

Lecture Notes¹ for the course
Introduction to Spectral Theory

Master Mathématiques et Applications
parcours *Analyse, Modélisation, Simulation* et
Analyse, Arithmétique, Géométrie

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Some notations

We list some notations used throughout the text.

The symbol \mathbb{N} denotes the set of the natural numbers starting from 0.

If (M, \mathcal{T}, μ) is a measure space and $f : M \rightarrow \mathbb{C}$ is a measurable function, then we denote the *essential range* and the *essential supremum* of f w.r.t. the measure μ :

$$\begin{aligned} \text{ess}_\mu \text{Ran } f &\stackrel{\text{def}}{=} \left\{ z \in \mathbb{C} : \mu\{x \in M : |z - f(x)| < \epsilon\} > 0 \text{ for all } \epsilon > 0 \right\}, \\ \text{ess}_\mu \sup |f| &\stackrel{\text{def}}{=} \inf \left\{ a \in \mathbb{R} : \mu\{x \in M : |f(x)| > a\} = 0 \right\}. \end{aligned}$$

If the measure μ is obvious in the context, we will omit to indicate it in the notations.

In the following, we will consider linear operators acting on a complex Banach space, which we will usually denote by the letter \mathcal{B} , but a large part of the notes will be focussed on the case of Hilbert spaces. What we call a *Hilbert space* will mean a *separable complex Hilbert space*, which we will generally denote by \mathcal{H} .

Because we'll have in mind mostly Hilbert spaces made of functions on \mathbb{R}^d or some domain $\Omega \subset \mathbb{R}^d$, we will denote the "vectors" of \mathcal{H} by u, v, w, \dots . For two vectors $u, v \in \mathcal{H}$, $\langle u, v \rangle$ will denote the sesquilinear scalar product of u and v . If several Hilbert spaces are considered in the problem, we will specify the scalar product with the notation $\langle u, v \rangle_{\mathcal{H}}$. To respect the convention in quantum mechanics, our scalar products will always be linear with respect to the *second* argument, and antilinear with respect to the first one:

$$\forall \alpha \in \mathbb{C} \quad \langle u, \alpha v \rangle = \langle \bar{\alpha} u, v \rangle = \alpha \langle u, v \rangle.$$

For example, the scalar product in the Lebesgue space $L^2(\mathbb{R})$ is defined by

$$\langle f, g \rangle_{L^2} = \int_{\mathbb{R}} \overline{f(x)} g(x) dx.$$

If A is a finite or countable set, $\ell^2(A)$ denotes the vector space of square-summable functions $u : A \rightarrow \mathbb{C}$:

$$\sum_{a \in A} |u(a)|^2 < \infty.$$

This forms a Hilbert space, equipped with the scalar product

$$\langle u, v \rangle = \sum_{a \in A} \overline{u(a)} v(a).$$

Note that when $A = \mathbb{N}$ or $A = \mathbb{Z}$ the functions u are sometimes written as sequences: $u(a) = u_a$.

$\mathcal{L}(\mathcal{B})$ and $\mathcal{K}(\mathcal{B})$ denote the spaces of continuous linear operators, respectively of compact operators from \mathcal{B} to \mathcal{B} . A similar notation applies also to bounded, resp. compact operators on a Hilbert space \mathcal{H} .

Some functional spaces

If $\Omega \subset \mathbb{R}^d$ is a domain (= convex open set) and $k \in \mathbb{N}$, then $H^k(\Omega)$ denotes the k th Sobolev space on Ω , i.e. the space of functions in L^2 , whose partial derivatives up to order k are also in $L^2(\Omega)$. The Sobolev space $H^k(\Omega)$ is equipped with the scalar product:

$$(0.0.1) \quad \langle u, v \rangle_{H^k} = \sum_{|\alpha| \leq k} \langle \partial^\alpha u, \partial^\alpha v \rangle_{L^2},$$

where $\alpha = (\alpha_1, \dots, \alpha_d) \in \mathbb{N}^d$ is a multiindex, and $\partial^\alpha = \partial_{x_1}^{\alpha_1} \dots \partial_{x_d}^{\alpha_d}$ is the multi-derivative operators. It is complete w.r.t. the norm associated with this scalar product.

We will use a notation frequent in the theory of partial differential equations: the symmetric derivative operator $D_x = \frac{1}{i} \partial_x$, as well as its multi-derivative version

$$D^\alpha = D_{x_1}^{\alpha_1} \dots D_{x_d}^{\alpha_d} = (-i)^{|\alpha|} \partial^\alpha, \quad \alpha \in \mathbb{N}^d.$$

By $H_0^k(\Omega)$ we denote the completion in $H^k(\Omega)$ of the subspace $C_c^\infty(\Omega)$ (with respect to the norm of $H^k(\Omega)$). The symbol $C^k(\Omega)$ denotes the space of functions on Ω whose partial derivatives up to order k are continuous; in particular, the set of the continuous functions is denoted as $C^0(\Omega)$. This should not be confused with the notation $C_0(\mathbb{R}^d)$ for the space of continuous functions $f : \mathbb{R}^d \rightarrow \mathbb{C}$ vanishing at infinity: $\lim_{|x| \rightarrow \infty} f(x) = 0$. The subscript $_{\text{comp}}$ on a functional space indicates that its elements have compact supports: for instance $H_{\text{comp}}^1(\mathbb{R}^d)$ is the space of functions in $H^1(\mathbb{R}^d)$ having compact supports.

We denote by $\mathcal{F} : L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)$ the Fourier transform, defined for $f \in \mathcal{S}(\mathbb{R}^d)$ by:

$$\mathcal{F}f(\xi) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} f(x) e^{-i\xi \cdot x} dx.$$

The normalization makes this transform unitary on $L^2(\mathbb{R}^d, dx)$. The Fourier transformed function $\mathcal{F}f$ will sometimes be denoted by \hat{f} .

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Recommended books

During the preparation of the notes, we used part of the lecture notes by Bernard Helffer [6]. Other recommended books are the one E. B. Davies [4] and the book of G. Teschl [13] (available online). A detailed account is given in the series by Reed&Simon, in particular [7, 8, 9].

Additional references for particular topics will be given throughout the text.

Chapter 1

What is a Spectrum ?

1.1 The spectrum in physics

The term "spectrum" first appeared in different domains of physics; originally it described the decomposition of the light observed from the spatial objects (like the sun, or other stars), when observed through a device able to separate the different colors (that is, the different frequencies of the received light). Quite often, one could observe peaks of luminosity at certain frequencies, above a more or less uniform "background". Chemists observed that the light emitted by some gases always produced peaks at the same frequencies: the emitted spectra were thus characteristic of chemical elements, and allow to identify the presence of these elements in distant bodies (e.g. stars).

In the study of electric circuits and electronics, one often observes a time signal (e.g. of the voltage along some part of the circuit). This time signal $S(t)$ can be analyzed through the Fourier transform, or the Laplace transform

$$\hat{S}(\omega) = \int_0^{\infty} e^{-i\omega t} S(t) dt$$

(we assume that the signal vanishes for negative times). Often one cannot detect the phase of $\hat{S}(\omega)$, but only observes $|\hat{S}(\omega)|^2$, which is called the *power spectrum* of the signal $S(t)$. For instance, the RLC circuit leads to a power spectrum which is peaked near the characteristic frequency $\omega_0 = \frac{1}{\sqrt{LC}}$, the width of the peak depending on the value of the resistance R (in case of vanishing resistance, the signal is a δ peak at $\omega = \omega_0$).

In both examples, the spectrum corresponds to a decomposition in frequency. The hope is to analyze a (possibly complicated) time signal, through a (hopefully small) set of characteristic frequencies, which would contain most of the "interesting" information of the signal.

1.2 An example: Schrödinger evolution in quantum mechanics

This analysis is most relevant when the dynamics under study can be modeled by a semigroup generated by a *linear operator*. We will take for example the case of Quantum Mechanics, where the notion

of spectrum acquired a central place, which acted as a strong incentive to the fast development of spectral theory in mathematics.

The state of a quantum particle evolving in some domain ("box") $\Omega \subset \mathbb{R}^d$ is represented by a time-dependent wavefunction

$$\psi : \mathbb{R} \ni t \mapsto \psi(t) \in L^2(\Omega).$$

The state of the particle at time $t \in \mathbb{R}$ is represented by the function $\psi(t) \in L^2(\Omega)$. Quantum mechanics is a probabilistic theory: if one uses a device to measure the position of the particle at time t , then $|\psi(t, x)|^2$ represents the probability density to detect the particle at the point x . With this probabilistic interpretation in mind, one needs to enforce the normalization:

$$\forall t \in \mathbb{R}, \quad \|\psi(t)\|_{L^2} = 1.$$

Quantum mechanics prescribes the law of evolution of $\psi(t)$: it is given by the (time dependent) Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \psi(t, x) = -\frac{\hbar^2}{2m} \Delta \psi(t, x) + V(x) \psi(t, x),$$

where $\Delta = \sum_{j=1}^d \frac{\partial^2}{\partial x_j^2}$ is the Laplacian, and the real valued function $V : \Omega \rightarrow \mathbb{R}$ represents the potential energy of the particle (e.g. the electric potential, if the particle carries an electric charge).

By rescaling the units of time and space, we can remove the physical constants, to obtain¹:

$$(1.2.1) \quad i \frac{\partial}{\partial t} \psi(t, x) = -\Delta \psi(t, x) + V(x) \psi(t, x) = [P \psi](t)$$

where $P = -\Delta + V$ appears as a linear operator acting on the Hilbert space $\mathcal{H} = L^2(\Omega)$; it is called a Schrödinger operator, or also the *Hamiltonian* of this quantum system. This equation therefore takes the form of a linear evolution equation, where the operator P acts as the generator of a semigroup on \mathcal{H} . The operator P is unbounded on \mathcal{H} .

Several mathematical questions pop up. A generic function $\psi \in L^2$ does not admit derivatives in L^2 , so $\Delta \psi$ is not well-defined on L^2 . This means that the operator Δ is not defined on the whole of L^2 , but only on a linear subspace of that space, namely the Sobolev space $H^2(\Omega)$. If the potential V is bounded on Ω , then P is still well-defined on $H^2(\Omega)$. We call $H^2(\Omega)$ the *domain* of the operator P , denoted by $D(P)$. In this course we will pay a special attention to the domains of operators.

Another question (both physical and mathematical) concerns the boundary behaviour of the functions $\psi(t)$: from physical ground, we may want to assume that the wavefunctions $\psi(t, x)$ vanish when x approaches the boundary of the box $\partial\Omega$. One may want to take into account such a physical constraint, when defining the domain of P .

1.2.1 The Schrödinger group

Semigroup theory, in particular the Hille-Yosida theorem, teaches us that, under favorable conditions on the operator $P : D(P) \rightarrow \mathcal{H}$, this operator will generate a semigroup of evolution, meaning that for

1. Implicitly, the functions ψ and V have been modified by the rescaling, but we keep the same notations.

any initial data $\psi(0) \in D(P)$, the equation (1.2.1) admits a unique solution $\psi \in C^1(\mathbb{R}_+, \mathcal{H})$, defined through a semigroup of bounded operators $S(t) : \mathcal{H} \rightarrow \mathcal{H} : \psi(t) = S(t)\psi(0)$. What is remarkable is that this semigroup extends to the full Hilbert space \mathcal{H} , namely the evolution is actually defined even for initial data $\psi(0) \notin D(P)$.

The “favorable conditions” on the operator H can be expressed in terms of the *resolvent* of the operator, which will play a crucial role in these notes. We will give a more formal definition of the resolvent, but roughly speaking it is a family of bounded operators $R(z) = (P - z)^{-1} : \mathcal{H} \rightarrow \mathcal{H}$, depending on complex parameter z defined on some open subset of \mathbb{C} .

In the case of the Schrödinger operator P acting on $L^2(\Omega)$, which is symmetric, these conditions can be replaced by a positivity argument, provided the potential V is bounded from below. We will see that, if one makes “good” choices of domain $D(P)$, the operator P is not only symmetric, but actually *selfadjoint*. In this case, the semigroup generated by P extends to a *unitary group* $(U^t)_{t \in \mathbb{R}}$ on $L^2(\Omega)$, which describes the quantum evolution:

$$\forall t \in \mathbb{R}, \quad \psi(t) = U^t \psi(0).$$

Formally, we will often write $U^t = e^{-itP}$, even though the exponential of P cannot be defined by a power series because the powers P^n have smaller and smaller domains when $n \rightarrow \infty$.

1.2.2 Spectral expansion

In order to describe more quantitatively the behaviour of $\psi(t) = U^t \psi(0)$, one is led to study the *spectrum* of the operator P . Let us restrict ourselves to the case where

- i) the “box” Ω is bounded,
- ii) one imposes Dirichlet boundary conditions on Ω ,
- iii) and the potential $V \in L^\infty(\Omega)$.

In that case, we will show that the spectrum of P is purely discrete: it is composed of a countable set of real eigenvalues $(\lambda_j)_{j \in \mathbb{N}}$ of finite multiplicities, associated with a family of eigenfunctions $(\varphi_j)_{j \in \mathbb{N}}$ which form an orthonormal Hilbert basis of $L^2(\Omega)$. This spectral information allows to expand the evolved state $\psi(t)$, taking into account the decomposition of $\psi(0)$ in this eigenbasis:

$$(1.2.2) \quad \psi(0) = \sum_{j \in \mathbb{N}} \langle \varphi_j, \psi(0) \rangle \varphi_j \quad \forall t \in \mathbb{R}, \quad \psi(t) = \sum_{j \in \mathbb{N}} e^{-it\lambda_j} \langle \varphi_j, \psi(0) \rangle \varphi_j.$$

We note that the spectrum of the differential operator P generally depends on the choice of its domain $D(P)$, and so does the expansion (1.2.2). For instance, requiring Dirichlet, vs. Neumann boundary conditions, leads to two different discrete spectra for P . This shows that the question of domain is not just a mathematical subtlety, but it directly impacts the evolution of the quantum state.

1.2.3 Stationary states

The above expansion shows that, if the initial state is an eigenstate of P , namely $\psi(0) = \varphi_j$ for some j , then the evolution of ψ is very simple:

$$\psi(t) = e^{-it\lambda_j} \psi(0) = e^{-it\lambda_j} \varphi_j.$$

The global phase factor $e^{-it\lambda_j}$ is not detectable physically, which explains why such a particle is said to occupy a *stationary* state. This solution shows that the system will remain for ever in the state φ_j . As a result, a large part of atomic and molecular physics consists in computing the eigenvalues (λ_j) and eigenstates (φ_j) of the corresponding Hamiltonian operator.

Yet, this description of atoms is too simplistic. Indeed, in atomic physics textbooks, the evolution of the atom (or molecule) is usually described as a sequence of “jumps” between different stationary states $\varphi_i \rightarrow \varphi_j$, induced by the absorption or emission of a photon of energy

$$h_{Planck} \nu_{ij} = |\lambda_j - \lambda_i|.$$

Such an evolution through “jumps” cannot simply result from the Schrödinger group described above, it requires to incorporate the interaction between the atom and the electromagnetic field embodied in the photons. We will not pursue this project in these notes. Still, the above equation shows that measuring the energy (\equiv frequency ν_{ij}) of emitted or absorbed photons allows to reconstruct the spectra of atoms and molecules.

1.3 Example of the heat equation

Let us briefly describe another equation making use of the spectral decomposition of the Laplacian on a bounded open set $\Omega \subset \mathbb{R}^d$. The heat equation

$$\partial_t \theta(t, x) = D \Delta \theta(t, x)$$

describes the evolution of the temperature $\theta(t, x)$ in a body Ω , when this body is inserted in a thermostat of given temperature $\theta_{th} \in \mathbb{R}$, starting from a given temperature distribution $\theta(0, x)$. Here $D > 0$ is a fixed parameter, called the diffusion constant; as above, by rescaling the space or time, we may assume that $D = 1$. The function $u(t) = \theta(t) - \theta_{th}$ describes the relative temperature wr.r.to the thermostat. The physical condition of thermal contact at the boundary of Ω imposes the constraint $\theta(t, x) = \theta_{th}$ for all $t > 0$, $x \in \partial\Omega$. It is easier to consider the relative temperature $u(t, x) \stackrel{\text{def}}{=} \theta(t, x) - \theta_{th}$, which satisfies the Dirichlet boundary conditions, and satisfies the same heat equation as θ . The discrete spectrum of $P = -\Delta$ implies the following spectral expansion for the function u :

$$(1.3.3) \quad u(t) = \sum_{j \in \mathbb{N}} e^{-t\lambda_j} \langle \varphi_j, u_0 \rangle \varphi_j.$$

As opposed to the expansion (1.2.2), we see that the above expansion is dominated by its first few terms when $t \rightarrow \infty$. To understand the long time behaviour of the heat equation, it is not necessary to identify the full spectrum, but only the “bottom” of the spectrum of P .

This example shows that, quite often, a partial description of the spectrum (like the identification of the bottom of the spectrum, or the presence of a *spectral gap* at the bottom), already provides relevant physical information for equations like the heat equation.

Focussing on selfadjoint operators on Hilbert spaces

In situations where the spectrum of P is not purely discrete, a similar (yet more complicated) decomposition can be written. Such a decomposition uses the *spectral theorem for selfadjoint operators*. The power of this theorem, and its relevance for quantum mechanics, induce us to devote a large part of the present notes to the specific case of selfadjoint operators defined on a Hilbert space. We will already see that the precise identification of such operators (including their domains) requires some care. A nice way to construct such selfadjoint operators is through the use of *quadratic forms*.

Yet, spectral expansions (possibly with some remainder term) can also be helpful in nonselfadjoint situations, for instance when the natural functional space is not a Hilbert space, but only a Banach space, for instance a space of Lebesgue type $L^p(\Omega)$, a Sobolev space based on such an L^p . Alternatively, the applications of spectral theory to statistical physics or dynamical systems theory, often use spaces of finitely differentiable functions $C^k(\Omega)$, or spaces of analytic functions $C^\omega(\Omega)$ and their variants.

Chapter 2

Bounded vs. Unbounded operators

In this section, after recalling the definition of a bounded operator on a Hilbert (or Banach) space, we start to describe a more general class of linear operators, namely (densely defined) unbounded operators, which will constitute the main focus of these notes. The Schrödinger operator $P = -\Delta + V$ on $L^2(\Omega)$ mentioned in the introduction is an example of such unbounded operators; actually, all differential operators belong to that class, which explains the importance of the study of these operators towards understanding linear (and actually, also nonlinear) Partial Differential Equations.

2.1 Some definitions

A *linear operator* T on a Banach space \mathcal{B} is a linear map from a subspace $D(T) \subset \mathcal{B}$ (called the *domain* of T) to \mathcal{B} . The domain is an important component of the definition of the operator, so one should actually denote the operator by the pair $(T, D(T))$. Yet, we will often omit to mention the domain, keeping the shorter notation T .

Across these notes, we will most of the time assume that the domain $D(T)$ is a *dense* subspace of \mathcal{B} (w.r.to the natural topology of \mathcal{B}). On a Hilbert space \mathcal{H} , a characterization of that density is the property $D(T)^\perp = \{0\}$, where \bullet^\perp is the orthogonal space to \bullet .

The *range* of $(T, D(T))$ is the set $\text{Ran } T \stackrel{\text{def}}{=} \{Tu : u \in D(T)\}$; this is obviously a linear subspace of \mathcal{B} . We say that a linear operator T is *bounded* if the quantity

$$\mu(T) \stackrel{\text{def}}{=} \sup_{\substack{u \in D(T) \\ u \neq 0}} \frac{\|Tu\|}{\|u\|}$$

is finite. On the opposite, an operator $(T, D(T))$ will be said to be *unbounded* if $\mu(T) = \infty$.

If $D(T) = \mathcal{B}$ and T is bounded, then the operator $T : \mathcal{B} \rightarrow \mathcal{B}$ is *continuous*. The set of continuous operators on \mathcal{B} forms a vector space, denoted by $\mathcal{L}(\mathcal{B})$. Equipped with the norm $\|T\| \stackrel{\text{def}}{=} \mu(T)$, this space has the structure of a *Banach algebra*: it is a Banach space, and also hosts an internal product $S, T \in \mathcal{L}(\mathcal{B}) \mapsto ST = S \circ T \in \mathcal{L}(\mathcal{B})$, with the inequality $\|ST\| \leq \|S\| \|T\|$.

Proposition 2.1.1 Assume $(T, D(T))$ is a *bounded* linear operator on \mathcal{B} with a dense domain $D(T)$. Then T can be *uniquely* extended to a continuous linear operator defined on all of \mathcal{B} . This extension is called the *closure* of T , and is usually denoted by \overline{T} .

