Cambridge University Press
978-1-107-03230-9 - Spectral Theory and its Applications
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Introduction

1.1 Spectral theory in action

In this book, we present the basic tools of spectral analysis and illustrate the theory by presenting many examples from the theory of Schrödinger operators and from various branches of physics, including statistical mechanics, superconductivity, fluid mechanics, and kinetic theory. Hence we shall alternately present parts of the theory and use applications in those fields as examples. In the final chapters, we also give an introduction to the theory of non-self-adjoint operators with an emphasis on the role of pseudospectra. Throughout the book, the reader is assumed to have some elementary knowledge of Hilbertian and functional analysis and, for many examples and exercises, to have had some practice in distribution theory and Sobolev spaces. This introduction is intended to be a rather informal walk through some questions in spectral theory. We shall answer these questions mainly "by hand" using examples, with the aim of showing the need for a general theory to explain the results. Only in Chapter 2 will we start to give precise definitions and statements.

Our starting point is the theory of Hermitian matrices, that is, the theory of matrices satisfying $A^\star = A$, where $A^\star$ is the adjoint matrix of A. When we are looking for eigenvectors and corresponding eigenvalues of A, that is, for pairs (u, λ) with $u \in \mathbb{C}^k$, $u \neq 0$, and $\lambda \in \mathbb{C}$ such that $Au = \lambda u$, we know that the eigenvalues will be real and that one can find an orthonormal basis of eigenvectors associated with those eigenvalues. In this case, we can speak of eigenpairs.

In order to extend this theory to the case of spaces with infinite dimension (that is, where the space $\mathbb{C}^m$ is replaced by a general Hilbert space $\mathcal{H}$), we might attempt to develop a theory of compact self-adjoint operators. But it would be a major task to cover all the interesting cases that arise in quantum mechanics. So, although our aim is to present a general theory, it is perhaps good to start by looking at specific operators and asking naive questions about the existence of eigenpairs (u, λ) with u in some suitable domain, $u \neq 0$ and

$\lambda \in \mathbb{C}$, such that $Au = \lambda u$. We shall discover in particular that the answers to these questions may depend strongly on the choice of the domain and on the precise definition of the operator.

1.2 The free Laplacian

In this spirit, let us start with the free Laplacian in $\mathbb{R}^m$. We denote by $L^2(\mathbb{R}^m)$ the space of (or class of) measurable functions on $\mathbb{R}^m$ that are square integrable with respect to the Lebesgue measure dx (for $dx_1, \ldots, dx_m$). The Laplacian

$$-\Delta = -\sum_{j=1}^{m} \frac{\partial^2}{\partial x_j^2}$$

has no eigenfunctions in $L^2(\mathbb{R}^m)$, i.e., there is not a pair (u, λ) with $\lambda \in \mathbb{C}$ and $u \neq 0$ in L^2 such that $-\Delta u = \lambda u$ in the sense of distributions.[1] But it has, for any $\lambda \in \mathbb{R}^+$, an eigenfunction in $\mathcal{S}'(\mathbb{R}^m)$ (the space of tempered distributions) (actually, in $L^\infty(\mathbb{R}^m)$) and, for any $\lambda \in \mathbb{C}$, an eigenfunction in $\mathcal{D}'(\mathbb{R}^m)$ (the space of distributions). So what is the right way to extend the theory of Hermitian matrices on $\mathbb{C}^k$?

On the other hand, it is easy to produce approximate eigenfunctions of the form $u_n(x) = n^{-m/2} e^{ix\cdot\xi} \chi(x/n)$, where χ is a compactly supported C^∞ function with an L^2-norm equal to 1 and $\xi \in \mathbb{R}^m$. By "approximate" we mean that if $\lambda = |\xi|^2$ and $A = -\Delta$, the norm in L^2 of $(A - \lambda)u_n$ tends to 0 as $n \to +\infty$.

