A} \text{Tr}(t) \leq C.$$

Similarly the upper bound on λ_j leads to

$$\liminf_{t \rightarrow 0} \frac{4\pi t}{A} \text{Tr}(t) \geq C^{-1}.$$

Letting $C \rightarrow 1$, we conclude $\lim_{t \rightarrow 0} \frac{4\pi t}{A} \text{Tr}(t) = 1$.

In dimensions $d \neq 2$ the short-time asymptotic can be proved the same way, with the help of the integral

$$\int_0^{\infty} e^{-z^{2/d}} dz = \frac{d}{2} \int_0^{\infty} e^{-\zeta} \zeta^{d/2-1} d\zeta = \frac{d}{2} \Gamma(d/2) = \Gamma(1 + d/2).$$

□

Higher order asymptotics as $t \rightarrow 0$

The short-time asymptotic in Proposition 14.2 can be improved to an infinite asymptotic series, analogous to a Taylor series.

Theorem 14.3 (Heat trace asymptotic). *If Ω has smooth boundary then*

$$\mathrm{Tr}(t) \sim \frac{1}{t^{d/2}} \sum_{n=0}^{\infty} c_n t^{n/2} \quad \text{as } t \rightarrow 0,$$

for certain constants $c_n = c_n(\Omega)$.

The meaning of the asymptotic series in the theorem is that

$$t^{d/2} \mathrm{Tr}(t) = \sum_{n=0}^N c_n t^{n/2} + O(t^{(N+1)/2}) \quad \text{as } t \rightarrow 0,$$

for each $N \geq 0$, and that the analogous formula holds for the derivative:

$$\frac{d}{dt} \left[t^{d/2} \mathrm{Tr}(t) \right] = \frac{d}{dt} \sum_{n=0}^N c_n t^{n/2} + O(t^{(N-1)/2}) \quad \text{as } t \rightarrow 0.$$

For the history and proof of this result, see the Notes at the end of the chapter. The constants c_n are known as the **heat invariants** of the domain. The zeroth coefficient depends only on the volume:

$$c_0 = \frac{|\Omega|}{(4\pi)^{d/2}}.$$

The leading heat invariants take a particularly simple form in 2-dimensions:

Corollary 14.4 (Heat trace asymptotic in the plane). *If $\Omega \subset \mathbb{R}^2$ has smooth boundary then*

$$\mathrm{Tr}(t) \sim \frac{\text{Area}}{4\pi t} - \frac{\text{Perimeter}}{8\sqrt{\pi t}} + \frac{1}{6}(1 - \#\text{holes}) + \frac{\sqrt{t}}{256\sqrt{\pi}} \int_{\partial\Omega} \kappa^2 ds + O(t) \quad \text{as } t \rightarrow 0,$$

where κ denotes the curvature of the boundary.

Readers familiar with topology might note that $(1 - \#\text{holes})$ equals the Euler characteristic of Ω .

Thus the spectrum of the Dirichlet Laplacian determines the following geometric quantities:

area, boundary length, connectivity, L^2 -norm of boundary curvature.

Remark. On manifolds with boundary, one obtains similar heat trace asymptotics.

On manifolds without boundary, the $1/2$ -order terms vanish from the asymptotic, meaning $c_n = 0$ for all odd n .

Higher order asymptotics for polygons

The heat trace asymptotic behaves quite differently for domains with corners.

Theorem 14.5 (Heat trace asymptotic for polygonal domain). *If $\Omega \subset \mathbb{R}^2$ is a polygon then*

$$\mathrm{Tr}(t) \sim \frac{\text{Area}}{4\pi t} - \frac{\text{Perimeter}}{8\sqrt{\pi t}} + \frac{1}{24} \sum_i \left(\frac{\pi}{\alpha_i} - \frac{\alpha_i}{\pi} \right) + O(e^{-b/t}) \quad \text{as } t \rightarrow 0,$$

where the α_i are the interior angles of the polygon and $b > 0$ is a constant.

This formula was stated by [McKean and Singer], and a proof can be found in [van den Berg and Srisatkunarajah]. Notice the asymptotic contains only three terms, after which the remainder term is exponentially small as $t \rightarrow 0$.

Inverse spectral problem — can you hear the shape of a drum?

The spectrum encodes a great deal of information about the domain, as we saw above from the heat trace. Inspired by this observation, Mark Kac asked in 1966

“Can one hear the shape of a drum?” [Kac]

That is, suppose you have perfect hearing, and can hear all the frequencies of a drum. Can you determine its shape? More mathematically, does the spectrum of the Dirichlet Laplacian determine the shape of the domain Ω ?

One can “hear” whether or not the domain is a disk, since the spectrum determines the area and the disk has the smallest λ_1 among all domains of the same area, by the Faber–Krahn Theorem mentioned in the Chapter 2 exercises.

In general, though, domains **cannot** be heard. A counterexample in 2-dimensions was found by [Gordon, Webb and Wolpert] in 1992, after many

years of effort by many authors. Their counterexample, and all subsequent counterexamples, are domains with corners. Thus nowadays one asks:

“Can one hear the shape of a smoothly bounded drum?”

This problem remains open. Recent progress of [Zelditch] handles the case of analytically bounded drums having some symmetry.

Triangular drums. Even a triangular drum is nontrivial to “hear”. In 1990, [Durso] showed that it can be done by wave trace methods (generally more difficult and powerful than heat trace methods). In other words, she showed if one knows the domain is a triangle, and if one knows its Dirichlet spectrum, then one can determine the shape of the triangle.

An easier proof of this fact using the heat trace asymptotic of Theorem 14.5 was found by [Grieser and Maronna]. The essence of their proof is as follows. The angles of a triangle add up to π , and so from the coefficients of the asymptotic in Theorem 14.5 one obtains the two quantities

$$\sum_{i=1}^3 \alpha_i \quad \text{and} \quad \sum_{i=1}^3 \frac{1}{\alpha_i}.$$

One also knows the perimeter P and area A , and hence $P^2/4A$, which equals (by an interesting identity for triangles) a third quantity involving the angles:

$$\sum_{i=1}^3 \cot \frac{\alpha_i}{2}.$$

From these last three quantities, Grieser and Maronna determine the three angles $\alpha_1, \alpha_2, \alpha_3$. Their argument is elementary yet elegant, relying on certain convexity and monotonicity properties. Then the angles determine the shape of the triangle. Lastly, the size of the triangle follows from knowing the area A .

Exercises

14.1 — *Heat trace on product domain.* Consider bounded domains $\Omega_1 \subset \mathbb{R}^{d_1}$ and $\Omega_2 \subset \mathbb{R}^{d_2}$. Write $\lambda_j^{(1)}$ and $\lambda_k^{(2)}$ for the eigenvalues of the Dirichlet

Laplacian on the two domains, and $\text{Tr}^{(1)}$ and $\text{Tr}^{(2)}$ for the corresponding heat traces. Show the heat trace on the product domain

$$\Omega = \Omega_1 \times \Omega_2.$$

is the product of the heat traces:

$$\text{Tr}(\mathbf{t}) = \text{Tr}^{(1)}(\mathbf{t}) \text{Tr}^{(2)}(\mathbf{t}), \quad \mathbf{t} > 0.$$

Notes and comments

Material to add: The heat trace asymptotic (Theorem 14.3) was first obtained by [Seeley] (with boundary as we need here, or without boundary???). For the geometric interpretation of heat invariants in terms of curvature in 2-dimensions (Corollary 14.4), see [Smith]. Need a reference that also proves the asymptotic for the derivative of $\mathbf{t}^{d/2} \text{Tr}(\mathbf{t})!!!$

On manifolds without boundary, [Polterovich] found a brief explicit formula for each heat invariant in terms of derivatives of powers of the distance function. His approach was simplified and generalized in [Weingart, Chapter 2].

Sometimes one wishes to perturb the boundary of a domain and obtain a formula for the resulting perturbation of the heat trace. Hadamard-type first and second variations of this kind were developed by [Ozawa].

Insert a picture for GWW — possibly use the homophonic drums from Buser, Conway, Doyle, and Semmler (1994), if the authors grant permission?

Mention extremal problems for the trace: Luttinger (connects Faber–Krahn to isoperimetric). Add exercises and open problems.

Chapter 15

Spectral zeta function

Goal

To develop the spectral zeta function as the Mellin transform of the heat trace, then show it is meromorphic, identify the residues, and find explicit formulas between the poles.

Definition

In this chapter, $\Omega \subset \mathbb{R}^d$ is a bounded domain with smooth boundary, and λ_j is the j -th eigenvalue of the Dirichlet Laplacian. Define the **spectral** zeta function

$$Z(s) = \sum_j \frac{1}{\lambda_j^s}, \quad \operatorname{Re} s > \frac{d}{2},$$

where s is a complex number. The series converges absolutely when $\operatorname{Re} s > d/2$, since $\lambda_j \sim (\operatorname{const.})j^{2/d}$ by the Weyl asymptotic in Theorem 12.1.

Example and motivation. The interval $\Omega = (0, \pi)$ in 1-dimension has Dirichlet eigenvalues $\lambda_j = j^2$, and so $Z(s) = \sum_{j=1}^{\infty} j^{-2s} = \zeta(2s)$, where ζ is the Riemann zeta function.

Relation to the heat trace

The spectral zeta function is a weighted mean of the heat trace.

Lemma 15.1 (Zeta function = Mellin transform of heat trace).

$$Z(s) = \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} \text{Tr}(t) dt, \quad \text{Re } s > \frac{d}{2}.$$

Here $\Gamma(s)$ is the Gamma function, which is defined for $\text{Re } s > 0$ by the formula $\Gamma(s) = \int_0^\infty z^{s-1} e^{-z} dz$ and then extends to all complex s by repeated use of the functional relation $s\Gamma(s) = \Gamma(s+1)$.

Proof. The integral on the right side of the lemma is

$$\begin{aligned} \int_0^\infty t^{s-1} \text{Tr}(t) dt &= \sum_j \int_0^\infty t^{s-1} e^{-\lambda_j t} dt && \text{by definition of } \text{Tr}(t) \\ &= \sum_j \frac{1}{\lambda_j^s} \int_0^\infty \tau^{s-1} e^{-\tau} d\tau && \text{where } \tau = \lambda_j t, \\ &= Z(s)\Gamma(s), \end{aligned}$$

which gives the desired formula. \square

Compact manifold without boundary. If Ω is a compact manifold without boundary then one defines the spectral zeta function similarly, except omitting the zero eigenvalue (traditionally labelled $\lambda_0 = 0$) so as not to divide by zero. In that case

$$Z(s) = \sum_{j>0} \frac{1}{\lambda_j^s} = \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} (\text{Tr}(t) - 1) dt, \quad \text{Re } s > \frac{d}{2}.$$

For example, the torus $\mathbb{R}/2\pi\mathbb{Z}$ has eigenvalues j^2 for $j \in \mathbb{Z}$, and so its zeta function is $\sum_{j \neq 0} j^{-2s} = 2\zeta(2s)$.

Extending the zeta function to all complex numbers

Just as the Riemann zeta function extends to a meromorphic function on the whole plane (complex analytic except for isolated poles), so does the spectral zeta function, as we proceed to show.

Theorem 15.2 (Spectral zeta in 2-dimensions). *Suppose $\Omega \subset \mathbb{R}^2$. Then the spectral zeta function $Z(s)$ has a meromorphic extension to \mathbb{C} with simple poles at $s = 1$ and $s = 1/2$:*

$$\begin{aligned} Z(s) &= \frac{\text{Area}}{4\pi} \frac{1}{s-1} + O(1) && \text{for } s \text{ near } 1, \\ Z(s) &= -\frac{\text{Perimeter}}{8\pi} \frac{1}{s-1/2} + O(1) && \text{for } s \text{ near } 1/2. \end{aligned}$$

The zeta function has simple poles also at $s = -1/2, -3/2, -5/2, \dots$, and is regular at every other $s \in \mathbb{C}$. Further, the zeta function is expressed by the formulas

$$\begin{aligned} Z(s) &= \Gamma(s)^{-1} \int_0^\infty t^{s-1} \text{Tr}(t) dt, && \text{Re } s \in (1, \infty), \\ &= \Gamma(s)^{-1} \int_0^\infty t^{s-1} \left[\text{Tr}(t) - \frac{\text{Area}}{4\pi t} \right] dt, && \text{Re } s \in \left(\frac{1}{2}, 1\right), \\ &= \Gamma(s)^{-1} \int_0^\infty t^{s-1} \left[\text{Tr}(t) - \frac{\text{Area}}{4\pi t} + \frac{\text{Perimeter}}{8\sqrt{\pi t}} \right] dt, && \text{Re } s \in \left(0, \frac{1}{2}\right), \end{aligned}$$

and also

$$Z(s) = \frac{-1}{\Gamma(s+1)} \int_0^\infty t^s \frac{d}{dt} \left[\text{Tr}(t) - \frac{\text{Area}}{4\pi t} + \frac{\text{Perimeter}}{8\sqrt{\pi t}} \right] dt, \quad \text{Re } s \in \left(-\frac{1}{2}, \frac{1}{2}\right).$$

At the origin, the spectral zeta function equals

$$Z(0) = \frac{1}{6}(1 - \#\text{holes}) = \frac{1}{6}(\text{Euler characteristic of } \Omega).$$

Already one can see patterns emerging in these formulas. The patterns appear even more strongly in the next theorem, when we treat domains in all dimensions. First, though, we establish the concrete 2-dimensional formulas in Theorem 15.2.

Proof. For $\text{Re } s \in (1, \infty)$, one has

$$\begin{aligned} \Gamma(s)Z(s) &= \int_0^\infty t^{s-2} t \text{Tr}(t) dt, \\ &= -(s-1)^{-1} \int_0^\infty t^{s-1} \frac{d}{dt} [t \text{Tr}(t)] dt \end{aligned} \quad (15.1)$$

by integration by parts, where the boundary terms vanish as follows for $\operatorname{Re} s > 1$:

$$(s-1)^{-1} t^{s-1} t \operatorname{Tr}(t) \Big|_0^\infty = 0 - 0$$

because $\operatorname{Tr}(t)$ decays exponentially as $t \rightarrow \infty$, and $t \operatorname{Tr}(t) = c_0 + O(t^{1/2})$ as $t \rightarrow 0$ by the heat trace asymptotic in Theorem 14.3.

The integral in (15.1) is an analytic function of s for $\operatorname{Re} s > 1/2$, since $\operatorname{Tr}(t)$ decays exponentially as $t \rightarrow \infty$ and $\frac{d}{dt} [t \operatorname{Tr}(t)] = O(t^{-1/2})$ as $t \rightarrow 0$ by Theorem 14.3. Therefore $Z(s)$ is meromorphic for $\operatorname{Re} s \in (1/2, \infty)$. The residue at $s = 1$ is obtained by evaluating (15.1) at $s = 1$ (except for the term $(s-1)^{-1}$, of course), which gives

$$\operatorname{Res}(Z, 1) = -\frac{1}{\Gamma(1)} \int_0^\infty \frac{d}{dt} [t \operatorname{Tr}(t)] dt = -[t \operatorname{Tr}(t)]_0^\infty = c_0 = \frac{\text{Area}}{4\pi}.$$

Notice (15.1) implies

$$\begin{aligned} \Gamma(s)Z(s) &= -(s-1)^{-1} \int_0^\infty t^{s-1} \frac{d}{dt} [t \operatorname{Tr}(t) - c_0] dt \\ &= \int_0^\infty t^{s-2} [t \operatorname{Tr}(t) - c_0] dt, \quad \operatorname{Re} s \in \left(\frac{1}{2}, 1\right), \end{aligned}$$

by integration by parts, where the boundary terms vanish as follows:

$$-(s-1)^{-1} t^{s-1} [t \operatorname{Tr}(t) - c_0] \Big|_0^\infty = 0 - 0$$

because

$$t \operatorname{Tr}(t) - c_0 = \begin{cases} O(1) & \text{as } t \rightarrow \infty, \\ O(t^{1/2}) & \text{as } t \rightarrow 0. \end{cases}$$

Thus we have proved the desired formula for $Z(s)$ in the theorem, when $\operatorname{Re} s \in (1/2, 1)$.

By continuing to integrate by parts and subtract terms of the heat trace asymptotic in the above fashion, one proves the rest of the claims in the theorem. The proof gives in principle that the zeta function has simple poles at $s = 1, \frac{1}{2}, 0, -\frac{1}{2}, -1, -\frac{3}{2}, \dots$, but the poles at $s = 0, -1, -2, \dots$ are eliminated by the zeros of $\Gamma(s)^{-1}$ at those points.

Note the final formula for $Z(s)$ in Theorem 15.2 can be evaluated at $s = 0$ to obtain

$$\begin{aligned} Z(0) &= \frac{-1}{\Gamma(1)} \int_0^\infty \frac{d}{dt} \left[\text{Tr}(t) - \frac{\text{Area}}{4\pi t} + \frac{\text{Perimeter}}{8\sqrt{\pi t}} \right] dt \\ &= - \left[\text{Tr}(t) - \frac{\text{Area}}{4\pi t} + \frac{\text{Perimeter}}{8\sqrt{\pi t}} \right]_0^\infty \\ &= -0 + c_2 = \frac{1}{6}(1 - \#\text{holes}) \end{aligned}$$

because

$$\text{Tr}(t) - \frac{\text{Area}}{4\pi t} + \frac{\text{Perimeter}}{8\sqrt{\pi t}} = \begin{cases} o(1) & \text{as } t \rightarrow \infty, \\ c_2 + o(1) & \text{as } t \rightarrow 0. \end{cases}$$

□

Next we develop formulas in all dimensions $d \geq 1$ for the zeta function between the poles.

Theorem 15.3 (Spectral zeta in d -dimensions). *Suppose $\Omega \subset \mathbb{R}^d$. Then the spectral zeta function $Z(s)$ has a meromorphic extension to \mathbb{C} with simple poles at $s = d/2, (d-1)/2, \dots, 1/2$ and at $s = -1/2, -3/2, -5/2, \dots$, with residues*

$$\text{Res}(Z, \frac{d-n}{2}) = c_n \Gamma(\frac{d-n}{2})^{-1}.$$

The zeta function is regular at all other $s \in \mathbb{C}$. In particular, it is finite at $s = 0, -1, -2, \dots$ with values

$$Z(-m) = (-1)^m m! c_{d+2m}, \quad m = 0, 1, 2, \dots$$

Around the pole at $s = (d-N)/2$ one has

$$\begin{aligned} Z(s) &= \frac{-1}{s - \frac{d-N}{2}} \frac{1}{\Gamma(s)} \int_0^\infty t^{s-(d-N)/2} \frac{d}{dt} \left(t^{-N/2} \left[t^{d/2} \text{Tr}(t) - \sum_{n=0}^N c_n t^{n/2} \right] \right) dt, \\ &\quad \frac{d-N-1}{2} < \text{Re } s < \frac{d-N+1}{2}, \end{aligned} \quad (15.2)$$

for $N = 0, 1, 2, \dots$, and between successive poles the zeta function is given by

$$\begin{aligned} Z(s) &= \frac{1}{\Gamma(s)} \int_0^\infty t^{s-d/2-1} \left[t^{d/2} \text{Tr}(t) - \sum_{n=0}^N c_n t^{n/2} \right] dt, \\ &\quad \frac{d-N-1}{2} < \text{Re } s < \frac{d-N}{2}. \end{aligned} \quad (15.3)$$

Proof. Write $P(N)$ for statement (15.2) and $Q(N)$ for statement (15.3), for $N \geq 0$. Also write $Q(-1)$ for the statement

$$Z(s) = \frac{1}{\Gamma(s)} \int_0^\infty t^{s-d/2-1} \left[t^{d/2} \operatorname{Tr}(t) \right] dt, \quad \operatorname{Re} s > \frac{d}{2},$$

which is true by definition of the zeta function.

We will prove that

$$Q(N-1) \implies P(N) \implies Q(N)$$

whenever $N \geq 0$. Then $P(N)$ and $Q(N)$ hold for all N by induction.