Proof.— Let us consider an element $u \in \mathcal{B} \setminus D(T)$. By the density of $D(T)$ in \mathcal{B} , we may consider a sequence $(u_n \in D(T))_{n \in \mathbb{N}}$ converging to u in \mathcal{B} . The sequence $(Tu_n)_{n \in \mathbb{N}}$ satisfies $\|Tu_n - Tu_m\| \leq \|T\| \|u_n - u_m\|$, hence it is a Cauchy sequence in \mathcal{B} , and admits a limit $w \in \mathcal{B}$. Let us decide that w is the image of u through an extended operator \overline{T} ; we need to check that this image does not depend on the choice of sequence converging to u . Indeed, if (\tilde{u}_n) is another sequence converging to u , with $T\tilde{u}_n$ converging to some $\tilde{w} \in \mathcal{B}$, then considering the alternating sequence $(u_0, \tilde{u}_0, u_1, \tilde{u}_1, \dots)$ shows that $w = \tilde{w}$, therefore the image of u is unique. It is easy to check that the resulting operator \overline{T} is linear, and bounded, with the same norm $\|\overline{T}\| = \|T\|$. \square

2.1.1 Closed unbounded operators

If $(T, D(T))$ is unbounded, it is not possible to extend it to all of \mathcal{B} in a natural way. Yet, we can aim at an alternative property, *closedness*, which refers to a topological property of the *graph* of T .

Definition 2.1.2 (Graph of a linear operator) The *graph* of a linear operator $(T, D(T))$ is the set

$$\text{gr } T \stackrel{\text{def}}{=} \{(u, Tu) : u \in D(T)\} \subset \mathcal{B} \times \mathcal{B}.$$

This is obviously a linear subspace of $\mathcal{B} \times \mathcal{B}$.

For two linear operators T_1 and T_2 in \mathcal{B} , we write $T_1 \subset T_2$ if $\text{gr } T_1 \subset \text{gr } T_2$. Namely, $T_1 \subset T_2$ means that $D(T_1) \subset D(T_2)$ and that $T_2 u = T_1 u$ for all $u \in D(T_1)$; the operator T_2 is then called an *extension* of T_1 , while T_1 is called a *restriction* of T_2 .

Definition 2.1.3 (Closed operator, closable operator)

- An operator $(T, D(T))$ on \mathcal{B} is called *closed* if its graph is a closed subspace in $\mathcal{B} \times \mathcal{B}$.
- An operator $(T, D(T))$ on \mathcal{B} is called *closable*, if the closure $\overline{\text{gr } T}$ of the graph of T in $\mathcal{B} \times \mathcal{B}$ is still the graph of a certain operator, which we call \overline{T} . The latter operator \overline{T} is called the *closure* of T .

An easy exercise shows that any continuous operator $T \in \mathcal{L}(\mathcal{B})$ is closed. Similarly, if we start from a bounded operator $(T, D(T))$ defined on a dense domain, the extension \overline{T} constructed in Proposition 2.1.1 is the closure of T .

The closedness property can be characterized in terms of sequences.

Proposition 2.1.4 A linear operator T in \mathcal{B} is closed if and only if, for any sequence $(u_n)_{n \in \mathbb{N}}$ satisfying the following two conditions:

- i) the sequence $(u_n)_{n \in \mathbb{N}}$ converges to some element $u \in \mathcal{B}$,
- ii) the sequence $(Tu_n)_{n \in \mathbb{N}}$ converges to $v \in \mathcal{B}$,

then one has $u \in D(T)$ and $v = Tu$.

In some sense, there is no natural way to extend a closed operator T .

Another characterization of the closedness can be obtained by introducing an auxiliary norm on $D(T)$, called the *graph norm*.

Definition 2.1.5 (Graph norm) Let $(T, D(T))$ be a linear operator on \mathcal{B} . We define on $D(T)$ the function:

$$u \mapsto \|u\|_T \stackrel{\text{def}}{=} \|u\|_{\mathcal{B}} + \|Tu\|_{\mathcal{B}}.$$

One easily checks that it makes up a norm on $D(T)$. We call it the *graph norm for T* .

If $\mathcal{B} = \mathcal{H}$ is a Hilbert space, the graph norm is usually defined alternatively as

$$\|u\|'_T \stackrel{\text{def}}{=} \sqrt{\|u\|_{\mathcal{H}}^2 + \|Tu\|_{\mathcal{H}}^2}$$

This definition has the advantage to be a Hilbert norm, associated with the scalar product $\langle u, v \rangle_T = \langle u, v \rangle + \langle Tu, Tv \rangle$. This norm is equivalent with $\|\cdot\|_T$.

If T is bounded, the graph norm is equivalent with the standard norm. But this is not the case for an unbounded operator.

The closedness property can then be characterized as follows.

Proposition 2.1.6 Let $(T, D(T))$ be a linear operator on \mathcal{B} .

- i) $(T, D(T))$ is closed iff the domain $D(T)$, equipped with the graph norm, is a complete Banach space.

ii) if $(T, D(T))$ is closable, then the domain $D(T)$, equipped with the graph norm, can be completed inside \mathcal{B} , namely its completion $\overline{D(T)}^{\|\cdot\|_T}$ can be identified with a certain subspace of \mathcal{B} , thereby extending the norm $\|\cdot\|_T$ to that subspace. This subspace is then the domain $D(\overline{T})$ of the operator \overline{T} .

The second point is a bit subtle: a normed space like $(D(T), \|\cdot\|_T)$ will always admit a formal completion, that is a Banach space $\tilde{\mathcal{B}}$ such that $D(T)$ embeds into $\tilde{\mathcal{B}}$ isometrically, and in a dense way. However, in general it is not clear whether $\tilde{\mathcal{B}}$ can be identified with a subspace of the initial Banach space \mathcal{B} . See Example 2.1.11 for a counter-example to this property.

Proposition 2.1.7 (Closed graph theorem) A linear operator T on \mathcal{B} with $D(T) = \mathcal{B}$ is closed if and only if it is bounded.

Proof.— The implication bounded \implies closed is obvious. Conversely, let us assume that T is closed with $D(T) = \mathcal{B}$. Its graph $\text{gr } T$ is thus a closed linear subspace of the Banach space $\mathcal{B} \times \mathcal{B}$, hence $\text{gr } T$ can be viewed itself as a Banach space. Consider the two natural projections $p_1, p_2 : \mathcal{B} \times \mathcal{B} \rightarrow \mathcal{B}$; they are obviously continuous linear maps. Their restrictions on $\text{gr } T \rightarrow \mathcal{B}$ are still continuous. In particular, the first projection $p_1 : \text{gr } T \rightarrow \mathcal{B}$ is a continuous bijection (because $D(T) = \mathcal{B}$). The *isomorphism theorem* then states that its inverse map $q : \mathcal{B} \rightarrow \text{gr } T$ is also a continuous bijection. Finally, the composition $p_2 \circ q : \mathcal{B} \rightarrow \mathcal{B}$ is continuous. But note that $p_2 \circ q$ is nothing but T itself.

$$\begin{array}{ccc} (u, Tu) & \xrightarrow{p_2} & Tu \\ q \uparrow \downarrow p_1 & \nearrow & T \\ u & & \end{array}$$

□

We now give some examples of closed unbounded operators.

Example 2.1.8 (Multiplication operator) Take $\mathcal{H} = L^2(\mathbb{R}^d)$ and pick $f \in L^\infty_{\text{loc}}(\mathbb{R}^d)$. Define a linear operator M_f in \mathcal{H} as follows:

$$D(M_f) = \{u \in L^2(\mathbb{R}^d) : fu \in L^2(\mathbb{R}^d)\} \text{ and } M_f u = fu \text{ for } u \in D(M_f).$$

It can be easily seen that $D(M_f)$, equipped with the graph norm $\|\cdot\|'_{M_f}$, coincides with the weighted space $L^2(\mathbb{R}^d, (1+|f|^2)dx)$, which is a Hilbert space, hence complete. This shows that M_f is closed.

Exercise 2.1.9 For any $p \in [1, \infty[$, one may define a closed multiplication operator M_f on $\mathcal{B} = L^p(\mathbb{R}^d)$ in a similar way.

Using the Fourier transform, we are able to transform certain multiplication operators on $\mathcal{H} = L^2$ into differential operators with constant coefficients. Let us start with the most famous one, the Laplacian on \mathbb{R}^d , which will appear many times in these notes.

Example 2.1.10 (Laplacians in \mathbb{R}^d) Take $\mathcal{H} = L^2(\mathbb{R}^d)$ and consider two operators in \mathcal{H} :

$$\begin{aligned} T_0 u &= -\Delta u, & D(T_0) &= C_c^\infty(\mathbb{R}^d), \\ T_1 u &= -\Delta u, & D(T_1) &= H^2(\mathbb{R}^d) \quad (\text{second Sobolev space}). \end{aligned}$$

We are going to show that $\overline{T_0} = T_1$ (this implies that T_1 is closed, while T_0 is not).

For this aim, we will use the Fourier transform to transform the differential operator Δ into a multiplication operator.

When acting on a function $f \in \mathcal{S}(\mathbb{R}^d)$, we have the identity

$$\mathcal{F}\Delta f(\xi) = -|\xi|^2 \mathcal{F}f(\xi), \quad \xi \in \mathbb{R}^d,$$

showing that $-\Delta$ is conjugate to the multiplication operator by $|\xi|^2$.

By duality, the above identity holds as well for distributions $f \in \mathcal{S}'(\mathbb{R}^d)$. But we would like to restrict $-\Delta$ to the Sobolev space $H^2(\mathbb{R}^d)$. How does this space translate on the Fourier side?

$$f \in H^2(\mathbb{R}^d) \iff \hat{f}, \xi_j \hat{f}, \xi_j \xi_k \hat{f} \in L^2(\mathbb{R}^d), \quad \text{for any indices } j, k.$$

The conditions on the right-hand side can be simplified. Indeed, the bounds:

$$(2.1.1) \quad \forall \xi \in \mathbb{R}^d, \forall j, k = 1, \dots, d, \quad |\xi_j \xi_k| \leq \frac{\xi_j^2 + \xi_k^2}{2} \leq |\xi|^2, \quad |\xi_j| \leq \frac{1 + \xi_j^2}{2} \leq (1 + |\xi|^2),$$

imply that

$$(2.1.2) \quad \begin{aligned} f \in H^2(\mathbb{R}^d) &\iff (1 + |\xi|^2) \hat{f} \in L^2(\mathbb{R}^d) \\ &\iff (1 - \Delta) f \in L^2(\mathbb{R}^d) \\ &\iff f, \Delta f \in L^2(\mathbb{R}^d). \end{aligned}$$

The first line shows that the operator T_1 , with domain $H^2(\mathbb{R}^d)$, is unitarily conjugate through the Fourier transform to the operator \hat{T} defined by

$$D(\hat{T}) = \{g \in L^2 : |\xi|^2 g \in L^2\}, \quad \hat{T}g(\xi) = |\xi|^2 g(\xi).$$

In other words, we have the exact conjugacy

$$T_1 = \mathcal{F}^{-1} \hat{T} \mathcal{F}, \quad D(T_1) = \mathcal{F}^{-1} D(\hat{T}).$$

This conjugacy shows the following relation between the graphs of the two operators:

$$\text{gr } T_1 = \{(\mathcal{F}^{-1}u, \mathcal{F}^{-1}\hat{T}u) : u \in D(\hat{T})\} = K(\text{gr } \hat{T}),$$

where K is the linear operator on $L^2 \times L^2$ defined by $K(u, v) = (\mathcal{F}^{-1}u, \mathcal{F}^{-1}v)$. The unitarity of \mathcal{F} implies that K acts unitarily on $L^2 \times L^2$, in particular it maps closed sets to closed sets.

Now, the example 2.1.8 shows that the multiplication operator \hat{T} is closed on $L^2(\mathbb{R}^d)$, which means that $\text{gr } \hat{T}$ is closed in $L^2 \times L^2$. Finally, $\text{gr } T_1 = K(\text{gr } \hat{T})$ is a closed set too, hence T_1 is closed.

Since T_0 is a restriction of the closed operator T_1 , namely $D(T_0) \subset D(T_1)$, it follows that $\overline{\text{gr } T_0}$ is a graph. Hence T_0 is closable, and the domain of its closure $D(\overline{T_0})$ is the closure of $D(T_0)$ in the graph norm of T_0 (Proposition 2.1.6).

What is this graph norm? The inequalities (2.1.1) show that the standard norm on H^2 , expressed through the Fourier conjugacy, reads:

$$\|f\|_{H^2}^2 = \|\hat{f}\|_{L^2}^2 + \sum_j \|\xi_j \hat{f}\|_{L^2}^2 + \sum_{j,k} \|\xi_j \xi_k \hat{f}\|_{L^2}^2,$$

This norm is equivalent with the modified norm

$$\|f\|_{\text{modif}}^2 \stackrel{\text{def}}{=} \|\hat{f}\|_{L^2}^2 + \|\xi^2 \hat{f}\|_{L^2}^2 = \|f\|_{L^2}^2 + \|\Delta f\|_{L^2}^2,$$

namely the graph norm of T_0 , so the two norms generate the same topology. The space $D(T_1) = H^2$ is hence complete w.r.to the norm $\|\cdot\|_{\text{modif}} = \|\cdot\|_{T_1} \sim \|\cdot\|_{H^2}$ (using the first item of Proposition 2.1.6, this is a second way to prove that T_1 is closed).

Finally, we know that $D(T_0) = C_c^\infty$ is a dense subspace in H^2 (w.r.to the corresponding Sobolev norm), hence its closure in H^2 is the full space $H^2 = D(T_1)$. In conclusion, $D(\overline{T_0}) = H^2 = D(T_1)$, or equivalently $\overline{T_0} = T_1$.

Let us now exhibit a simple operator which does NOT admit a closure.

Example 2.1.11 (Non-closable operator) Take $\mathcal{B} = L^p(\mathbb{R})$ for some $p \in [1, \infty[$, and pick a nontrivial function $g \in \mathcal{B}$. Consider the rank-1 operator L defined on $D(L) = C^0(\mathbb{R}) \cap L^p(\mathbb{R})$ by $Lf = f(0)g$. Let us show that this operator is *not* closable.

Choose some nontrivial function $f \in D(L)$. It is easy to construct two sequences $(f_n)_{n \in \mathbb{N}}$, $(g_n)_{n \in \mathbb{N}}$ in $D(L)$ such that both converge in L^p to f , but with $f_n(0) = 0$ and $g_n(0) = 1$ for all n . Then for all n we have $Lf_n = 0$, while $Lg_n = g$: both sequences Lf_n and Lg_n converge to different limits. This shows that the closure of $\text{gr } L$ in $\mathcal{B} \times \mathcal{B}$ is not a graph, since it contains both elements $(f, 0)$ and (f, g) . Hence L is not closable.

If we try to complete $D(L)$ w.r.to the graph norm $\|\cdot\|_L$, we will obtain a space $\tilde{\mathcal{B}}$ isometric to $L^p(\mathbb{R}) \times \mathbb{R}$, which takes into account both the limiting function $\lim_n f \in L^p(\mathbb{R})$, and the limiting values $\lim_n f_n(0)$. The space $\tilde{\mathcal{B}}$ is “larger” than $L^p(\mathbb{R})$, since it records the extra information of the value taken by the function at zero.

The next example generalizes the case of the Laplacian, and shows that considering differential operators acting on a domain $\Omega \subsetneq \mathbb{R}^d$ with boundaries makes the analysis more tricky.

2.1.2 Partial differential operators

Let Ω be an open subset of \mathbb{R}^d and $P(x, D_x)$ be a partial differential expression with C^∞ coefficients:

$$P(x, D_x) = \sum_{|\alpha| \leq m} a_\alpha(x) D^\alpha, \quad a_\alpha \in C^\infty(\Omega),$$

where we use the notation $D_x = \frac{1}{i} \partial_x$, and $D^\alpha = D_{x_1}^{\alpha_1} \cdots D_{x_d}^{\alpha_d}$ for multiple derivatives. Choosing as reference space $\mathcal{H} = L^2(\Omega)$, this differential expression defines a linear operator P on the domain $D(P) = C_c^\infty(\Omega)$, $Pu(x) = P(x, D_x)u(x)$. Like in the example of the Laplacian, we try to extend P to some larger subspace of L^2 .

The theory of distributions teaches us that, for any $u \in L^2$, the expression $P(x, D_x)u$ makes sense as a well-defined distribution in $\mathcal{D}'(\Omega)$, yet generally this distribution is not in L^2 . However, if a sequence $(u_n \in D(P))$ converges to u in L^2 , and satisfies $Pu_n \rightarrow v$ in L^2 , then the two limits hold as well in \mathcal{D}' . Because P acts continuously $\mathcal{D}' \rightarrow \mathcal{D}'$, the limit v must be equal to the (unique) distribution defined by Pu . Hence, the limit v is independent of the sequence (u_n) converging towards u . This shows that the closure of $\text{gr } P$ in $L^2 \times L^2$ is a graph, hence that P is closable. Its closure $\overline{P} =: P_{\min}$ is called the minimal closed extension of P , or the *minimal operator*. The above reasoning also shows that $\text{gr } \overline{P} = \overline{\text{gr } P}$ must be included in the set

$$(2.1.3) \quad \{(u, f) \in \mathcal{H} \times \mathcal{H} : P(x, D_x)u = f \text{ in } \mathcal{D}'(\Omega)\}.$$

The above set defines a closed graph in $L^2 \times L^2$, the corresponding operator is called the maximal extension of P , or the *maximal operator*, and is denoted by P_{\max} . Its domain is

$$D(P_{\max}) = \{u \in \mathcal{H} : P(x, D_x)u \in \mathcal{H}\},$$

where, as above, $P(x, D_x)u$ is understood in the sense of distributions.

We have already shown the inclusion $P_{\min} \subset P_{\max}$, and we saw in the Example 2.1.10 of the Laplacian on \mathbb{R}^d , that one can have $P_{\min} = P_{\max}$. But one may easily find examples where this equality does not hold, and the inclusion $P_{\min} \subset P_{\max}$ is strict.

Example 2.1.12 If we take $P(x, D_x) = d/dx$ and $\Omega = \mathbb{R}_+^*$, with domain $D(P) = C_c^\infty(\mathbb{R}_+^*)$, we find for the minimal closed extension

$$D(P_{\min}) = \overline{C_c^\infty(\mathbb{R}_+^*)}^{H^1} = H_0^1(\mathbb{R}_+^*),$$

(the space of functions in $H^1(\mathbb{R}_+^*)$ vanishing at $x = 0$), since the graph norm $\|\cdot\|_P$ is equivalent with the H^1 norm. On the other hand,

$$D(P_{\max}) = \{u \in L^2(\mathbb{R}_+^*), u' \in L^2(\mathbb{R}_+^*)\} = H^1(\mathbb{R}_+^*)$$

(with no condition at $x = 0$). which is strictly larger than $H_0^1(\mathbb{R}_+^*)$.

In general, one may expect that $P_{\min} \subsetneq P_{\max}$ if Ω has a boundary.

Such questions become more involved if one studies partial differential operators with more singular coefficients (e.g. with coefficients which are not smooth but just belong to some L^p), since one cannot easily define their action on distributions. During the course, we will nevertheless deal with certain classes of such operators (one easy case is the multiplication operator by an L_{loc}^∞ function of Example 2.1.8).

In the next section, we restrict ourselves to operators P defined on a *Hilbert space*. In this framework, we will define and study the *adjoint operator* of P ; we will see that the very definition of the adjoint is not obvious, in cases where P is unbounded on \mathcal{H} .

Note that adjoints can also be defined on Banach space \mathcal{B} , yet the adjoint operator then acts on the dual space \mathcal{B}' , which is generally different from \mathcal{B} . We will not address this situation in these notes.

2.2 Adjoint of an operator on a Hilbert space

In this section all operators are defined on a Hilbert space \mathcal{H} .

2.2.1 Adjoint of a continuous operator

For a continuous operator $T \in \mathcal{L}(\mathcal{H})$, its adjoint T^* is defined by the identity

$$(2.2.4) \quad \langle u, Tv \rangle = \langle T^*u, v \rangle \text{ for all } u, v \in \mathcal{H}.$$

The fact that these identities uniquely define the operator T^* comes from the Riesz representation theorem: for each $u \in \mathcal{H}$ the map $\mathcal{H} \ni v \mapsto \langle u, Tv \rangle \in \mathbb{C}$ is a *continuous* linear functional; the Riesz theorem states that there exists a unique vector $w \in \mathcal{H}$ such that $\langle u, Tv \rangle = \langle w, v \rangle$ for all $v \in \mathcal{H}$. One can then easily check that the map $u \mapsto w$ is linear, and by estimating the above scalar product with $v = w$, one finds that this map is bounded:

$$\langle w, w \rangle = \langle u, Tw \rangle \implies \|w\|^2 \leq \|u\| \|T\| \|w\| \implies \|w\| \leq \|T\| \|u\|$$

We may hence denote this map by: $w = T^*u$, thus defining the continuous linear operator T^* . The above bound shows that $\|T^*\| \leq \|T\|$. Actually, the symmetry of (2.2.4) shows that $(T^*)^* = T$, hence we actually have $\|T^*\| = \|T\|$.

2.2.2 Adjoint of an unbounded operator

Let us try to generalize this construction to an unbounded operator T . As we will see, the main difficulty consists in properly defining the domain of T^* .

Definition 2.2.1 (Adjoint operator) Let $(T, D(T))$ be a linear operator in \mathcal{H} , with $D(T)$ dense in \mathcal{H} . We then define its *adjoint operator* $(T^*, D(T^*))$ as follows.