1.3 The harmonic oscillator

As we shall see, the operator of the harmonic oscillator (referred to simply as the "harmonic oscillator" from now on),

$$H = -\frac{d^2}{dx^2} + x^2,$$

plays a central role in the theory of quantum mechanics. When we look for eigenfunctions in $\mathcal{S}(\mathbb{R})$ (the Schwartz space of C^∞ rapidly decreasing functions at ∞, together with all derivatives), we can show that there is a sequence of eigenvalues λ_n $(n \in \mathbb{N}^*)$,

$$\lambda_n = (2n - 1).$$

[1] This means in this case that $-\int u(x)(\Delta\phi)\, dx = \lambda \int u(x)\phi(x)\, dx$, for any function ϕ in $C_0^\infty(\mathbb{R}^m)$. Some other authors use the notion of a weak solution.

In particular, the fundamental level (in other words, the lowest eigenvalue) is $\lambda_1 = 1$ and the splitting between the first two eigenvalues is 2.

The first (normalized) eigenfunction is given by

$$\phi_1(x) = \pi^{-1/2} \exp -\frac{x^2}{2}, \tag{1.3.1}$$

and the other eigenfunctions are obtained by applying the so-called[2] creation operator

$$L^+ = -\frac{d}{dx} + x. \tag{1.3.2}$$

We observe that

$$H = L^+ \cdot L^- + 1, \tag{1.3.3}$$

where

$$L^- = \frac{d}{dx} + x, \tag{1.3.4}$$

and L^- has the property

$$L^- \phi_1 = 0. \tag{1.3.5}$$

Note that if $u \in L^2$ is a distributional solution of $L^+ u = 0$, then $u = 0$. Also, if $u \in L^2$ is a distributional solution of $L^- u = 0$, then $u = \mu \phi_1$ for some $\mu \in \mathbb{R}$.

The nth eigenfunction is then given by

$$\phi_n = 2^{-(n-1)/2} \left((n-1)!\right)^{-1/2} (L^+)^{n-1} \phi_1. \tag{1.3.6}$$

This can be shown by recursion using the identity

$$L^+(H + 2) = H L^+. \tag{1.3.7}$$

It is easy to see that

$$\phi_n(x) = P_n(x) \exp -\frac{x^2}{2}, \tag{1.3.8}$$

where $P_n(x)$ is a polynomial of order $n - 1$. It can also be shown that the ϕ_n are mutually orthogonal. The proof of this point is identical to the

[2] In quantum mechanics.

finite-dimensional case, if we observe the following identity (expressing the fact that H is symmetric):

$$\langle Hu, v\rangle_{L^2} = \langle u, Hv\rangle_{L^2}, \forall u \in \mathcal{S}(\mathbb{R}), \forall v \in \mathcal{S}(\mathbb{R}), \tag{1.3.9}$$

which is obtained by an integration by parts.

We also observe that, by recursion, $||\phi_n|| = 1$. It is then a standard exercise to show that the family $(\phi_n)_{n\in\mathbb{N}}$ is total in $L^2(\mathbb{R})$ (i.e., the vector space generated by finite linear combinations of elements of the family is dense in L^2). A direct way is to analyze, for any $g \in L^2$, the function $\mathbb{R} \ni \xi \mapsto F_g(\xi) = \int_{\mathbb{R}} \exp -ix\xi\, g(x)\phi_1(x)\, dx$, and to observe that, owing to the Gaussian decay of ϕ_1, this is a real analytic function on $\mathbb{R}$. Moreover, if g is orthogonal to all of the ϕ_n, then $F_g^{(k)}(0) = 0$ for any k. This implies $F_g(\xi) = 0$, $\forall \xi \in \mathbb{R}$. But $F_g(\xi)$ is the Fourier transform of $g\phi_1$, and hence $g = 0$. Hence we have obtained an orthonormal Hilbertian basis of $L^2(\mathbb{R})$, which in some sense permits us to diagonalize the operator H.

Another way to understand this completeness is to show that if we start with an eigenfunction u in $\mathcal{S}'(\mathbb{R})$ associated with $\lambda \in \mathbb{R}$ that is a solution (in the sense of distributions) of

$$Hu = \lambda u,$$

then there exist $k \in \mathbb{N}$ and $c_k \neq 0$ such that $(L^-)^k u = c_k\phi_1$ and that the corresponding λ is equal to $(2k + 1)$. For the proof of this, we have to assume that any eigenfunction is in $\mathcal{S}(\mathbb{R})$ (this can be proven independently of any explicit knowledge of the eigenfunctions) and use the identity

$$L^-(H - 2) = HL^- \tag{1.3.10}$$

and the inequality

$$\langle Hu, u\rangle \geq 0, \forall u \in \mathcal{S}(\mathbb{R}). \tag{1.3.11}$$

This last property is called the "nonnegativity" of the operator.