PROOF THAT $Q(N-1) \implies P(N)$. Statement $Q(N-1)$ can be rewritten to say

$$\Gamma(s)Z(s) = \int_0^\infty t^{s-(d-N)/2-1} t^{-N/2} \left[t^{d/2} \operatorname{Tr}(t) - \sum_{n=0}^{N-1} c_n t^{n/2} \right] dt$$

whenever

$$\frac{d-N}{2} < \operatorname{Re} s < \frac{d-N+1}{2}. \quad (15.4)$$

Integrating by parts gives

$$\Gamma(s)Z(s) = \frac{-1}{s - \frac{d-N}{2}} \int_0^\infty t^{s-(d-N)/2} \frac{d}{dt} \left(t^{-N/2} \left[t^{d/2} \operatorname{Tr}(t) - \sum_{n=0}^{N-1} c_n t^{n/2} \right] \right) dt \quad (15.5)$$

because the boundary term

$$t^{s-d/2} \left[t^{d/2} \operatorname{Tr}(t) - \sum_{n=0}^{N-1} c_n t^{n/2} \right]$$

vanishes as $t \rightarrow \infty$ and as $t \rightarrow 0$, as we now show. As $t \rightarrow \infty$ it vanishes because

$$t^{d/2} \operatorname{Tr}(t) - \sum_{n=0}^{N-1} c_n t^{n/2} = O(t^{(N-1)/2})$$

and $\operatorname{Re}(s - d/2) < -(N-1)/2$ by (15.4). The boundary term vanishes as $t \rightarrow 0$ because

$$t^{d/2} \operatorname{Tr}(t) - \sum_{n=0}^{N-1} c_n t^{n/2} = O(t^{N/2})$$

by the heat trace asymptotic in Theorem 14.3, and $\operatorname{Re}(s - d/2) > -N/2$ by (15.4).

In formula (15.5) we may extend the range of summation up to $n = N$, because doing so merely adds a constant term c_N inside the derivative and thus has no effect on the formula. Thus we obtain (15.2), for the range of s -values in (15.4).

Formula (15.2) is an analytic function of s for the larger range

$$\frac{d - N - 1}{2} < \operatorname{Re} s < \frac{d - N + 1}{2} \quad (15.6)$$

because

$$\frac{d}{dt} \left(t^{-N/2} \left[t^{d/2} \operatorname{Tr}(t) - \sum_{n=0}^N c_n t^{n/2} \right] \right) = \begin{cases} O(t^{-3/2}) & \text{as } t \rightarrow \infty, \\ O(t^{-1/2}) & \text{as } t \rightarrow 0, \end{cases}$$

where the decay is proved directly as $t \rightarrow \infty$ and follows from the heat trace asymptotic Theorem 14.3 as $t \rightarrow 0$. Thus formula (15.2) provides an analytic extension of $\Gamma(s)Z(s)$ to the larger range (15.6), and thus proves statement $P(N)$.

PROOF THAT $P(N) \implies Q(N)$. Integrating (15.2) by parts gives (15.2), provided we prove the boundary term

$$t^{s-d/2} \left[t^{d/2} \operatorname{Tr}(t) - \sum_{n=0}^N c_n t^{n/2} \right]$$

vanishes as $t \rightarrow \infty$ and as $t \rightarrow 0$ under the assumption

$$\frac{d - N - 1}{2} < \operatorname{Re} s < \frac{d - N}{2}. \quad (15.7)$$

As $t \rightarrow \infty$ it vanishes because

$$t^{d/2} \operatorname{Tr}(t) - \sum_{n=0}^N c_n t^{n/2} = O(t^{N/2})$$

and $\operatorname{Re}(s - d/2) < -N/2$ by (15.7). The boundary term vanishes as $t \rightarrow 0$ because

$$t^{d/2} \operatorname{Tr}(t) - \sum_{n=0}^N c_n t^{n/2} = O(t^{(N+1)/2})$$

by the heat trace asymptotic in Theorem 14.3, and $\operatorname{Re}(s - d/2) > -(N+1)/2$ by (15.7).

INSERT REST OF PROOF HERE!!! □

Exercises

15.1 — *Relative zeta function on domains.* Suppose Ω_1 and Ω_2 are smoothly bounded domains in \mathbb{R}^d with the same area. Show that the difference of their spectral zeta functions can be written

$$Z_1(s) - Z_2(s) = \Gamma(s)^{-1} \int_0^\infty t^{s-1} (\text{Tr}_1(t) - \text{Tr}_2(t)) dt, \quad \text{Re } s > \frac{d-1}{2}.$$

Hint. The $t^{-d/2}$ term is absent from the asymptotic for $\text{Tr}_1(t) - \text{Tr}_2(t)$ as $t \rightarrow 0$, due to the two domains having the same area.

15.2 — *Zeta function on compact surface without boundary.* As remarked in Chapter 14, on a manifold without boundary the $1/2$ -order terms vanish from the heat trace asymptotic, meaning $c_n = 0$ for all odd n . Use this fact to state and prove a meromorphic extension result (analogous to Theorem 15.2) for the spectral zeta function of a smooth compact surface ($d = 2$) without boundary.

15.3 — *Relative zeta function on compact surfaces.* Suppose Ω_1 and Ω_2 are smooth, compact 2-dimensional surfaces without boundary that have the same area and same Euler characteristic. (For example, one might apply two different conformal factors to a metric on an underlying surface, with the conformal factors normalized to have the same integral.)

Show that the difference of the spectral zeta functions of the two surfaces can be written

$$Z_1(s) - Z_2(s) = \Gamma(s)^{-1} \int_0^\infty t^{s-1} (\text{Tr}_1(t) - \text{Tr}_2(t)) dt, \quad \text{Re } s > -1,$$

and that $Z_1(s) - Z_2(s)$ is entire, that is, analytic for all $s \in \mathbb{C}$.

Hint. The t^{-1} and t^0 terms are absent from the asymptotic for $\text{Tr}_1(t) - \text{Tr}_2(t)$ as $t \rightarrow 0$, due to the two surfaces having the same area and same Euler characteristic.

Notes and comments

The formulas for the spectral zeta function between successive poles and around each pole, in Theorems 15.2 and 15.3, might be somewhat new. I have not seen these formulas elsewhere since discovering them while working with Carlo Morpurgo in the mid-1990s.

The standard method for proving the meromorphic extension of the zeta function is less elegant: one splits the integral into \int_0^1 and \int_1^∞ and then uses the heat trace asymptotic only in the first integral.

Chapter 16

Case study: stability of steady states for reaction–diffusion PDEs

Goal

To linearize a nonlinear reaction–diffusion PDE around a steady state, and determine stability using the spectral theory of the linearized operator.

Reaction–diffusion PDEs

Assume throughout this section that $f : \mathbb{R} \rightarrow \mathbb{R}$ is a smooth function with f' bounded above. Let $X > 0$. We study the reaction–diffusion PDE

$$\mathbf{u}_t = \mathbf{u}_{xx} + f(\mathbf{u}) \tag{16.1}$$

on the interval $(0, X)$ with Dirichlet boundary conditions $\mathbf{u}(0) = \mathbf{u}(X) = 0$.

Physical interpretations include:

- (i) \mathbf{u} = temperature and f = rate of heat generation,
- (ii) \mathbf{u} = chemical concentration and f = reaction rate of chemical creation.

Intuitively, the 2nd order diffusion term in the PDE is **stabilizing** (since $\mathbf{u}_t = \mathbf{u}_{xx}$ is the usual diffusion equation), whereas the 0th order reaction term can be **destabilizing** (since solutions to $\mathbf{u}_t = f(\mathbf{u})$ will grow, when f is positive). Thus the reaction–diffusion PDE features a competition between stabilizing

and destabilizing effects. This competition can lead to nonconstant steady states, and interesting stability behavior.

Next we characterize the steady states of the reaction-diffusion equation, and investigate their stability.

Steady states

$U(x)$ is a steady state if

$$U'' + f(U) = 0, \quad 0 < x < X. \quad (16.2)$$

More than one steady state can exist. For example if $f(y) = y$ and $X = \pi$, then $U(x) \equiv 0$ is a steady state and so is $U(x) = \sin x$.

The nonlinear oscillator equation (16.2) can in principle be solved by multiplying by U' and integrating to obtain

$$\frac{1}{2}(U')^2 + F(U) = c,$$

where F is an antiderivative of f and c is constant. Then one rearranges to the form $dx/dU = \pm 1/\sqrt{2(c - F(U))}$ which can be integrated to obtain x as a function of U .

Linearizing the PDE

Perturb a steady state by considering

$$u = U + \varepsilon\phi,$$

where the perturbation $\phi(x, t)$ is assumed to satisfy the Dirichlet BC $\phi = 0$ at $x = 0$ and $x = X$, for each t . Substituting u into the reaction-diffusion equation (16.1) gives

$$\begin{aligned} u_t &= u_{xx} + f(u) \\ 0 + \varepsilon\phi_t &= U_{xx} + \varepsilon\phi_{xx} + f(U + \varepsilon\phi) \\ &= U_{xx} + \varepsilon\phi_{xx} + f(U) + f'(U)\varepsilon\phi + O(\varepsilon^2). \end{aligned}$$

The terms of order ε^0 on the right side equal zero by the steady state equation $U_{xx} + f(U) = 0$. We discard terms of order ε^2 and higher. (This approximation seems reasonable when ε is small and ϕ is not too large. To justify the

approximation rigorously, one would need to prove a linearization theorem for the reaction diffusion PDE.)

The remaining terms, which have order ε^1 , give the linearized equation

$$\phi_t = \phi_{xx} + f'(\mathbf{U})\phi. \quad (16.3)$$

That is,

$$\phi_t = L\phi$$

where L is the second order linear operator

$$Lw = w_{xx} + f'(\mathbf{U})w.$$

Separation of variables gives (formally) solutions of the form

$$\phi(x, t) = \sum_j c_j e^{-\tau_j t} w_j(x),$$

where the eigenvalues τ_j and Dirichlet eigenfunctions w_j satisfy

$$-Lw_j = \tau_j w_j$$

with $w_j(0) = w_j(X) = 0$.

The steady state \mathbf{U} of the reaction–diffusion PDE is called

- **linearly stable** if $\tau_1 \geq 0$, because in that case all coefficients in ϕ remain bounded as t increases,
- **linearly unstable** if $\tau_1 < 0$, because in that case the first coefficient $c_1 e^{-\tau_1 t}$ grows as t increases.

Thus the task is to investigate the spectrum of L and the sign of its first eigenvalue τ_1 .

Spectrum of linearized operator L

We take:

$$\Omega = (0, X),$$

$$\mathcal{H} = L^2(0, X), \text{ inner product } \langle \mathbf{u}, \mathbf{v} \rangle_{L^2} = \int_0^X \mathbf{u}\mathbf{v} \, dx,$$

$$\mathcal{K} = H_0^1(0, X), \text{ inner product}$$

$$\langle \mathbf{u}, \mathbf{v} \rangle_{H^1} = \int_0^X (\mathbf{u}'\mathbf{v}' + \mathbf{u}\mathbf{v}) \, dx.$$

Compact imbedding $H_0^1 \hookrightarrow L^2$ by Rellich's Theorem B.4.
Symmetric sesquilinear form

$$a(\mathbf{u}, \mathbf{v}) = \int_0^X (\mathbf{u}'\mathbf{v}' - f'(\mathbf{U})\mathbf{u}\mathbf{v} + C\mathbf{u}\mathbf{v}) \, dx$$

where $C = 1 + \sup f'$.

Coercivity: the definition of C insures

$$a(\mathbf{u}, \mathbf{u}) \geq \int_0^X ((\mathbf{u}')^2 + \mathbf{u}^2) \, dx = \|\mathbf{u}\|_{H^1}^2.$$

The discrete spectral Theorem 4.1 now yields an ONB of eigenfunctions $\{\mathbf{w}_j\}$ with eigenvalues γ_j such that

$$a(\mathbf{w}_j, \mathbf{v}) = \gamma_j \langle \mathbf{w}_j, \mathbf{v} \rangle_{L^2} \quad \forall \mathbf{v} \in H_0^1(0, X).$$

Writing $\gamma_j = \tau_j + C$ we get

$$\int_0^X (\mathbf{w}_j'\mathbf{v}' - f'(\mathbf{U})\mathbf{w}_j\mathbf{v}) \, dx = \tau_j \int_0^X \mathbf{w}_j\mathbf{v} \, dx \quad \forall \mathbf{v} \in H_0^1(0, X).$$

That is, the eigenfunctions satisfy

$$-L\mathbf{w}_j = \tau_j\mathbf{w}_j \quad \text{weakly}$$

and hence also classically.

Stability of the zero steady state

Assume $f(0) = 0$, so that $\mathbf{U} \equiv 0$ is a steady state. The linearized operator is $L\mathbf{w} = \mathbf{w}'' + f'(0)\mathbf{w}$, which on the interval $(0, X)$ has Dirichlet eigenvalues

$$\tau_j = \left(\frac{j\pi}{X}\right)^2 - f'(0)$$

with eigenfunctions $\sin(j\pi x/X)$, for $j \geq 1$. The first eigenvalue is $\tau_1 = (\pi/X)^2 - f'(0)$, from which one deduces:

Proposition 16.1 (Stability of the zero steady state).

- (a) If $f(0) = 0$ and $f'(0) \leq 0$ then the zero steady state is linearly stable.
(b) If $f(0) = 0$ and $f'(0) > 0$ then the zero steady state is linearly stable on short intervals ($X \leq \pi/\sqrt{f'(0)}$), but is linearly unstable when the interval is long ($X > \pi/\sqrt{f'(0)}$).

The reaction-diffusion equation is called long-wave unstable, in case (b).

Instability of sign-changing steady states

The next criterion depends on a sign-changing property of the steady state.

Theorem 16.2 (Linear instability [Schaaf2, Proposition 4.1.2]). *If the steady state \mathbf{U} changes sign on $(0, X)$ then $\tau_1 < 0$.*

For example, suppose $f(\mathbf{y}) = \mathbf{y}$ so that the steady state equation is $\mathbf{U}'' + \mathbf{U} = 0$. If $X = 2\pi$ then the steady state $\mathbf{U} = \sin x$ is linearly unstable, by the theorem. In this example we can compute the spectrum of \mathbf{L} exactly: the lowest eigenfunction is $w = \sin(x/2)$ with eigenvalue $\tau_1 = (\frac{1}{2})^2 - 1 < 0$.

Proof. If \mathbf{U} changes sign then it has a positive local maximum and a negative local minimum in $(0, X)$, recalling that $\mathbf{U} = 0$ at the endpoints. Obviously \mathbf{U}' must be nonzero at some point between these local extrema, and so there exist points $0 < x_1 < x_2 < X$ such that

$$\mathbf{U}'(x_1) = \mathbf{U}'(x_2) = 0$$

and $\mathbf{U}' \neq 0$ on (x_1, x_2) . Define a trial function

$$w = \begin{cases} \mathbf{U}' & \text{on } (x_1, x_2), \\ 0 & \text{elsewhere.} \end{cases}$$

(We motivate this choice of trial function at the end of the proof.) Then w is piecewise smooth, and is continuous since $w = \mathbf{U}' = 0$ at x_1 and x_2 . Therefore $w \in H_0^1(0, X)$, and $w \not\equiv 0$ since $\mathbf{U}' \neq 0$ on (x_1, x_2) .

The numerator of the Rayleigh quotient for w is

$$\begin{aligned} \int_0^X ((w')^2 - f'(\mathbf{U})w^2) dx &= \int_{x_1}^{x_2} (-w'' - f'(\mathbf{U})w)w dx && \text{by parts} \\ &= 0 \end{aligned}$$

since

$$-w'' = -\mathbf{U}''' = (f(\mathbf{U}))' = f'(\mathbf{U})\mathbf{U}' = f'(\mathbf{U})w. \quad (16.4)$$

Hence $\tau_1 \leq 0$, by using w as a trial function in the Rayleigh principle for the first eigenvalue.

Suppose $\tau_1 = 0$. Then w is an eigenfunction with eigenvalue 0, by the condition for equality in the Rayleigh quotient (10.1). Since eigenfunctions are smooth, one has $w'(x_2) = 0$ by taking the derivative from the right. Then $w(x_2) = w'(x_2) = 0$, and so $w \equiv 0$ by uniqueness for the second order linear ODE (16.4). On the other hand, $w \not\equiv 0$ by construction. Hence $\tau_1 < 0$. \square

Motivation for the choice of trial function. The derivative \mathbf{U}' lies in the nullspace of \mathbf{L} since

$$\mathbf{L}\mathbf{U}' = (\mathbf{U}')'' + f'(\mathbf{U})\mathbf{U}' = (\mathbf{U}'' + f(\mathbf{U}))' = 0.$$

In other words, \mathbf{U}' is an eigenfunction with eigenvalue 0, which almost proves instability, since instability would correspond to a negative eigenvalue. Of course, \mathbf{U}' does not satisfy the Dirichlet boundary conditions at the endpoints, which is why we restrict to the subinterval (x_1, x_2) in the proof above in order to obtain a valid trial function.

Structural conditions for linearized instability

Our next instability criterion is *structural*, meaning it depends on properties of the reaction function f rather than on properties of the particular steady state \mathbf{U} .

Theorem 16.3 (Linear instability). *Assume the steady state \mathbf{U} is nonconstant, and that*

$$f(0) = 0, \quad f''(0) = 0, \quad f''' > 0.$$

Then $\tau_1 < 0$.

For example, every nonconstant steady state is unstable if $f(y) = y^3 - y$. (The derivative $f'(y) = 3y^2 - 1$ admittedly has no upper bound, but one may make it bounded by modifying f outside a neighborhood of \mathbf{U} ; the instability proof below is unaffected.)

Proof. First we collect facts about boundary values, to be used later when integrating by parts:

$$\begin{array}{ll} \mathbf{U} = 0 \text{ at } x = 0, X & \text{by the Dirichlet BC,} \\ f(\mathbf{U}) = 0 \text{ at } x = 0, X & \text{since } f(0) = 0, \\ \mathbf{U}'' = 0 \text{ at } x = 0, X & \text{because } \mathbf{U}'' = -f(\mathbf{U}), \\ f''(\mathbf{U}) = 0 \text{ at } x = 0, X & \text{since } f''(0) = 0. \end{array}$$

The Rayleigh principle for \mathbf{L} says that

$$\tau_1 = \min \left\{ \frac{\int_0^X ((w')^2 - f'(\mathbf{U})w^2) dx}{\int_0^X w^2 dx} : w \in H_0^1(0, X) \right\}.$$

Choose a trial function

$$w = U''$$

for reasons explained after the proof. Notice w is not the zero function, since U is not linear. The numerator of the Rayleigh quotient for w is

$$\begin{aligned} & \int_0^X ((U''')^2 - f'(U)(U'')^2) dx \\ &= \int_0^X (-U'''' - f'(U)U'')U'' dx \quad \text{by parts on the first term} \\ &= \int_0^X f''(U)(U')^2U'' dx \quad \begin{array}{l} \text{by substituting for } U'''' \text{ from the second} \\ \text{derivative of steady state equation (16.2)} \end{array} \\ &= \frac{1}{3} \int_0^X f''(U)[(U')^3]' dx \\ &= -\frac{1}{3} \int_0^X f'''(U)(U')^4 dx \quad \text{by parts} \\ &< 0 \end{aligned}$$

since $f''' > 0$ and U is nonconstant. Hence $\tau_1 < 0$, by the Rayleigh principle. \square

Motivation for the choice of trial function. Our trial function $w = U''$ corresponds to a perturbation $u = U + \varepsilon\phi \approx U + \varepsilon e^{-\tau_1 t}U''$, which will want to evolve (assuming $\varepsilon > 0$ and the steady state U looks something like a sine function) from the steady state towards the constant function.

Time map criteria for linearized in/stability

Next we derive structural instability criteria that are almost necessary and sufficient. These conditions depend on the *time map* for a family of steady states.