The domain $D(T^*)$ consists of the vectors $u \in \mathcal{H}$ for which the map $D(T) \ni v \mapsto \langle u, Tv \rangle \in \mathbb{C}$ is a *bounded* linear form on \mathcal{H} . For such u there exists, by the Riesz theorem, a unique vector (which we denote by T^*u) such that $\langle u, Tv \rangle = \langle T^*u, v \rangle$ for all $v \in D(T)$.

We notice that our assumption of a *dense* domain $\overline{D(T)} = \mathcal{H}$ is crucial here: if it is not satisfied, then there are several ways to extend the linear form defined on $D(T)$, into a bounded linear form on \mathcal{H} . Equivalently, the vector T^*u is not uniquely determined, since one can add to T^*u an arbitrary vector in $D(T)^\perp$. Hence, when we mention the adjoint of an operator T , we always (implicitly or explicitly) assume that $D(T)$ is dense.

Let us give a *geometric* interpretation of the adjoint operator. Consider the linear “ $-\pi/2$ rotation” operator

$$J : \mathcal{H} \times \mathcal{H} \rightarrow \mathcal{H} \times \mathcal{H}, \quad J(u, v) = (v, -u).$$

We notice that J commutes with taking the orthogonal complement in $\mathcal{H} \times \mathcal{H}$: for any subset $V \subset \mathcal{H} \times \mathcal{H}$, $J(V)^\perp = J(V^\perp)$.

Proposition 2.2.2 (Geometric interpretation of the adjoint) Let T be a linear operator in \mathcal{H} , with dense domain $D(T)$. Then the graph of the adjoint operator T^* is given by:

$$(2.2.5) \quad \text{gr } T^* = J(\text{gr } T)^\perp = J((\text{gr } T)^\perp).$$

Proof.— By definition, $u \in D(T^*)$ iff there exists a vector T^*u such that, for any $v \in D(T)$,

$$(2.2.6) \quad \begin{aligned} 0 &= \langle u, Tv \rangle_{\mathcal{H}} - \langle T^*u, v \rangle_{\mathcal{H}} \\ &= \langle (u, T^*u), (Tv, -v) \rangle_{\mathcal{H} \times \mathcal{H}} \\ &= \langle (u, T^*u), J(v, Tv) \rangle_{\mathcal{H} \times \mathcal{H}}. \end{aligned}$$

Equivalently, $u \in D(T^*)$ iff there exists $T^*u \in \mathcal{H}$ such that (u, T^*u) is orthogonal to the subspace $J(\text{gr } T)$. Hence, the set of admissible pairs (u, T^*u) is given by the orthogonal complement to $J(\text{gr } T)$. We know that these pairs form a graph (due to the density of $D(T)$, to each admissible u corresponds a unique T^*u). We finally get the required identity $\text{gr } T^* = J(\text{gr } T)^\perp$. \square

A byproduct of the equalities (2.2.6) is the identity

$$(2.2.7) \quad \text{Ker } T^* = (\text{Ran } T)^\perp.$$

As a simple application we obtain

Proposition 2.2.3 *i)* The adjoint T^* is a closed operator.

ii) If T is closable, then $T^* = (\overline{T})^*$.

Proof.— In (2.2.5), we remember that the orthogonal complement of a subspace is always a *closed* subspace, so $\text{gr } T^*$ is closed, meaning that T^* is a closed operator.

Besides, the map J is continuous, and the orthogonal complement of a subspace is equal to the orthogonal complement of its closure, so

$$J(\text{gr } T)^\perp = \overline{J(\text{gr } T)}^\perp = J(\overline{\text{gr } T})^\perp = J(\text{gr } \overline{T})^\perp,$$

which proves the second item. \square

So far, we do not know if the domain of the adjoint operator could be nontrivial. This is discussed in the following proposition.

Proposition 2.2.4 (Domain of the adjoint) Let $(T, D(T))$ be a *closable* operator on \mathcal{H} , with dense domain. Then

- i)* $D(T^*)$ is a dense subspace of \mathcal{H} ;
- ii)* $T^{**} \stackrel{\text{def}}{=} (T^*)^* = \overline{T}$.

Proof.— The item *ii)* easily follows from *i)* and Eq. (2.2.5): one remarks that $J^2 = -1$, and that taking twice the orthogonal complement results in taking the closure of the graph, hence $\text{gr } \overline{T}$.

Now let us prove *i)*. Assume the opposite conclusion, namely that some nonzero vector $w \in \mathcal{H}$ is orthogonal to $D(T^*)$: $\langle u, w \rangle = 0$ for all $u \in D(T^*)$. Then for all $u \in D(T^*)$ one has

$$\langle J(u, T^*u), (0, w) \rangle_{\mathcal{H} \times \mathcal{H}} = \langle u, w \rangle + \langle T^*u, 0 \rangle = 0,$$

which means that $(0, w) \in J(\text{gr } T^*)^\perp = \overline{\text{gr } T}$. Since the operator T is closable, the closure $\overline{\text{gr } T}$ must be a graph, which imposes $w = 0$, so we have a contradiction. \square

Remark 2.2.5 In the above Proposition, the closability of T is a necessary assumption. Indeed, let us come back to the Example 2.1.11 of the nonclosable operator L . The adjoint of this operator has for domain $D(L^*) = \{g\}^\perp$, a closed subspace of codimension 1, hence not dense on L^2 . Note that the operator L^* vanishes on this domain.

Let us consider some examples of adjoints of closable operators.

Example 2.2.6 (Adjoint of a bounded operator) The general definition (2.2.1) for the adjoint operator is compatible with the definition of the adjoint of a continuous linear operators given in section 2.2.1: in case T is bounded and $D(T) = \mathcal{H}$, the domain of the adjoint is $D(T^*) = \mathcal{H}$, and the relation $\langle u, Tv \rangle = \langle T^*u, v \rangle$ for all $u, v \in \mathcal{H}$ fully defines T^* .

Example 2.2.7 (Laplacian on \mathbb{R}^d) Let us consider again the operators T_0 and T_1 from Example 2.1.10, and show that $T_0^* = T_1$.

By definition, the domain $D(T_0^*)$ consists of the functions $u \in L^2(\mathbb{R}^d)$ for which there exists a vector $f \in L^2(\mathbb{R}^d)$ such that

$$\forall v \in D(T_0) = C_c^\infty(\mathbb{R}^d), \quad \int_{\mathbb{R}^d} \overline{u(x)}(-\Delta v)(x)dx = \int_{\mathbb{R}^d} \overline{f(x)}v(x)dx.$$

This equation exactly means that $f = -\Delta u$ in $\mathcal{D}'(\mathbb{R}^d)$. Therefore, $D(T_0^*)$ consists of the functions $u \in L^2$ such that the distribution $-\Delta u$ is actually in L^2 . The identities (2.1.2) showed that this is exactly the space $H^2(\mathbb{R}^d) = D(T_1)$. So $D(T_0^*) = D(T_1)$, and the two operators both act by $u \mapsto -\Delta u$, they are thus identical.

Let us come back to the simplest differential operator, which appeared in Example 2.1.12.

Example 2.2.8 Consider the operator A_0 acting through $A_0 u = D_x u \stackrel{\text{def}}{=} -i \frac{d}{dx} u$ for $u \in D(A_0) = C_c^\infty(]0, 1[)$. In Example 2.1.12 we showed that the “minimal operator” $\overline{A_0} = A_{0,\min}$ admits the domain $D(\overline{A_0}) = H_0^1(]0, 1[)$.

Let us show that the adjoint A_0^* admits the larger domain $D(A_0^*) = H^1(]0, 1[)$. Indeed, if $v \in C_c^\infty(]0, 1[)$, the equation

$$\langle u, D_x v \rangle = \langle D_x u, v \rangle$$

holds for any $u \in C^\infty(]0, 1[)$ thanks to an integration by parts, and the resulting linear form in v can be continuously extended to all of $v \in L^2$, as long as $D_x u \in L^2$, hence as long as $u \in H^1(]0, 1[)$. The action of A_0^* is also by $A_0^* u = D_x u$, so A_0^* is equal to the maximal operator $A_{0,\max}$.

To anticipate the Definition 2.2.10 below, the operator A_0 is symmetric, but not essentially self-adjoint, since $\overline{A_0} \subsetneq A_0^*$. Equivalently, the non-inclusion $A_0^* \not\subset A_0^{**} = \overline{A_0}$ shows that the operator A_0^* is *not* symmetric.

Exercise 2.2.9 Remember the multiplication operator M_f from Example 2.1.8, for a complex valued function $f \in L_{loc}^\infty$. Show that $(M_f)^* = M_{\bar{f}}$.

2.2.3 Symmetric and Selfadjoint operators

The following definition introduces classes of linear operators defined on a Hilbert space, which will be studied intensively in this course.

Definition 2.2.10 (Symmetric, self-adjoint, essentially self-adjoint ops) An operator $(T, D(T))$ on a Hilbert space is said to be *symmetric* (or *Hermitian*) if

$$\langle u, Tv \rangle = \langle Tu, v \rangle \quad \text{for all } u, v \in D(T).$$

Equivalently, T is symmetric iff $T \subset T^*$ (that is, T^* is an extension of T).

- T is called *selfadjoint* if $T = T^*$ (in particular, $D(T) = D(T^*)$)
- T is called *essentially selfadjoint* if T is closable and \overline{T} is self-adjoint: $\overline{T} = (\overline{T})^* = T^*$.

An important feature of symmetric operators is their closability:

Proposition 2.2.11 A symmetric operator $(T, D(T))$ is necessarily closable.

Proof.— Indeed, for a symmetric operator T we have $\text{gr } T \subset \text{gr } T^*$ and, due to the closedness of T^* , $\overline{\text{gr } T} \subset \text{gr } T^*$ is a graph, the graph of the closure \overline{T} . \square

Example 2.2.12 (Free Laplacian on \mathbb{R}^d) The Laplacian T_1 from Example 2.1.10 is selfadjoint. Indeed, we have shown in Ex. 2.2.7 that $T_0^* = T_1$, hence $T_1^* = T_0^{**} = \overline{T_0} = T_1$, where the last equality uses Ex. 2.1.10. This shows that T_1 is selfadjoint, while its restriction T_0 is essentially selfadjoint.

The operator T_1 is called the *free Laplacian* on \mathbb{R}^d .

Example 2.2.13 (Continuous symmetric operators are selfadjoint) For $T \in \mathcal{L}(\mathcal{H})$, being symmetric is equivalent to being selfadjoint, since the domains of T and T^* are both the full space \mathcal{H} .

Example 2.2.14 (Selfadjoint multiplication operators) As follows from example 2.2.9, the multiplication operator M_f on $L^2(\mathbb{R}^d)$ from example 2.1.8, with $D(M_f) = \{u \in L^2, fu \in L^2\}$ is self-adjoint iff $f(x) \in \mathbb{R}$ for a.e. $x \in \mathbb{R}^d$.

The following proposition will allow to construct a large class of self-adjoint operators.

Proposition 2.2.15 Let T be an *injective* selfadjoint operator, then its inverse T^{-1} is also self-adjoint (notice that the inverse may be unbounded).

Proof.— Let us first show that $D(T^{-1}) \stackrel{\text{def}}{=} \text{Ran } T$ is dense in \mathcal{H} . Let $u \perp \text{Ran } T$, then $\langle u, Tv \rangle = 0$ for all $v \in D(T)$. This can be rewritten as $\langle u, Tv \rangle = \langle 0, v \rangle$ for all $v \in D(T)$, which shows that $u \in D(T^*)$, with image $T^*u = 0$. Since by assumption $T^* = T$, we have $u \in D(T)$ and $Tu = 0$. Since T is injective, the vector u must be trivial. Hence $\text{Ran } T$ is dense.

Now consider the “switch operator” $S : \mathcal{H} \times \mathcal{H} \rightarrow \mathcal{H} \times \mathcal{H}$ given by $S(u, v) = (v, u)$. One has then $\text{gr } T^{-1} = S(\text{gr } T)$. We conclude the proof by noting that S commutes with the operation of the orthogonal complement in $\mathcal{H} \times \mathcal{H}$ and anticommutes with J . From the assumption $\text{gr } T = \text{gr } T^* = J(\text{gr } T)^\perp$, we draw:

$$\begin{aligned} \text{gr } T^{-1} &\stackrel{\text{def}}{=} S(\text{gr } T) \stackrel{\text{a.s.s.}}{=} S(\text{gr } T^*) = S(J(\text{gr } T)^\perp) \\ &= -JS((\text{gr } T)^\perp) = J(S \text{gr } T)^\perp = J(\text{gr } T^{-1})^\perp = \text{gr}(T^{-1})^*. \end{aligned}$$

□

Proving the symmetry of an unbounded operator is often easy (for differential operators, this fact often involves some integration by parts); but proving selfadjointness requires a precise identification of the domains, which may be quite difficult in general. This is a reason why, in the next section, we will appeal to quadratic forms to construct selfadjoint operators.

Yet, one may use the following criteria to check essential selfadjointness, or selfadjointness.

Proposition 2.2.16 (Criteria for selfadjointness) Assume the operator $(T, D(T))$ is *symmetric* on the Hilbert space \mathcal{H} . Then the following properties are equivalent:

- i) $(T, D(T))$ is essentially selfadjoint (selfadjoint);

- ii) $\text{Ker}(T^* + i) = \text{Ker}(T^* - i) = \{0\}$ (and furthermore $(T, D(T))$ is closed);
 iii) $\text{Ran}(T + i), \text{Ran}(T - i)$ are dense in \mathcal{H} (are equal to \mathcal{H}).

Proof.— We will give the proofs for the selfadjoint case only, the small adaptations necessary for the essentially selfadjoint case being left to the reader.

i) \implies ii): easy.

ii) \implies iii): we have $0 = \text{Ker}(T^* \pm i) = \text{Ran}(T \mp i)^\perp$, which shows that $\text{Ran}(T \pm i)$ is dense. Assuming the closedness of T , we want to show the closedness of $\text{Ran}(T \pm i)$. For this, we use “Pythagore’s theorem”:

$$\|(T + i)u\|^2 = \langle (T + i)u, (T + i)u \rangle = \langle Tu, Tu \rangle + \langle u, u \rangle$$

Assume that a sequence $(u_n \in D(T))$ is such that the sequence $((T + i)u_n)$ is Cauchy. The above equality then shows that so are (u_n) and (Tu_n) . The closedness of T then implies that $u_n \rightarrow u$ and $Tu_n \rightarrow Tu$, hence $(T + i)u_n \rightarrow (T + i)u \in \text{Ran}(T + i)$. As a result, $\text{Ran}(T + i)$ is closed, and is equal to \mathcal{H} . The proof for $\text{Ran}(T - i)$ is identical.

iii) \implies i) The symmetry means that $T \subset T^*$, and we want to show the inverse inclusion $T^* \subset T$.

Take any $v \in D(T^*)$; one then has $(T^* + i)v \in \mathcal{H}$. From the assumption that $\text{Ran}(T + i) = \mathcal{H}$, there exists $u \in D(T)$ such that $(T^* + i)v = (T + i)u$; since $T \subset T^*$ (T is symmetric), this identity also reads $(T^* + i)u = (T^* + i)v$, hence $v - u \in \text{Ker}(T^* + i) = \text{Ran}(T - i)^\perp$. The assumption $\text{Ran}(T - i) = \mathcal{H}$ shows that $u = v$, so that $v \in D(T)$, and finally $D(T^*) \subset D(T)$. \square

Remark 2.2.17 (Why focus on selfadjoint operators?) As mentioned in the introduction, selfadjoint operators lie at the heart of quantum mechanics, not just in as Hamiltonians generating the quantum evolution, but also as *quantum observables*, selfadjoint operators representing the quantities which can (in theory) be measured in an experiment.

Mathematically, selfadjoint operators enjoy a very special spectral structure: we will establish in Chapter 5 the *spectral theorem* for selfadjoint operators, which provides a general description of these operators, in terms of their spectral measure. From this theorem we will also construct a *functional calculus* for selfadjoint operators, that is define operators of the form $f(T)$, for T selfadjoint and $f : \mathbb{R} \rightarrow \mathbb{C}$ is an arbitrary function.

2.3 Exercises

Exercise 2.3.1 (a) Let \mathcal{H}_1 and \mathcal{H}_2 be Hilbert spaces. Let A be a linear operator in \mathcal{H}_1 , B be a linear operator in \mathcal{H}_2 . Assume that there exists a unitary operator $U : \mathcal{H}_2 \rightarrow \mathcal{H}_1$ such that $D(A) = UD(B)$ and that $U^*AUf = Bf$ for all $f \in D(B)$; such A and B are called *unitary equivalent*.

Let two operators A and B be unitarily equivalent. Show that A is closed/symmetric/self-adjoint iff B has the same property.

(b) Let (λ_n) be an arbitrary sequence of complex numbers, $n \in \mathbb{N}$. In the Hilbert space $\ell^2(\mathbb{N})$ consider the operator S :

$$D(S) = \{(x_n) : \text{there exists } N \text{ such that } x_n = 0 \text{ for } n > N\}, \quad S(x_n) = (\lambda_n x_n).$$

Describe the closure of S .

(c) Now let \mathcal{H} be a separable Hilbert space and T be a linear operator in \mathcal{H} with the following property: there exists an orthonormal basis $(e_n)_{n \in \mathbb{N}}$ of \mathcal{H} with $e_n \in D(T)$ and $Te_n = \lambda_n e_n$ for all $n \in \mathbb{N}$, where λ_n are some complex numbers. We take as $D(T)$ the finite linear combinations of the (e_n) .

i) Describe the closure \overline{T} of T . Hint: one may use (a) and (b).

ii) Describe the adjoint T^* of T .

iii) Let all λ_n be real. Show that the operator \overline{T} is self-adjoint.

Exercise 2.3.2 Let A and B be self-adjoint operators in a Hilbert space H such that $D(A) \subset D(B)$ and $Au = Bu$ for all $u \in D(A)$. Show that $D(A) = D(B)$. (This property is called the *maximality* of self-adjoint operators.)

Exercise 2.3.3 We consider a linear operator A on a Hilbert space \mathcal{H} , and a *continuous* operator B on the same space; we define their sum $A + B$ as the operator S with domain $D(S) = D(A)$, such that $Su \stackrel{\text{def}}{=} Au + Bu$ for each $u \in D(S)$. (We note that defining the sum of two unbounded operators is a nontrivial task in general, due to questions of domains.)

(a) Assume A is a closed operator and B is continuous. Show that $A + B$ is closed.

(b) Assume, in addition, that A is densely defined. Show that $(A + B)^* = A^* + B^*$ (here the sum $A^* + B^*$ is defined similarly as $A + B$).

Exercise 2.3.4 Let $\mathcal{H} = L^2(]0, 1[)$. For $\alpha \in \mathbb{C}$, consider the operator T_α acting as $T_\alpha f = if'$ on the domain

$$D(T_\alpha) = \left\{ f \in C^\infty([0, 1]) : f(1) = \alpha f(0) \right\}.$$

(a) Describe the adjoint of T_α .

(b) Describe the closure $S_\alpha \stackrel{\text{def}}{=} \overline{T_\alpha}$.

(c) Find all α for which S_α is selfadjoint.

Chapter 3

Operators and quadratic forms

In this section, we will focus on operators defined on a Hilbert space. In many situations, the action of the operator is clear (typically it is a differential operator), but the difficult point is to identify the domain of the operator which provides it with “good properties”, namely selfadjointness.

To construct such a “good domain”, we will start by defining a *quadratic form* on \mathcal{H} (more precisely, the form will be defined on a dense subspace of \mathcal{H}). Provided this form enjoys some properties (which are usually easy to verify), we will extract from the form an operator which will automatically be selfadjoint. The advantage of this procedure is that the domain of the quadratic form is usually easier to construct, or describe, than the domain of the resulting operator. This procedure can thus be seen as a “fast track” to construct selfadjoint operators, without need to explicitly describe their domains.

3.1 From quadratic form to operator

A *sesquilinear form* q on a Hilbert space \mathcal{H} , with domain $D(q) \subset \mathcal{H}$, is a map

$$q : D(q) \times D(q) \rightarrow \mathbb{C},$$

which is linear with respect to the second argument and antilinear with respect to the first one. By default we assume that $D(q)$ is a dense subspace of \mathcal{H} . (In the literature, one uses also the terms *bilinear form* and *quadratic form*.) The sesquilinear form q is said to be:

- *bounded*, if $D(q) = \mathcal{H}$ and there exists $M > 0$ such that $|q(u, v)| \leq M\|u\| \cdot \|v\|$ for all $u, v \in \mathcal{H}$;
- *elliptic* (or *coercive*), if it is *bounded* and there exists $\alpha > 0$ such that $|q(u, u)| \geq \alpha\|u\|^2$ for all $u \in \mathcal{H}$;
- *symmetric* if $q(v, u) = \overline{q(u, v)}$ for all $u, v \in D(q)$,
- *semibounded from below* if for some $c \in \mathbb{R}$ one has $q(u, u) \geq c\|u\|^2$ for all $u \in D(q)$; in this case we write $q \geq c$; by polarization, one checks that q is then necessarily symmetric;

- *positive* or *non-negative*, if one can take $c = 0$ in the previous item;
- *positive definite* or *strictly positive*, if one can take $c > 0$ in the previous item.