Actually, it can be shown in various ways that

$$\langle Hu, u\rangle \geq ||u||^2, \forall u \in \mathcal{S}(\mathbb{R}). \tag{1.3.12}$$

One way is to first establish the Heisenberg uncertainty principle,

$$||u||^2_{L^2(\mathbb{R})} \leq 2||xu||_{L^2}||u'||_{L^2}, \forall u \in \mathcal{S}(\mathbb{R}). \tag{1.3.13}$$

Before we describe the trick behind the proof, however, let us give a more "physical" version.

If u is normalized by $||u||_{L^2(\mathbb{R})} = 1$, the measure $|u|^2\,dx$ is a probability measure. One can then define the mean value of the position by

$$\langle x\rangle = \int x|u|^2\,dx$$

and the variance by

$$\sigma_x = \langle (x - \langle x\rangle)^2\rangle.$$

Similarly, we can consider

$$\langle D_x\rangle := \int (D_x u)\cdot \bar{u}(x)\,dx$$

(with $D_x = -i d/dx$) and

$$\sigma_{D_x} := ||(D_x - \langle D_x\rangle)u||^2.$$

Then (1.3.13) can be extended in the form

$$\sigma_x \cdot \sigma_{D_x} \geq \frac{1}{4}.$$

The trick is to observe the identity

$$1 = \frac{d}{dx}\cdot x - x\cdot \frac{d}{dx}. \tag{1.3.14}$$

We then write, for $u \in \mathcal{S}(\mathbb{R})$,

$$u(x)\,\bar{u}(x) = \left(\left(\frac{d}{dx}\cdot x - x\cdot\frac{d}{dx}\right)u(x)\right)\,\bar{u}(x),$$

and then integrate over $\mathbb{R}$:

$$\int_{\mathbb{R}} |u(x)|^2\,dx = \int (xu)'\,\bar{u}(x)\,dx - \int xu'(x)\,\bar{u}(x)\,dx.$$

After an integration by parts, we obtain

$$\int_{\mathbb{R}} |u(x)|^2\,dx = -\int xu'(x)\bar{u}(x)\,dx - \int xu(x)\bar{u}'(x)\,dx.$$

(1.3.13) is then a consequence of the Cauchy–Schwarz inequality.

The inequality (1.3.12) is simply a consequence of the identity

$$\langle Hu, u\rangle = ||u'||^2 + ||xu||^2, \tag{1.3.15}$$

which can be proved by an integration by parts, and of the application in (1.3.13) of the Cauchy–Schwarz inequality. Another way is to directly observe the identity

$$\langle Hu, u\rangle = ||L^- u||^2 + ||u||^2, \ \forall u \in \mathcal{S}(\mathbb{R}). \tag{1.3.16}$$

1.4 The problem of the boundary

We consider mainly ordinary differential operators of first or second order on an interval $]0, 1[$ and look at various questions that can be asked naively about the existence of eigenfunctions for the problem in $L^2(]0, 1[)$.

1.4.1 Preliminary discussion

We look first at pairs $(u, \lambda) \in H^1(]0, 1[) \times \mathbb{C}$ $(u \neq 0)$ such that

$$-\frac{du}{dx} = \lambda u, \ u(0) = 0,$$

where $H^1(]0, 1[)$ is the Sobolev space

$$H^1(]0, 1[) = \{u \in L^2(]0, 1[) \,|\, u' \in L^2(]0, 1[)\}.$$

Here we recall that $H^1(]0, 1[)$ is included in $C^0([0, 1])$, by the Sobolev injection theorem. It can be seen immediately that no such pairs exist. We shall come back to this example later when we analyze non-self-adjoint problems.

We now look at pairs $(u, \lambda) \in H^2(]0, 1[) \times \mathbb{C}$ $(u \neq 0)$ such that

$$-\frac{d^2u}{dx^2} = \lambda u.$$

For any λ, we can find two linearly independent solutions.