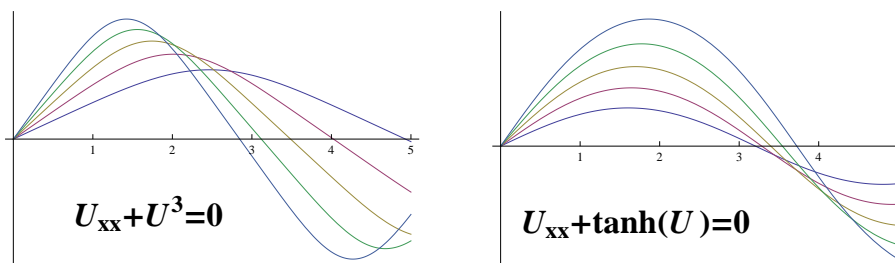
Parameterize the steady states by the slope s at the left endpoint: write $U_s(x)$ for the steady state on \mathbb{R} (if it exists) satisfying

$$U_s(0) = 0, \quad U'_s(0) = s, \quad U_s(x) = 0 \text{ for some } x > 0.$$

Define the *time map* $\mathbb{T}(s)$ to give the first point or “time” x at which the steady state hits the axis:

$$\mathbb{T}(s) = \min\{x > 0 : \mathbf{U}_s(x) = 0\}.$$

If \mathbf{U}_s exists for some $s \neq 0$ then it exists for all nearby s -values, and $\mathbf{U}_s(x)$ is jointly smooth in (x, s) and the time map $\mathbb{T}(s)$ is smooth [Schaaf2, Proposition 4.1.1]. The time map can be determined numerically by plotting solutions with different initial slopes, as the figures below show. In the first figure the time map is decreasing, whereas in the second it increases.



Monotonicity of the time maps determines stability of the steady state:

Theorem 16.4 ([Schaaf2, Proposition 4.1.3]). *The steady state \mathbf{U}_s on the interval $(0, \mathbb{T}(s))$ is:*

- *linearly unstable if $s\mathbb{T}'(s) < 0$,*
- *linearly stable if $s\mathbb{T}'(s) > 0$.*

Proof. We begin by differentiating the family of steady states with respect to the parameter s . Then we treat the “instability” and “stability” parts of the theorem separately.

Write $s_0 \neq 0$ for a specific value of s , in order to reduce notational confusion. Let $X = \mathbb{T}(s_0)$. Define a function

$$\mathbf{v} = \left. \frac{\partial \mathbf{U}_s}{\partial s} \right|_{s=s_0}$$

on $(0, X)$. Then

$$\mathbf{v}'' + f'(\mathbf{U})\mathbf{v} = 0 \tag{16.5}$$

as one sees by differentiating the steady state equation (16.2) with respect to s , and writing \mathbf{U} for \mathbf{U}_{s_0} .

At the left endpoint,

$$v(0) = 0 \quad \text{and} \quad v'(0) = 1$$

because $\mathbf{U}_s(0) = 0$ and $\mathbf{U}'_s(0) = s$ for all s by definition of the steady state.

We do not expect v to vanish at the right endpoint, but its value there can be calculated as follows. Differentiating the identity $0 = \mathbf{U}_s(T(s))$ gives

$$\begin{aligned} 0 &= \frac{\partial}{\partial s} \mathbf{U}_s(T(s)) \\ &= \frac{\partial \mathbf{U}_s}{\partial s}(T(s)) + \mathbf{U}'_s(T(s))T'(s) \\ &= v(T(s)) + \mathbf{U}'_s(T(s))T'(s). \end{aligned}$$

Note the steady state \mathbf{U}_s is symmetric about the midpoint of the interval $(0, T(s))$ (exercise; use that $\mathbf{U}_s = 0$ at both endpoints and that the steady state equation is invariant under $x \mapsto -x$, so that steady states must be symmetric about any local maximum point). Thus $\mathbf{U}'_s(T(s)) = -\mathbf{U}'_s(0) = -s$, and evaluating the last displayed formula at $s = s_0$ then gives that $0 = v(X) - s_0 T'(s_0)$, so that v has value

$$v(X) = s_0 T'(s_0).$$

Proof of instability. Assume $s_0 T'(s_0) < 0$. Then $v(X) < 0$. Since $v'(0) = 1$ we know $v(x)$ is positive for small values of x , and so an $x_2 \in (0, X)$ exists at which $v(x_2) = 0$. Define a trial function

$$w = \begin{cases} v & \text{on } [0, x_2), \\ 0 & \text{elsewhere.} \end{cases}$$

Then w is piecewise smooth, and is continuous since $v = 0$ at x_2 . Note $w(0) = 0$. Therefore $w \in H_0^1(0, X)$, and $w \not\equiv 0$.

Hence $\tau_1 < 0$ by arguing as in the proof of Theorem 16.2 with $x_1 = 0$.

Motivation for the choice of trial function above. Differentiating the steady state equation $\mathbf{U}'' + f(\mathbf{U}) = 0$ with respect to s shows that $v = \partial \mathbf{U} / \partial s$ is an eigenfunction with eigenvalue zero:

$$L v = \left(\frac{\partial \mathbf{U}}{\partial s} \right)'' + f'(\mathbf{U}) \frac{\partial \mathbf{U}}{\partial s} = \frac{\partial}{\partial s} \left(\mathbf{U}'' + f(\mathbf{U}) \right) = 0.$$

In other words, v lies in the nullspace of the linearized operator. Although v does not satisfy the Dirichlet boundary condition at the right endpoint, we handled that issue in the proof above by restricting to the subinterval $(0, x_2)$, in order to obtain a valid trial function with $w = 0$ at the right endpoint.

Proof of stability. Assume $s_0 T'(s_0) > 0$, so that $v(X) > 0$. Define $\sigma = -v'(X)/v(X)$. Then

$$v(0) = 0, \quad v'(X) + \sigma v(X) = 0,$$

which is a mixed Dirichlet–Robin boundary condition. We will show later that v is a first eigenfunction for L , under this mixed condition, with eigenvalue $\rho_1 = 0$ (since $Lv = 0$ by (16.5)).

By adapting our Dirichlet-to-Robin monotonicity result (Theorem 11.1) one deduces that

$$\tau_1 \geq \rho_1 = 0,$$

which gives linearized stability of the steady state \mathbf{U} .

To show v is a first eigenfunction for L , as used above, we start by showing v is positive on $(0, X)$. Apply the steady state equation (16.2) to \mathbf{U}_s , and multiply by \mathbf{U}'_s and integrate to obtain the energy equation

$$\frac{1}{2}(\mathbf{U}'_s)^2 + F(\mathbf{U}_s) = \frac{1}{2}s^2, \quad (16.6)$$

where F is an antiderivative of f chosen with $F(0) = 0$. Differentiating with respect to s at $s = s_0$ gives that

$$\mathbf{U}'v' + f(\mathbf{U})v = s_0.$$

Hence if v vanishes at some $x_* \in (0, X)$ then $\mathbf{U}'(x_*)v'(x_*) = s_0 \neq 0$. Thus at any two successive zeros of v , we know v' is nonzero and has opposite signs, and so \mathbf{U}' is nonzero has opposite signs too. It is straightforward to show from (16.6) that if $s_0 > 0$ then \mathbf{U} increases on $[0, X/2]$ and decreases on $[X/2, X]$, while if $s_0 < 0$ then \mathbf{U} decreases on $[0, X/2]$ and increases on $[X/2, X]$. Either way, in order for $\mathbf{U}'(x)$ to change sign, x must increase past $X/2$. Thus after the zero of v at $x = 0$, the next zero (if it exists) must be greater than $X/2$, and the one after that (if it exists) must be greater than X . Since we know $v(x)$ is positive for small x and that $v(X) > 0$, we conclude v has no zeros in $(0, X)$ and hence is positive there.

The first eigenfunction of L with mixed Dirichlet–Robin boundary condition is positive, and it is the unique positive eigenfunction (adapt the argument in [Gilbarg and Trudinger, Theorem 8.38]). Since the eigenfunction v is positive, we conclude that it is the first Dirichlet–Robin eigenfunction, as desired. \square

Notes and comments

Monotonicity criteria for the time map (or “period map”) can be found in [Chicone, Schaaf1, Schaaf2]. See the overview and extensions in [Laugesen and Pugh 1, Section 7]. These monotonicity criteria combine with Theorem 16.4 to provide structural stability results for steady states of reaction–diffusion equations.

Exercises

16.1 — Show that Theorem 16.3 (linear instability for nonconstant steady states) continues to hold under the alternative assumptions

$$f(0) = 0, \quad f(y)f''(y) > 0 \quad \text{for all } y \neq 0.$$

Verify those assumptions when

$$f(y) = 2y - \int_0^y e^{-z^2} dz,$$

and show f''' changes sign in this example, so that Theorem 16.3 does not apply.

16.2 — Prove linear instability of every nonconstant steady state of the reaction-diffusion equation under the Neumann boundary conditions $\mathbf{u}'(0) = \mathbf{u}'(X) = 0$, assuming either

$$f''' > 0 \quad \text{or} \quad f(y)f''(y) > 0 \quad \text{for all } y \neq 0.$$

Chapter 17

Case study: stability of steady states for thin fluid film PDEs

Goal

To linearize a particular fourth order nonlinear PDE around a steady state, and develop the spectral theory of the linearized operator.

Thin fluid film PDE

The evolution of a thin layer of fluid (such as paint) on a flat substrate (such as the ceiling) can be modeled using the *thin fluid film PDE*:

$$h_t = -(f(h)h_{xxx})_x - (g(h)h_x)_x$$

where $h(x, t) > 0$ measures the thickness of the fluid, and the positive smooth coefficient functions f and g represent surface tension and gravitational effects (or substrate-fluid interactions), respectively. For simplicity we assume $f \equiv 1$, so that the equation becomes

$$h_t = -h_{xxxx} - (g(h)h_x)_x. \quad (17.1)$$

We will treat the case of general g , but readers are welcome to focus on the special case $g(y) = y^p$ for some $p \in \mathbb{R}$.

Intuitively, the fourth order term in the PDE is stabilizing (since $h_t = -h_{xxxx}$ is the standard fourth order diffusion equation) whereas the second order term is destabilizing (since $h_t = -h_{xx}$ is the time-backwards heat

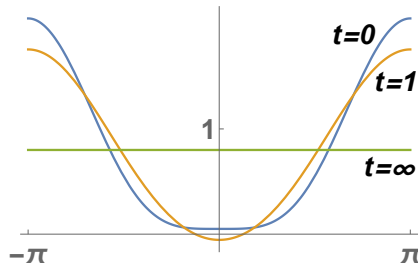
equation). Thus the thin film PDE features a competition between stabilizing and destabilizing effects such as surface tension and gravity. This competition leads to nonconstant steady states, and interesting stability behavior.

Positivity preservation

Solutions of the PDE are known to exist for small time, given positive smooth initial data. Films can rupture in finite time, though, meaning that $h(x, t) \searrow 0$ as $t \nearrow T$. That is, the minimum principle can fail for these fourth order equations: a solution that starts out positive need not remain positive. For example, the 2π -periodic function

$$h(x, t) = \frac{4}{5} - e^{-t} \cos x + \frac{1}{4} e^{-16t} \cos 2x$$

satisfies the fourth order diffusion equation $h_t = -h_{xxxx}$ and is positive everywhere at $t = 0$. By time $t = 1/10$, the solution has become negative at $x = 0$. Then as $t \rightarrow \infty$, the solution relaxes to its mean value $4/5$ and regains positivity. The key to this example is the observation that $h_t(0, 0) = -3 < 0$,



and so the solution is pushed downward initially before relaxing to the mean as $t \rightarrow \infty$.

Positivity can be preserved if the diffusion slows down sufficiently when the film thickness approaches 0. The fourth order porous medium type equation $h_t = -(h^4 h_{xxx})_x$ was shown by [Bernis and Friedman] to preserve positivity of initial data. Their intuition is that because the diffusivity h^4 approaches 0 as the film thickness h approaches 0, nearby fluid has enough time to diffuse and prevent the film from rupturing.

Periodic BCs and conservation of fluid

The thin fluid film PDE is derived from the Navier–Stokes equation via the lubrication approximation. Thus one would expect the equation to conserve the total volume of fluid. Indeed, if we fix $X > 0$ and assume h is X -periodic with respect to x , then

$$\begin{aligned} \frac{d}{dt} \int_0^X h(x, t) \, dx &= - \int_0^X (h_{xxx} + g(h)h_x)_x \, dx \\ &= -(h_{xxx} + g(h)h_x) \Big|_{x=0}^{x=X} \\ &= 0 \end{aligned}$$

by periodicity.

Stability of constant steady states

Let $\bar{H} > 0$. The constant function \bar{H} is a steady state, whose stability is determined as follows.

Linearizing (17.1) with $h = \bar{H} + \varepsilon\phi$, where $\phi(x, t)$ is X -periodic in x , gives

$$\begin{aligned} \phi_t &= -\phi_{xxxx} - g(\bar{H})\phi_{xx} \\ &= -\bar{L}\phi \end{aligned}$$

where the fourth order, constant coefficient, symmetric linear operator \bar{L} is defined by

$$\bar{L}w = w_{xxxx} + g(\bar{H})w_{xx}.$$

Separation of variables gives (formally) solutions of the form

$$\phi(x, t) = \sum_j c_j e^{-\tau_j t} w_j(x),$$

where the eigenvalues τ_j and X -periodic eigenfunctions w_j satisfy

$$\bar{L}w_j = \tau_j w_j.$$

The constant steady state \bar{H} is

- **linearly stable** if $\tau_1 \geq 0$,

- **linearly unstable** if $\tau_1 < 0$.

Our task is to investigate the spectrum of \bar{L} and the sign of τ_1 .

The eigenfunctions of \bar{L} are the Fourier modes

$$v_k(x) = \exp(2\pi i k x / X), \quad k \in \mathbb{Z} \setminus \{0\},$$

noting $k \neq 0$ because our perturbations must have mean value zero in order to conserve fluid volume (that is, to insure $\int_0^X \phi(x, t) dx = 0$). The corresponding eigenvalues are

$$\tau_k = \left(\frac{2\pi k}{X}\right)^2 \left(\left(\frac{2\pi k}{X}\right)^2 - g(\bar{H})\right), \quad k \neq 0.$$

If $g \leq 0$ (in which case the second order term in the thin film PDE behaves like a forwards heat equation), then $\tau \geq 0$ for each k , and so all constant steady states are linearly stable.

If $\left(\frac{2\pi}{X}\right)^2 \geq g(\bar{H}) > 0$ then $\tau \geq 0$ for each k , and so the constant steady state \bar{H} is linearly stable.

If $\left(\frac{2\pi}{X}\right)^2 < g(\bar{H})$ then the constant steady state \bar{H} is linearly unstable with respect to the $k = \pm 1$ modes (and possibly other modes too). In particular, this occurs if X is large enough. Hence the thin film PDE is “long-wave unstable” if $g > 0$, because constant steady states are unstable with respect to perturbations of sufficiently long wavelength X .

Nonconstant steady states — existence

To find nonconstant steady states, substitute $h = H(x)$ and solve:

$$\begin{aligned} -H_{xxxx} - (g(H)H_x)_x &= 0 \\ H_{xxx} + g(H)H_x &= \alpha \\ H_{xx} + G(H) &= \beta + \alpha x \end{aligned} \tag{17.2}$$

where G is an antiderivative of g . In fact, $\alpha = 0$ because the left side of the equation (which is $H_{xx} + G(H)$) is periodic and so the right side must be periodic also. Thus

$$H'' + G(H) = \beta.$$

This equation describes a nonlinear oscillator. To construct solutions one multiplies by H' and integrates, as explained in Chapter 16.

Assume from now on that $H(x)$ is a nonconstant steady state with period X .

Linearized PDE

Perturb the nonconstant steady state H by considering

$$h = H + \varepsilon\phi$$

where the perturbation $\phi(x, t)$ is assumed to be X -periodic in x and have mean value zero ($\int_0^X \phi(x, t) dx = 0$), so that fluid volume is conserved. Substituting h into the equation (17.1) gives

$$\begin{aligned} 0 + \varepsilon\phi_t &= -(H_{xxxx} + \varepsilon\phi_{xxxx}) - (g(H + \varepsilon\phi)(H_x + \varepsilon\phi_x))_x \\ &= -H_{xxxx} - (g(H)H_x)_x - \varepsilon[\phi_{xxx} + g(H)\phi_x + g'(H)H_x\phi]_x + O(\varepsilon^2). \end{aligned}$$

The terms of order ε^0 equal zero by the steady state equation for H . We discard terms of order ε^2 and higher. The remaining terms, of order ε^1 , give the linearized equation:

$$\phi_t = -(\phi_{xx} + g(H)\phi)_{xx}. \quad (17.3)$$

The fourth order operator on the right side is not symmetric, meaning it does not equal its formal adjoint. To make it symmetric, we “integrate up” the equation as follows. Write

$$\psi_x = \phi$$

and notice ψ is X -periodic: integrating the equation from x to $x + X$ gives

$$\psi(x + X, t) - \psi(x, t) = \int_x^{x+X} \phi(\tilde{x}, t) d\tilde{x} = 0$$

since ϕ has mean value zero at each time. We may also suppose ψ has mean value zero at each time, by subtracting from it a suitable function of t (which does not affect the condition $\psi_x = \phi$).

Substituting $\phi = \psi_x$ into (17.3) gives that

$$\begin{aligned} \psi_{tx} &= -(\psi_{xxx} + g(H)\psi_x)_{xx} \\ \psi_t &= -(\psi_{xxx} + g(H)\psi_x)_x \end{aligned}$$

where we note the constant of integration must equal 0 since $\frac{d}{dt} \int_0^X \psi(x, t) dx = 0$. Thus

$$\psi_t + L\psi = 0$$

where L is the fourth order symmetric linear operator

$$Lw = w_{xxxx} + (g(H)w_x)_x.$$

Separation of variables gives (formally) solutions of the form

$$\psi = \sum_j c_j e^{-\tau_j t} w_j(x), \quad \phi = \sum_j c_j e^{-\tau_j t} w_j'(x),$$

where the eigenvalues τ_j and periodic eigenfunctions w_j satisfy

$$Lw_j = \tau_j w_j.$$

The steady state H is

- **linearly stable** if $\tau_1 \geq 0$,
- **linearly unstable** if $\tau_1 < 0$.

Recall this definition of stability relates only to zero-mean (volume preserving) perturbations of H .

To determine the stability of the steady state H , we investigate the eigenvalue problem for L .

Spectrum of linearized operator L

We take:

$\Omega = \mathbb{T} = \mathbb{R}/(X\mathbb{Z}) =$ torus of length X , meaning functions are X -periodic,

$\mathcal{H} = L^2(\mathbb{T})$, inner product $\langle u, v \rangle_{L^2} = \int_0^X uv \, dx$,

$\mathcal{K} = H^2(\mathbb{T})$, with inner product

$$\langle u, v \rangle_{H^2} = \int_0^X (u''v'' + u'v' + uv) \, dx.$$

Compact imbedding $\mathcal{K} \hookrightarrow H^1(\mathbb{T}) \hookrightarrow L^2$ is compact by a suitable adaptation of Rellich's Theorem B.6.

Symmetric sesquilinear form

$$a(u, v) = \int_0^X (u''v'' - g(H)u'v' + Cuv) \, dx$$

where $C > 0$ is a sufficiently large constant to be chosen below.