Notice the subtle differences between ellipticity and strict positivity. It is important to notice that the above properties refer to the Hilbert norm on \mathcal{H} . Later we will introduce a second norm, in general stronger than $\|\cdot\|_{\mathcal{H}}$; when mentioning one of the above properties, it will be important to specify w.r.to which norm the form q is bounded, or semibounded below etc.

3.1.1 Starting from an elliptic form on \mathcal{V}

One may canonically associate a linear operator to any bounded form. For a moment we switch notations, and call A our operator, defined on a Hilbert space \mathcal{V} .

Definition 3.1.1 (Operator associated with a bounded form)

Let \mathcal{V} be a Hilbert space and let q be a *bounded* sesquilinear form on \mathcal{V} . Then, by the Riesz representation theorem, there is a unique operator $A_q \in \mathcal{L}(\mathcal{V})$ such that

$$q(u, v) = \langle u, A_q v \rangle_{\mathcal{V}} \quad \text{for all } u, v \in \mathcal{V}.$$

In the sequel we will often drop the subscript q , and write A instead of A_q .

The following theorem will be crucial for our constructions, it relates ellipticity of the quadratic form with invertibility of the operator.

Theorem 3.1.2 (Lax-Milgram theorem) If a quadratic form q on \mathcal{V} is *elliptic*, then the associated operator $A_q \in \mathcal{L}(\mathcal{V})$ is an isomorphism of \mathcal{V} , that is, A_q is invertible and $A_q^{-1} \in \mathcal{L}(\mathcal{V})$.

Proof.— By assumption, one can find two constants $\alpha, C > 0$ such that

$$\alpha\|v\|^2 \leq |q(v, v)| \leq C\|v\|^2 \quad \text{for all } v \in \mathcal{V}.$$

This implies $\alpha\|v\|^2 \leq |q(v, v)| = |\langle v, Av \rangle| \leq \|v\| \cdot \|Av\|$. Hence,

$$(3.1.1) \quad \|Av\| \geq \alpha\|v\| \quad \text{for all } v \in \mathcal{V}.$$

Step 1. The above inequality shows that A is injective.

Step 2. Let us show that $\text{Ran } A$ is closed. Assume that $f_n \in \text{Ran } A$ and that f_n converge to f in \mathcal{V} . By the result of step 1, there are uniquely determined vectors $v_n \in \mathcal{V}$ with $f_n = Av_n$. The sequence $(f_n) = (Av_n)$ is convergent, hence is Cauchy. By (3.1.1), the sequence (v_n) is also Cauchy, hence, due to the completeness of \mathcal{V} , it converges to some $v \in \mathcal{V}$. Since A is continuous, Av_n converges to Av . Hence, $f = Av$, which shows that $f \in \text{Ran } A$.

Step 3. Let us finally show that $\text{Ran } A = \mathcal{V}$. Since we already showed that $\text{Ran } A$ is closed, it is sufficient to show that $(\text{Ran } A)^\perp = \{0\}$. Let $u \perp \text{Ran } A$, then $q(u, v) = \langle u, Av \rangle = 0$ for all $v \in \mathcal{V}$. Taking $v = u$ we obtain $q(u, u) = 0$, hence $u = 0$ by ellipticity of q . \square

3.1.2 From \mathcal{V} to \mathcal{H}

We now extend the above construction to unbounded forms.

Definition 3.1.3 (Operator defined by a quadratic form)

Like in Theorem 3.1.2, consider an *elliptic* quadratic form q on a Hilbert space \mathcal{V} . Moreover, assume that \mathcal{V} densely embeds into another Hilbert space \mathcal{H} , and that there exists a constant $c > 0$ such that

$$\|u\|_{\mathcal{H}} \leq c\|u\|_{\mathcal{V}} \quad \text{for all } u \in \mathcal{V}$$

(that is, the \mathcal{V} -norm is stronger than the \mathcal{H} -norm).

Let us construct a linear operator $T = T_q$ on the larger space \mathcal{H} , associated with q as follows.

1. The domain $D(T)$ consists of the vectors $v \in \mathcal{V} \subset \mathcal{H}$ for which the map $\mathcal{V} \ni u \mapsto q(u, v)$ can be extended to a continuous antilinear map $\mathcal{H} \rightarrow \mathbb{C}$.
2. By the Riesz representation theorem, for such v there exists a unique $f_v \in \mathcal{H}$ such that $q(u, v) = \langle u, f_v \rangle_{\mathcal{H}}$ for all $u \in \mathcal{V}$; we then set $Tv \stackrel{\text{def}}{=} f_v$.

Notice the difference between the operator $T : D(T) \subset \mathcal{H} \rightarrow \mathcal{H}$ constructed above, and the bounded operator $A : \mathcal{V} \rightarrow \mathcal{V}$ constructed in Definition (3.1.1): the duality defining these operators comes from different scalar products, namely the one on \mathcal{H} for T , resp. the one on \mathcal{V} for A . So the actions of the two operators are genuinely different, even if both of them are well-defined on $D(T)$:

$$\text{for any } u, v \in D(T) \subset \mathcal{V}, \quad q(u, v) = \langle u, Av \rangle_{\mathcal{V}} = \langle u, Tv \rangle_{\mathcal{H}}.$$

The subtlety of the construction comes from the different vector spaces which are into play:

- the “large” Hilbert space \mathcal{H} , equipped with its scalar product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ and norm $\|\cdot\|_{\mathcal{H}}$;
- the “small” Hilbert space $\mathcal{V} \subset \mathcal{H}$, which is the domain of q , equipped with the scalar product $\langle \cdot, \cdot \rangle_{\mathcal{V}}$ and norm $\|\cdot\|_{\mathcal{V}}$; the quadratic form q is elliptic on this Hilbert space \mathcal{V} , but generally not on \mathcal{H} !
- the domain $D(T) \subset \mathcal{V}$ of the operator T .

To avoid confusions, we will keep on the scalar products the subscripts \mathcal{H} or \mathcal{V} .

Theorem 3.1.4 The operator constructed in Definition 3.1.3 satisfies the following properties.

- i) the domain of T is dense in \mathcal{H} ;
- ii) $T : D(T) \rightarrow \mathcal{H}$ is bijective;
- iii) $T^{-1} \in \mathcal{L}(\mathcal{H})$.

Proof.— Let $v \in D(T)$. Using the \mathcal{V} -ellipticity of q and the relation between \mathcal{V} and \mathcal{H} , we find:

$$\alpha \|v\|_{\mathcal{H}}^2 \leq \alpha c^2 \|v\|_{\mathcal{V}}^2 \stackrel{\text{ellip.}}{\leq} c^2 |q(v, v)| \stackrel{CS}{\leq} c^2 |\langle v, Tv \rangle_{\mathcal{H}}| \leq c^2 \|v\|_{\mathcal{H}} \cdot \|Tv\|_{\mathcal{H}},$$

showing that

$$(3.1.2) \quad \|Tv\|_{\mathcal{H}} \geq \frac{\alpha}{c^2} \|v\|_{\mathcal{H}}.$$

This inequality shows that T is injective.

Let us show that $T : D(T) \rightarrow \mathcal{H}$ is surjective. Let $h \in \mathcal{H}$ and let $A \in \mathcal{L}(\mathcal{V})$ be the operator associated with q . The map $\mathcal{V} \ni u \mapsto \langle u, h \rangle_{\mathcal{H}} \in \mathbb{C}$ is a continuous antilinear map $\mathcal{V} \rightarrow \mathbb{C}$, so from Riesz's theorem, one can find $w \in \mathcal{V}$ such that

$$\langle u, h \rangle_{\mathcal{H}} = \langle u, w \rangle_{\mathcal{V}} \quad \text{for all } u \in \mathcal{V}.$$

Denote $v \stackrel{\text{def}}{=} A^{-1}w \in \mathcal{V}$, then

$$\langle u, h \rangle_{\mathcal{H}} = \langle u, Av \rangle_{\mathcal{V}} = q(u, v).$$

By definition this means that $v \in D(T)$ and $h = Tv$. Hence, T is surjective and injective, and the inverse is bounded by (3.1.2): $\|T^{-1}\| \leq c^2/\alpha$.

It remains to show that the domain of T is dense in \mathcal{H} . Let $h \in \mathcal{H}$ with $\langle u, h \rangle_{\mathcal{H}} = 0$ for all $u \in D(T)$. Since T is surjective, there exists $v \in D(T)$ with $h = Tv$. Taking now $u = v$ we obtain $0 = \langle v, Tv \rangle_{\mathcal{H}} = q(v, v)$; the \mathcal{V} -ellipticity of q finally gives $v = 0$, and $h = 0$. \square

If the form q enjoys some additional properties, the associated operators T do so as well. Our main constructions of selfadjoint operators will come from the following theorem.

Theorem 3.1.5 (Selfadjoint operators defined by forms) In Definition 3.1.3, assume furthermore that the sesquilinear form q is *symmetric*. Then the associated operator T satisfies:

- i) T is a *selfadjoint* operator on \mathcal{H} ;
- ii) $D(T)$ is a dense subspace of the Hilbert space \mathcal{V} (and therefore, is also dense in \mathcal{H}).

Proof.— For any $u, v \in D(T)$ we have:

$$\langle u, Tv \rangle_{\mathcal{H}} \stackrel{\text{def}}{=} q(u, v) \stackrel{\text{symmetry}}{=} \overline{q(v, u)} = \overline{\langle v, Tu \rangle_{\mathcal{H}}} = \langle Tu, v \rangle_{\mathcal{H}}.$$

This shows that T is symmetric: $T \subset T^*$.

Take $v \in D(T^*)$. We know from the previous theorem that T is surjective. This means that we can find $v_0 \in D(T)$ such that $Tv_0 = T^*v$. Then for all $u \in D(T)$ we have:

$$\langle Tu, v \rangle_{\mathcal{H}} = \langle u, T^*v \rangle_{\mathcal{H}} = \langle u, Tv_0 \rangle_{\mathcal{H}} = \langle Tu, v_0 \rangle_{\mathcal{H}}.$$

Since T is surjective, this implies that $v = v_0 \in D(T)$, hence $T = T^*$.

Let us now show the density of $D(T)$ in \mathcal{V} . Let $h \in \mathcal{V}$ such that $\langle v, h \rangle_{\mathcal{V}} = 0$ for all $v \in D(T)$. Since the operator $A \in \mathcal{L}(\mathcal{V})$ associated with q is invertible, we may define $f = A^{-1}h \in \mathcal{V}$. We then have the equalities

$$0 = \langle v, h \rangle_{\mathcal{V}} = \langle v, Af \rangle_{\mathcal{V}} = q(v, f) \stackrel{\text{symm.}}{=} \overline{q(f, v)} = \overline{\langle f, Tv \rangle_{\mathcal{H}}} = \langle Tv, f \rangle_{\mathcal{H}}.$$

Since the vectors Tv cover the full space \mathcal{H} when v runs over $D(T)$, this implies $f = 0$ and $h = Af = 0$. This proves that $D(T)$ is dense in \mathcal{V} . \square

3.1.3 Starting from a quadratic form on \mathcal{H}

In the above definitions, the Hilbert space \mathcal{V} preceded the appearance of \mathcal{H} . The space \mathcal{V} also coincides with the domain of the form q . In practice, \mathcal{H} is usually defined beforehand, and one has to identify \mathcal{V} , together with its Hilbert structure, so as to make the form q \mathcal{V} -elliptic.

This motivates the following definition:

Definition 3.1.6 (Closed quadratic form) A sesquilinear form q on a Hilbert space \mathcal{H} with a dense domain $D(q) \subset \mathcal{H}$ is said to be *closed* if the following properties are satisfied:

- q is symmetric;
- q is semibounded from below: there exists $C \geq 0$ such that $q(u, u) \geq -C\|u\|_{\mathcal{H}}^2$ for all $u \in D(q)$;
- The domain $D(q)$, equipped with the scalar product

$$(3.1.3) \quad \langle u, v \rangle_q \stackrel{\text{def}}{=} q(u, v) + (C + 1)\langle u, v \rangle_{\mathcal{H}}$$

is a Hilbert space.

As opposed to our previous construction, this definition starts from the “large” Hilbert space, and constructs an auxiliary norm $\|\cdot\|_q$ on the domain $D(q)$, making this domain complete.

Notice that the notion of *closed form* is quite different with that of a *closed operator*, which already makes sense on a Banach space. In the case of forms, closedness requests symmetry and semiboundedness.

Proposition 3.1.7 (Operators defined by closed forms) Let q be a *closed* sesquilinear form in \mathcal{H} . Then the associated linear operator $(T, D(T))$ is *selfadjoint* on \mathcal{H} . This operator is also automatically bounded from below:

$$\langle u, Tu \rangle_{\mathcal{H}} \geq -C\|u\|_{\mathcal{H}}^2, \quad \text{for any } u \in D(T).$$

Proof.— If q is closed, one simply takes $(D(q), \langle \cdot, \cdot \rangle_q)$ as the auxiliary Hilbert space $\mathcal{V} \subset \mathcal{H}$ in Def. 3.1.3, with the norm $\|\cdot\|_{\mathcal{V}} = \|\cdot\|_q$. One has indeed $\|u\|_q^2 = q(u, u) + (C+1)\|u\|_{\mathcal{H}}^2 \geq \|u\|_{\mathcal{H}}^2$, showing that $\|\cdot\|_{\mathcal{V}}$ is stronger than $\|\cdot\|_{\mathcal{H}}$.

The modified form $\tilde{q} : \mathcal{V} \times \mathcal{V} \rightarrow \mathbb{C}$ defined by $\tilde{q} = q(u, v) + (C+1)\langle u, v \rangle_{\mathcal{H}}$ is \mathcal{V} -bounded:

$$|\tilde{q}(u, v)| = |\langle u, v \rangle_q| \leq \|u\|_q \|v\|_q,$$

and \mathcal{V} -elliptic:

$$\tilde{q}(u, u) = \|u\|_q^2.$$

The operator \tilde{T} constructed from \tilde{q} is hence selfadjoint on \mathcal{H} , with domain $D(\tilde{T}) \subset \mathcal{V}$. Finally, we notice that $T = \tilde{T} - (C+1)Id$ is the operator associated with q ; as a sum of a selfadjoint operator with a bounded selfadjoint operator, it is also selfadjoint, with the same domain $D(T) = D(\tilde{T})$. \square

Like in the case of operators, the forms we will encounter will not always be closed. The main question is whether they can be made so, up to an extension of their domain.

Definition 3.1.8 (Closable form) We say that a *symmetric* sesquilinear form q is *closable*, if there exists a closed form on \mathcal{H} which extends q . The closed sesquilinear form with the above property and with the minimal domain is called the *closure* of q , and is denoted by \bar{q} .

In the case of a closable semibounded form q , the following proposition identifies the domain of \bar{q} .

Proposition 3.1.9 (Domain of the closure of a form) If $q(u, u) \geq -C\|u\|_{\mathcal{H}}^2$, for some $C \in \mathbb{R}_+$, and q is a closable form, then $D(\bar{q})$ is exactly the completion of $D(q)$ with respect to the scalar product $\langle u, v \rangle_q \stackrel{\text{def}}{=} q(u, v) + (C+1)\langle u, v \rangle_{\mathcal{H}}$ (this completion is a subspace of \mathcal{H}).

Proof.— In the proof we assume for simplicity that $q \geq 1$, therefore we may take for the norm $\|u\|_q = \sqrt[q]{q(u, u)}$.

Since the domain $D(\bar{q})$ of the closure of q must be a Hilbert space w.r.t. the norm $\|\cdot\|_{\bar{q}}$, it must contain the limits of all the sequences $(u_n) \subset D(\bar{q})$ which are Cauchy w.r.t. the norm $\|\cdot\|_{\bar{q}}$, in particular the limits of the sequences $(u_n) \subset D(q)$ which are Cauchy w.r.t. the norm $\|\cdot\|_q$ (we will call those “ q -Cauchy sequences” in the following).

The abstract completion of $D(q)$ w.r.t. $\|\cdot\|_q$ is given by the equivalence classes of q -Cauchy sequences in $D(q)$, with the equivalence relation

$$(3.1.4) \quad (u_n) \sim (\tilde{u}_n) \quad \text{iff} \quad \|u_n - \tilde{u}_n\|_q \rightarrow 0.$$

This completion is denoted by $\overline{D(q)}^{\|\cdot\|_q}$.

The question is whether this completion does injectively embed in \mathcal{H} . Namely, any q -Cauchy sequence (u_n) is also a Cauchy sequence for the weaker \mathcal{H} -norm, hence it \mathcal{H} -converges to some $u \in \mathcal{H}$. To ensure that $\overline{D(q)}^{\|\cdot\|_q}$ embeds in \mathcal{H} , we must check that if two q -Cauchy sequences $(u_n), (\tilde{u}_n)$ \mathcal{H} -converge to the same $u \in \mathcal{H}$, then they must be equivalent in the above sense, namely define the same element of $\overline{D(q)}^{\|\cdot\|_q}$. This element can be identified with that $u \in \mathcal{H}$. The domain of the closure \bar{q} is made of those \mathcal{H} -limits u of q -Cauchy sequences.

The abstract completion $\overline{D(q)}^{\|\cdot\|_q}$ is naturally equipped with an extension of the quadratic form q . In case $\overline{D(q)}^{\|\cdot\|_q}$ forms a subspace of \mathcal{H} , this extended form is the closure \bar{q} of q . \square

Let us now exhibit a non-closable quadratic form.

Example 3.1.10 (Non-closable form) Take $\mathcal{H} = L^2(\mathbb{R})$ and consider the form defined on $D(q) = L^2(\mathbb{R}) \cap C^0(\mathbb{R})$ by $q(u, v) = \overline{u(0)}v(0)$; it is obviously symmetric and positive. Let us show that it is not closable, using the proof of the preceding proposition. We take the q -norm $\|u\|_q^2 = q(u, u) + \|u\|^2$.

Let us exhibit two q -Cauchy sequences $(u_n), (\tilde{u}_n)$ which have the same limit in \mathcal{H} , but are not equivalent in the sense of (3.1.4). By contradiction, let us assume that q can be extended to a closed form \bar{q} .

Let us choose some $u_0 \in D(\bar{q})$. We may easily construct two sequences $(u_n)_{n \geq 1}$ and $(\tilde{u}_n)_{n \geq 1}$ in $D(q)$ with the following properties:

- both sequences converge to u_0 in the \mathcal{H} -norm,
- $u_n(0) = 1$ and $v_n(0) = 0$ for all n .

These two properties show that these two sequences are indeed q -Cauchy, and they converge in \mathcal{H} to u_0 . But they are not equivalent, since

$$\|u_n - \tilde{u}_n\|_q^2 = 1 + \|u_n - \tilde{u}_n\|^2 \rightarrow 1.$$

The existence of these sequences shows that q is not closable.

Remark that this counter-example is based on the same phenomenon as the non-closable operator of Example 2.1.11, namely the fact that L^2 functions are not defined pointwise.

3.1.4 Various Laplacians

Let us give some “canonical” examples of forms, from which we will extract selfadjoint operators. We focus on various versions of the Laplacian.

Example 3.1.11 (Dirichlet forms) Consider the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^d)$ and the Dirichlet form

$$q(u, v) = \int_{\mathbb{R}^d} \overline{\nabla u} \nabla v \, dx, \quad \text{with domain } D(q) = H^1(\mathbb{R}^d).$$

This form is closed, since $\|\cdot\|_q = \|\cdot\|_{H^1}$, and $H^1(\mathbb{R}^d)$ is known to be complete. Let us find the associated operator T , which will automatically be selfadjoint.

Let $f \in D(T)$ and $g \stackrel{\text{def}}{=} Tf$, then for any $u \in H^1(\mathbb{R}^d)$ we have

$$\int_{\mathbb{R}^d} \overline{\nabla u} \nabla f \, dx = \int_{\mathbb{R}^d} \overline{u} g \, dx.$$

In particular, this equality holds for $u \in C_c^\infty(\mathbb{R}^d)$, which gives

$$\int_{\mathbb{R}^d} \overline{u} g \, dx = \int_{\mathbb{R}^d} \overline{\nabla u} \nabla f \, dx = \int_{\mathbb{R}^d} \overline{(-\Delta u)} f \, dx = \langle f, \overline{-\Delta u} \rangle_{\mathcal{D}', \mathcal{D}} = \langle -\Delta f, \overline{u} \rangle_{\mathcal{D}', \mathcal{D}}.$$

It follows that $g = -\Delta f$ in $\mathcal{D}'(\mathbb{R}^d)$. Therefore, for each $f \in D(T)$ we must have $\Delta f \in L^2(\mathbb{R}^d)$, which by (2.1.2) means that $f \in H^2(\mathbb{R}^d)$. Conversely, $f \in H^2$ is a sufficient condition to extend the antilinear form

$$u \mapsto q(u, f) = \int_{\mathbb{R}^d} \overline{u} (-\Delta f) \, dx$$

to all $u \in L^2$. According to the Definition 3.1.3, this shows that $D(T) = H^2(\mathbb{R}^d)$.

In other words, the operator T constructed from the form q is $T = T_1$, where T_1 is the free Laplacian in \mathbb{R}^d (see Definition 2.2.12). We thus recover the fact that the free Laplacian on \mathbb{R}^d is selfadjoint.