1.4.2 The periodic problem

We consider pairs $(u, \lambda) \in H^{2,\mathrm{per}}(]0, 1[) \times \mathbb{C}$ $(u \neq 0)$ such that

$$-\frac{d^2u}{dx^2} = \lambda u.$$

Here,

$$H^{2,\mathrm{per}}(]0,1[) = \{u \in H^2(]0,1[),\ u(0) = u(1) \text{ and } u'(0) = u'(1)\},$$

where $H^2(]0,1[)$ is the Sobolev space

$$H^2(]0,1[) = \{u \in H^1(]0,1[) \mid u' \in H^1(]0,1[)\}.$$

Here we recall that $H^2(]0,1[)$ is included in $C^1([0,1])$, by the Sobolev injection theorem. It is an easy exercise to show that the pairs are described by two families:

- $\lambda = 4\pi^2 n^2,\ u_n = \mu \cos 2\pi n x,\ \text{ for } n \in \mathbb{N},\ \mu \in \mathbb{R} \setminus \{0\},$
- $\lambda = 4\pi^2 n^2,\ v_n = \mu \sin 2\pi n x,\ \text{ for } n \in \mathbb{N}^*,\ \mu \in \mathbb{R} \setminus \{0\}.$

We observe that $\lambda = 0$ is the lowest eigenvalue and that its multiplicity is one. This means that the corresponding eigenspace is of dimension one (the other eigenspaces are of dimension 2). Moreover, an eigenfunction in this subspace never vanishes in $]0,1[$. This is quite evident, because $u_0 = \mu \neq 0$. One can also obtain an orthonormal basis of eigenfunctions in $L^2(]0,1[)$ by normalizing the family $(\cos 2\pi n x\ (n \in \mathbb{N}), \sin 2\pi n x\ (n \in \mathbb{N}^*))$ or the family $\exp 2\pi i n x\ (n \in \mathbb{Z})$.

We are merely recovering the L^2-theory of Fourier series here.

1.4.3 The Dirichlet problem

Here we consider spectral pairs $(u, \lambda) \in H^{2,D}(]0,1[) \times \mathbb{C}$ $(u \neq 0)$ such that $-d^2u/dx^2 = \lambda u$, with $H^{2,D}(]0,1[) = \{u \in H^2(]0,1[),\ u(0) = u(1) = 0\}$. It is again an easy exercise to show that these pairs are described by

$$\lambda = \pi^2 n^2,\ v_n = \mu \sin \pi n x,\ \text{ for } n \in \mathbb{N}^*,\ \mu \in \mathbb{R} \setminus \{0\}.$$

We observe that $\lambda = \pi^2$ is the lowest eigenvalue, that its multiplicity is one (here, all the eigenspaces are one dimensional), and that an eigenfunction in this subspace does not vanish in $]0,1[$.

1.4.4 The Neumann problem

Here we consider eigenpairs $(u, \lambda) \in H^{2,N}(]0,1[) \times \mathbb{C}$ $(u \neq 0)$, such that

$$-d^2u/dx^2 = \lambda u,$$

where

$$H^{2,N}(]0,1[) = \{u \in H^2(]0,1[),\ u'(0) = u'(1) = 0\}.$$

It is again an easy exercise to show that these pairs are described by

$$\lambda = \pi^2 n^2,\ v_n = \mu \cos \pi n x, \quad \text{for} \quad n \in \mathbb{N},\ \mu \in \mathbb{R} \setminus \{0\}.$$

We observe that $\lambda = 0$ is the lowest eigenvalue, that its multiplicity is one (here, again, all the eigenspaces are one dimensional), and that the corresponding eigenspace is of dimension one and that an eigenfunction in this subspace does not vanish in $]0, 1[$.

1.5 Aim and organization of the book

By looking at some rather simple operators, we have demonstrated various problems that occur when one tries to extend the notion of an eigenpair of a matrix. Many of the examples involving second-order ordinary differential operators can be treated by the so-called Sturm–Liouville theory. Our goal in this book is to develop a theory that is not limited to 1D problems and not based on explicit computations.

The book is organized into 16 chapters, which are mainly of two types: the first type presents an introduction to a theory (we sometimes choose to skip some of the proofs presented in standard, more complete textbooks), and the second type presents applications, without being afraid to give explicit computations. Hence we hope that the reader will always see how the theory can be used.