Coercivity: The quantity $\mathbf{a}(\mathbf{u}, \mathbf{u})$ has a term of the form $-(\mathbf{u}')^2$, whereas for $\|\mathbf{u}\|_{\mathbb{H}^2}^2$ we need $+(\mathbf{u}')^2$. To get around this obstacle we “hide” the $-(\mathbf{u}')^2$ term inside the terms $(\mathbf{u}'')^2$ and \mathbf{u}^2 . Specifically,

$$\begin{aligned} \int_0^x (\mathbf{u}')^2 \, dx &= - \int_0^x \mathbf{u}'' \mathbf{u} \, dx \\ &\leq \int_0^x (\delta^2 (\mathbf{u}'')^2 + \frac{1}{4\delta^2} \mathbf{u}^2) \, dx \end{aligned} \quad (17.4)$$

whenever $\delta > 0$ by “Cauchy-with- δ ”, which says:

$$0 \leq (\alpha\delta \mp \beta/2\delta)^2 \quad \implies \quad \pm\alpha\beta \leq \delta^2\alpha^2 + \frac{1}{4\delta^2}\beta^2$$

for all $\alpha, \beta \in \mathbb{R}$. Hence

$$\begin{aligned} \mathbf{a}(\mathbf{u}, \mathbf{u}) &\geq \int_0^x ((\mathbf{u}'')^2 - (\|\mathbf{g}(\mathbf{H})\|_{L^\infty} + \frac{1}{2})(\mathbf{u}')^2 + \frac{1}{2}(\mathbf{u}')^2 + C\mathbf{u}^2) \, dx \\ &\geq \int_0^x \left([1 - (\|\mathbf{g}(\mathbf{H})\|_{L^\infty} + \frac{1}{2})\delta^2] (\mathbf{u}'')^2 + \frac{1}{2}(\mathbf{u}')^2 + [C - (\|\mathbf{g}(\mathbf{H})\|_{L^\infty} + \frac{1}{2})\frac{1}{4\delta^2}] \mathbf{u}^2 \right) \, dx \\ &\quad \text{by (17.4)} \\ &\geq \frac{1}{2} \|\mathbf{u}\|_{\mathbb{H}^2}^2 \end{aligned}$$

provided we choose δ sufficiently small, depending on $\mathbf{g}(\mathbf{H})$, and then choose C sufficiently large. Thus coercivity holds.

The discrete spectral Theorem 4.1 now yields an ONB of eigenfunctions $\{\mathbf{w}_j\}$ with eigenvalues γ_j such that

$$\mathbf{a}(\mathbf{w}_j, \mathbf{v}) = \gamma_j \langle \mathbf{w}_j, \mathbf{v} \rangle_{L^2} \quad \forall \mathbf{v} \in \mathcal{K}.$$

Writing $\gamma_j = \tau_j + C$ we get

$$\int_0^x (\mathbf{w}_j'' \mathbf{v}'' - \mathbf{g}(\mathbf{H}) \mathbf{w}_j' \mathbf{v}') \, dx = \tau_j \int_0^x \mathbf{w}_j \mathbf{v} \, dx \quad \forall \mathbf{v} \in \mathbb{H}^2(\mathbb{T}).$$

These eigenfunctions satisfy $L\mathbf{w}_j = \tau_j \mathbf{w}_j$ weakly, and hence also classically (by elliptic regularity, since \mathbf{H} and \mathbf{g} are smooth).

Zero eigenvalues: the constant, and translational symmetry

The constant function $\mathbf{1}$ is an eigenfunction with eigenvalue 0 , since $L\mathbf{1} = 0$. This constant mode is irrelevant, since the ψ 's in which we are interested have mean value zero and thus are orthogonal to the constant.

More interestingly, $\tau = 0$ has another eigenfunction $w = H - \bar{H}$, where \bar{H} is the mean value of the steady state H . Indeed,

$$Lw = L(H - \bar{H}) = H_{xxxx} + (g(H)H_x)_x = 0$$

by the steady state equation (17.2). Notice this w is orthogonal in L^2 to the constant function $\mathbf{1}$.

This zero mode $w = H - \bar{H}$ arises from a *translational perturbation* of the steady state, because choosing

$$H(x + \varepsilon) = H(x) + \varepsilon H'(x) + O(\varepsilon^2)$$

corresponds to a perturbation $\phi = H'$, which integrates up to give $\psi = H - \bar{H}$.

Instability of nonconstant steady state H

Theorem 17.1 ([Laugesen and Pugh 2, Th. 3]). *If $g'' > 0$ then $\tau_1 < 0$.*

For example, if $g(y) = y^p$ with $p > 1$ or $p < 0$ then the theorem shows that each nonconstant steady state is unstable with respect to volume-preserving perturbations.

The theorem is essentially the same as Theorem 16.3 for the reaction–diffusion PDE, by writing g instead of f' and noting that periodicity handles all boundary terms in the integrations by parts, in the argument below.

Proof. The Rayleigh principle for L says that

$$\tau_1 = \min \left\{ \frac{\int_0^X ((w'')^2 - g(H)(w')^2) dx}{\int_0^X w^2 dx} : w \in H^2(\mathbb{T}) \setminus \{0\} \right\}.$$

We choose

$$w = H',$$

which is not the zero function since H is nonconstant. The numerator of the Rayleigh quotient for w is

$$\begin{aligned}
 & \int_0^X ((H''')^2 - g(H)(H'')^2) \, dx \\
 &= \int_0^X (-H'''' - g(H)H'')H'' \, dx && \text{by parts} \\
 &= \int_0^X g'(H)(H')^2H'' \, dx && \text{by the steady state equation (17.2)} \\
 &= \frac{1}{3} \int_0^X g'(H)[(H')^3]' \, dx \\
 &= -\frac{1}{3} \int_0^X g''(H)(H')^4 \, dx && \text{by parts} \\
 &< 0
 \end{aligned}$$

by strong convexity of g and since $H' \not\equiv 0$. Hence $\tau_1 < 0$, by the Rayleigh principle. \square

Motivation for the choice of trial function. Our trial function $w = H'$ corresponds to $\phi = H''$. This perturbation $H + \varepsilon\phi = H + \varepsilon H''$ tends to push the periodic steady state towards the constant function. The opposite perturbation $H - \varepsilon H''$ would tend to push the steady state towards a “droplet” solution that is supported on some interval. Thus our instability proof in Theorem 17.1 suggests (in the language of dynamical systems) that a heteroclinic connection might exist between the nonconstant steady state and the constant steady state, and similarly between the nonconstant steady state and a droplet steady state. Such connections are explored numerically in [Laugesen and Pugh 4].

Stability of nonconstant steady states

It is more difficult to prove stability results, because lower bounds on the first eigenvalue are generally more difficult to prove than upper bounds. See [Laugesen and Pugh 2, §3.2] for some stability results when $g(y) = y^p$, $0 < p \leq 3/4$, based on time-map monotonicity ideas from the theory of reaction diffusion equations, similar to Chapter 16.

Notes and comments

This chapter is drawn from [Laugesen and Pugh 1] and [Laugesen and Pugh 2], which treat steady states and their stability. For the dynamics of thin fluid film equations and existence of heteroclinic connections, see [Laugesen and Pugh 3] and [Laugesen and Pugh 4]. The references in those papers provide an entry point into the vibrant literature of this field.

Part II

Continuous Spectrum

Looking ahead to continuous spectrum

The discrete spectral theory in Part I of the course generated, in each application:

- eigenfunctions $\{\mathbf{u}_j\}$ with “discrete” spectrum $\lambda_1, \lambda_2, \lambda_3, \dots$ satisfying $L\mathbf{u}_j = \lambda_j\mathbf{u}_j$ where L is a symmetric differential operator, together with
- a spectral decomposition (or “resolution”) of each $f \in L^2$ into a sum of eigenfunctions: $f = \sum_j \langle f, \mathbf{u}_j \rangle \mathbf{u}_j$.

These constructions depended heavily on symmetry of the differential operator L (which ensured symmetry of the sesquilinear form \mathbf{a}) and on compactness of the imbedding of the Hilbert space \mathcal{K} into \mathcal{H} .

For the remainder of the course we retain the symmetry assumption on the operator, but drop the compact imbedding assumption. The resulting “continuous” spectrum leads to a decomposition of $f \in L^2$ into an integral of “almost eigenfunctions”.

We begin with examples, and later put the examples in context by developing some general spectral theory for unbounded, selfadjoint differential operators.

Chapter 18

Computable example: Laplacian (free Schrödinger) on all of space

Goal

To develop a spectral decomposition of $L^2(\mathbb{R}^d)$ associated with the Laplacian, determine the continuous spectrum $[0, \infty)$, and introduce Weyl sequences.

Spectral decomposition

The Laplacian $L = -\Delta$ on a domain of finite volume has discrete spectrum, as we saw in Chapters 2 and 5. When the domain expands to all of space, the Laplacian has no eigenvalues at all. For example in 1 dimension, solutions of $-u'' = \lambda u$ are linear combinations of $e^{+i\sqrt{\lambda}x}$ and $e^{-i\sqrt{\lambda}x}$, which oscillate if $\lambda > 0$, or are constant if $\lambda = 0$ (with the other solution being x), or grow in one direction or the other if $\lambda \in \mathbb{C} \setminus [0, \infty)$. In none of these situations can u belong to L^2 .

In any dimension, the non-existence of L^2 -eigenfunctions can be seen as follows. If $-\Delta u = \lambda u$ and $u \in L^2$ then by taking Fourier transforms, $4\pi^2|\xi|^2\widehat{u}(\xi) = \lambda\widehat{u}(\xi)$ a.e., and so the only place \widehat{u} can be nonzero is on the sphere $\{|\xi| = \sqrt{\lambda}/2\pi\}$, which has measure zero; hence $\widehat{u} = 0$ a.e. and so $u = 0$ a.e. and thus no L^2 -eigenfunction exists.

A fundamental difference between the case of finite-volume domains and the whole space case is that the imbedding $H^1(\mathbb{R}^d) \hookrightarrow L^2(\mathbb{R}^d)$ is not compact.

For example, given a nonzero function $f \in H^1(\mathbb{R})$, the translated functions $f(x - k)$ form a bounded sequence in $L^2(\mathbb{R})$ but have no L^2 -convergent subsequence as $k \rightarrow \infty$. Hence the discrete spectral theorem (Theorem 4.1) does not apply.

Nevertheless, the Laplacian $-\Delta$ on \mathbb{R}^d has **generalized eigenfunctions** and a **spectral decomposition**:

1. Generalized eigenfunctions:

$$v_\omega(x) = e^{2\pi i \omega \cdot x}, \quad \omega \in \mathbb{R}^d.$$

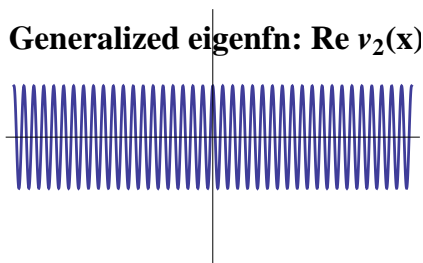
Note v_ω is bounded and satisfies the eigenfunction equation

$$-\Delta v_\omega = \lambda v_\omega$$

with generalized eigenvalue

$$\lambda = \lambda(\omega) = 4\pi^2 |\omega|^2,$$

but is not an eigenfunction since $v_\omega \notin L^2$.



2. Spectral decomposition:

$$f = \int_{\mathbb{R}^d} \langle f, v_\omega \rangle v_\omega \, d\omega, \quad \forall f \in L^2(\mathbb{R}^d).$$

Proof.

$$\langle f, v_\omega \rangle = \int_{\mathbb{R}^d} f(x) e^{-2\pi i \omega \cdot x} \, dx = \widehat{f}(\omega),$$

and so the spectral decomposition simply says

$$f(x) = \int_{\mathbb{R}^d} \widehat{f}(\omega) e^{2\pi i \omega \cdot x} \, d\omega,$$

which is the Fourier inversion formula on L^2 .

Application of spectral decomposition

One may solve evolution equations by separating variables: for example, the heat equation $\mathbf{u}_t = \Delta \mathbf{u}$ with initial condition $\mathbf{h}(\mathbf{x})$ has solution

$$\mathbf{u}(\mathbf{x}, t) = \int_{\mathbb{R}^d} \widehat{\mathbf{h}}(\boldsymbol{\omega}) e^{-\lambda(\boldsymbol{\omega})t} \mathbf{v}_{\boldsymbol{\omega}}(\mathbf{x}) \, d\boldsymbol{\omega}.$$

Notice the analogy to the series solution obtained by separation of variables, in the case of discrete spectrum.

Aside. One can evaluate the last integral (an inverse Fourier transform) as the convolution of the initial data \mathbf{h} with the fundamental solution of the heat equation, which is the inverse transform of $e^{-\lambda(\boldsymbol{\omega})t}$.

Continuous spectrum = $[0, \infty)$

The generalized eigenvalue $\lambda \geq 0$ is “almost” an eigenvalue, in two senses:

- the eigenfunction equation $(-\Delta - \lambda)\mathbf{u} = \mathbf{0}$ does not have a solution in L^2 , but it does have a solution $\mathbf{v}_{\boldsymbol{\omega}} \in L^\infty$ where $\boldsymbol{\omega}$ is chosen with $\lambda = 4\pi^2|\boldsymbol{\omega}|^2$,
- λ has a **Weyl sequence**: as we will prove, a sequence of functions $\mathbf{w}_n \in L^2$ exists such that

$$(W1) \quad \|(-\Delta - \lambda)\mathbf{w}_n\|_{L^2} \rightarrow 0 \text{ as } n \rightarrow \infty,$$

$$(W2) \quad \|\mathbf{w}_n\|_{L^2} = 1,$$

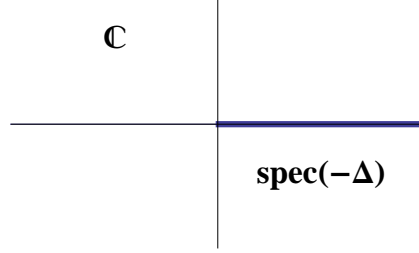
$$(W3) \quad \mathbf{w}_n \rightarrow \mathbf{0} \text{ weakly in } L^2 \text{ as } n \rightarrow \infty.$$

See Proposition 18.1 below. Later we will define the **continuous spectrum** to consist of those $\lambda \in \mathbb{C}$ for which a Weyl sequence exists.

Remark. Existence of a Weyl sequence ensures that $(-\Delta - \lambda)$ does not have a bounded inverse from $L^2 \rightarrow L^2$, for if we write $\mathbf{f}_n = (-\Delta - \lambda)\mathbf{w}_n$ then

$$\frac{\|(-\Delta - \lambda)^{-1}\mathbf{f}_n\|_{L^2}}{\|\mathbf{f}_n\|_{L^2}} = \frac{\|\mathbf{w}_n\|_{L^2}}{\|(-\Delta - \lambda)\mathbf{w}_n\|_{L^2}} \rightarrow \infty$$

as $n \rightarrow \infty$, by (W1) and (W2). In this way, existence of a Weyl sequence is similar to existence of an eigenfunction, which also prevents invertibility of $(-\Delta - \lambda)$.



Proposition 18.1 (Weyl sequences for negative Laplacian). *A Weyl sequence exists for $-\Delta$ and $\lambda \in \mathbb{C}$ if and only if $\lambda \in [0, \infty)$.*

Thus the continuous spectrum of $-\Delta$ consists of precisely the nonnegative real axis. Those values $\lambda \geq 0$ featured in our spectral decomposition earlier in the chapter.

Proof. “ \Leftarrow ” Fix $\lambda \in [0, \infty)$ and choose $\omega \in \mathbb{R}^d$ with

$$\lambda = 4\pi^2|\omega|^2.$$

Take a cut-off function $\kappa \in C_0^\infty(\mathbb{R}^d)$ such that $\kappa \equiv 1$ on the unit ball $B(1)$ and $\kappa \equiv 0$ on $\mathbb{R}^d \setminus B(2)$. Define a cut-off version of the generalized eigenfunction, by

$$w_n = c_n \kappa\left(\frac{x}{n}\right) v_\omega(x)$$

where the normalizing constant is

$$c_n = \frac{1}{n^{d/2} \|\kappa\|_{L^2}}.$$

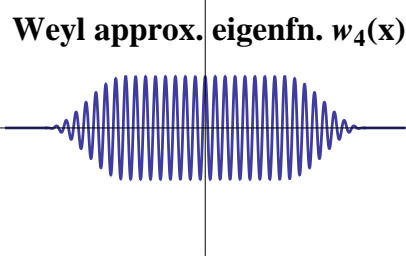
Then (W2) holds because $|v_\omega(x)| = 1$ pointwise and so $\|w_n\|_{L^2} = 1$ by a change of variable, using the definition of c_n .

Next we prove (W1). We have

$$\begin{aligned} & (\lambda + \Delta)w_n \\ &= c_n(\lambda v_\omega + \Delta v_\omega) \kappa\left(\frac{x}{n}\right) + 2\frac{c_n}{n} \nabla v_\omega(x) \cdot (\nabla \kappa)\left(\frac{x}{n}\right) + \frac{c_n}{n^2} v_\omega(x) (\Delta \kappa)\left(\frac{x}{n}\right). \end{aligned}$$

The first term vanishes because $\Delta v_\omega = -4\pi|\omega|^2 v_\omega = -\lambda v_\omega$. In the third term, note v_ω is a bounded function and a change of variable shows

$$\frac{c_n}{n^2} \|(\Delta \kappa)\left(\frac{x}{n}\right)\|_{L^2} = \frac{1}{n^2} \frac{\|\Delta \kappa\|_{L^2}}{\|\kappa\|_{L^2}} \rightarrow 0.$$



The second term similarly vanishes in the limit, as $n \rightarrow \infty$. Hence $(\lambda + \Delta)w_n \rightarrow 0$ in L^2 , which is (W1).

To prove (W3), take an arbitrary $f \in L^2$. Let $R > 0$ and decompose f into “near” and “far” components as $f = g + h$ where $g = f1_{B(R)}$ and $h = f1_{\mathbb{R}^d \setminus B(R)}$. Then

$$\langle f, w_n \rangle_{L^2} = \langle g, w_n \rangle_{L^2} + \langle h, w_n \rangle_{L^2}.$$

We have

$$|\langle g, w_n \rangle_{L^2}| \leq c_n \|\kappa\|_{L^\infty} \|g\|_{L^1} \rightarrow 0$$

as $n \rightarrow \infty$, since $c_n \rightarrow 0$. Also, by Cauchy–Schwarz and (W2) we see

$$\limsup_{n \rightarrow \infty} |\langle h, w_n \rangle_{L^2}| \leq \|h\|_{L^2}.$$

This last quantity can be made arbitrarily small by letting $R \rightarrow \infty$, and so $\lim_{n \rightarrow \infty} \langle f, w_n \rangle_{L^2} = 0$. That is, $w_n \rightarrow 0$ weakly.

“ \implies by contrapositive” Assume $\lambda \in \mathbb{C} \setminus [0, \infty)$, and let

$$\delta = \text{dist}(\lambda, [0, \infty))$$

so that $\delta > 0$. Suppose (W1) holds for some functions $w_n \in L^2$. Write $g_n = (-\Delta - \lambda)w_n$ so that $\|g_n\|_{L^2} \rightarrow 0$ by (W1). Then

$$\begin{aligned} \widehat{g}_n(\xi) &= (4\pi^2|\xi|^2 - \lambda)\widehat{w}_n(\xi) \\ \widehat{w}_n(\xi) &= \frac{1}{(4\pi^2|\xi|^2 - \lambda)}\widehat{g}_n(\xi) \\ |\widehat{w}_n(\xi)| &\leq \delta^{-1}|\widehat{g}_n(\xi)| \end{aligned}$$

and hence

$$\begin{aligned}\|\mathcal{W}_n\|_{L^2} &= \|\widehat{\mathcal{W}}_n\|_{L^2} \leq \delta^{-1} \|\widehat{\mathcal{G}}_n\|_{L^2} \\ &= \delta^{-1} \|\mathcal{G}_n\|_{L^2} \\ &\rightarrow 0.\end{aligned}$$

Thus (W2) does not hold, completing our proof that if $\lambda \notin [0, \infty)$ then λ has no Weyl sequence.