Example 3.1.12 (Neumann boundary condition on the halfline) Take $\mathcal{H} = L^2(]0, \infty[)$, and consider the form

$$(3.1.5) \quad q(u, v) = \int_0^\infty \overline{u'(x)} v'(x) \, dx, \quad D(q) = H^1(]0, \infty[).$$

This form is semibounded below and closed (this is due to the completeness of H^1 w.r.to the norm $\|\cdot\|_{H^1} = \|\cdot\|_q$). Let us describe the associated operator T .

For $v \in D(T)$, there exists $f_v \in \mathcal{H}$ such that

$$\int_0^\infty \overline{u'(x)} v'(x) \, dx = \int_0^\infty \overline{u(x)} f_v(x) \, dx$$

for all $u \in H^1$. Taking here $u \in C_c^\infty$, we obtain just the definition of the distributional derivative: $f_v = -(v')' = -v''$ in $\mathcal{D}'(]0, \infty[)$. As we require $f_v \in L^2$, the function v must be in $H^2(]0, \infty[)$, and $Tv = f_v = -v''$.

Now, notice that for $v \in H^2(]0, \infty[)$ and $u \in H^1(]0, \infty[)$ the integration by parts gives:

$$\int_0^\infty \overline{u'(x)v'(x)} dx = \overline{u(x)v'(x)} \Big|_{x=0}^{x=\infty} - \int_0^\infty \overline{u(x)v''(x)} dx.$$

If we want the identity $q(u, v) = \langle u, Tv \rangle_{\mathcal{H}}$ to be continuously extended to all $u \in L^2$, the boundary term at $x = 0$ must vanish; this will be the case if we ensure the additional condition $v'(0) = 0$ (remember that for $v \in H^2(]0, \infty[)$, we have $v' \in H^1(]0, \infty[) \subset C^0([0, \infty[)$, so the value $v'(0)$ is well-defined). This condition is necessary and sufficient for this extension to hold.

In conclusion, the operator associated with the form (3.1.5) is $T \stackrel{\text{def}}{=} T_N$, which acts as $T_N v = -v''$ on the domain $D(T_N) = \{v \in H^2(0, \infty) : v'(0) = 0\}$. It will be referred to as the (positive) Laplacian with the *Neumann* boundary condition, or simply the Neumann Laplacian on $]0, \infty[$. It is automatically selfadjoint on L^2 .

The following example starts with a slight modification of the form (3.1.5).

Example 3.1.13 (Dirichlet boundary condition on the halfline) Take $\mathcal{H} = L^2(0, \infty)$. Consider the following form, which is a restriction of the previous one,

$$(3.1.6) \quad q_0(u, v) = \int_0^\infty \overline{u'(x)v'(x)} dx, \quad \text{with the domain } D(q_0) = H_0^1(0, \infty).$$

This form, which is a restriction of (3.1.5), is still semibounded below and closed (because H_0^1 is complete with respect to the H^1 -norm). Due to this restricted domain, no boundary term appears when integrating by parts, which means that the associated operator T_D acts as $T_D v = -v''$ on the domain $D(T_D) = H^2(0, \infty) \cap H_0^1(0, \infty) = \{v \in H^2(0, \infty) : v(0) = 0\}$. This operator will be referred to as the (positive) Laplacian with the Dirichlet boundary condition, or Dirichlet Laplacian for short.

Remark 3.1.14 In the two previous examples we see an important feature: the fact that one closed form extends another closed form (here, $D(q_0) \subset D(q)$) does *not* imply the same ordering between the associated operators: $D(T_D) \not\subset D(T_N)$.

Example 3.1.15 (Neumann/Dirichlet Laplacians: general case) The two previous examples can be generalized to the multidimensional case. Let Ω be an open subset of \mathbb{R}^d with a sufficiently regular boundary $\partial\Omega$ (for example, a compact Lipschitz one). In $\mathcal{H} = L^2(\Omega)$, consider two sesquilinear forms:

$$\begin{aligned} q_0(u, v) &= \int_{\Omega} \overline{\nabla u} \nabla v dx, & D(q_0) &= H_0^1(\Omega), \\ q(u, v) &= \int_{\Omega} \overline{\nabla u} \nabla v dx, & D(q) &= H^1(\Omega). \end{aligned}$$

Both these forms are closed and semibounded from below, and one can easily show that the respective operators T_D and T_N act both as $u \mapsto -\Delta u$. By a more careful analysis and, for example, for a smooth $\partial\Omega$, one can show that

$$\begin{aligned} D(T_D) &= H^2(\Omega) \cap H_0^1(\Omega) = \{u \in H^2(\Omega) : u|_{\partial\Omega} = 0\}, \\ D(T_N) &= \{u \in H^2(\Omega) : \frac{\partial u}{\partial n} \Big|_{\partial\Omega} = 0\}, \end{aligned}$$

where $n = n(x)$ denotes the outward pointing unit normal vector on $\partial\Omega \ni x$, and the restrictions to the boundary should be understood as the respective traces of the functions on the boundary. If the boundary is not regular, the domains become more complicated, in particular, the domains of T_D and T_N are not necessarily included in $H^2(\Omega)$, see e.g. detailed results in Grisvard's book [5]. Nevertheless, the operator T_D is called the *Dirichlet Laplacian* in Ω and T_N is called the *Neumann Laplacian*.

These constructions are relevant only if the boundary of Ω is non-empty: if $\Omega = \mathbb{R}^d$, then $q = q_0$, because as $H^1(\mathbb{R}^d) = H_0^1(\mathbb{R}^d)$, hence $T_D = T_N = T_1$ the free Laplacian.

3.2 Semibounded operators and Friedrichs extensions

The goal of this section is to start from a linear operator T on \mathcal{H} enjoying "good" properties (namely, symmetric and semibounded from below), and construct an extension of this operator which is self-adjoint, called the Friedrichs extension of T . The strategy is to make a "detour" through quadratic forms: schematically, the construction goes as follows:

$$(T, D(T)) \rightarrow (q, D(q)) \rightarrow (\bar{q}, D(\bar{q})) \rightarrow (T_F, D(T_F)).$$

Let us start with the definition of the "good properties" we require T to enjoy. In Section 3.1 we have seen the definition of a quadratic form being semibounded from below. A similar notion exists for linear operators:

Definition 3.2.1 (Semibounded operator) Let T be a symmetric operator T on \mathcal{H} . T is said to be *semibounded from below* if there exists a constant $C \in \mathbb{R}$ such that

$$\langle u, Tu \rangle \geq C \langle u, u \rangle \text{ for all } u \in D(T),$$

and in that case we write $T \geq C$, or $T \geq C Id$.

From an operator T we naturally induce a sesquilinear form $q = q_T$ on \mathcal{H} , with domain $D(q) = D(T)$:

$$q(u, v) \stackrel{\text{def}}{=} \langle u, Tv \rangle, \quad \forall u, v \in D(T).$$

Proposition 3.2.2 If T is semibounded from below, then the associated sesquilinear form q_T is semibounded from below and closable (see Def. 3.1.8).

Proof.— The semiboundedness of q directly follows from the analogous property of T . For simplicity, we will consider in the proof that $T \geq 1$, so that the q -norm can simply be chosen as $\|u\|_q = q(u, u)^{1/2}$.

To show the closability of q , we come back to the proof of Proposition 3.1.9, which attempted to construct the closed extension \bar{q} to the form q . The construction went by considering q -Cauchy sequences $(u_n)_n \subset D(T)$. Each such sequence converges to a limit $u \in \mathcal{H}$ in the \mathcal{H} -norm. As noticed in that proof, to show the closability of q we must check that two q -Cauchy sequences $(u_n), (\tilde{u}_n)$ which \mathcal{H} -converge to the same $u \in \mathcal{H}$ must also be equivalent in the sense of (3.1.4).

Let us show that in the present situation ($q = q_T$), this is indeed the case. The sequence $(w_n = u_n - \tilde{u}_n)_n$ is obviously a q -Cauchy sequence (since both (u_n) and (\tilde{u}_n) are so, and \mathcal{H} -converges to zero. The following Assertion shows that it must also q -converge to zero, showing that (u_n) and (\tilde{u}_n) are equivalent.

Assertion. If $(w_n) \subset D(q)$ is a q -Cauchy sequence converging to zero in \mathcal{H} , then $\lim_{n \rightarrow \infty} \|w_n\|_q = 0$.

We already noticed that $(\|w_n\|_q)_{n \in \mathbb{N}}$ is a nonnegative Cauchy sequence, so it converges to some limit $N_w \geq 0$. Suppose by contradiction that $N_w > 0$. Now let us split

$$q(w_n, w_m) = q(w_n, w_n) + q(w_n, w_m - w_n),$$

and consider the Cauchy-Schwarz inequality:

$$|q(w_n, w_m - w_n)| \leq \|w_n\|_q \|w_m - w_n\|_q \leq C \|w_m - w_n\|_q.$$

Combining these two expressions with the fact that w_n is q -Cauchy, we see that for any $\epsilon > 0$ there exists $n_\epsilon > 0$ such that $|q(w_n, w_m) - N_w^2| \leq \epsilon$ for all $n, m > n_\epsilon$. We now use the definition of the form q , and take $\epsilon = N_w^2/2$. Then, for $n, m > n_\epsilon$ we have

$$|\langle w_n, Tw_m \rangle_{\mathcal{H}}| = |q(w_n, w_m)| \geq \frac{N_w^2}{2}.$$

On the other hand, if we fix some $m \geq n_\epsilon$ and take the limit $n \rightarrow \infty$, the left-hand side goes to 0 since $w_n \xrightarrow{\mathcal{H}} 0$, so we obtain a contradiction. The Assertion is proved, and thus the Proposition as well. \square

The closability of q , together with Prop. 3.1.7 allows us to construct a selfadjoint extension of T .

Definition 3.2.3 (Friedrichs extensions) Let T be a linear operator in \mathcal{H} which is semi-bounded from below. Consider the sesquilinear form q associated with T , and its closure \bar{q} . The selfadjoint operator T_F associated with the form \bar{q} is called the *Friedrichs extension* of T .

Let us notice that, in general, such an operator T could admit *several* selfadjoint extensions. The above procedure selects one of these extensions.

Proposition 3.2.4 If T is a selfadjoint operator and is semibounded from below, then it is equal to its own Friedrichs extension.

Proof.— Let q be the sesquilinear form associated with T . It is closable, and the domain of its closure $\mathcal{V} \stackrel{\text{def}}{=} D(\bar{q})$ is given by the closure of $D(T)$ w.r.t. the norm $\|\cdot\|_q$. By definition, the domain $D(T_F)$ is the set of $v \in \mathcal{V}$ s.t. the map $u \in \mathcal{V} \mapsto \bar{q}(u, v)$ extends to a bounded antilinear form on \mathcal{H} ; hence $D(T_F) \supset D(T)$. On the other hand, $v \in D(T^*)$ iff $u \in D(T) \mapsto \langle Tu, v \rangle$ extends to a bounded antilinear form on \mathcal{H} . Since $u \in \mathcal{V} \mapsto \bar{q}(u, v)$ is already an extension of $u \in D(T) \mapsto \langle Tu, v \rangle$, we see that extending the latter allows to extend the former: this means that $D(T_F) \subset D(T^*)$. Since T is selfadjoint, we draw $D(T) = D(T_F)$, hence $T = T_F$. \square

Remark 3.2.5 (Form domain) The domain of the associated closed form \bar{q} is usually called the *form domain* of T , and is denoted by $Q(T)$. The form domain plays an important role in the analysis of selfadjoint operators, see e.g. the Chapter 8 on variational methods.

By construction, this form domain $Q(T)$ contains the operator domain $D(T)$, and this inclusion is often a *strict* one. Yet, for $u, v \in Q(T)$ one sometimes uses the abusive notation $\langle u, Tv \rangle$ to denote $\bar{q}(u, v)$, eventhough v may not belong to $D(T)$.

Example 3.2.6 (Semibounded Schrödinger operators) A basic example for the Friedrichs extension is delivered by Schrödinger operators with semibounded potentials. Let $W \in L^2_{\text{loc}}(\mathbb{R}^d, \mathbb{R})$ and $W \geq -C$, $C \in \mathbb{R}$ (i.e. W is semibounded from below). On $\mathcal{H} = L^2(\mathbb{R}^d)$, we consider the operator T acting as $Tu(x) = -\Delta u(x) + W(x)u(x)$ on the domain $D(T) = C_c^\infty(\mathbb{R}^d)$. This operator is clearly symmetric and semibounded from below:

$$(3.2.7) \quad \forall u \in C_c^\infty(\mathbb{R}^d), \quad \langle u, Tu \rangle = \|\nabla u\|^2 + \int W|u|^2 dx \geq -C\|u\|^2.$$

The Friedrichs extension T_F of T will be called the *Schrödinger operator* with potential W . Note that the expression in the middle of (3.2.7) allows to define the sesquilinear form q associated with T :

$$q(u, v) = \int_{\mathbb{R}^d} \overline{\nabla u} \nabla v dx + \int_{\mathbb{R}^d} W \bar{u} v dx.$$

Let us denote by \bar{q} the closure of q . For u to be in $D(\bar{q})$, both terms in the above expression must be finite, so $D(\bar{q})$ is included in the following weighted Sobolev space:

$$D(\bar{q}) \subset H^1_W(\mathbb{R}^d) \stackrel{\text{def}}{=} \left\{ u \in H^1(\mathbb{R}^d) : \int |W||u|^2 dx < \infty \right\}.$$

We actually have the equality $D(\bar{q}) = H^1_W(\mathbb{R}^d)$ (see Theorem 8.2.1 in Davies's book [4] for a rather technical proof), but the inclusion will suffice for our purposes.

We now extend the construction of Schrödinger operators to a class of potentials which are *not* semibounded from below, but which are still bounded from below by a specific negative function (see Corollary 3.2.9). The main interest of this class of potentials is that they include the physically relevant *Coulomb potential*.

Proposition 3.2.7 (Hardy's inequality) Let $d \geq 3$. Then, for any $u \in C_c^\infty(\mathbb{R}^d)$, the following inequality holds:

$$\int_{\mathbb{R}^d} |\nabla u(x)|^2 dx \geq \frac{(d-2)^2}{4} \int_{\mathbb{R}^d} \frac{|u(x)|^2}{|x|^2} dx.$$

The restriction on the dimension is necessary to make the function $x \mapsto |x|^{-2}$ locally integrable near the origin.

Remark 3.2.8 (Uncertainty principles) Before proving Hardy's inequality, let us argue that this inequality can be interpreted as a form of uncertainty principle, similar to the well-known Heisenberg uncertainty principle in quantum mechanics or harmonic analysis. The latter takes the following form: for any $u \in C_c^\infty(\mathbb{R}^d)$ normalized as $\|u\|_{L^2} = 1$, one has

$$\|\nabla u\|_{L^2} \|x|u|\|_{L^2} \geq C_0, \quad \text{with the constant } C_0 = \frac{d}{4}.$$

The interpretation is the following: a function which is very localized near $x = 0$, thus for which $\|x|u|\|_{L^2}$ is much smaller than $\|u\|_{L^2} = 1$, must have a large gradient (in the L^2 sense). Conversely, a very "flat" function, for which $\|\nabla u\| \ll \|u\|$, must be quite delocalized, forcing $\|x|u|\|_{L^2}$ to be large.

In quantum mechanics, the two above factors can be interpreted as the *quantum averages*, for the normalized state u , of the positive Laplacian (the "kinetic energy" operator), respectively of the operator of multiplication by $|x|^2$:

$$\begin{aligned} \|\nabla u\|^2 &= \langle u, -\Delta u \rangle = \langle u, (-i\nabla)^2 u \rangle \stackrel{\text{def}}{=} \mathbb{E}_u(D_x^2), \\ \|x|u|\|^2 &= \langle u, |x|^2 u \rangle \stackrel{\text{def}}{=} \mathbb{E}_u(|x|^2). \end{aligned}$$

Written in these probabilistic notations, the uncertainty principle reads:

$$\mathbb{E}_u((-i\nabla)^2) \mathbb{E}_u(|x|^2) \geq C_0 \iff \mathbb{E}_u((-i\nabla)^2) \geq \frac{C_0}{\mathbb{E}_u(|x|^2)}, \quad \text{for all normalized } u.$$

Expressed in these notations, the right-hand side in Hardy's inequality takes the form of the quantum average of the operator of multiplication by $\frac{1}{|x|^2}$:

$$\mathbb{E}_u((-i\nabla)^2) \geq C_1 \mathbb{E}_u\left(\frac{1}{|x|^2}\right), \quad \text{with the constant } C_1 = \frac{(d-2)^2}{4}.$$

Hence, Hardy's inequality essentially amounts to replacing, on the right-hand side, the inverse average $\frac{1}{\mathbb{E}_u(|x|^2)}$, by the average of the inverse, $\mathbb{E}_u\left(\frac{1}{|x|^2}\right)$. Both inequalities have a similar meaning: a function with a small gradient $\mathbb{E}_u((-i\nabla)^2)$ must be delocalized, hence it cannot concentrate too much at the origin, which prevents $\mathbb{E}_u\left(\frac{1}{|x|^2}\right)$ from exploding.

Proof.— The proof of the Hardy inequality borrows the same methods as the proof of the Heisenberg uncertainty principle. For any $\gamma \in \mathbb{R}$, we construct the mixed operator

$$u \in C_c^\infty(\mathbb{R}^d) \mapsto P_\gamma u(x) \stackrel{\text{def}}{=} \frac{1}{i} \nabla u(x) + i\gamma \frac{x}{|x|^2} u(x),$$

Now, the obvious inequality

$$\|P_\gamma u\|_{L^2}^2 \geq 0, \quad \text{for any } u \in C_c^\infty(\mathbb{R}^d),$$

may be expanded into:

$$(3.2.8) \quad \int_{\mathbb{R}^d} |\nabla u(x)|^2 dx + \gamma^2 \int_{\mathbb{R}^d} \frac{|u(x)|^2}{|x|^2} dx \geq \gamma \int_{\mathbb{R}^d} \left(x \cdot \overline{\nabla u(x)} \frac{u(x)}{|x|^2} + x \cdot \nabla u(x) \frac{\overline{u(x)}}{|x|^2} \right) dx.$$

Using the identities

$$\nabla |u|^2 = \overline{u} \nabla u + u \overline{\nabla u}, \quad \operatorname{div} \left(\frac{x}{|x|^2} \right) = \frac{d-2}{|x|^2},$$

and integration by parts, the integral in the right-hand side of (3.2.8) becomes

$$\begin{aligned} \int_{\mathbb{R}^d} \left(\frac{x}{|x|^2} \cdot \left(\overline{\nabla u(x)} u(x) + \nabla u(x) \overline{u(x)} \right) \right) dx &= \int_{\mathbb{R}^d} \frac{x}{|x|^2} \cdot \nabla |u(x)|^2 dx \\ &= - \int_{\mathbb{R}^d} \operatorname{div} \left(\frac{x}{|x|^2} \right) |u(x)|^2 dx = -(d-2) \int_{\mathbb{R}^d} \frac{|u(x)|^2}{|x|^2} dx. \end{aligned}$$

The above expression could be recast into the “magic fact” that sum of commutators $\sum_{j=1}^d [\frac{1}{i} \partial_j, \frac{x_j}{|x|^2}]$ gives back a multiple of the operator $\frac{1}{|x|^2}$, which already appears on the left-hand side of (3.2.8). Finally, inserting this equality into (3.2.8) gives

$$\int_{\mathbb{R}^d} |\nabla u(x)|^2 dx \geq \gamma((d-2) + \gamma) \int_{\mathbb{R}^d} \frac{|u(x)|^2}{|x|^2} dx.$$

In order to maximize the coefficient before the integral, we adjust the parameter γ to the value $\gamma = -(d-2)/2$, which gives our result. \square

From Hardy’s inequality, we draw the following criterium for a semibounded Schrödinger operator.

Corollary 3.2.9 Let $d \geq 3$ and $W \in L_{\text{loc}}^2(\mathbb{R}^d)$ be real valued, with $W(x) \geq -\frac{(d-2)^2}{4|x|^2}$. Then the operator $T = -\Delta + W$ defined on the domain $C_c^\infty(\mathbb{R}^d \setminus 0)$, is semibounded from below, hence it admits a selfadjoint extension.

Notice that we need to be careful when multiplying by the potential W : applying this multiplication to a function $u \in C_c^\infty(\mathbb{R}^d)$ with $u(0) \neq 0$ will not produce a function in $L^2(\mathbb{R}^d)$ if $d \leq 4$, since $\frac{1}{|x|^4}$ is not locally integrable at the origin. This is why we need to define the operator T on $C_c^\infty(\mathbb{R}^d \setminus 0)$.

Example 3.2.10 (Coulomb potential) In the ambient space \mathbb{R}^3 , the Coulomb potential generated by a charge placed at the origin, is of the form $W(x) = \frac{C}{|x|}$, where $C \in \mathbb{R}$ is the product of the charges of the particle at the origin and of the particle at the point x . If both particles have charges of the same sign, they repel each other, implying that $W(x)$ grows to $+\infty$ when $|x| \rightarrow 0$. In the case of opposite charges, $C < 0$, and the potential energy goes to $-\infty$ when $|x| \rightarrow 0$: the particles attract each other.