Chapter 2 is an introduction to the theory of unbounded operators. We assume here that the reader is familiar with basic Hilbertian and Banach theory, together with the theory of linear bounded operators on Hilbert and Banach spaces.

Chapter 3 presents the Lax–Milgram theorem, which is simply a useful variant of Riesz's theorem characterizing the dual of a Hilbert space.

Chapter 4 introduces the notion of semibounded operators (most of the time semibounded from below) and treats many examples, mainly from quantum mechanics. On the way, the reader will encounter inequalities that belong to the common background of the analyst, such as Hardy's inequality and Kato's inequality, which are of interest in their own right.

Chapter 5 recalls some rather basic material on compact operators and emphasizes examples. We also recall some tools from functional analysis that permit one to recognize if an operator is compact (precompactness criteria).

Chapter 6 also presents some basic material, about the spectral theory of bounded operators. This also provides us with an occasion to visit (sometimes only briefly) various aspects of functional analysis, such as Fredholm theory, index theory, subclasses of the space of compact operators, and the Krein–Rutman theorem.

Chapter 7 describes applications. The first of these is from statistical mechanics (continuous models). The other applications describe cases where the operators involved are unbounded but where one can come back, by considering the inverse, to the spectral theory of compact operators recalled in Chapters 5 and 6.

Chapter 8 returns to the more general spectral theory of unbounded operators, and is mainly standard and devoted to the presentation of an almost complete proof of the spectral theorem. We focus on elementary consequences of this theorem for functional calculus and for the determination of approximate eigenvalues.

Chapter 9, in some sense, answers some of the questions asked in Chapter 1. We give some rather explicit criteria for determining whether an operator is self-adjoint or whether it can be naturally extended to a self-adjoint operator. Again, we discuss some examples (mainly Schrödinger operators) thoroughly.

There are several different ways to distinguish between different subsets of a spectrum. We have chosen in Chapter 10 to present the decomposition of a spectrum into two parts: the essential spectrum and the discrete spectrum. As an application, we consider the case of the Schrödinger operator with a constant magnetic field.

In many situations, the problems considered depend on various parameters, and a comparison of the spectra of different problems could be difficult without a variational characterization of the eigenvalues, which is the subject of Chapter 11. This point of view is useful for finite-dimensional matrices.

Chapter 12 presents a short walk through the theory of fluid mechanics, and this permits us to see "spectral theory in action" with a rather explicit computation.

Chapter 13 is devoted to some ideas that appear to be important when we are no longer in the self-adjoint case. We give some basic properties of some specific families of neighborhoods of the spectrum computed by analyzing the growth of the resolvent. After recalling some elements of the theory of semigroups and their generators, we present some recent improvements on the Gearhart–Prüss theorem.

Since most of the books devoted to the material presented in Chapter 13 are written in a rather abstract way, we have chosen in Chapters 14 and 15 to discuss how the theorems can be applied in interesting cases. Here, "interesting" may mean either that one can compute everything in great detail or that an apparently simple model plays an important role in the explanation of a physical phenomenon, for example in the theory of superconductivity, in fluid mechanics, or in kinetic theory.

Although many examples are given in the body of and at the end of each chapter, in the last chapter we present various problems that should be solvable after the reader has understood, say, the first ten chapters.

Instead of giving references in the body of the chapters, we give references together with remarks and comments at the end of each chapter, in a section entitled "Notes."

Acknowledgments Some of the material for this book was prepared together with colleagues for specific lectures or courses. I would like particularly to thank S. Fournais in this respect. Some other material has come rather directly from collaborations and discussions with Ph.D. students and colleagues: I would like in particular to thank Y. Almog, W. Bordeaux-Montrieux, T. Gallay, R. Henry, J. Martinet, F. Nier, X. Pan, and J. Sjöstrand for the part related to non-self-adjoint problems. Discussions (sometimes a long time ago) with B. Davies, A. Laptev, O. Lafitte, P. Lévy-Bruhl, and D. Robert were also very useful. Finally, I would like to thank R. Henry, F. Hérau, and C. Lena for their critical reading of chapters of the book.