(*Aside.* The calculations above show, in fact, that $(-\Delta - \lambda)^{-1}$ is bounded from $L^2 \rightarrow L^2$ with norm bound δ^{-1} .) \square

Chapter 19

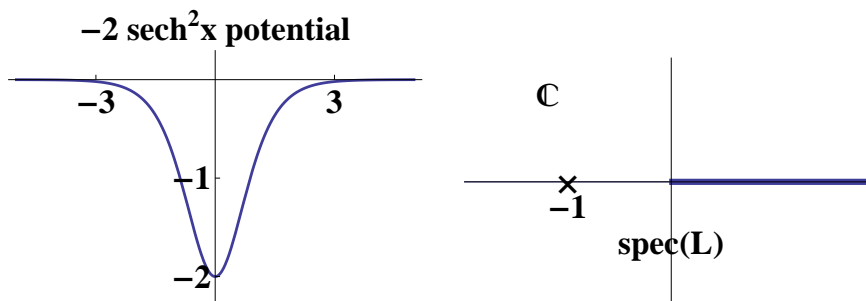
Computable example: Schrödinger with a bounded potential well

Goal

To show that the 1-dimensional Schrödinger operator

$$L = -\frac{d^2}{dx^2} - 2 \operatorname{sech}^2 x$$

has both continuous and discrete spectrum, with a single negative eigenvalue and nonnegative continuous spectrum $[0, \infty)$. The spectral decomposition will show the potential is reflectionless.



Discrete spectrum = $\{-1\}$

We claim -1 is an eigenvalue of L with eigenfunction $\operatorname{sech} x$. This fact can be checked directly, but we will proceed more systematically by factoring the Schrödinger operator with the help of the first order operators

$$\begin{aligned} L^+ &= -\frac{d}{dx} + \tanh x, \\ L^- &= \frac{d}{dx} + \tanh x. \end{aligned}$$

We compute

$$\begin{aligned} L^+L^- - 1 &= \left(-\frac{d}{dx} + \tanh x\right)\left(\frac{d}{dx} + \tanh x\right) - 1 \\ &= -\frac{d^2}{dx^2} - (\tanh x)' + \tanh^2 x - 1 \\ &= -\frac{d^2}{dx^2} - 2\operatorname{sech}^2 x \\ &= L \end{aligned}$$

since $(\tanh)' = \operatorname{sech}^2$ and $1 - \tanh^2 = \operatorname{sech}^2$. Thus

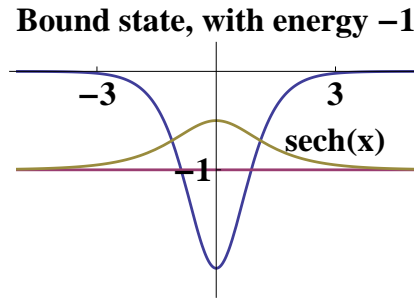
$$L = L^+L^- - 1. \tag{19.1}$$

It follows that functions in the kernel of L^- are eigenfunctions of L with eigenvalue $\lambda = -1$. To find the kernel we solve:

$$\begin{aligned} L^-v &= 0 \\ v' + (\tanh x)v &= 0 \\ (\cosh x)v' + (\sinh x)v &= 0 \\ (\cosh x)v &= \text{const.} \\ v &= c \operatorname{sech} x \end{aligned}$$

Clearly $\operatorname{sech} x \in L^2(\mathbb{R})$, since sech decays exponentially. Thus -1 lies in the discrete spectrum of L , with eigenfunction $\operatorname{sech} x$.

Are there any other eigenvalues? No! Argue as follows. By composing



L^+ and L^- in the reverse order we find

$$\begin{aligned}
 L^-L^+ - 1 &= \left(\frac{d}{dx} + \tanh x \right) \left(-\frac{d}{dx} + \tanh x \right) - 1 \\
 &= -\frac{d^2}{dx^2} + (\tanh x)' + \tanh^2 x - 1 \\
 &= -\frac{d^2}{dx^2}.
 \end{aligned} \tag{19.2}$$

From (19.1) and (19.2) we deduce

$$-\frac{d^2}{dx^2}L^- = L^-L.$$

Thus if $Lv = \lambda v$ then $-\frac{d^2}{dx^2}(L^-v) = L^-Lv = \lambda(L^-v)$. By solving for L^-v in terms of $e^{\pm i\sqrt{\lambda}x}$, and then integrating to obtain v , we conclude after some thought (omitted) that the only way for v to belong to $L^2(\mathbb{R})$ is to have $L^-v = 0$ and hence $v = c \operatorname{sech} x$, so that $\lambda = -1$.

Continuous spectrum $\supset [0, \infty)$

Let $\lambda \in [0, \infty)$. Generalized eigenfunctions with $Lv = \lambda v$ certainly exist: choose $\omega \in \mathbb{R}$ with $\lambda = 4\pi^2\omega^2$ and define

$$v(x) = L^+(e^{2\pi i\omega x}) = (\tanh x - 2\pi i\omega)e^{2\pi i\omega x},$$

which is bounded but not square integrable. We compute

$$\begin{aligned}
L\mathbf{v} &= (L^+L^- - 1)L^+(e^{2\pi i\omega x}) && \text{by (19.1)} \\
&= L^+(L^-L^+ - 1)(e^{2\pi i\omega x}) \\
&= -L^+\frac{d^2}{dx^2}(e^{2\pi i\omega x}) && \text{by (19.2)} \\
&= L^+(4\pi^2\omega^2 e^{2\pi i\omega x}) \\
&= \lambda\mathbf{v},
\end{aligned}$$

which verifies that $\mathbf{v}(x)$ is a generalized eigenfunction.

We can further prove existence of a Weyl sequence for L and λ by adapting Lemma 18.1 “ \Leftarrow ”, using the same Weyl functions $w_n(x)$ as for the free Schrödinger operator $-\Delta$. The only new step in the proof, for proving $\|(L - \lambda)w_n\|_{L^2} \rightarrow 0$ in (W1), is to observe that

$$\begin{aligned}
|2\text{sech}^2 x w_n(x)| &= 2c_n |\kappa(\frac{x}{n}) e^{2\pi i\omega x}| \text{sech}^2 x \\
&\leq 2c_n \|\kappa\|_{L^\infty} \text{sech}^2 x \\
&\rightarrow 0
\end{aligned}$$

in $L^2(\mathbb{R})$ as $n \rightarrow \infty$, because $c_n \rightarrow 0$. (*Note.* This part of the proof works not only for the sech^2 potential, but for any potential belonging to L^2 .)

We have shown that the continuous spectrum contains $[0, \infty)$. We will prove the reverse inclusion at the end of the chapter.

Generalized eigenfunctions as traveling waves

The eigenfunction (“bound state”) $\mathbf{v}(x) = \text{sech } x$ with eigenvalue (“energy”) -1 produces a standing wavefunction

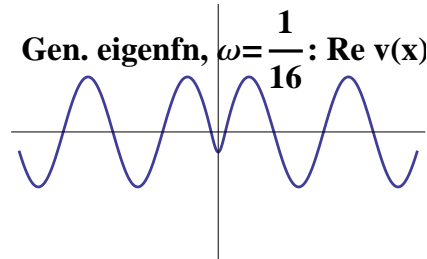
$$\mathbf{u} = e^{it} \text{sech } x$$

satisfying the time-dependent Schrödinger equation

$$i\mathbf{u}_t = L\mathbf{u}.$$

The generalized eigenfunction

$$\mathbf{v}(x) = (\tanh x - 2\pi i\omega) e^{2\pi i\omega x} \tag{19.3}$$



with generalized eigenvalue $\lambda = 4\pi^2\omega^2$ similarly produces a standing wave

$$\mathbf{u} = e^{-i4\pi^2\omega^2 t} (\tanh x - 2\pi i\omega) e^{2\pi i\omega x}.$$

More usefully, we rewrite this formula as a traveling plane wave multiplied by an x -dependent amplitude:

$$\mathbf{u} = (\tanh x - 2\pi i\omega) e^{2\pi i\omega(x-2\pi\omega t)}. \quad (19.4)$$

The amplitude factor serves to quantify the effect of the potential on the traveling wave: in the absence of a potential, the amplitude would be identically 1, since the plane wave $e^{2\pi i\omega(x-2\pi\omega t)}$ solves the free Schrödinger equation $i\mathbf{u}_t = -\Delta\mathbf{u}$.

Reflectionless nature of the potential, and a nod to scattering theory. One calls the potential $-2\text{sech}^2 x$ “reflectionless” because the right-moving wave in (19.4) passes through the potential with none of its energy reflected into a left-moving wave. In other words, the generalized eigenfunction (19.3) has the form $\mathbf{c}e^{2\pi i\omega x}$ both as $x \rightarrow -\infty$ and as $x \rightarrow \infty$ (with different constants, it turns out, although the constants are equal in magnitude).

This reflectionless property is unusual. A typical Schrödinger potential would produce generalized eigenfunctions equalling approximately

$$\mathbf{c}_I e^{2\pi i\omega x} + \mathbf{c}_R e^{-2\pi i\omega x} \quad \text{as } x \rightarrow -\infty$$

and

$$\mathbf{c}_T e^{2\pi i\omega x} \quad \text{as } x \rightarrow \infty$$

(or similarly with the roles of $\pm\infty$ interchanged). Here $|\mathbf{c}_I|$ is the amplitude of the *incident* right-moving wave, $|\mathbf{c}_R|$ is the amplitude of the left-moving

wave *reflected* by the potential, and $|c_T|$ is the amplitude of the right-moving wave *transmitted* through the potential. Conservation of L^2 -energy demands that

$$|c_I|^2 = |c_R|^2 + |c_T|^2.$$

For a gentle introduction to this “scattering theory” see [Keener, Section 7.5]. Then one can proceed to the book-length treatment in [Reed and Simon 3].

Spectral decomposition of L^2

Analogous to an orthonormal expansion in terms of eigenfunctions, we have:

Theorem 19.1.

$$f = \frac{1}{2} \langle f, \text{sech} \rangle \text{sech} + \int_{\mathbb{R}} \langle f, L^+ v_\omega \rangle L^+ v_\omega \frac{d\omega}{1 + 4\pi^2 \omega^2}, \quad \forall f \in L^2(\mathbb{R}),$$

where $L^+ v_\omega(x) = (\tanh x - 2\pi i \omega) e^{2\pi i \omega x}$ is the generalized eigenfunction at frequency ω .

The discrete part of the decomposition has the same form as the continuous part, in fact, because $\text{sech} = -L^+(\sinh)$.

Proof. We will sketch the main idea of the proof, and leave it to the reader to make the argument rigorous.

By analogy with an orthonormal expansion in the discrete case, we assume that $f \in L^2(\mathbb{R})$ has a decomposition in terms of the eigenfunction $\text{sech} x$ and the generalized eigenfunctions $L^+ v_\omega$ in the form

$$f = c \langle f, \text{sech} \rangle \text{sech} + \int_{\mathbb{R}} m_f(\omega) \langle f, L^+ v_\omega \rangle L^+ v_\omega d\omega,$$

where the coefficient c and multiplier $m_f(\omega)$ are to be determined.

Taking the inner product with $\text{sech} x$ implies that $c = \frac{1}{2}$, since $\|\text{sech}\|_{L^2(\mathbb{R})}^2 = 2$ and $\langle L^+ v_\omega, \text{sech} \rangle = \langle v_\omega, L^- \text{sech} \rangle = 0$.

Next we annihilate the sech term by applying L^- to both sides:

$$L^- f = L^- \left(\int_{\mathbb{R}} m_f(\omega) \langle f, L^+ v_\omega \rangle L^+ v_\omega d\omega \right).$$

Note that by integration by parts,

$$\langle f, L^+ v_\omega \rangle = \langle L^- f, v_\omega \rangle = \widehat{(L^- f)}(\omega).$$

Hence

$$\begin{aligned} \mathbf{L}^{-}\mathbf{f} &= \mathbf{L}^{-}\left(\int_{\mathbb{R}} \mathbf{m}_f(\omega)(\widehat{\mathbf{L}^{-}\mathbf{f}})(\omega)\mathbf{L}^{+}\mathbf{v}_\omega \, d\omega\right) \\ &= \int_{\mathbb{R}} \mathbf{m}_f(\omega)(\widehat{\mathbf{L}^{-}\mathbf{f}})(\omega)\mathbf{L}^{-}\mathbf{L}^{+}\mathbf{v}_\omega \, d\omega \\ &= \int_{\mathbb{R}} \mathbf{m}_f(\omega)(\widehat{\mathbf{L}^{-}\mathbf{f}})(\omega)(1 + 4\pi^2\omega^2)\mathbf{v}_\omega \, d\omega \end{aligned}$$

by (19.2). Thus the multiplier should be $\mathbf{m}_f(\omega) = 1/(1 + 4\pi^2\omega^2)$, in order for Fourier inversion to hold. This argument shows the necessity of the formula in the theorem, and one can show sufficiency by suitably reversing the steps. \square

The theorem implies a Plancherel type identity.

Corollary 19.2.

$$\|\mathbf{f}\|_{\mathbf{L}^2}^2 = \frac{1}{2}|\langle \mathbf{f}, \text{sech} \rangle|^2 + \int_{\mathbb{R}} |\langle \mathbf{f}, \mathbf{L}^{+}\mathbf{v}_\omega \rangle|^2 \frac{d\omega}{1 + 4\pi^2\omega^2}, \quad \forall \mathbf{f} \in \mathbf{L}^2(\mathbb{R}).$$

Proof. Take the inner product of \mathbf{f} with the formula in Theorem 19.1. \square

Continuous spectrum = $[0, \infty)$

Earlier we showed that the continuous spectrum contains $[0, \infty)$. For the reverse containment, suppose $\lambda \notin [0, \infty)$ and $\lambda \neq -1$. Then $\mathbf{L} - \lambda$ is invertible on \mathbf{L}^2 , with

$$(\mathbf{L} - \lambda)^{-1}\mathbf{f} = -\frac{1}{\lambda + 1} \frac{1}{2} \langle \mathbf{f}, \text{sech} \rangle \text{sech} + \int_{\mathbb{R}} \frac{\langle \mathbf{f}, \mathbf{L}^{+}\mathbf{v}_\omega \rangle}{4\pi^2\omega^2 - \lambda} \mathbf{L}^{+}\mathbf{v}_\omega \frac{d\omega}{1 + 4\pi^2\omega^2}$$

as one sees by applying $\mathbf{L} - \lambda$ to both sides and recalling Theorem 19.1. To check the boundedness of this inverse, note that

$$\begin{aligned} \|(\mathbf{L} - \lambda)^{-1}\mathbf{f}\|_{\mathbf{L}^2}^2 &= \frac{1}{|\lambda + 1|^2} \frac{1}{2} |\langle \mathbf{f}, \text{sech} \rangle|^2 + \int_{\mathbb{R}} \frac{|\langle \mathbf{f}, \mathbf{L}^{+}\mathbf{v}_\omega \rangle|^2}{|4\pi^2\omega^2 - \lambda|^2} \frac{d\omega}{1 + 4\pi^2\omega^2} \\ &\leq \frac{1}{|\lambda + 1|^2} \frac{1}{2} |\langle \mathbf{f}, \text{sech} \rangle|^2 + \frac{1}{\text{dist}(\lambda, [0, \infty))^2} \int_{\mathbb{R}} |\langle \mathbf{f}, \mathbf{L}^{+}\mathbf{v}_\omega \rangle|^2 \frac{d\omega}{1 + 4\pi^2\omega^2} \\ &\leq (\text{const.}) \|\mathbf{f}\|_{\mathbf{L}^2}^2, \end{aligned}$$

where we used Corollary 19.2.

The boundedness of $(L - \lambda)^{-1}$ implies that the Weyl conditions (W1) and (W2) cannot both hold. Thus no Weyl sequence can exist for λ , so that λ does not belong to the continuous spectrum.

Next suppose $\lambda = -1$. If a Weyl sequence w_n exists, then

$$\langle w_n, \text{sech} \rangle_{L^2} \rightarrow 0 \quad \text{as } n \rightarrow \infty,$$

by the weak convergence in (W3). Hence if we project away from the $\lambda = -1$ eigenspace by defining

$$y_n = w_n - \frac{1}{2} \langle w_n, \text{sech} \rangle_{L^2} \text{sech} \quad \text{and} \quad z_n = y_n / \|y_n\|_{L^2},$$

then we find $\|y_n\|_{L^2} \rightarrow 1$ and $\|z_n\|_{L^2} = 1$, with $\langle z_n, \text{sech} \rangle_{L^2} = 0$. Also

$$(L + 1)z_n = (L + 1)y_n / \|y_n\|_{L^2} = (L + 1)w_n / \|y_n\|_{L^2} \rightarrow 0$$

in L^2 . Thus z_n satisfies (W1) and (W2) and lies in the orthogonal complement of the eigenspace spanned by sech . A contradiction now follows from the boundedness of $(L + 1)^{-1}$ on that orthogonal complement (with the boundedness being proved by the same argument as above for $\lambda \neq -1$). This contradiction shows that no such Weyl sequence w_n can exist, and so -1 does not belong to the continuous spectrum.

Note. The parallels with our derivation of the continuous spectrum for the Laplacian in Chapter 18 are instructive.

Notes and comments

The treatment in this chapter was drawn from [Keener] Section 7.5.

Chapter 20

Selfadjoint, unbounded linear operators

Goal

To develop the theory of unbounded linear operators on a Hilbert space, and to define selfadjointness for such operators.

References [Gustafson and Sigal] Sections 1.5, 2.4
[Hislop and Sigal] Chapters 4, 5

Motivation

Now we should develop some general theory, to provide context for the examples computed in Chapters 18 and 19.

We begin with a basic principle of calculus:

integration makes functions better, while differentiation makes them worse.

More precisely, integral operators are bounded (generally speaking), while differential operators are unbounded. For example, $e^{2\pi i n x}$ has norm 1 in $L^2[0, 1]$ while its derivative $\frac{d}{dx} e^{2\pi i n x} = 2\pi i n e^{2\pi i n x}$ has norm that grows with n . The unboundedness of such operators prevents us from applying the spectral theory of bounded operators on a Hilbert space.

Further, differential operators are usually defined only on a (dense) subspace of our natural function spaces. In particular, we saw in our study

of discrete spectra that the Laplacian is most naturally studied using the Sobolev space H^1 , even though the Laplacian involves two derivatives and H^1 -functions are guaranteed only to possess a single derivative.

To meet these challenges, we will develop the theory of densely defined, unbounded linear operators, along with the notion of adjoints and selfadjointness for such operators.

Domains and inverses of (unbounded) operators

Take a complex Hilbert space \mathcal{H} with inner product $\langle \cdot, \cdot \rangle$. Suppose A is a linear operator (not necessarily bounded) from a subspace $D(A) \subset \mathcal{H}$ into \mathcal{H} :

$$A : D(A) \rightarrow \mathcal{H}.$$

Call $D(A)$ the **domain** of A .

An operator B with domain $D(B)$ is called the **inverse** of A if

- $D(B) = \text{Ran}(A)$, $D(A) = \text{Ran}(B)$, and
- $BA = \text{id}_{\text{Ran}(B)}$, $AB = \text{id}_{\text{Ran}(A)}$.

Write A^{-1} for this inverse, if it exists. Obviously A^{-1} is unique, if it exists, because in that case A is bijective.

Further say A is **invertible** if A^{-1} exists and is bounded on \mathcal{H} (meaning that A^{-1} exists, $\text{Ran}(A) = \mathcal{H}$, and $A^{-1} : \mathcal{H} \rightarrow \mathcal{H}$ is a bounded linear operator).

Example. Consider the operator $A = -\Delta + 1$ with domain $H^2(\mathbb{R}^d) \subset L^2(\mathbb{R}^d)$. Invertibility is proved using the Fourier transform: let $D(B) = L^2(\mathbb{R}^d)$, and define a bounded operator $B : L^2 \rightarrow L^2$ by

$$\widehat{Bf}(\xi) = (1 + 4\pi^2|\xi|^2)^{-1}\widehat{f}(\xi).$$

One can check that $\text{Ran}(B) = H^2(\mathbb{R}^d) = D(A)$. Notice $BA = \text{id}_{H^2}$, $AB = \text{id}_{L^2}$. The second identity implies that $\text{Ran}(A) = L^2 = D(B)$.