We want to show that whatever the value of $C \in \mathbb{R}$, the operator $T = -\Delta + C/|x|$ acting on $C_c^\infty(\mathbb{R}^3)$ is semibounded from below. In the “repulsive situation” $C \geq 0$, we are in the situation of Example 3.2.6, since the potential is positive; the operator is then positive as well (the sum of two positive operators is obviously positive). On the opposite, in the case $C < 0$, it is not clear whether the operator is bounded from below: could the quantum particle “collapse” to the origin under the attraction of the charge at the origin, leading to arbitrary negative values of $\langle u, Tu \rangle$?

We are going to show that this collapse is impossible: eventhough $W(x) \rightarrow -\infty$ when $|x| \rightarrow 0$, the operator $T = -\Delta + \frac{C}{|x|}$ will be bounded from below, due to the uncertainty principle embodied in Hardy’s inequality.

For any $u \in C_c^\infty(\mathbb{R}^3)$ and any $p \in \mathbb{R}^*$, we may write:

$$\begin{aligned} \int_{\mathbb{R}^3} \frac{|u|^2}{|x|} dx &= \int_{\mathbb{R}^3} p|u| \frac{|u|}{p|x|} dx \leq \frac{p^2}{2} \int_{\mathbb{R}^3} |u|^2 dx + \frac{1}{2p^2} \int_{\mathbb{R}^3} \frac{|u|^2}{|x|^2} dx \\ &\stackrel{\text{Hardy}}{\leq} \frac{p^2}{2} \int_{\mathbb{R}^3} |u|^2 dx + \frac{1}{8p^2} \int_{\mathbb{R}^3} |\nabla u|^2 dx. \end{aligned}$$

As a consequence (remember that $C < 0$):

$$\langle u, Tu \rangle = \int_{\mathbb{R}^3} |\nabla u|^2 dx - |C| \int_{\mathbb{R}^3} \frac{|u|^2}{|x|} dx \geq \left(1 - \frac{|C|}{8p^2}\right) \int_{\mathbb{R}^3} |\nabla u|^2 dx - \frac{|C|p^2}{2} \int_{\mathbb{R}^3} |u|^2 dx.$$

We may now pick $p = \sqrt{\frac{|C|}{8}}$ to make the operator T bounded from below by $-\frac{|C|^2}{16}$.

As a consequence, for any $C \in \mathbb{R}$ the above operator T can be extended to a selfadjoint Friedrichs extension.

3.3 Exercises

Exercise 3.3.1 Show that the following sesquilinear forms q are closed and semibounded from below, and describe the associated selfadjoint operators on \mathcal{H} ($\alpha \in \mathbb{R}$ is a fixed parameter):

(a) $\mathcal{H} = L^2([0, \infty[)$, $D(q) = H^1([0, \infty[)$, $q(u, v) = \int_0^\infty \overline{u'(s)}v'(s) ds + \alpha \overline{u(0)}v(0)$.

(b) $\mathcal{H} = L^2(\mathbb{R})$, $D(q) = H^1(\mathbb{R})$, $q(u, v) = \int_{\mathbb{R}} \overline{u'(s)}v'(s) ds + \alpha \overline{u(0)}v(0)$.

(c) $\mathcal{H} = L^2([0, 1])$, $D(q) = \{u \in H^1([0, 1]) : u(0) = u(1)\}$, $q(u, v) = \int_0^1 \overline{u'(s)}v'(s) ds$.

Exercise 3.3.2 This exercise shows a possible way of constructing the sum of two unbounded operators under the assumption that one of them is “smaller” than the other one. In a sense, we are going to extend the construction of Exercise 1.4.

Let \mathcal{H} be a Hilbert space, q be a closed sesquilinear form on \mathcal{H} , and T the self-adjoint operator on \mathcal{H} associated with q . Let B be a symmetric linear operator in \mathcal{H} such that $D(q) \subset D(B)$ and such that there exist $\alpha, \beta > 0$ with $\|Bu\|^2 \leq \alpha q(u, u) + \beta \|u\|^2$ for all $u \in D(q)$. Consider the operator S on $D(S) = D(T)$ defined by $Su = Tu + Bu$. We are going to show that S is self-adjoint.

(a) Consider the sesquilinear form $s(u, v) = q(u, v) + \langle u, Bv \rangle$, $D(s) = D(q)$. Show that s is closed.

(b) Let \tilde{S} be the operator associated with s . Show that $D(\tilde{S}) = D(T)$ and that $\tilde{S}u = Tu + Bu$ for all $u \in D(T)$.

(c) Show that S is self-adjoint.

Exercise 3.3.3 In the examples below the Sobolev embedding theorem and the previous exercise can be of use.

(a) Let $v \in L^2(\mathbb{R})$ be real-valued. Show that the operator A having as domain $D(A) = H^2(\mathbb{R})$ and acting by $Af(x) = -f''(x) + v(x)f(x)$ is a self-adjoint operator on $L^2(\mathbb{R})$.

(b) Let $v \in L^2_{\text{loc}}(\mathbb{R})$ be real-valued and 1-periodic, i.e. $v(x+1) = v(x)$ for all $x \in \mathbb{R}$. Show that the operator A with the domain $D(A) = H^2(\mathbb{R})$ acting by $Af(x) = -f''(x) + v(x)f(x)$ is self-adjoint.

(c) Let $\mathcal{H} = L^2(\mathbb{R}^3)$. Suggest a class of unbounded potentials $v : \mathbb{R}^3 \rightarrow \mathbb{R}$ such that the operator $Af(x) = -\Delta f(x) + v(x)f(x)$, with the domain $D(A) = H^2(\mathbb{R}^3)$, is self-adjoint on \mathcal{H} .

Exercise 3.3.4 (a) Let \mathcal{H} be a Hilbert space and A be a closed densely defined operator in \mathcal{H} (not necessarily symmetric). Consider the operator L given by

$$Lu = A^*Au, \quad u \in D(L) = \{u \in D(A) : Au \in D(A^*)\}.$$

We will write simply $L = A^*A$ having in mind the above precise definition. While the above is a natural definition of the product of two operators, it is not clear if the domain $D(L)$ is sufficiently large. We are going to study this question.

i) Consider the sesquilinear form $b(u, v) = \langle Au, Av \rangle + \langle u, v \rangle$ on \mathcal{H} defined on $D(b) = D(A)$. Show that this form is closed.

ii) Let B be the self-adjoint operator associated with the form b . Find a relation between L and B and show that L is densely defined, self-adjoint and positive.

iii) Let A_0 denote the restriction of A to $D(L)$. Show that $\overline{A_0} = A$.

(b) A linear operator A acting in a Hilbert space \mathcal{H} is called *normal* if $D(A) = D(A^*)$ and $\|Ax\| = \|A^*x\|$ for all $x \in D(A)$.

- i)* Show that any normal operator is closed.
- ii)* Let A be a closed operator. Show: A is normal iff A^* is normal.
- iii)* Let A be a normal operator. Show: $\langle Ax, Ay \rangle = \langle A^*x, A^*y \rangle$ for all $x, y \in D(A) \equiv D(A^*)$.
- iv)* Let A be a closed operator. Show: A is normal iff $AA^* = A^*A$. Here the both operators are defined as in (a), the operator AA^* being understood as $(A^*)^*A^*$.

Chapter 4

Spectrum and resolvent

We will now focus on the central topic of this course, namely the spectrum of (mostly unbounded) linear operators.

4.1 Definitions

In this section we will consider operators $(T, D(T))$ defined on a Banach space \mathcal{B} , or sometimes only a Hilbert space \mathcal{H} , and with dense domain $D(T)$.

On a d -dimensional vector space, the spectrum of an operator (which can be represented as a matrix) is identical to the union of all eigenvalues of the operator; it is composed of at most d complex numbers.

On infinite dimensional vector spaces, the situation is more complicated: the eigenvalues of the operator are usually only one part of the spectrum, namely the *point spectrum*, while the full spectrum can be more easily defined through its complement, called the *resolvent set* of the operator.

Definition 4.1.1 (Resolvent set, spectrum, point spectrum) Let $(T, D(T))$ be a linear operator on a Banach space \mathcal{B} . The *resolvent set* $\text{res } T$ consists of the complex numbers $z \in \mathbb{C}$ for which the operator $T - z : D(T) \rightarrow \mathcal{B}$ is bijective, and with inverse $(T - z)^{-1} : \mathcal{B} \rightarrow \mathcal{B}$ a continuous operator.

The *spectrum* $\text{spec } T$ of T is defined by $\text{spec } T \stackrel{\text{def}}{=} \mathbb{C} \setminus \text{res } T$. The *point spectrum* $\text{spec}_p T$ is the set of eigenvalues of T , namely the set of points $z \in \mathbb{C}$ such that $\text{Ker}(T - z) \neq \{0\}$. The dimension of $\text{Ker}(T - z)$ is called the *geometric multiplicity* of the eigenvalue z .

The resolvent set, respectively the spectrum of T are often denoted by $\rho(T)$, resp. $\sigma(T) = \text{spec}(T)$.

Proposition 4.1.2 If $\text{res } T \neq \emptyset$, then T must be a closed operator.

Proof.— Let $z \in \text{res } T$, then the graph $\text{gr}(T - z)^{-1}$ of the continuous operator $(T - z)^{-1}$ is closed (by the closed graph theorem). Since $\text{gr}(T - z) = S(\text{gr}(T - z)^{-1})$ where $S(u, v) = (v, u)$, the graph of $T - z$ is also closed, since the involution S is continuous. \square

Proposition 4.1.3 Let T be a *closed* operator on \mathcal{B} . Then one has the following equivalence:

$$z \in \text{res } T \iff \{ \text{Ker}(T - z) = \{0\} \text{ and } \text{Ran}(T - z) = \mathcal{B} \}.$$

Proof.— The \Rightarrow direction follows from the definition.

Assume $(T, D(T))$ is a closed operator, and $z \in \mathbb{C}$ such that $\text{Ker}(T - z) = \{0\}$ and $\text{Ran}(T - z) = \mathcal{H}$. The operator $(T - z)^{-1}$ is then well-defined on the whole of \mathcal{B} , and has a closed graph (since the graph of $T - z$ is closed); by the closed graph theorem, this operator is continuous. \square

Notice that, as opposed to finite-dimensional situations, the condition $\text{Ker}(T - z) = \{0\}$ alone does not suffice to characterize the spectrum; it only characterizes the point spectrum of T .

The resolvent is a family of operators $\{(T - z)^{-1}; z \in \text{res } T\}$, which enjoys interesting properties. It will be very important in the rest of these lectures. We first recall a few facts:

Lemma 4.1.4 (Neumann series inversion) Assume $A \in \mathcal{L}(\mathcal{B})$ is such that $\|A\| < 1$. Then the operator $(I - A) \in \mathcal{L}(\mathcal{B})$ is invertible, and its inverse can be expressed as a Neumann series:

$$(I - A)^{-1} = \sum_{n \geq 0} A^n.$$

As a first application, let us observe the case of bounded operators.

Proposition 4.1.5 (Spectrum of bounded operators) Let T be a continuous operator on \mathcal{B} . Then the resolvent set of T is not empty. More precisely, it contains $\{z \in \mathbb{C}; |z| > \|T\|_{\mathcal{L}(\mathcal{B})}\}$.

Proof.— If $|z| > \|T\|$, then the operator $(zI - T) = z(I - z^{-1}T)$ can be inverted by Neumann series:

$$|z| > \|T\| \implies (zI - T)^{-1} = z^{-1} \sum_{n \geq 0} (z^{-1}T)^n.$$

\square

The resolvent is a function of $z \in \text{res } T$, valued in $\mathcal{L}(\mathcal{B})$. An important property will be the holomorphy of this function, a notion which directly generalizes the holomorphy of complex valued functions.

Definition 4.1.6 Let $\Omega \subset \mathbb{C}$ be open. An operator valued function $z \in \Omega \mapsto A(z) \in \mathcal{L}(\mathcal{B})$ is said to be holomorphic (or strongly analytic) at a point $z_0 \in \Omega$ if the ratio $\frac{A(z)-A(z_0)}{z-z_0}$ admits a limit in $\mathcal{L}(\mathcal{B})$ when $z \rightarrow z_0$ in Ω . The limit, denoted $A'(z_0)$, is the (holomorphic) derivative of $A(z)$ at the point z_0 .

Lemma 4.1.7 If $z \mapsto A(z)$ is holomorphic in all points of a ball $B(z_0, r)$, $r > 0$, then the function $A(z)$ admits a convergent Taylor series at the point z_0 .

Like for scalar valued holomorphic functions, the coefficients $A^{(n)}(z_0)/n!$ of the Taylor series can be obtained by the Cauchy formula centered at z_0 :

$$\frac{1}{n!}A^{(n)}(z_0) = \frac{1}{2i\pi} \oint_{|z-z_0|=r-\epsilon} \frac{A(z)}{z-z_0} dz.$$

Proposition 4.1.8 (Elementary properties of the resolvent) The set $\text{res } T$ is open, so its complement $\text{spec } T$ is closed. The operator function

$$\text{res } T \ni z \mapsto R_T(z) \stackrel{\text{def}}{=} (T - z)^{-1} \in \mathcal{L}(\mathcal{B}),$$

called the *resolvent* of T , is holomorphic and satisfies the following identities:

$$(4.1.1) \quad R_T(z_1) - R_T(z_2) = (z_1 - z_2)R_T(z_1)R_T(z_2), \quad (\text{Resolvent identity})$$

$$(4.1.2) \quad R_T(z_1)R_T(z_2) = R_T(z_2)R_T(z_1), \quad (\text{commutative family})$$

$$(4.1.3) \quad \frac{d}{dz}R_T(z) = R_T(z)^2,$$

for all $z, z_1, z_2 \in \text{res } T$.

Proof.— Let $z_0 \in \text{res } T$. The obvious equality

$$(T - z_0)(T - z_0)^{-1} = I : \mathcal{B} \rightarrow \mathcal{B},$$

implies the following one:

$$T - z = (T - z_0)(I - (z - z_0)R_T(z_0)).$$

If $|z - z_0| < 1/\|R_T(z_0)\|$, then the operator on the right-hand side admits a bounded inverse, which can be obtained through a Neumann series. This implies that such values $z \in \text{res } T$. Moreover, one has the series representation

$$(4.1.4) \quad R_T(z) = (I - (z - z_0)R_T(z_0))^{-1}R_T(z_0) = \sum_{j=0}^{\infty} (z - z_0)^j R_T(z_0)^{j+1},$$

This representation shows that R_T exists in a neighbourhood of z_0 , and that it depends *holomorphically* on z in this neighbourhood.

The resolvent identity (4.1.1) is obtained through easy manipulations:

$$\begin{aligned} I - (T - z_2)R_T(z_2) &= 0 \\ \iff I - \{(T - z_2) + (z_2 - z_1)\}R_T(z_2) &= (z_1 - z_2)R_T(z_2) \\ \iff I - (T - z_1)R_T(z_2) &= (z_1 - z_2)R_T(z_2) \\ \iff R_T(z_1) - R_T(z_2) &= (z_1 - z_2)R_T(z_1)R_T(z_2). \end{aligned}$$

The commutativity of the family $\{R_T(z), z \in \text{res}(T)\}$ directly follows from this identity. Besides, taking z_2 in a ball $B(z_1, r) \subset \text{res}(T)$ and taking $z_2 \rightarrow z_1$ in this ball, we draw from this identity, and the continuity of R_T w.r.t. z , the derivative identity (4.1.3). \square

4.2 Examples

Let us consider a series of examples featuring various situations where an explicit calculation of the spectrum is possible. We emphasize that the point spectrum is usually a proper subset of the spectrum!

4.2.1 Spectrum of bounded operators

We start by a simple, yet not completely obvious fact.

Proposition 4.2.1 Let T be a continuous operator on a Banach space \mathcal{B} . Then its spectrum is nonempty: $\text{spec } T \neq \emptyset$.

Proof.— We know that for $|z| > \|T\|_{\mathcal{L}(\mathcal{B})}$, the operator $(z - T)^{-1}$ can be represented by a Neumann series, and is holomorphic. Assuming that $\text{res}(T) = \mathbb{C}$ means that this operator valued holomorphic function can be continued to all of \mathbb{C} . For any vectors $v \in \mathcal{B}$ and continuous linear form $L \in \mathcal{B}^*$, the function $z \mapsto \langle L((z - T)^{-1}v) \rangle$ is thus entire and bounded; besides, it decays to zero when $|z| \rightarrow \infty$. Liouville's theorem then implies that this function vanishes identically. Since it is the case for any u, L , the operator $(z - T)^{-1}$ vanishes identically, which is a contradiction. \square

Proposition 4.2.2 (Invertible continuous operator) Assume $T \in \mathcal{L}(\mathcal{B})$ is invertible with bounded inverse. Then $\text{spec}(T^{-1}) = \frac{1}{\text{spec}(T)} = \{\frac{1}{z}; z \in \text{spec}(T)\}$.

Proof.— For any $0 \neq z \in \text{res}(T)$, we may write

$$(T - z)^{-1} = (zT(z^{-1} - T^{-1}))^{-1} = (z^{-1} - T^{-1})^{-1}z^{-1}T^{-1},$$

which shows that $(z^{-1} - T^{-1})^{-1}$ is bounded, hence $z^{-1} \in \text{res}(T^{-1})$. Besides, T^{-1} is invertible, hence $0 \in \text{res}(T^{-1})$. We have shown that $0 \neq z \in \text{res} T \implies z^{-1} \in \text{res} T^{-1}$. Exchanging the roles of T and T^{-1} , we obtain the reverse inclusion. Finally, 0 is in the resolvent sets of T and T^{-1} , hence

$$\text{res}(T^{-1}) = \{z^{-1}; z \in \text{res}(T)\} \cup \{0\},$$

from where we deduce the statement. □

This proposition allows to constrain the spectrum of unitary operators on a Hilbert space \mathcal{H} .

Corollary 4.2.3 Let \mathcal{H} be a Hilbert space, and $U : \mathcal{H} \rightarrow \mathcal{H}$ be a unitary operator. Then $\text{spec}(U) \subset \{z \in \mathbb{C}; |z| = 1\}$.

Example 4.2.4 Let us define the *shift operator* on \mathbb{Z} , $S : \ell^2(\mathbb{Z}) \rightarrow \ell^2(\mathbb{Z})$ by $(Su)(n) = u(n+1)$. Then $\text{spec}(S) = \{z \in \mathbb{C}; |z| = 1\}$.

Proof.— The above corollary shows the inclusion. To show that $e^{i\theta} \in \text{spec}(S)$ for any $\theta \in [0, 2\pi[$, we will construct *quasimodes* associated with the spectral value $e^{i\theta}$. Namely, for any small $\varepsilon > 0$, there exists a nonzero $u_{\theta, \varepsilon} \in \ell^2$, such that

$$(4.2.5) \quad \|(S - e^{i\theta})u_{\theta, \varepsilon}\| \leq \varepsilon \|u_{\theta, \varepsilon}\|.$$

The sequence $(u_{\theta, 1/m})_{m \geq 1}$ then shows that $(S - e^{i\theta})$ is not invertible with bounded inverse, hence $e^{i\theta} \in \text{spec}(S)$.

Definition 4.2.5 Nontrivial vectors $u_{\theta, \varepsilon}$ satisfying (4.2.5) are called *quasimodes* of S , with quasi-eigenvalue $e^{i\theta}$, and *error* (or *discrepancy*) ε .

How to construct such quasimodes? If we tried to construct an eigenstate $(S - e^{i\theta})u = 0$, it would necessarily take the form

$$u_{\theta}(n) = e^{i\theta} u_{\theta}(n-1) = e^{in\theta} u_{\theta}(0),$$

which gives a sequence $u_{\theta} \notin \ell^2$. Hence $e^{i\theta}$ is not in the point spectrum, which shows that the point spectrum is empty.

In order to construct a quasimode, we may truncate the formal eigenvector u_{θ} , taking for some $N > 0$ the vector

$$u_{\theta, N}(n) = \mathbb{1}_{|n| \leq N} e^{in\theta}.$$

An easy computation shows that $\|u_{\theta, N}\| = \sqrt{2N+1}$ while $\|(S - e^{i\theta})u_{\theta, N}\| = \sqrt{2}$, so this state is an ε -quasimode for $\varepsilon = N^{-1/2}$.