Adjoint of an (unbounded) operator

Call A **symmetric** if

$$\langle Af, g \rangle = \langle f, Ag \rangle, \quad \forall f, g \in D(A). \quad (20.1)$$

Symmetry is a simpler concept than **selfadjointness**, which requires the operator and its adjoint to have the same domain, as we now explain.

First we define a subspace

$$D(A^*) = \{f \in \mathcal{H} : \text{the linear functional } g \mapsto \langle f, Ag \rangle \text{ is bounded on } D(A)\}.$$

Assume from now on that A is **densely defined**, meaning $D(A)$ is dense in \mathcal{H} . Then for each $f \in D(A^*)$, the bounded linear functional $g \mapsto \langle f, Ag \rangle$ is defined on a dense subspace of \mathcal{H} and hence extends uniquely to a bounded linear functional on all of \mathcal{H} . By the Riesz Representation Theorem, that linear functional can be represented as the inner product of g against a unique element of \mathcal{H} , which we call A^*f . Hence

$$\langle f, Ag \rangle = \langle A^*f, g \rangle, \quad \forall f \in D(A^*), \quad g \in D(A). \quad (20.2)$$

Clearly this operator $A^* : D(A^*) \rightarrow \mathcal{H}$ is linear. We call it the **adjoint** of A .

Lemma 20.1. *If A is a densely defined linear operator and $\lambda \in \mathbb{C}$, then $(A - \lambda)^* = A^* - \bar{\lambda}$.*

We leave the (easy) proof to the reader. Implicit in the proof is that domains are unchanged by subtracting a constant: $D(A - \lambda) = D(A)$ and $D(((A - \lambda)^*)) = D(A^*)$.

The kernel of the adjoint complements the range of the original operator, as follows.

Proposition 20.2. *If A is a densely defined linear operator then $\overline{\text{Ran}(A)} \oplus \ker(A^*) = \mathcal{H}$.*

Proof. Clearly $\ker(A^*) \subset \text{Ran}(A)^\perp$, because if $f \in \ker(A^*)$ then $A^*f = 0$ and so for all $g \in D(A)$ we have

$$\langle f, Ag \rangle = \langle A^*f, g \rangle = 0.$$

To prove the reverse inclusion, $\text{Ran}(A)^\perp \subset \ker(A^*)$, suppose $h \in \text{Ran}(A)^\perp$. For all $g \in D(A)$ we have $\langle h, Ag \rangle = 0$. In particular, $h \in D(A^*)$. Hence

$$\langle A^*h, g \rangle = \langle h, Ag \rangle = 0 \quad \forall g \in D(A),$$

and so from density of $D(A)$ we conclude $A^*h = 0$. That is, $h \in \ker(A^*)$.

We have shown $\text{Ran}(A)^\perp = \ker(A^*)$, and so (since the orthogonal complement is unaffected by taking the closure) $\overline{\text{Ran}(A)}^\perp = \ker(A^*)$. The proposition follows immediately. \square

We will need later that the graph of the adjoint, $\{(f, A^*f) : f \in D(A^*)\}$, is closed in $\mathcal{H} \times \mathcal{H}$.

Theorem 20.3. *If A is a densely defined linear operator then A^* is a closed operator.*

Proof. Suppose $f_n \in D(A^*)$ with $f_n \rightarrow f, A^*f_n \rightarrow g$, for some $f, g \in \mathcal{H}$. To prove the graph of A^* is closed, we must show $f \in D(A^*)$ with $A^*f = g$.

For each $h \in D(A)$ we have

$$\langle f, Ah \rangle = \lim_n \langle f_n, Ah \rangle = \lim_n \langle A^*f_n, h \rangle = \langle g, h \rangle.$$

Thus the map $h \mapsto \langle f, Ah \rangle$ is bounded for $h \in D(A)$. Hence $f \in D(A^*)$, and using the last calculation we see

$$\langle A^*f, h \rangle = \langle f, Ah \rangle = \langle g, h \rangle$$

for all $h \in D(A)$. Density of the domain implies $A^*f = g$, as we wanted. \square

Selfadjointness

Call A **selfadjoint** if $A^* = A$, meaning $D(A^*) = D(A)$ and $A^* = A$ on their common domain.

Selfadjoint operators have closed graphs, due to closedness of the adjoint in Theorem 20.3. Thus:

Corollary 20.4. *If a densely defined linear operator A is selfadjoint then it is closed.*

The relation between selfadjointness and symmetry is clear:

Proposition 20.5. *The densely defined linear operator A is selfadjoint if and only if it is symmetric and $D(A) = D(A^*)$.*

Proof. “ \implies ” If $A^* = A$ then the adjoint relation (20.2) reduces immediately to the symmetry relation (20.1).

“ \impliedby ” The symmetry relation (20.1) together with the adjoint relation (20.2) implies that $\langle Af, g \rangle = \langle A^*f, g \rangle$ for all $f, g \in D(A) = D(A^*)$. Since $D(A)$ is dense in \mathcal{H} , we conclude $Af = A^*f$. \square

For bounded operators, selfadjointness and symmetry are equivalent.

Lemma 20.6. *If a linear operator A is bounded on \mathcal{H} , then it is selfadjoint if and only if it is symmetric.*

Proof. Boundedness of A ensures that $D(A^*) = \mathcal{H} = D(A)$, and so the adjoint relation (20.2) holds for all $f, g \in \mathcal{H}$. Thus $A^* = A$ is equivalent to symmetry. \square

Example: selfadjointness for Schrödinger operators

Let $L = -\Delta + V$ be a Schrödinger operator with potential $V(x)$ that is bounded and real valued. Choose the domain to be $D(L) = H^2(\mathbb{R}^d)$ in the Hilbert space $L^2(\mathbb{R}^d)$. This Schrödinger operator is selfadjoint.

Proof. Density of $D(L)$ follows from density in L^2 of the smooth functions with compact support.

Our main task is to determine the domain of L^* . Fix $f, g \in H^2(\mathbb{R}^d)$. From the integration by parts formula $\langle f, \Delta g \rangle_{L^2} = \langle \Delta f, g \rangle_{L^2}$ (which one may alternatively prove with the help of the Fourier transform), one deduces that

$$|\langle f, \Delta g \rangle_{L^2}| = |\langle \Delta f, g \rangle_{L^2}| \leq \|f\|_{H^2} \|g\|_{L^2}.$$

Also $|\langle f, Vg \rangle_{L^2}| \leq \|f\|_{L^2} \|V\|_{L^\infty} \|g\|_{L^2}$. Hence the linear functional $g \mapsto \langle f, Lg \rangle_{L^2}$ is bounded on $g \in D(L)$. Therefore $f \in D(L^*)$, which tells us $H^2(\mathbb{R}^d) \subset D(L^*)$.

To prove the reverse inclusion, fix $f \in D(L^*)$. Then

$$|\langle f, Lg \rangle_{L^2}| \leq (\text{const.}) \|g\|_{L^2}, \quad \forall g \in D(L) = H^2(\mathbb{R}^d).$$

Since the potential V is bounded, the last formula still holds if we replace V with 1 , so that

$$|\langle f, (-\Delta + 1)g \rangle_{L^2}| \leq (\text{const.}) \|g\|_{L^2}, \quad \forall g \in H^2(\mathbb{R}^d).$$

Taking Fourier transforms gives

$$|\langle \widehat{f}, (1 + 4\pi^2|\xi|^2)\widehat{g} \rangle_{L^2}| \leq (\text{const.}) \|\widehat{g}\|_{L^2}, \quad \forall g \in H^2(\mathbb{R}^d).$$

In particular, we may suppose $\widehat{g} = h \in C_0^\infty(\mathbb{R}^d)$, since every such \widehat{g} gives $g \in H^2(\mathbb{R}^d)$. Hence

$$|\langle (1 + 4\pi^2|\xi|^2)\widehat{f}, h \rangle_{L^2}| \leq (\text{const.}) \|h\|_{L^2}, \quad \forall h \in C_0^\infty(\mathbb{R}^d).$$

Taking the supremum of the left side over all \mathbf{h} with L^2 -norm equal to 1 shows that

$$\|(1 + 4\pi^2|\xi|^2)\widehat{f}\|_{L^2} \leq (\text{const.})$$

Hence $(1 + |\xi|)^2 \widehat{f} \in L^2(\mathbb{R}^d)$, which means $f \in H^2(\mathbb{R}^d)$. Thus $D(L^*) \subset H^2(\mathbb{R}^d)$.

Now that we know the domains of L and L^* agree, we have only to check symmetry, and that is straightforward. When $f, g \in H^2(\mathbb{R}^d)$ we have

$$\begin{aligned} \langle Lf, g \rangle &= -\langle \Delta f, g \rangle_{L^2} + \langle Vf, g \rangle_{L^2} \\ &= -\langle f, \Delta g \rangle_{L^2} + \langle f, Vg \rangle_{L^2} \\ &= \langle f, Lg \rangle_{L^2} \end{aligned}$$

where we integrated by parts and used that $V(x)$ is real valued. □

Chapter 21

Spectra: discrete and continuous

Goal

To develop the spectral theory of selfadjoint unbounded linear operators.

References [Gustafson and Sigal] Sections 2.4, 5.1
[Hislop and Sigal] Chapters 1, 5, 7
[Rudin] Chapter 13

Resolvent set, and spectrum

Let A be a densely defined linear operator on a complex Hilbert space \mathcal{H} , as in the preceding chapter. The operator $A - \lambda$ has domain $D(A)$, for each constant $\lambda \in \mathbb{C}$. Define the **resolvent set**

$\text{res}(A) = \{\lambda \in \mathbb{C} : A - \lambda \text{ is invertible (has a bounded inverse defined on } \mathcal{H})\}$.

For λ in the resolvent set, we call the inverse $(A - \lambda)^{-1}$ the **resolvent operator**.

The **spectrum** is defined as the complement of the resolvent set:

$$\text{spec}(A) = \mathbb{C} \setminus \text{res}(A).$$

For example, if λ is an eigenvalue of A then $\lambda \in \text{spec}(A)$, because if $Af = \lambda f$ for some $f \neq 0$, then $(A - \lambda)f = 0$ and so $A - \lambda$ is not injective, and hence is not invertible.

Proposition 21.1 ([Hislop and Sigal, Theorem 1.2]). *The resolvent set is open, and hence the spectrum is closed.*

We omit the proof.

The next result generalizes the fact that Hermitian matrices have only real eigenvalues.

Theorem 21.2. *If A is selfadjoint then its spectrum is real: $\text{spec}(A) \subset \mathbb{R}$.*

Proof. We prove the contrapositive. Suppose $\lambda \in \mathbb{C}$ has nonzero imaginary part, $\text{Im } \lambda \neq 0$. We will show $\lambda \in \text{res}(A)$.

The first step is to show $A - \lambda$ is injective. For all $f \in D(A)$,

$$\|(A - \lambda)f\|^2 = \|Af\|^2 - 2(\text{Re } \lambda)\langle f, Af \rangle + |\lambda|^2\|f\|^2$$

and so

$$\begin{aligned} \|(A - \lambda)f\|^2 &\geq \|Af\|^2 - 2|\text{Re } \lambda|\|f\|\|Af\| + |\lambda|^2\|f\|^2 \\ &= (\|Af\| - |\text{Re } \lambda|\|f\|)^2 + |\text{Im } \lambda|^2\|f\|^2 \\ &\geq |\text{Im } \lambda|^2\|f\|^2. \end{aligned} \tag{21.1}$$

The last inequality implies that $A - \lambda$ is injective, using here that $|\text{Im } \lambda| > 0$. That is, $\ker(A - \lambda) = \{0\}$.

Selfadjointness ($A^* = A$) now gives $\ker(A^* - \lambda) = 0$, and so $\overline{\text{Ran}(A - \lambda)} = \mathcal{H}$ by Proposition 20.2. That is, $A - \lambda$ has dense range.

Next we show $\text{Ran}(A - \lambda) = \mathcal{H}$. Let $g \in \mathcal{H}$. By density of the range, we may take a sequence $f_n \in D(A)$ such that $(A - \lambda)f_n \rightarrow g$. The sequence f_n is Cauchy, in view of (21.1). Hence the sequence $(f_n, (A - \lambda)f_n)$ is Cauchy in $\mathcal{H} \times \mathcal{H}$, and so converges to (f, g) for some $f \in \mathcal{H}$. Note each ordered pair $(f_n, (A - \lambda)f_n)$ lies in the graph of $A - \lambda$, and this graph is closed by Corollary 20.4 (relying here on selfadjointness again). Therefore (f, g) belongs to the graph of $A - \lambda$, and so $g \in \text{Ran}(A - \lambda)$. Thus $A - \lambda$ has full range.

To summarize: we have shown $A - \lambda$ is injective and surjective, and so it has an inverse operator

$$(A - \lambda)^{-1} : \mathcal{H} \rightarrow D(A) \subset \mathcal{H}.$$

This inverse is bounded with

$$\|(A - \lambda)^{-1}g\| \leq |\text{Im } \lambda|^{-1}\|g\|, \quad \forall g \in \mathcal{H},$$

by taking $f = (A - \lambda)^{-1}g$ in estimate (21.1). The proof is thus complete. \square

Characterizing the spectrum

We will characterize the spectrum in terms of approximate eigenfunctions. Given a number $\lambda \in \mathbb{C}$ and a sequence $w_n \in D(A)$, consider three conditions:

$$(W1) \quad \|(A - \lambda)w_n\|_{\mathcal{H}} \rightarrow 0 \text{ as } n \rightarrow \infty,$$

$$(W2) \quad \|w_n\|_{\mathcal{H}} = 1,$$

$$(W3) \quad w_n \rightharpoonup 0 \text{ weakly in } \mathcal{H} \text{ as } n \rightarrow \infty.$$

(We considered these conditions in Chapter 18 for the special case of the Laplacian).

Condition (W1) says w_n is an “approximate eigenfunction”, and condition (W2) simply normalizes the sequence. These conditions characterize the spectrum, for a selfadjoint operator.

Theorem 21.3. *If A is selfadjoint then*

$$\text{spec}(A) = \{\lambda \in \mathbb{C} : (W1) \text{ and } (W2) \text{ hold for some sequence } w_n \in D(A)\}.$$

Proof. “ \supset ” Assume (W1) and (W2) hold for λ , and that $A - \lambda$ has an inverse defined on \mathcal{H} . Then for $f_n = (A - \lambda)w_n$ we find

$$\frac{\|(A - \lambda)^{-1}f_n\|_{\mathcal{H}}}{\|f_n\|_{\mathcal{H}}} = \frac{\|w_n\|_{\mathcal{H}}}{\|(A - \lambda)w_n\|_{\mathcal{H}}} \rightarrow \infty$$

as $n \rightarrow \infty$, by (W1) and (W2). Thus the inverse operator is not bounded, and so $\lambda \in \text{spec}(A)$.

“ \subset ” Assume $\lambda \in \text{spec}(A)$, so that λ is real by Theorem 21.2. If λ is an eigenvalue, say with normalized eigenvector f , then we simply choose $w_n = f$ for each n , and (W1) and (W2) hold trivially.

Suppose λ is not an eigenvalue. Then $A - \lambda$ is injective, hence so is $(A - \lambda)^*$, which equals $A - \lambda$ by selfadjointness of A and reality of λ . Thus $\ker((A - \lambda)^*) = \{0\}$, and so $\text{Ran}(A - \lambda)$ is dense in \mathcal{H} by Proposition 20.2.

Injectivity ensures that $(A - \lambda)^{-1}$ exists on $\text{Ran}(A - \lambda)$. If it is unbounded there, then we may choose a sequence $f_n \in \text{Ran}(A - \lambda)$ with $\|(A - \lambda)^{-1}f_n\|_{\mathcal{H}} = 1$ and $\|f_n\|_{\mathcal{H}} \rightarrow 0$. Letting $w_n = (A - \lambda)^{-1}f_n$ gives (W1) and (W2) as desired. Suppose on the other hand that $(A - \lambda)^{-1}$ is bounded on $\text{Ran}(A - \lambda)$. Then the argument in the proof of Theorem 21.2 shows that $\text{Ran}(A - \lambda) = \mathcal{H}$, which means λ belongs to the resolvent set, and not the spectrum. Thus this case cannot occur. \square

Discrete and continuous spectra

Define the **discrete spectrum**

$$\begin{aligned} \text{spec}_{\text{disc}}(\mathbf{A}) \\ = \{\lambda \in \text{spec}(\mathbf{A}) : \lambda \text{ is an isolated eigenvalue of } \mathbf{A} \text{ having finite multiplicity}\}, \end{aligned}$$

where “isolated” means that some neighborhood of λ in the complex plane intersects $\text{spec}(\mathbf{A})$ only at λ . By “multiplicity” we mean the geometric multiplicity (dimension of the eigenspace); if \mathbf{A} is not selfadjoint then we should use instead the algebraic multiplicity [Hislop and Sigal].

Next define the **continuous spectrum**

$$\begin{aligned} \text{spec}_{\text{cont}}(\mathbf{A}) \\ = \{\lambda \in \mathbb{C} : (\text{W1}), (\text{W2}) \text{ and } (\text{W3}) \text{ hold for some sequence } w_n \in \mathbf{D}(\mathbf{A})\}. \end{aligned}$$

The continuous spectrum lies within the spectrum, by Theorem 21.3. The characterization in that theorem required only (W1) and (W2), whereas the continuous spectrum imposes in addition the “weak convergence” condition (W3).

A **Weyl sequence** for \mathbf{A} and λ is a sequence $w_n \in \mathbf{D}(\mathbf{A})$ such that (W1), (W2) and (W3) hold. Thus the preceding definition says the continuous spectrum consists of λ -values for which Weyl sequences exist.

The continuous spectrum can contain eigenvalues that are not isolated (“imbedded eigenvalues”) or which have infinite multiplicity.

A famous theorem of Weyl says that for selfadjoint operators, the entire spectrum is covered by the discrete and continuous spectra.

Theorem 21.4. *If \mathbf{A} is selfadjoint then*

$$\text{spec}(\mathbf{A}) = \text{spec}_{\text{disc}}(\mathbf{A}) \cup \text{spec}_{\text{cont}}(\mathbf{A}).$$

(Further, the discrete and continuous spectra are disjoint.)

We omit the proof. See [Hislop and Sigal, Theorem 7.2].

Applications to Schrödinger operators

The continuous spectrum of the Laplacian $-\Delta$ equals $[0, \infty)$, and the spectrum contains no eigenvalues, as we saw in Chapter 18.

The hydrogen atom too has continuous spectrum $[0, \infty)$, with its Schrödinger operator $L = -\Delta - 2/|x|$ on \mathbb{R}^3 having domain $H^2(\mathbb{R}^d) \subset L^2(\mathbb{R}^d)$; see [Taylor, Section 8.7]. The discrete spectrum $\{-1/n^2 : n \geq 1\}$ of the hydrogen atom was stated in Chapter 3.

As the hydrogen atom example suggests, potentials vanishing at infinity generate continuous spectrum that includes all nonnegative numbers:

Theorem 21.5. *Assume $V(x)$ is real valued, continuous, and vanishes at infinity ($V(x) \rightarrow 0$ as $|x| \rightarrow \infty$).*

Then the Schrödinger operator $-\Delta + V$ is selfadjoint (with domain $H^2(\mathbb{R}^d) \subset L^2(\mathbb{R}^d)$) and has continuous spectrum $= [0, \infty)$.

For a proof see [Hislop and Sigal, Corollary 14.10], where a stronger theorem is proved that covers also the Coulomb potential $-2/|x|$ for the hydrogen atom. Note the Coulomb potential vanishes at infinity but is discontinuous at the origin, where it blows up. The stronger version of the theorem requires (instead of continuity and vanishing at infinity) that for each $\varepsilon > 0$, the potential $V(x)$ be decomposable as $V = V_2 + V_\infty$ where $V_2 \in L^2$ and $\|V_\infty\|_{L^\infty} < \varepsilon$. This decomposition can easily be verified for the Coulomb potential, by “cutting off” the potential near infinity.