One can obtain a smaller error by *smoothly* truncating the above formal eigenstate. Namely, we fix some auxiliary function $\chi \in C_c^1([-1, 1])$, and define

$$u_\varepsilon(n) \stackrel{\text{def}}{=} \chi(n\varepsilon) e^{in\theta}.$$

We notice that this sequence is supported in the interval $\{|n| \leq 1/\varepsilon\}$. We then check that

$$u_\varepsilon(n+1) - e^{i\theta}u_\varepsilon(n) = e^{i(n+1)\theta} \left(\chi((n+1)\varepsilon) - \chi(n\varepsilon) \right) \implies |Su_\varepsilon - e^{i\theta}u_\varepsilon|(n) \leq \varepsilon \sup_{t \in [n\varepsilon; (n+1)\varepsilon]} |\chi'(t)|$$

Squaring this expression and summing over $n \in \mathbb{Z}$, we find that

$$\|Su_\varepsilon - e^{i\theta}u_\varepsilon\|^2 \leq \varepsilon \sum_{n \in \mathbb{Z}} \sup_{t \in [n\varepsilon; (n+1)\varepsilon]} |\chi'(t)|^2.$$

The sum on the RHS converges to $C_\chi \stackrel{\text{def}}{=} \int_{\mathbb{R}} |\chi'(t)|^2 dt < \infty$ when $\varepsilon \rightarrow 0$, so for $\varepsilon > 0$ small enough we have:

$$\|Su_\varepsilon - e^{i\theta}u_\varepsilon\|^2 \leq \varepsilon 2C_\chi.$$

On the other hand, we check that

$$\|u_\varepsilon\|^2 = \sum_{n \in \mathbb{Z}} |\chi(n\varepsilon)|^2 = \varepsilon^{-1} \left(\int_{\mathbb{R}} |\chi(t)|^2 dt + o(1)_{\varepsilon \rightarrow 0} \right).$$

Comparing the two expressions, we see that there exists $C > 0$ such that, for $\varepsilon > 0$ small enough,

$$\|Su_\varepsilon - e^{i\theta}u_\varepsilon\| \leq C \varepsilon \|u_\varepsilon\|.$$

□

Another method of proof will be presented later, which uses the fact that the Fourier transform maps S to a simple multiplication operator on $[0, 1[$.

Example 4.2.6 Let us now consider the shift operator acting on the single-sided sequences $\ell^2(\mathbb{N})$. It is still defined by $Tu(n) = u(n+1)$. This operator is not an isometry on $\ell^2(\mathbb{N})$, it is a contraction of norm $\|T\| = 1$

We claim that $\text{spec}(T) = \{|z| \leq 1\}$, and most it consists in eigenvalues: $\text{spec}_p(T) = \{|z| < 1\}$.

The adjoint of this operator is given by $T^*(u(0), u(1), u(2) \dots) = (0, u(0), u(1), u(2) \dots)$. Its spectrum can be obtained through the following general

Proposition 4.2.7 Let $(T, D(T))$ be a closed operator on some Hilbert space \mathcal{H} . Then

$$\text{spec}(T^*) = \overline{\text{spec } T} = \{\bar{z}; z \in \text{spec}(T)\}.$$

Proof.— For any $z \in \text{res}(T)$, the operator $[(z - T)^{-1}]^*$ satisfies

$$\begin{aligned} \forall v \in \mathcal{H}, \forall u \in D(T^*), \quad \langle [(z - T)^{-1}]^*(\bar{z} - T^*)u, v \rangle &= \langle (\bar{z} - T^*)u, (z - T)^{-1}v \rangle \\ &= \langle u, (z - T)(z - T)^{-1}v \rangle = \langle u, v \rangle \end{aligned}$$

(notice that $(z - T)^{-1}v$ is automatically in $D(T)$). This shows that $[(z - T)^{-1}]^*(\bar{z} - T^*) = I_{D(T^*)}$. The equality $(\bar{z} - T^*)[(z - T)^{-1}]^* = I_{\mathcal{H}}$ is proved similarly. This shows that $\bar{z} \in \text{res}(T^*)$, and therefore $\overline{\text{res}T} \subset \text{res}(T^*)$. Since for a closed operator $T^{**} = T$, we obtain the reverse inclusion, hence the equality for the resolvent sets. The statement is obtained by taking the complementary sets. \square

If we apply the above Proposition to our continuous operator T of Ex.4.2.6, we find that $\text{spec}(T^*) = \{|z| \leq 1\}$. However, that spectrum is not of the same nature as $\text{spec}(T)$. A simple computation shows that for any $z \in \mathbb{C}$, $\text{Ker}(T^* - z) = \{0\}$, so $\text{spec}_p(T^*) = \emptyset$. On the other hand, for $|z| < 1$ we have $\text{Ker}(T^* - z) = \{0\}$ and $\text{Ran}(\bar{z} - T^*) = \text{Ker}(z - T)^\perp$ has codimension one. In this situation we say that \bar{z} belongs to the *residual spectrum* of T^* .

Definition 4.2.8 (Residual spectrum) Let $(T, D(T))$ be a closed linear operator on \mathcal{H} . We say that z lies in the residual spectrum of T if $\text{Ker}(T - z) = \{0\}$ and $\text{Ran}(T - z)$ is not dense in \mathcal{H} .

4.2.2 Evolution operators

Let us consider a situation where a continuous operator $T \in \mathcal{L}(\mathcal{B})$ models the *evolution* of a state $u_0 \in \mathcal{B}$, that is it embodies a certain *dynamical system*. One is then interested by the evolution of the state for long times, that is the behaviour of $T^n u_0$ when $n \rightarrow \infty$. An important information is then the spectral radius of the operator T .

Definition 4.2.9 Let $T \in \mathcal{L}(\mathcal{B})$. We define the spectral radius of T by:

$$r(T) \stackrel{\text{def}}{=} \sup\{|z|; z \in \text{spec}(T)\}.$$

Notice that the supremum is well-defined, since we know that $\text{spec}(T) \neq \emptyset$. The Proposition 4.1.5 already shows that $r(T) \leq \|T\|$. The following theorem connects this radius with the long time iterates of the operator.

Theorem 4.2.10 Let $T \in \mathcal{L}(\mathcal{B})$. Then $r(T) = \lim_{n \rightarrow \infty} \|T^n\|^{1/n}$.

Proof.— The inequality $\|T^{n+m}\| \leq \|T^n\| \|T^m\|$ shows that the sequence $t_n \stackrel{\text{def}}{=} \log \|T^n\|$ is subadditive. As a result, the sequence (t_n/n) converges to a limit, hence its exponential is the limit of $\|T^n\|^{1/n}$, which we call r . Let us check that this limit is the spectral radius.

Take $z \in \mathbb{C}$ such that $|z| > r$. then for any $0 < \epsilon < |z| - r$, there exists $n_\epsilon \in \mathbb{N}$ such that for any $n \geq n_\epsilon$, $\|T^n\| \leq (|z| - \epsilon)^n$. As a result, the series $\sum_{n \in \mathbb{N}} \frac{T^n}{z^n}$ converges, which shows that $z \in \text{res}(T)$. This shows that $r(T) \leq r$.

On the opposite, since $\{|z| > r\} \subset \text{res } T$, the function $w \mapsto (I - wT)^{-1}$ is well-defined and analytic in the disk $\{|w| < r(T)^{-1}\}$, so its series expansion converges in this disk. Take any $r_0 > r(T)$. The Cauchy formula then allows to compute T^n by integrating on the circle $\{|z| = r_0\}$:

$$(4.2.6) \quad T^n = \frac{1}{2i\pi} \oint_{|z|=r_0} (z - T)^{-1} z^n dz.$$

Since $\|(z - T)^{-1}\| \leq C$ on the circle $|z| = r_0$, we find the bounds $\|T^n\| \leq C' r_0^n$ for all $n \in \mathbb{N}$, and thus $r \leq r_0$. \square

For an initial state $u_0 \in \mathcal{B}$, we then have, for any $\epsilon > 0$ and n large enough, the bound

$$\|T^n u_0\| \leq (r(T) + \epsilon)^n \|u_0\|.$$

If we have more informations on the spectrum, the long time behaviour can be made more precise. This is the case if the external spectrum is discrete.

Definition 4.2.11 (Discrete vs. essential spectrum) The spectrum of an operator $(T, D(T))$ splits into two parts:

1. the discrete spectrum $\text{spec}_d(T)$ made of eigenvalues with finite algebraic multiplicities, which are isolated from the rest of the spectrum;
2. the essential spectrum $\text{spec}_{ess}(T) = \text{spec}(T) \setminus \text{spec}_d(T)$.

We recall that the algebraic multiplicity of an eigenvalue z is the dimension of $\bigcup_{n \geq 1} [\text{Ker}(T - z)^n]$.

By "isolated from the rest of the spectrum", we mean that for each such eigenvalue z_i , there is some radius $r_i > 0$ s.t. $\{0 < |z| < r_i\} \cap \text{spec}(T) = \emptyset$.

In general $\text{spec}_d(T)$ is a subset of $\text{spec}_p(T)$; for instance, the shift operator T on $\ell^2(\mathbb{N})$ has no discrete spectrum, but the open unit disk is made of eigenvalues.

Let us assume that the "external spectrum" of a bounded evolution operator T is discrete, which means that for some $r_{int} < r(T)$ we have

$$\text{spec}(T) \cap \{r_{int} \leq |z| \leq r(T)\} = \text{spec}_d(T) \cap \{r_{int} \leq |z| \leq r(T)\},$$

then this external (and compact) part of the spectrum contains only finitely many eigenvalues, all of finite multiplicities. We assume that $\{|z| = r_{int}\} \cap \text{spec}(T) = \emptyset$. It is then possible to take into account these external eigenvalues in the description of $T^n u_0$, starting from the integral representation (4.2.6). The discrete external spectrum shows that $(z - T)^{-1}$ is holomorphic in $\{r_{int} \leq |z|\} \setminus \text{spec}_d(T)$. It

is then possible to deform the contour $\{|z| = r(T) + \epsilon\}$ into the union of $\{|z| = r_f\}$ with the small circles $\{|z - z_i| = r_i\}$:

$$T^n = \frac{1}{2i\pi} \oint_{|z|=r_{int}} (z - T)^{-1} z^n dz + \sum_i \frac{1}{2i\pi} \oint_{|z-z_i|=r_i} (z - T)^{-1} z^n dz.$$

For $n = 0$, the integral around the eigenvalue z_i produces the spectral projector

$$\Pi_i = \frac{1}{2i\pi} \oint_{|z-z_i|=r_i} (z - T)^{-1} dz.$$

The fact that Π_i is a projector can be shown by using the resolvent identity (Exercise).

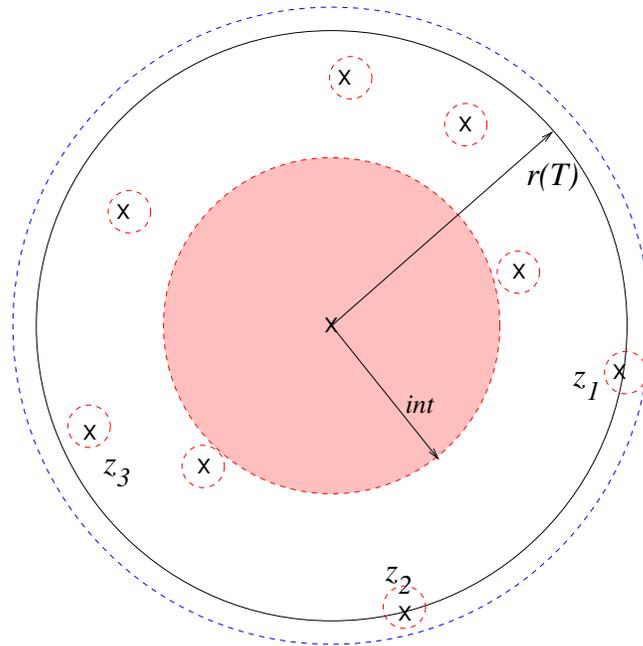


Figure 4.1: Spectrum of a quasicompact operator.

This spectral projector naturally commutes with T : $[T, \Pi_i] = 0$, implying that T preserves the generalized eigenstate $\mathcal{V}_i = \text{Ran } \Pi_i$. We may then call this finite rank operator $T_i = T|_{\mathcal{V}_i}$. It admits as only eigenvalue z_i , but can feature a nontrivial Jordan structure. In the simple case where there is no Jordan structure, then $T^n \Pi_i = (T_i)^n \Pi_i = z_i^n \Pi_i$. In the limit $n \rightarrow \infty$, these external eigenvalues allow to expand T^n as:

$$T^n = \sum_i z_i^n \Pi_i + \mathcal{O}(r_{int}^n)_{\mathcal{L}(\mathcal{B})}, \quad n \rightarrow \infty,$$

where the sum over eigenvalues is finite. In the case of nontrivial Jordan blocks, the operator T_i takes the form of $(z_i + J_i) \Pi_i$, where $J_i : \mathcal{V}_i \rightarrow \mathcal{V}_i$ is nilpotent, so that

$$(T_i)^n = (z_i + J_i)^n \Pi_i = z_i^n \sum_{k=0}^n \binom{n}{k} \left(\frac{1}{z_i} J_i\right)^k \Pi_i$$

The nilpotency of J_i implies that for some $d_i > 1$, $J_i^{d_i} = 0$, hence the above sum actually stops at the order $k = \min(n, d_i - 1)$. As a function of n , the sum is a product of z_i^n with an operator-valued polynomial in n of degree $\leq d_i - 1$.

An operator T with such an external discrete spectrum is said to be *quasicompact*.

Let us now restrict ourselves to operators acting on a Hilbert space \mathcal{H} . The spectral radius of a bounded selfadjoint operator is easy to determine.

Proposition 4.2.12 Let $T \in \mathcal{L}(\mathcal{H})$ be selfadjoint. Then its spectral radius $r(T) = \|T\|$.

Proof.— The statement just comes from the following variational identification:

$$\|T\|^2 = \sup_{u \in \mathcal{H}, \|u\|=1} \|Tu\|^2 = \sup_{u \in \mathcal{H}, \|u\|=1} \langle Tu, Tu \rangle = \sup_{u \in \mathcal{H}, \|u\|=1} \langle T^2 u, u \rangle \leq \|T^2\|.$$

On the other hand, $\|T^2\| \leq \|T\|^2$, so finally we have for any selfadjoint continuous operator $\|T^2\| = \|T\|^2$. Since T^2 is itself selfadjoint, we have then $\|T^4\| = \|T^2\|^2 = \|T\|^4$. Iterating this procedure, we see that for any $j \geq 1$, $\|T^{2^j}\| = \|T\|^{2^j}$. We thus deduce that

$$r(T) = \lim_{j \rightarrow \infty} \|T^{2^j}\|^{2^{-j}} = \|T\|.$$

□

4.2.3 Unbounded operators

All the following examples live on a Hilbert space.

Example 4.2.13 (Multiplication operator) Consider the measured space (\mathbb{R}^d, μ) equipped with a locally finite measure on the Borel σ -algebra. Let $f : (\mathbb{R}^d, \mu) \rightarrow \mathbb{C}$ be a borelian function. The *essential range* of f is defined by: by

$$\text{ess-ran}_\mu f = \left\{ z \in \mathbb{C} : \mu\{x \in \mathbb{R}^d : |f(x) - z| < \epsilon\} > 0 \text{ for all } \epsilon > 0 \right\}.$$

Proposition 4.2.14 (Spectrum of a multiplication operator) Let $f \in L^\infty_{\text{loc}}(\mathbb{R}^d, \mu; \mathbb{C})$, and consider the multiplication operator M_f acting on $L^2(\mathbb{R}^d, \mu)$, as defined in Example 2.1.8. Then,

$$\begin{aligned} \text{spec } M_f &= \text{ess-ran}_\mu f, \\ \text{spec}_p M_f &= \{z \in \mathbb{C} : \mu\{x \in \mathbb{R}^d : f(x) = z\} > 0\}. \end{aligned}$$

Proof.— Let $z \notin \text{ess-ran}_\mu f$, showing that for some $\epsilon > 0$, $|f(x) - z| \geq \epsilon$ for μ -a.e. x . The function $x \mapsto (f(x) - z)^{-1}$ is therefore in $L^\infty(\mathbb{R}^d, \mu)$. As a result, the multiplication operator $M_{1/(f-z)}$ is bounded on $L^2(\mathbb{R}^d, \mu)$, and one easily checks that it is the inverse of the operator $(M_f - z)$.

On the other hand, let $z \in \text{ess-ran}_\mu f$. For any $m \in \mathbb{N}$ denote

$$\tilde{S}_m \stackrel{\text{def}}{=} \{x \in \mathbb{R}^d : |f(x) - z| < 2^{-m}\}$$

and choose a subset $S_m \subset \tilde{S}_m$ of strictly positive but finite measure. If ϕ_m is the characteristic function of S_m , one has

$$(4.2.7) \quad \|(M_f - z)\phi_m\|^2 = \int_{S_m} |f(x) - z|^2 |\phi_m(x)|^2 d\mu(x) \leq 2^{-2m} \|\phi_m\|^2.$$

The vector ϕ_m is a quasimode of M_f , of quasi-eigenvalue z and error 2^{-m} . Since the error can be chosen arbitrary small, the operator $(M_f - z)$ cannot be inverted with bounded inverse. Indeed, if this were the case, there would be some $C > 0$ such that

$$\forall m \geq 1, \quad \|\phi_m\| = \|(M_f - z)^{-1}(M_f - z)\phi_m\| \leq C \|(M_f - z)\phi_m\|.$$

For m large enough, these inequalities contradict the ones above. This shows the statement on $\text{spec } M_f$.

To prove the assertion on the point spectrum, we remark that the condition $z \in \text{spec}_p M_f$ is equivalent to the existence of $\phi \in L^2(\mathbb{R}^d, \mu)$ such that $(f(x) - z)\phi(x) = 0$ for μ -a.e. x . This means that $\phi(x) = 0$ for μ -a.e. x in $\{f(x) \neq z\}$. If we further assume that $\{x; f(x) = z\}$ is negligible, then we would have $\phi(x) = 0$ for μ -a.e. x , or $\phi = 0$ in $L^2(\mu)$, so ϕ cannot be an eigenstate. We deduce that $\mu(f^{-1}(z)) = 0$ implies that $z \notin \text{spec}_p(M_f)$.

On the opposite, if $\mu(f^{-1}(z)) > 0$, one can choose a measurable subset $\Sigma \subset \{x : f(x) = z\}$ of strictly positive but finite measure. The function $\phi = \mathbb{1}_\Sigma$ is then an element of $L^2(\mathbb{R}^d)$, and it is an eigenfunction of M_f with eigenvalue z . \square

We notice that the above example is already nontrivial when the function $f \in L^\infty(\mathbb{R}^d, \mu)$, and the operator $M_f : L^2(\mathbb{R}^d, \mu) \rightarrow L^2(\mathbb{R}^d, \mu)$ is bounded.

Exercise 4.2.15 If μ is the Lebesgue measure and $f \in C(\mathbb{R}^d, \mathbb{C})$, then its essential range coincides with the closure of its range.

But if $(x_n \in \mathbb{R}^d)_{n \in S}$ is a finite or countable family with no accumulation point, and $\mu = \sum_{n \in S} \delta_{x_n}$, then $\text{ess-ran}_\mu f = \overline{\bigcup_{n \in S} \{f(x_n)\}}$.

In the Hilbert space context, an important property of the spectrum of an operator $(T, D(T))$ is its invariance through unitary conjugacy.

Proposition 4.2.16 (Spectrum and unitary conjugacy) Let two operators $(A, D(A))$ and $(B, D(B))$ defined on a Hilbert space \mathcal{H} be unitarily conjugate: there exists a unitary operator $U : \mathcal{H} \rightarrow \mathcal{H}$ such that $D(B) = UD(A)$ and $A = U^*BU$.

Then $\text{spec } A = \text{spec } B$ and $\text{spec}_p A = \text{spec}_p B$.

Proof.— See Exercise 4.3.7. □

Let us make use of this unitary invariance of the spectrum, to analyze our old friend, the free laplacian on \mathbb{R}^d .

Example 4.2.17 Let $T = T_1$ be the (positive) free Laplacian on \mathbb{R}^d (see Definition 2.2.12). As seen above, through the Fourier transform on $L^2(\mathbb{R}^d)$, T is unitarily equivalent to the multiplication operator by the function $f(\xi) = |\xi|^2$. By Propositions 4.2.14 and 4.2.16, we find $\text{spec } T_1 = [0, +\infty)$ and $\text{spec}_p T_1 = \emptyset$.

An interesting example of space $L^2(\mathbb{R}, \mu)$ is the case of the discrete measure $\mu = \sum_{n \in \mathbb{Z}} \delta_n$. This space is equivalent with the Hilbert space $\ell^2(\mathbb{Z})$.

Example 4.2.18 (Discrete multiplication operator) Take $\mathcal{H} = \ell^2(\mathbb{Z})$. Consider an arbitrary function $a : \mathbb{Z} \rightarrow \mathbb{C}$, $n \mapsto a_n$, and the associated multiplication operator M_a :

$$D(M_a) = \{(u_n) \in \ell^2(\mathbb{Z}) : (a_n u_n) \in \ell^2(\mathbb{Z})\}, \quad (M_a u)_n = a_n u_n.$$

Similarly to Example 2.1.8, one can show that M_a is a closed operator. Applying the rule of Example 4.2.14, we may extend the function a to all of \mathbb{R} (ex. by $\tilde{a}(x) = 0$ for $x \notin \mathbb{Z}$), and then view M_a as the multiplication operator $M_{\tilde{a}}$ by this function $\tilde{a} : \mathbb{R} \rightarrow \mathbb{C}$. Because $\text{ess-ran}_\mu(\tilde{a}) = \overline{\{a_n : n \in \mathbb{Z}\}}$, while $\tilde{a}^{-1}(z)$ has positive measure only if $z = a_n$ for some $n \in \mathbb{Z}$, we then find that

$$\text{spec } M_a = \text{spec } M_{\tilde{a}} = \text{ess-ran}_\mu(\tilde{a}) = \overline{\{a_n : n \in \mathbb{Z}\}}, \quad \text{spec}_p M_a = \{a_n : n \in \mathbb{Z}\}.$$

For each value a_{n_0} , set $\Lambda(a_{n_0}) = \{m \in \mathbb{Z} : a_m = a_{n_0}\}$. The eigenspace associated with the eigenvalue a_{n_0} is easy to describe:

$$\text{Ker}(M_a - a_{n_0}) = \overline{\text{span}\{\delta_m : m \in \Lambda(a_{n_0})\}},$$

where the vector $(\delta_m)_n = \delta_{mn}$ (Kronecker symbol).