Theorem 21.5 implies that any isolated eigenvalues of L must lie on the negative real axis (possibly accumulating at 0). For example, the $-2 \operatorname{sech}^2$ potential in Chapter 19 generates a negative eigenvalue at -1 .

Connection to generalized eigenvalues and eigenfunctions

Just as the discrete spectrum is characterized by eigenfunctions in L^2 , so the full spectrum is characterized by existence of a generalized eigenfunction that grows at most polynomially at infinity.

Theorem 21.6. *Assume $V(x)$ is real valued and bounded on \mathbb{R}^d . Then the Schrödinger operator $-\Delta + V$ has spectrum*

$$\operatorname{spec}(-\Delta + V) = \text{closure of } \{\lambda \in \mathbb{C} : (-\Delta + V)\mathbf{u} = \lambda\mathbf{u} \text{ for some polynomially bounded } \mathbf{u}\}.$$

We omit the proof; see [Gustafson and Sigal, Theorem 5.22].

Further reading

A wealth of information on spectral theory, especially for Schrödinger operators, can be found in the books [Gustafson and Sigal, Hislop and Sigal, Reed and Simon 2, Reed and Simon 4].

Chapter 22

Discrete spectrum revisited

Goal

To fit the discrete spectral Theorem 4.1 (from Part I of the course) into the spectral theory of selfadjoint operators and, in particular, to prove the absence of continuous spectrum in that situation.

Discrete spectral theorem

The discrete spectral Theorem 4.1 concerns a symmetric, coercive, bounded sesquilinear form $\mathfrak{a}(\mathbf{u}, \mathbf{v})$ on an infinite dimensional Hilbert space \mathcal{K} , where \mathcal{K} imbeds compactly and densely into the Hilbert space \mathcal{H} . The theorem guarantees existence of an ONB for \mathcal{H} consisting of eigenvectors of \mathfrak{a} :

$$\mathfrak{a}(\mathbf{u}_j, \mathbf{v}) = \gamma_j \langle \mathbf{u}_j, \mathbf{v} \rangle_{\mathcal{H}} \quad \forall \mathbf{v} \in \mathcal{K},$$

where the eigenvalues satisfy

$$0 < \gamma_1 \leq \gamma_2 \leq \gamma_3 \leq \cdots \rightarrow \infty.$$

We want to interpret these eigenvalues as the discrete spectrum of some selfadjoint, densely defined linear operator on \mathcal{H} . By doing so, we will link the discrete spectral theory in Part I of the course with the spectral theory of unbounded operators in Part II.

Our tasks are to identify the operator \mathbf{A} and its domain, to prove \mathbf{A} is symmetric, to determine the domain of the adjoint, to conclude selfadjointness, and finally to show that the spectrum of \mathbf{A} consists precisely of the eigenvalues γ_j .

Operator A and its domain

In the proof of Theorem 4.1 we found a bounded, selfadjoint linear operator $B : \mathcal{H} \rightarrow \mathcal{K} \subset \mathcal{H}$ with eigenvalues $1/\gamma_j$ and eigenvectors \mathbf{u}_j :

$$B\mathbf{u}_j = \frac{1}{\gamma_j}\mathbf{u}_j.$$

We showed B is injective (meaning its eigenvalues are nonzero). Notice B has dense range because its eigenvectors \mathbf{u}_j span \mathcal{H} .

(*Aside.* This operator B relates to the sesquilinear form \mathbf{a} by satisfying $\mathbf{a}(B\mathbf{f}, \mathbf{v}) = \langle \mathbf{f}, \mathbf{v} \rangle_{\mathcal{H}}$ for all $\mathbf{v} \in \mathcal{K}$. We will not need that formula below.)

Define

$$A = B^{-1} : \text{Ran}(B) \rightarrow \mathcal{H}.$$

Then A is a linear operator, and its domain

$$D(A) = \text{Ran}(B)$$

is dense in \mathcal{H} .

Symmetry of A

Let $\mathbf{u}, \mathbf{v} \in D(A)$. Then

$$\begin{aligned} \langle A\mathbf{u}, \mathbf{v} \rangle_{\mathcal{H}} &= \langle A\mathbf{u}, B\mathbf{A}\mathbf{v} \rangle_{\mathcal{H}} && \text{since } B\mathbf{A} = \text{Id}, \\ &= \langle B\mathbf{A}\mathbf{u}, \mathbf{A}\mathbf{v} \rangle_{\mathcal{H}} && \text{since } B \text{ is selfadjoint,} \\ &= \langle \mathbf{u}, \mathbf{A}\mathbf{v} \rangle_{\mathcal{H}} && \text{since } B\mathbf{A} = \text{Id}. \end{aligned}$$

Domain of the adjoint

First we show $D(A) \subset D(A^*)$. Let $\mathbf{u} \in D(A)$. For all $\mathbf{v} \in D(A)$ we have

$$\begin{aligned} |\langle \mathbf{u}, \mathbf{A}\mathbf{v} \rangle_{\mathcal{H}}| &= |\langle A\mathbf{u}, \mathbf{v} \rangle_{\mathcal{H}}| && \text{by symmetry} \\ &\leq \|A\mathbf{u}\|_{\mathcal{H}} \|\mathbf{v}\|_{\mathcal{H}}. \end{aligned}$$

Hence the functional $\mathbf{v} \mapsto \langle \mathbf{u}, \mathbf{A}\mathbf{v} \rangle_{\mathcal{H}}$ is bounded on $D(A)$ with respect to the \mathcal{H} -norm, so that \mathbf{u} belongs to the domain of the adjoint A^* .

Next we show $D(A^*) \subset D(A)$. Let $\mathbf{u} \in D(A^*) \subset \mathcal{H}$. We have

$$|\langle \mathbf{u}, \mathbf{A}\mathbf{v} \rangle_{\mathcal{H}}| \leq (\text{const.}) \|\mathbf{v}\|_{\mathcal{H}} \quad \forall \mathbf{v} \in D(A) = \text{Ran}(B).$$

Writing $\mathbf{v} = \mathbf{B}\mathbf{g}$ gives

$$|\langle \mathbf{u}, \mathbf{g} \rangle_{\mathcal{H}}| \leq (\text{const.}) \|\mathbf{B}\mathbf{g}\|_{\mathcal{H}} \quad \forall \mathbf{g} \in \mathcal{H}.$$

One can express \mathbf{u} in terms of the ONB as $\mathbf{u} = \sum_j \mathbf{d}_j \mathbf{u}_j$. Fix $J \geq 1$ and choose $\mathbf{g} = \sum_{j=1}^J \gamma_j^2 \mathbf{d}_j \mathbf{u}_j \in \mathcal{H}$, so that $\mathbf{B}\mathbf{g} = \sum_{j=1}^J \gamma_j \mathbf{d}_j \mathbf{u}_j$. We deduce from the last inequality that

$$\sum_{j=1}^J \gamma_j^2 |\mathbf{d}_j|^2 \leq (\text{const.}) \left(\sum_{j=1}^J \gamma_j^2 |\mathbf{d}_j|^2 \right)^{1/2},$$

and so

$$\sum_{j=1}^J \gamma_j^2 |\mathbf{d}_j|^2 \leq (\text{const.})^2$$

Letting $J \rightarrow \infty$ implies that

$$\sum_j \gamma_j^2 |\mathbf{d}_j|^2 \leq (\text{const.})^2$$

and so the sequence $\{\gamma_j \mathbf{d}_j\}$ belongs to ℓ^2 . Put $\mathbf{f} = \sum_j \gamma_j \mathbf{d}_j \mathbf{u}_j \in \mathcal{H}$. Then $\mathbf{B}\mathbf{f} = \sum_j \mathbf{d}_j \mathbf{u}_j = \mathbf{u}$, and so $\mathbf{u} \in \text{Ran}(\mathbf{B}) = \mathbf{D}(\mathbf{A})$, as desired.

Selfadjointness, and discreteness of the spectrum

Theorem 22.1. *A is selfadjoint, with domain*

$$\mathbf{D}(\mathbf{A}) = \text{Ran}(\mathbf{B}) = \left\{ \sum_j \gamma_j^{-1} \mathbf{c}_j \mathbf{u}_j : \{\mathbf{c}_j\} \in \ell^2 \right\}.$$

Furthermore, $\text{spec}(\mathbf{A}) = \text{spec}_{\text{disc}}(\mathbf{A}) = \{\gamma_j : j \geq 1\}$.

Proof. We have shown above that \mathbf{A} is symmetric and $\mathbf{D}(\mathbf{A}^*) = \mathbf{D}(\mathbf{A})$, which together imply that \mathbf{A} is selfadjoint.

We will show that if

$$\lambda \in \mathbb{C} \setminus \{\gamma_1, \gamma_2, \gamma_3, \dots\}$$

then $\mathbf{A} - \lambda$ is invertible, so that λ belongs to the resolvent set. Thus the spectrum consists of precisely the eigenvalues γ_j . Note each eigenvalue has finite

multiplicity by Theorem 4.1, and is isolated from the rest of the spectrum; hence A has purely discrete spectrum.

The inverse of $A - \lambda$ can be defined explicitly, as follows. Define a bounded operator $C : \mathcal{H} \rightarrow \mathcal{H}$ on $f = \sum_j c_j u_j \in \mathcal{H}$ by

$$Cf = \sum_j (\gamma_j - \lambda)^{-1} c_j u_j,$$

where we note that $(\gamma_j - \lambda)^{-1}$ is bounded for all j , and in fact approaches 0 as $j \rightarrow \infty$, because $|\gamma_j - \lambda|$ is never zero and tends to ∞ as $j \rightarrow \infty$. This new operator has range $\text{Ran}(C) = \text{Ran}(B)$, because $(\gamma_j - \lambda)^{-1}$ is comparable to γ_j^{-1} (referring here to the characterization of $\text{Ran}(B)$ in Theorem 22.1). Thus $\text{Ran}(C) = D(A)$.

Clearly $(A - \lambda)Cf = f$ by definition of A , and so $\text{Ran}(A - \lambda) = \mathcal{H}$. Similarly one finds that $C(A - \lambda)u = u$ for all $u \in D(A)$. Thus C is the inverse operator of $A - \lambda$. Because C is bounded on all of \mathcal{H} we conclude $A - \lambda$ is invertible, according to the definition in Chapter 20. \square

Example: Laplacian on a bounded domain

To animate the preceding theory, let us consider the Laplacian on a bounded domain $\Omega \subset \mathbb{R}^d$, with Dirichlet boundary conditions. We work with the Hilbert spaces

$$\mathcal{H} = L^2(\Omega), \quad \mathcal{K} = H_0^1(\Omega),$$

and the sesquilinear form

$$a(u, v) = \int_{\Omega} \nabla u \cdot \nabla v \, dx + \int_{\Omega} uv \, dx = \langle u, v \rangle_{H^1},$$

which in Chapter 5 gave eigenfunctions satisfying $(-\Delta + 1)u = (\lambda + 1)u$ weakly. In this setting, $u = Bf$ means that $(-\Delta + 1)u = f$ weakly. Note $B : L^2(\Omega) \rightarrow H_0^1(\Omega)$, and recall that $A = B^{-1}$.

Proposition 22.2. *The domain of the operator A contains $H^2(\Omega) \cap H_0^1(\Omega)$, and*

$$A = -\Delta + 1$$

on $H^2(\Omega) \cap H_0^1(\Omega)$.

Furthermore, if $\partial\Omega$ is smooth then $D(A) = H^2(\Omega) \cap H_0^1(\Omega)$, in which case $A = -\Delta + 1$ on all of its domain.

Proof. For all $\mathbf{u} \in H^2(\Omega) \cap H_0^1(\Omega)$, $\mathbf{v} \in H_0^1(\Omega)$, we have

$$\begin{aligned} \langle \mathbf{u}, \mathbf{v} \rangle_{H^1} &= \langle -\Delta \mathbf{u} + \mathbf{u}, \mathbf{v} \rangle_{L^2} && \text{by parts} \\ &= \langle \mathbf{B}(-\Delta \mathbf{u} + \mathbf{u}), \mathbf{v} \rangle_{H^1} && \text{by definition of } \mathbf{B}. \end{aligned}$$

Since both \mathbf{u} and $\mathbf{B}(-\Delta \mathbf{u} + \mathbf{u})$ belong to $H_0^1(\Omega)$, and $\mathbf{v} \in H_0^1(\Omega)$ is arbitrary, we conclude from above that $\mathbf{u} = \mathbf{B}(-\Delta \mathbf{u} + \mathbf{u})$. Therefore $\mathbf{u} \in \text{Ran}(\mathbf{B}) = \mathbf{D}(\mathbf{A})$, and so $H^2(\Omega) \cap H_0^1(\Omega) \subset \mathbf{D}(\mathbf{A})$.

Further, we find $\mathbf{A}\mathbf{u} = -\Delta \mathbf{u} + \mathbf{u}$ because $\mathbf{B} = \mathbf{A}^{-1}$, and so

$$\mathbf{A} = -\Delta + 1 \quad \text{on } H^2(\Omega) \cap H_0^1(\Omega).$$

Finally we note that if $\partial\Omega$ is C^2 -smooth then by elliptic regularity the weak solution \mathbf{u} of $(-\Delta + 1)\mathbf{u} = \mathbf{f}$ belongs to $H^2(\Omega)$, so that $\text{Ran}(\mathbf{B}) \subset H^2(\Omega) \cap H_0^1(\Omega)$. Thus

$$\mathbf{D}(\mathbf{A}) = H^2(\Omega) \cap H_0^1(\Omega)$$

when $\partial\Omega$ is smooth enough. In that case $\mathbf{A} = -\Delta + 1$ on all of its domain. \square

Compact resolvents

The essence of the proof of the discrete spectral Theorem 4.1 is to show that the inverse operator \mathbf{B} is compact, which means for our differential operators that the inverse is a compact integral operator. For example, in the Neumann Laplacian application we see that $(-\Delta + 1)^{-1}$ is compact from $L^2(\Omega)$ to $H^1(\Omega)$. So is $(-\Delta + \alpha)^{-1}$ for any positive α , but $\alpha = 0$ does not give an invertible operator because the Neumann Laplacian has nontrivial kernel, with $-\Delta(\mathbf{c}) = 0$ for every constant \mathbf{c} .

Thus for the Neumann Laplacian, the *resolvent operator*

$$\mathbf{R}_\lambda = (-\Delta - \lambda)^{-1}$$

is compact whenever λ is negative.

Part III
Appendix

Appendix A

Spectral theorem for compact selfadjoint operators

Goal

State and prove the spectral theorem for compact selfadjoint linear operators on a Hilbert space, as used in Chapter 4.

Let \mathcal{H} be a Hilbert space with either real or complex scalars. We begin with two useful lemmas about weakly convergent sequences.

Lemma A.1 (Continuous linear maps preserve weak convergence). *Suppose $T : \mathcal{H} \rightarrow \mathcal{H}$ is linear and bounded. If $\mathbf{u}_k \rightharpoonup \mathbf{u}$ weakly then $T\mathbf{u}_k \rightharpoonup T\mathbf{u}$ weakly.*

Proof. For all $\mathbf{v} \in \mathcal{H}$ we have

$$\begin{aligned}\langle T\mathbf{u}_k, \mathbf{v} \rangle &= \langle \mathbf{u}_k, T^*\mathbf{v} \rangle && \text{where } T^* \text{ is the Hilbert space adjoint of } T \\ &\rightarrow \langle \mathbf{u}, T^*\mathbf{v} \rangle && \text{since } \mathbf{u}_k \rightharpoonup \mathbf{u} \text{ weakly} \\ &= \langle T\mathbf{u}, \mathbf{v} \rangle.\end{aligned}$$

□

Lemma A.2 (Compact linear maps transform weak convergence into norm convergence). *Suppose $T : \mathcal{H} \rightarrow \mathcal{H}$ is linear and compact. If $\mathbf{u}_k \rightharpoonup \mathbf{u}$ weakly then $T\mathbf{u}_k \rightarrow T\mathbf{u}$ in norm. Also $\langle \mathbf{u}_k, T\mathbf{u}_k \rangle \rightarrow \langle \mathbf{u}, T\mathbf{u} \rangle$.*

Proof. Consider an arbitrary subsequence $\{\mathbf{u}_{k_\ell}\}$, which for notational simplicity we write as $\{\mathbf{v}_\ell\}$. Since $T\mathbf{u}_k \rightharpoonup T\mathbf{u}$ weakly by Lemma A.1, in particular we have $T\mathbf{v}_\ell \rightharpoonup T\mathbf{u}$ weakly.

The sequence $\{\mathbf{u}_k\}$ is bounded since it is weakly convergent. Compactness of T therefore implies norm convergence of some subsequence of $\{T\mathbf{v}_\ell\}$, say $T\mathbf{v}_{\ell_m} \rightarrow \mathbf{v}$ for some $\mathbf{v} \in \mathcal{H}$. This norm convergence implies also the weak convergence $T\mathbf{v}_{\ell_m} \rightharpoonup \mathbf{v}$.

Combining the last two paragraphs shows that $T\mathbf{u} = \mathbf{v}$, and so $T\mathbf{v}_{\ell_m} \rightarrow T\mathbf{u}$ in norm. Thus each subsequence of $\{\mathbf{u}_k\}$ has a further subsequence whose image under T converges to $T\mathbf{u}$. Therefore $T\mathbf{u}_k \rightarrow T\mathbf{u}$.

Further,

$$\langle \mathbf{u}_k, T\mathbf{u}_k \rangle - \langle \mathbf{u}, T\mathbf{u} \rangle = \langle \mathbf{u}_k, T\mathbf{u}_k - T\mathbf{u} \rangle + \langle \mathbf{u}_k - \mathbf{u}, T\mathbf{u} \rangle.$$

The first inner product on the right converges to 0 because $\{\mathbf{u}_k\}$ is bounded and $T\mathbf{u}_k - T\mathbf{u} \rightarrow 0$. The second inner product converges to 0 because $\mathbf{u}_k \rightharpoonup \mathbf{u}$ weakly. \square

Now comes the main result of the section, giving an ONB of eigenvectors.

Theorem A.3 (Spectral theorem for compact selfadjoint operators). *Assume \mathcal{H} is a separable, infinite dimensional Hilbert space, and $B : \mathcal{H} \rightarrow \mathcal{H}$ is a linear, compact, selfadjoint operator.*

Then \mathcal{H} has a countable ONB $\{\mathbf{u}_k\}_{k=1}^\infty$ consisting of eigenvectors of B , with

$$B\mathbf{u}_k = \beta_k \mathbf{u}_k,$$

for some real eigenvalues β_k .

Further, if infinitely many of the β_k are nonzero then they can be arranged as a sequence converging to 0. In particular, each nonzero eigenvalue has finite multiplicity (the corresponding eigenspace is finite dimensional).

The finite dimensional version of the theorem simply says that a selfadjoint matrix (either real symmetric or complex Hermitian) possesses an ONB of eigenvectors.

Proof. Notice $\langle \mathbf{u}, B\mathbf{u} \rangle$ is real, because selfadjointness of B implies

$$\langle \mathbf{u}, B\mathbf{u} \rangle = \langle \mathbf{u}, B^*\mathbf{u} \rangle = \langle B\mathbf{u}, \mathbf{u} \rangle = \overline{\langle \mathbf{u}, B\mathbf{u} \rangle}$$

for each $\mathbf{u} \in \mathcal{H}$. Define

$$m = \inf_{\mathbf{u} \neq 0} \frac{\langle \mathbf{u}, B\mathbf{u} \rangle}{\langle \mathbf{u}, \mathbf{u} \rangle}, \quad M = \sup_{\mathbf{u} \neq 0} \frac{\langle \mathbf{u}, B\mathbf{u} \rangle}{\langle \mathbf{u}, \mathbf{u} \rangle},$$

so that $-\infty < m \leq M < \infty$.

STEP 1 — Finding the largest eigenvalue. We will show that if $M > 0$ then M is an eigenvalue of B . First we prove the supremum for M is attained at some vector \mathbf{u} . Then we show \mathbf{u} is an eigenvector with eigenvalue M .

Take a supremizing sequence $\{\mathbf{u}_k\}$, normalized by $\|\mathbf{u}_k\| = 1$, such that

$$\langle \mathbf{u}_k, B\mathbf{u}_k \rangle \rightarrow M.$$

After passing to a subsequence we may suppose $\mathbf{u}_k \rightharpoonup \mathbf{u}$ weakly for some $\mathbf{u} \in \mathcal{H}$, by weak sequential compactness of the closed unit ball. Then

$$\langle \mathbf{u}_k, B\mathbf{u}_k \rangle \rightarrow \langle \mathbf{u}, B\mathbf{u} \rangle$$

by Lemma A.2, since B is compact. Thus $\langle \mathbf{u}, B\mathbf{u} \rangle = M > 0$, and so $\mathbf{u} \neq 0$.

Notice $\|\mathbf{u}\| \leq 1$ because

$$\|\mathbf{u}\|^2 = \langle \mathbf{u}, \mathbf{u} \rangle = \lim_k \langle \mathbf{u}_k, \mathbf{u} \rangle \leq \|\mathbf{u}\|.$$

Also $\|\mathbf{u}\| \geq 1$ because

$$M \geq \frac{\langle \mathbf{u}, B\mathbf{u} \rangle}{\langle \mathbf{u}, \mathbf{u} \rangle} = \frac{M}{\|\mathbf{u}\|^2} > 0.$$

Hence $\|\mathbf{u}\| = 1$, and so the supremum for M is attained at \mathbf{u} .

Now we show that this maximizing vector \mathbf{u} is an eigenvector with eigenvalue M . Fix $\mathbf{v} \in \mathcal{H}$ (the “variation direction”) and define a real valued function

$$g(t) = \frac{\langle \mathbf{u} + t\mathbf{v}, B(\mathbf{u} + t\mathbf{v}) \rangle}{\langle \mathbf{u} + t\mathbf{v}, \mathbf{u} + t\mathbf{v} \rangle},$$

where we assume $t \in \mathbb{R}$ is small enough that $\mathbf{u} + t\mathbf{v} \neq 0$ in the denominator. Notice g is maximal at $t = 0$, since the supremum M is attained at \mathbf{u} . Hence by the first derivative test,

$$\begin{aligned} 0 &= g'(0) \\ &= \frac{d}{dt} \frac{\langle \mathbf{u}, B\mathbf{u} \rangle + 2t \operatorname{Re} \langle \mathbf{v}, B\mathbf{u} \rangle + t^2 \langle \mathbf{v}, B\mathbf{v} \rangle}{\langle \mathbf{u}, \mathbf{u} \rangle + 2t \operatorname{Re} \langle \mathbf{v}, \mathbf{u} \rangle + t^2 \langle \mathbf{v}, \mathbf{v} \rangle} \Big|_{t=0} \\ &= 2(\operatorname{Re} \langle \mathbf{v}, B\mathbf{u} \rangle - M \operatorname{Re} \langle \mathbf{v}, \mathbf{u} \rangle) \end{aligned}$$

where we used that $\langle \mathbf{u}, B\mathbf{u} \rangle = M$ and $\langle \mathbf{u}, \mathbf{u} \rangle = 1$.

For a real Hilbert space one dispenses with the “Re” parts, getting just

$$\langle \mathbf{v}, \mathbf{B}\mathbf{u} \rangle - M\langle \mathbf{v}, \mathbf{u} \rangle = 0.$$

The “Re” parts may be removed on a complex Hilbert space too, since one may repeat the above argument with \mathbf{v} replaced by $i\mathbf{v}$ in the definition of \mathbf{g} , which changes the real part to an imaginary part. Hence $\langle \mathbf{v}, \mathbf{B}\mathbf{u} - M\mathbf{u} \rangle = 0$ for all $\mathbf{v} \in \mathcal{H}$, and so $\mathbf{B}\mathbf{u} - M\mathbf{u} = \mathbf{0}$. Thus \mathbf{u} is an eigenvector with eigenvalue M , as we wanted to show.

Similarly, one finds that if $m < 0$ then m is an eigenvalue of \mathbf{B} .

STEP 2 — Finding the largest-magnitude eigenvalue. Let

$$\alpha_1 = \sup_{\mathbf{u} \neq \mathbf{0}} \frac{|\langle \mathbf{u}, \mathbf{B}\mathbf{u} \rangle|}{\langle \mathbf{u}, \mathbf{u} \rangle}$$

so that $\alpha_1 = \max(|m|, |M|)$. Step 1 shows that if $\alpha_1 \neq 0$ then α_1 or $-\alpha_1$ is an eigenvalue of \mathbf{B} . Denote the eigenvalue by β_1 , and the corresponding eigenvector by \mathbf{u}_1 , so that $\mathbf{B}\mathbf{u}_1 = \beta_1\mathbf{u}_1$.

STEP 3 — Repeat on the orthogonal complement. Let \mathcal{H}_1 be the span of the eigenvector \mathbf{u}_1 (that is, the subspace of all scalar multiples of \mathbf{u}_1), so that \mathcal{H}_1 is a closed subspace of \mathcal{H} . Decompose the Hilbert space as

$$\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_1^\perp.$$

Notice \mathbf{B} maps \mathcal{H}_1^\perp to \mathcal{H}_1^\perp , since if $\mathbf{w} \in \mathcal{H}_1^\perp$ then $\langle \mathbf{w}, \mathbf{u}_1 \rangle = 0$ and so

$$\langle \mathbf{B}\mathbf{w}, \mathbf{u}_1 \rangle = \langle \mathbf{w}, \mathbf{B}\mathbf{u}_1 \rangle = \beta_1 \langle \mathbf{w}, \mathbf{u}_1 \rangle = 0,$$

where we used once again the selfadjointness of \mathbf{B} .

Hence \mathcal{H}_1^\perp is a separable, infinite dimensional Hilbert space and $\mathbf{B} : \mathcal{H}_1^\perp \rightarrow \mathcal{H}_1^\perp$ is a linear, compact, selfadjoint operator. Thus Step 2 applies to the operator \mathbf{B} restricted to \mathcal{H}_1^\perp , and in this fashion we continue iteratively generating eigenvalues $\beta_1, \beta_2, \beta_3, \dots$ with decreasing magnitudes $|\beta_1| \geq |\beta_2| \geq |\beta_3| \geq \dots$. The corresponding eigenvectors are orthonormal by construction, and so at each stage of the construction

$$\mathcal{H} = (\mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \dots \oplus \mathcal{H}_k) \oplus (\mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \dots \oplus \mathcal{H}_k)^\perp.$$

The process terminates after $k \geq 0$ iterations if $\alpha_{k+1} = 0$ where

$$\alpha_{k+1} = \sup_{\mathbf{u} \perp (\mathcal{H}_1 \oplus \dots \oplus \mathcal{H}_k)} \frac{|\langle \mathbf{u}, \mathbf{B}\mathbf{u} \rangle|}{\langle \mathbf{u}, \mathbf{u} \rangle}.$$

Otherwise the process continues for all k .

STEP 4 — Suppose the process terminates after $k \geq 0$ iterations. Let $K = (\mathcal{H}_1 \oplus \cdots \oplus \mathcal{H}_k)^\perp$. The condition $\alpha_{k+1} = 0$ gives

$$\langle \mathbf{u}, \mathbf{B}\mathbf{u} \rangle = 0, \quad \mathbf{u} \in K. \quad (\text{A.1})$$

Then

$$\langle \mathbf{v}, \mathbf{B}\mathbf{u} \rangle = 0, \quad \mathbf{u}, \mathbf{v} \in K, \quad (\text{A.2})$$

because

$$\begin{aligned} 2 \operatorname{Re} \langle \mathbf{v}, \mathbf{B}\mathbf{u} \rangle &= \langle \mathbf{v}, \mathbf{B}\mathbf{u} \rangle + \langle \mathbf{B}\mathbf{u}, \mathbf{v} \rangle \\ &= \langle \mathbf{v}, \mathbf{B}\mathbf{u} \rangle + \langle \mathbf{u}, \mathbf{B}\mathbf{v} \rangle \quad \text{by selfadjointness of } \mathbf{B} \\ &= \langle \mathbf{u} + \mathbf{v}, \mathbf{B}(\mathbf{u} + \mathbf{v}) \rangle - \langle \mathbf{u}, \mathbf{B}\mathbf{u} \rangle - \langle \mathbf{v}, \mathbf{B}\mathbf{v} \rangle \\ &= 0 \end{aligned}$$

by (A.1), with the imaginary part vanishing similarly after replacing \mathbf{v} with $i\mathbf{v}$ (in the complex case).

Choosing $\mathbf{v} = \mathbf{B}\mathbf{u}$ in (A.2) shows $\mathbf{B}\mathbf{u} = \mathbf{0}$ for all $\mathbf{u} \in K$. Thus K is the kernel or zero eigenspace of the operator \mathbf{B} . It has a countable ONB, since \mathcal{H} is separable by hypothesis. Combining this basis with the eigenvectors $\mathbf{u}_1, \dots, \mathbf{u}_k$ yields an ONB for the whole space \mathcal{H} .

STEP 5 — Suppose the process continues for all k . Then $\beta_k \rightarrow 0$, as follows. The orthonormal sequence $\{\mathbf{u}_k\}$ converges weakly to $\mathbf{0}$ because $\langle \mathbf{u}_k, \mathbf{v} \rangle \rightarrow 0$ for each $\mathbf{v} \in \mathcal{H}$, which follows from Bessel's inequality

$$\sum_k |\langle \mathbf{u}_k, \mathbf{v} \rangle|^2 \leq \|\mathbf{v}\|^2.$$

Hence $\mathbf{B}\mathbf{u}_k$ converges in norm to $\mathbf{0}$, by Lemma A.2, and so

$$|\beta_k| = \|\beta_k \mathbf{u}_k\| = \|\mathbf{B}\mathbf{u}_k\| \rightarrow 0$$

as we wanted to show.

Let $K = \{\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3, \dots\}^\perp$.

If $K = \{\mathbf{0}\}$ then $\{\mathbf{u}_k\}$ is complete and so forms an ONB for \mathcal{H} . Suppose $K \neq \{\mathbf{0}\}$. Observe $\langle \mathbf{u}, \mathbf{B}\mathbf{u} \rangle = 0$ for all $\mathbf{u} \in K$ because

$$\frac{|\langle \mathbf{u}, \mathbf{B}\mathbf{u} \rangle|}{\langle \mathbf{u}, \mathbf{u} \rangle} \leq \alpha_{k+1} \rightarrow 0.$$

Hence $B\mathbf{u} = \mathbf{0}$ by arguing as in Step 4. Thus \mathbf{K} is the zero eigenspace. To finish the proof one chooses a countable ONB for \mathbf{K} and combines it with the $\{\mathbf{u}_k\}$ to get a countable ONB for \mathcal{H} . \square

Appendix B

Compact imbeddings of Sobolev space into L^2

Goal

Develop compact imbedding theorems of Rellich type for $H_0^1 \hookrightarrow L^2$ on domains of finite volume, and $H^1 \hookrightarrow L^2$ on bounded Lipschitz domains, as used in Chapters 5–9.

Fourier multiplier operators

Boundedness and compactness properties of Fourier multipliers are established in the next lemmas, to be used later when proving compact imbeddings of Sobolev space.

All functions in this appendix are complex valued unless specified otherwise, and $L^2(\Omega)$ means $L^2(\Omega; \mathbb{C})$ and so on.

Write M_w for the Fourier multiplier operator

$$M_w f = \mathcal{F}^{-1}(w\mathcal{F}f)$$

where \mathcal{F} is the Fourier transform.

Lemma B.1 (Boundedness). *If $g, w \in L^\infty(\mathbb{R}^d)$ then*

$$gM_w : L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)$$

is linear and bounded.

Proof. Since the Fourier transform acts isometrically on L^2 , it is obvious from the definition of $M_w f = \mathcal{F}^{-1}(w\mathcal{F}f)$ and boundedness of the functions g and w that gM_w is a bounded operator, with norm at most $\|g\|_{L^\infty}\|w\|_{L^\infty}$. \square

Lemma B.2 (Compactness). *If $g, w \in L^2(\mathbb{R}^d)$ then*

$$gM_w : L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)$$

is linear and compact.

Proof. First we show the operator is well defined and bounded. Since $w \in L^2$, the multiplier can be written as a convolution, namely

$$M_w f = \mathcal{F}^{-1}(w\mathcal{F}f) = (\mathcal{F}^{-1}w) * f, \quad f \in L^2(\mathbb{R}^d),$$

and so

$$\|gM_w f\|_{L^2} \leq \|g\|_{L^2}\|M_w f\|_{L^\infty} \leq \|g\|_{L^2}\|w\|_{L^2}\|f\|_{L^2}.$$

Thus gM_w is bounded on L^2 . Further, it is Hilbert–Schmidt and therefore compact, because the operator

$$(gM_w f)(x) = g(x) \int_{\mathbb{R}^d} (\mathcal{F}^{-1}w)(x-y)f(y) dy$$

has integral kernel $K(x, y) = g(x)(\mathcal{F}^{-1}w)(x-y)$, which is square integrable:

$$\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} K(x, y)^2 dx dy = \|g\|_{L^2}^2 \|w\|_{L^2}^2.$$

\square

Lemma B.3. *If $g \in L^2 \cap L^\infty(\mathbb{R}^d)$, $w \in L^\infty(\mathbb{R}^d)$ and $w(\xi) \rightarrow 0$ as $|\xi| \rightarrow \infty$, then*

$$gM_w : L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)$$

is linear and compact.

Proof. First, gM_w is bounded on L^2 by Lemma B.1, since g and w are bounded. For compactness, write

$$w_n = w \mathbf{1}_{B(n)}$$

where $B(\mathbf{n})$ is the ball of radius \mathbf{n} in \mathbb{R}^d . Then $w_{\mathbf{n}}$ is a bounded function with compact support, and so belongs to $L^2(\mathbb{R}^d)$. Since $g \in L^2$ by hypothesis, Lemma B.2 now yields compactness of $gM_{w_{\mathbf{n}}}$.

We will show $gM_{w_{\mathbf{n}}} \rightarrow gM_w$ in the operator norm, so that gM_w is compact. Indeed,

$$\begin{aligned} \|(gM_{w_{\mathbf{n}}} - gM_w)f\|_{L^2} &\leq \|g\|_{L^\infty} \|(M_{w_{\mathbf{n}}} - M_w)f\|_{L^2} \\ &= \|g\|_{L^\infty} \|(w_{\mathbf{n}} - w)\mathcal{F}f\|_{L^2} \\ &\leq \|g\|_{L^\infty} \sup_{|\xi| \geq \mathbf{n}} |w(\xi)| \|\mathcal{F}f\|_{L^2} \end{aligned}$$

and so as $\mathbf{n} \rightarrow \infty$,

$$\|gM_{w_{\mathbf{n}}} - gM_w\|_{L^2 \rightarrow L^2} \leq \|g\|_{L^\infty} \sup_{|\xi| \geq \mathbf{n}} |w(\xi)| \rightarrow 0.$$

□

Compactness of $H_0^1 \hookrightarrow L^2$ on finite volume domains

Now comes the main result of the chapter.

Theorem B.4 (Rellich for H_0^1). *If $\Omega \subset \mathbb{R}^d$ is open with finite volume then the imbedding*

$$H_0^1(\Omega) \hookrightarrow L^2(\Omega)$$

is compact.

This appendix treats complex valued functions. Real valued functions are a special case.

Proof. Step 1. Consider a bounded sequence $\{f_k\}$ in $H^1(\mathbb{R}^d)$, say with $\|f_k\|_{H^1(\mathbb{R}^d)} \leq C$. Define $F_k \in L^2(\mathbb{R}^d)$ by

$$\mathcal{F} F_k = (1 + 4\pi^2|\xi|^2)^{1/2} \mathcal{F} f_k,$$

where we observe

$$\|F_k\|_{L^2(\mathbb{R}^d)} = \|f_k\|_{H^1(\mathbb{R}^d)} \leq C,$$

so that the sequence $\{F_k\}$ is bounded in $L^2(\mathbb{R}^d)$.

Let $g = 1_\Omega$ where $\Omega \subset \mathbb{R}^d$ is measurable with finite volume. (We do not assume Ω is open, in this step of the proof.) Notice $g \in L^1 \cap L^\infty(\mathbb{R}^d)$

since Ω has finite volume, so that in particular $\mathbf{g} \in L^2(\mathbb{R}^d)$. Next let $\mathbf{w}(\xi) = (1 + 4\pi^2|\xi|^2)^{-1/2}$, so that $\mathbf{w} \in L^\infty(\mathbb{R}^d)$ and $\mathbf{w}(\xi) \rightarrow 0$ as $|\xi| \rightarrow \infty$. Hence \mathbf{gM}_w is compact on $L^2(\mathbb{R}^d)$ by Lemma B.3.

Applying this compact operator to F_k yields existence of a subsequence of $\{\mathbf{gM}_w F_k\}$ that converges in $L^2(\mathbb{R}^d)$. Since

$$\mathbf{gM}_w F_k = 1_\Omega f_k,$$

we have a subsequence of $\{f_k\}$ whose restrictions to Ω converge in $L^2(\Omega)$. Thus the restriction map from $H^1(\mathbb{R}^d)$ to $L^2(\Omega)$ is compact.

Step 2. Now take a bounded sequence $\{f_k\}$ in $H_0^1(\Omega)$, where Ω is open with finite volume, and extend f_k to equal 0 outside Ω so that the extended function belongs to $H^1(\mathbb{R}^d)$. Step 1 yields a subsequence of $\{f_k\}$ that converges in $L^2(\Omega)$, proving compactness of the imbedding $H_0^1(\Omega) \hookrightarrow L^2(\Omega)$. \square

A useful fact was established by Step 1 of the last proof.

Theorem B.5 (Restriction of H^1 to L^2). *If $\Omega \subset \mathbb{R}^d$ is measurable with finite volume then the restriction map*

$$\begin{aligned} H^1(\mathbb{R}^d) &\rightarrow L^2(\Omega) \\ f &\mapsto f|_\Omega \end{aligned}$$

is compact.

Compactness of $H^1 \hookrightarrow L^2$ on Lipschitz domains

The imbedding of H_0^1 implies an imbedding of H^1 .

Theorem B.6 (Rellich for H^1). *If $\Omega \subset \mathbb{R}^d$ is a bounded domain with Lipschitz boundary then the imbedding*

$$H^1(\Omega) \hookrightarrow L^2(\Omega)$$

is compact.

Proof. Choose a bounded domain Ω_0 that contains the closure of Ω , and write

$$E : H^1(\Omega) \rightarrow H_0^1(\Omega_0)$$

for the extension operator [Evans and Gariepy]. A bounded sequence $\{f_k\}$ in $H^1(\Omega)$ gives a bounded sequence $\{Ef_k\}$ in $H_0^1(\Omega_0)$. Some subsequence of the Ef_k converges in $L^2(\Omega_0)$ by Rellich's Theorem B.4, and restricting to Ω (where $Ef_k = f_k$) shows convergence of the subsequence in $L^2(\Omega)$. \square

Notes and comments

The proof by Fourier transform and Hilbert–Schmidt operators of the compact imbedding $H_0^1 \hookrightarrow L^2$ (Rellich’s Theorem for finite volume domains) was shown to me by Dirk Hundertmark.

The proof extends straightforwardly to give compactness of the imbedding for fractional order Sobolev spaces too: $H_0^s(\Omega) \hookrightarrow L^2(\Omega)$ compactly for all $s > 0$, whenever Ω has finite volume. Hence one obtains discrete spectrum for the fractional Laplacian on domains of finite volume. For more on spectral theory of the fractional Laplacian, see the review article [Frank].

Further, the proof of Theorem B.5 adapts easily to show that $H^s(\mathbb{R}^d)$ restricts compactly into $L^2(\Omega)$, whenever the set Ω has finite volume.

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