Example 4.2.19 (Harmonic oscillator) Let $\mathcal{H} = L^2(\mathbb{R})$. Consider the operator $T_0 = -d^2/dx^2 + x^2$ defined on the Schwartz space $\mathcal{S}(\mathbb{R})$. We see that this operator is semibounded from below and denote by T its Friedrichs extension. The operator $(T, D(T))$ is called the *quantum harmonic oscillator*; it is one of the basic operators appearing in quantum mechanics.

One can easily see that the numbers $\lambda_n = 2n - 1$ are eigenvalues of T_0 , $n \in \mathbb{N}^*$, and the associated eigenfunctions ϕ_n are given by

$$\phi_1(x) = c_1 \exp(-x^2/2), \quad \phi_n(x) = c_n (-d/dx + x)^{n-1} \phi_1(x), \quad n \geq 2,$$

where c_n are normalization constants. It is known that the functions (ϕ_n) (called *Hermite functions*) form an orthonormal basis in $L^2(\mathbb{R})$. We remark that $\phi_n \in D(T_0)$ for all n , hence, T_0 is essentially self-adjoint (see Exercise 2.3.1c). This means, in particular, that $T = \overline{T_0}$.

Furthermore, using the unitary map $U : L^2(\mathbb{R}) \rightarrow \ell^2(\mathbb{N})$, $Uf(n) = \langle \phi_n, f \rangle$, one easily checks that the operator T is unitarily equivalent to the operator of multiplication by (λ_n) in $\ell^2(\mathbb{N})$, cf. Example 4.2.18, which gives

$$\text{spec } T = \text{spec}_p T = \{2n - 1 : n \in \mathbb{N}^*\}.$$

Hence, for this operator, the spectrum is only composed of the point spectrum.

Example 4.2.20 (A finite-difference operator) Consider again the Hilbert space $\mathcal{H} = \ell^2(\mathbb{Z})$ and the operator T in \mathcal{H} acting as $(Tu)_n = u_{n-1} + u_{n+1}$. Clearly, $T \in \mathcal{L}(\mathcal{H})$. To find its spectrum, we consider the map

$$\Phi : \ell^2(\mathbb{Z}) \rightarrow L^2([0, 1[, dx), \quad (\Phi u)(x) = \sum_{n \in \mathbb{Z}} u_n e^{2\pi i n x},$$

where the sum on the right-hand side should be understood as a series in L^2 . Φ is the inverse of the Fourier series expansion of a function in $L^2([0, 1[)$. From Plancherel's identity, this map is unitary. On the other hand, for any $u \in \ell^2(\mathbb{Z})$ supported at a finite number of points we have

$$\begin{aligned} \Phi(Tu)(x) &= \sum_n (Tu)_n e^{2\pi i n x} \\ &= \sum_n u_{n-1} e^{2\pi i n x} + \sum_n u_{n+1} e^{2\pi i n x} \\ &= \sum_n u_n e^{2\pi i (n+1)x} + \sum_n u_n e^{2\pi i (n-1)x} \\ &= e^{2\pi i x} \sum_n u_n e^{2\pi i n x} + e^{-2\pi i x} \sum_n u_n e^{2\pi i n x} \\ &= 2 \cos(2\pi x) (\Phi u)(x). \end{aligned}$$

This shows that the operator $\Phi T \Phi^*$ is exactly the multiplication by $f(x) = 2 \cos(2\pi x)$ on the space $L^2([0, 1[)$; its spectrum coincides with the segment $[-2, 2]$, i.e. with the essential range of f . So we have $\text{spec } T = [-2, 2]$ and $\text{spec}_p T = \emptyset$.

Notice that, by using the same unitary transformation, one shows that the shift operator $(Su)_n = u_{n+1}$ on $\ell^2(\mathbb{Z})$ is conjugate to the multiplication by $e^{2i\pi x}$ on $L^2([0, 1[, dx)$. We thus easily recover that $\text{spec}(S) = \{e^{2i\pi x}, x \in [0, 1[\}$, with no point spectrum.

The next example shows that, as opposed to the case of bounded operators, nontrivial unbounded operators may have an empty spectrum.

Example 4.2.21 (Empty spectrum) Take $\mathcal{H} = L^2([0, 1[, dx)$ and consider the operator T defined on the domain $D(T) = \{f \in H^1(0, 1) : f(0) = 0\}$, acting as $Tf = f'$. One can easily see that for any $g \in L^2(0, 1)$ and any $z \in \mathbb{C}$ the equation $(T - z)f = g$ admits the unique solution in $D(T)$, given by

$$f(x) = \int_0^x e^{z(x-t)} g(t) dt, \quad \forall x \in [0, 1[.$$

This shows that $(T - z) : D(T) \rightarrow \mathcal{H}$ is a bijection, and one easily checks that this inverse map $(T - z)^{-1} : g \in \mathcal{H} \mapsto f \in \mathcal{H}$ is a bounded operator on \mathcal{H} . So we have obtained $\text{res } T = \mathbb{C}$ and thus $\text{spec } T = \emptyset$.

Example 4.2.22 (Empty resolvent set) Let us modify the previous example. Take $\mathcal{H} = L^2([0, 1[, dx)$ and consider the operator T acting as $Tf = f'$ on the domain $D(T) = H^1([0, 1])$. Now, for any $z \in \mathbb{C}$ we see that the function $\phi_z(x) = e^{zx}$ belongs to $D(T)$ and satisfies $(T - z)\phi_z = 0$. Therefore, $\text{spec}_p T = \text{spec } T = \mathbb{C}$.

As we can see in the two last examples, for general operators one cannot say much on the location of the spectrum. In what follows we will study mostly self-adjoint operators on a Hilbert space \mathcal{H} , whose spectral theory is much better understood than in the nonselfadjoint case.

4.3 Basic facts on the spectra of self-adjoint operators

In this section we will “prepare the ground” for the spectral theorem of selfadjoint operators, and the associated functional calculus. The following two propositions will be of importance during the whole course.

Proposition 4.3.1 Let T be a closable operator acting on a Hilbert space \mathcal{H} , and $z \in \mathbb{C}$. Then

$$(4.3.8) \quad \text{Ker}(T^* - \bar{z}) = \text{Ran}(T - z)^\perp,$$

$$(4.3.9) \quad \overline{\text{Ran}(T - z)} = \text{Ker}(T^* - \bar{z})^\perp.$$

Proof.— Note that the second equality can be obtained from the first one by taking the orthogonal complement in the both parts. Let us prove the first equality. Since $D(T)$ is dense, the condition $f \in \text{Ker}(T^* - \bar{z})$ is equivalent to $\langle (T^* - \bar{z})f, g \rangle = 0$ for all $g \in D(T)$, which can be also rewritten as

$$\langle T^*f, g \rangle = z\langle f, g \rangle \text{ for all } g \in D(T).$$

By the definition of T^* , one has $\langle T^*f, g \rangle = \langle f, Tg \rangle$ and

$$\langle f, Tg \rangle - z\langle f, g \rangle \equiv \langle f, (T - z)g \rangle = 0 \text{ for all } g \in D(T),$$

i.e. $f \perp \text{Ran}(T - z)$, using the density of $D(T)$. □

Proposition 4.3.2 (The spectrum of a selfadjoint operator is real) Let T be a selfadjoint operator in a Hilbert space \mathcal{H} , then $\text{spec } T \subset \mathbb{R}$, and for any $z \in \mathbb{C} \setminus \mathbb{R}$, the norm of the resolvent is bounded by:

$$(4.3.10) \quad \|(T - z)^{-1}\| \leq \frac{1}{|\text{Im } z|}.$$

Proof.— Let $z \in \mathbb{C} \setminus \mathbb{R}$ and $u \in D(T)$. We have

$$\langle u, (T - z)u \rangle = \langle u, Tu \rangle - \text{Re } z\langle u, u \rangle - i \text{Im } z\langle u, u \rangle.$$

Since T is self-adjoint, the number $\langle u, Tu \rangle$ is real. Therefore,

$$|\text{Im } z|\|u\|^2 \leq |\langle u, (T - z)u \rangle| \leq \|(T - z)u\| \cdot \|u\|,$$

which shows that

$$(4.3.11) \quad \|(T - z)u\| \geq |\operatorname{Im} z| \cdot \|u\|.$$

It follows from here that $\operatorname{Ran}(T - z)$ is closed, that $\operatorname{Ker}(T - z) = \{0\}$ and, by proposition 4.3.1, that $\operatorname{Ran}(T - z) = \mathcal{H}$. Therefore, $(T - z)^{-1} \in \mathcal{L}(\mathcal{H})$, and the estimate (4.3.10) follows from (4.3.11). \square

We have already mentioned that the spectral radius of a bounded selfadjoint operator is equal to $r(T) = \|T\|$. Since the spectrum is real, the spectral radius corresponds to $\max(|\min \operatorname{spec}(T)|, \max \operatorname{spec}(T))$, so $\operatorname{spec}(T) \subset [-\|T\|, \|T\|]$, and at least one of the boundaries of the interval belong to the spectrum. We can be a bit more precise:

Proposition 4.3.3 (Location of the spectrum of self-adjoint operators) Let $T \in \mathcal{L}(\mathcal{H})$ be selfadjoint. Denote

$$m = m(T) = \inf_{u \neq 0} \frac{\langle u, Tu \rangle}{\langle u, u \rangle}, \quad M = M(T) = \sup_{u \neq 0} \frac{\langle u, Tu \rangle}{\langle u, u \rangle},$$

then $\operatorname{spec} T \subset [m, M]$ and $\{m, M\} \subset \operatorname{spec} T$. We also have $\|T\| = \max(|m|, |M|)$.

Proof.— We already proved that $\operatorname{spec} T \subset \mathbb{R}$. For $\lambda \in]M, +\infty[$ we have

$$|\langle u, (\lambda - T)u \rangle| \geq (\lambda - M)\|u\|^2,$$

so by the Lax-Milgram theorem, $(T - \lambda)^{-1} \in \mathcal{L}(\mathcal{H})$. In the same way one shows that $\operatorname{spec} T \cap (-\infty, m) = \emptyset$.

Let us show that $M \in \operatorname{spec} T$ (for m the proof is similar). The quadratic form $(u, v) \mapsto \langle u, (M - T)v \rangle$ is nonnegative, it is called a *semi-scalar product*, and satisfies as well a Cauchy-Schwarz inequality:

$$|\langle u, (M - T)v \rangle|^2 \leq \langle u, (M - T)u \rangle \cdot \langle v, (M - T)v \rangle.$$

Taking the supremum over all $u \in \mathcal{H}$ with $\|u\| \leq 1$ we obtain

$$\|(M - T)v\| \leq \|M - T\| \cdot \langle v, (M - T)v \rangle.$$

By assumption, one can construct a sequence (v_n) with $\|v_n\| = 1$ such that $\langle v_n, Tv_n \rangle \rightarrow M$ as $n \rightarrow \infty$. By the above inequality we have then $(M - T)v_n \rightarrow 0$, so the operator $M - T$ cannot have bounded inverse. Thus $M \in \operatorname{spec} T$. \square

Corollary 4.3.4 If $T = T^* \in \mathcal{L}(\mathcal{H})$ and $\operatorname{spec} T = \{0\}$, then $T = 0$.

Proof.— By proposition 4.3.3 we have $m(T) = M(T) = 0$. This means that $\langle u, Tu \rangle = 0$ for all $u \in \mathcal{H}$, and by polarization, $\langle u, Tv \rangle = 0$ for all $u, v \in \mathcal{H}$. \square

Notice that the conclusion does not apply for a general bounded operator (think of a nilpotent finite rank operator).

Let us combine all of the above to show the following

Theorem 4.3.5 (Non-emptiness of spectrum) The spectrum of a selfadjoint operator $(T, D(T))$ on a Hilbert space \mathcal{H} is a non-empty closed subset of the real line.

Proof.— In view of the preceding discussion, it remains to show the non-emptiness of the spectrum. Let T be a self-adjoint operator in a Hilbert space \mathcal{H} . By contradiction, assume that $\text{spec } T = \emptyset$. Then, first of all, $T^{-1} \in \mathcal{L}(\mathcal{H})$. Let $z \in \mathbb{C} \setminus \{0\}$. One can easily show that the operator

$$L_z \stackrel{\text{def}}{=} -\frac{T}{z} \left(T - \frac{1}{z}\right)^{-1} \equiv -\frac{1}{z} - \frac{1}{z^2} \left(T - \frac{1}{z}\right)^{-1}$$

belongs to $\mathcal{L}(\mathcal{H})$, and that $(T^{-1} - z)L_z = L_z(T^{-1} - z) = I_{\mathcal{H}}$. Therefore, $z \in \text{res}(T^{-1})$. Since z was an arbitrary non-zero complex number, we have $\text{spec}(T^{-1}) \subset \{0\}$. Since T^{-1} is bounded, Prop. 4.2.1 shows that its spectrum is non-empty, hence we must have $\text{spec } T^{-1} = \{0\}$. On the other hand, T^{-1} is selfadjoint by Proposition 2.2.15, so Corollary 4.3.4 imposes that $T^{-1} = 0$, which contradicts the definition of the inverse operator. \square

4.3.1 Exercises

Exercise 4.3.6 [Jordan block of an isolated eigenvalue] Let $T \in \mathcal{L}(\mathcal{B})$, and let z_1 be one isolated eigenvalue of finite multiplicity, so that for $r > 0$ small enough, $\text{spec}(T) \cap \{|z - z_1| \leq r\} = \{z_1\}$.

i) show that

$$\Pi \stackrel{\text{def}}{=} \frac{1}{2i\pi} \oint_{|z-z_1|=r} (z - T)^{-1} dz$$

is a projector, namely it satisfies $\Pi^2 = \Pi$. For this, express Π^2 by a double contour integral, and use the resolvent identity.

ii) show that Π commutes with T , hence that T preserves $\mathcal{V} \stackrel{\text{def}}{=} \text{Ran}(\Pi)$. Show that

$$T\Pi = \Pi T = \Pi T \Pi = \frac{1}{2i\pi} \oint_{|z-z_1|=r} (z - T)^{-1} z dz$$

iii) We call the finite rank operator $T_1 = \Pi T \Pi$. Show that for any $z \in \text{res}(T)$, the resolvent satisfies

$$(z - T)^{-1} \Pi = (z - T_1)^{-1} \Pi.$$

Deduce that the spectrum of T_1 in $\{0 \leq |z| < r\}$ reduces to $\{z_i\}$, and therefore that T_1 takes the form $T_1 = z_1 I_{\mathcal{V}} + J$, where $J : \mathcal{V} \rightarrow \mathcal{V}$ is nilpotent of order $\leq D$ (that is, $J^D = 0$), where $D = \dim \mathcal{V}$.

iv) Compute T_1^n for any $n \geq 1$.

Exercise 4.3.7 i) Let two operators A and B be unitarily equivalent (see Exercise 2.3.1). Show that the $\text{spec } A = \text{spec } B$ and $\text{spec}_p A = \text{spec}_p B$.

ii) Let $\mu \in \text{res } A \cap \text{res } B$. Show that A and B are unitarily equivalent iff their resolvents $R_A(\mu)$ and $R_B(\mu)$ are unitarily equivalent.

iii) Let A be a closed operator. Show that $\text{spec } A^* = \{\bar{z} : z \in \text{spec } A\}$ and that the resolvent identity $R_A(z)^* = R_{A^*}(\bar{z})$ holds for any $z \in \text{res } A$.

iv) Let $k \in L^1(\mathbb{R})$. Consider on $L^2(\mathbb{R})$ the operator A , $Af(x) = \int_{\mathbb{R}} k(x-y)f(y) dy$. Show: (i) the operator A is well-defined and bounded, (ii) the spectrum of A is a connected set.

Exercise 4.3.8 i) Let $\Omega \subset \mathbb{R}^n$ be a non-empty open set and let $L : \Omega \rightarrow M_2(\mathbb{C})$ be a continuous matrix valued function such that $L(x)^* = L(x)$ for all $x \in \Omega$. Define an operator A in $H = L^2(\Omega, \mathbb{C}^2)$ by

$$Af(x) = L(x)f(x), \quad D(A) = \left\{ f \in H : \int_{\Omega} \|L(x)f(x)\|_{\mathbb{C}^2}^2 dx < +\infty \right\}.$$

Show that A is self-adjoint and explain how to calculate its spectrum using the eigenvalues of $L(x)$.

Hint: For each $x \in \Omega$, let $\xi_1(x)$ and $\xi_2(x)$ be suitably chosen eigenvectors of $L(x)$ forming an orthonormal basis of \mathbb{C}^2 . Consider the map

$$U : H \rightarrow H, \quad Uf(x) = \begin{pmatrix} \langle \xi_1(x), f(x) \rangle_{\mathbb{C}^2} \\ \langle \xi_2(x), f(x) \rangle_{\mathbb{C}^2} \end{pmatrix}$$

and the operator $M = UAU^*$.

ii) In $\mathcal{H} = \ell^2(\mathbb{Z})$ consider the operator T given by

$$Tf(n) = f(n-1) + f(n+1) + V(n)f(n), \quad V(n) = \begin{cases} 4 & \text{if } n \text{ is even,} \\ -2 & \text{if } n \text{ is odd.} \end{cases}$$

Calculate its spectrum.

Hint: Consider the operators

$$U : \ell^2(\mathbb{Z}) \rightarrow \ell^2(\mathbb{Z}, \mathbb{C}^2), \quad Uf(n) := \begin{pmatrix} f(2n) \\ f(2n+1) \end{pmatrix}, \quad n \in \mathbb{Z},$$

$$F : \ell^2(\mathbb{Z}, \mathbb{C}^2) \rightarrow L^2((0, 1), \mathbb{C}^2), \quad (Ff)(\theta) = \sum_{n \in \mathbb{Z}} f(n)e^{2\pi i n \theta}.$$

Write explicit expressions for the operators $S := UTU^*$ and $\widehat{S} := FSF^*$ and use the item i).

Exercise 4.3.9 On \mathcal{H} , let A be a semibounded from below selfadjoint operator. Show:

$$i) \inf \operatorname{spec} A = \inf_{\substack{x \in D(A) \\ x \neq 0}} \frac{\langle x, Ax \rangle}{\langle x, x \rangle}.$$

$$ii) \inf \operatorname{spec} A = \inf_{\substack{x \in Q(A) \\ x \neq 0}} \frac{\langle x, Ax \rangle}{\langle x, x \rangle}, \text{ where } Q(A) \text{ is the form domain of } A.$$

Chapter 5

Spectral theory of compact operators

5.1 Definitions and elementary properties

It is assumed that the the reader already has some knowledge of compact operators. We recall briefly the key points. Recall first that any Hilbert space is locally compact in the weak topology:

Proposition 5.1.1 Let \mathcal{H} be a Hilbert space. Then:

i) Any bounded sequence $(u_n)_{n \in \mathbb{N}}$ in \mathcal{H} contains a weakly convergent subsequence: one can extract a subsequence $(u_{n_k})_{k \geq 1}$ converging weakly to some $u \in \mathcal{H}$, that is such that

$$\forall v \in \mathcal{H}, \quad \langle v, u_{n_k} \rangle \xrightarrow{k \rightarrow \infty} \langle v, u \rangle.$$

ii) Conversely, any weakly converging subsequence is necessarily bounded.

Before introducing the concept of compact operator, let us recall Riesz's theorem:

Theorem 5.1.2 (Riesz's theorem) In a Banach space \mathcal{B} , for $\mathcal{V} \subset \mathcal{B}$ a subspace, the intersection $\mathcal{V} \cap \overline{B_{\mathcal{B}}(0, 1)}$ is compact iff \mathcal{V} is finite dimensional.

We now recall the definition of compact operators.

Definition 5.1.3 A linear operator $T : \mathcal{B}_1 \rightarrow \mathcal{B}_2$ is called compact, if the image of the unit ball in \mathcal{B}_1 is relatively compact in \mathcal{B}_2 . In particular, T is continuous.

We denote by $\mathcal{K}(\mathcal{B}_1, \mathcal{B}_2)$ the subspace of $\mathcal{L}(\mathcal{B}_1, \mathcal{B}_2)$ formed by the compact operators.

As a first property of compact operators, we check that limits of compact operators are compact.

Proposition 5.1.4 The space $\mathcal{K}(\mathcal{B}_1, \mathcal{B}_2)$ is closed in $\mathcal{L}(\mathcal{B}_1, \mathcal{B}_2)$.

Proof.— Assume that $(T_j)_{j \geq 1}$ are a family of compact operators, and that $\|T_j - T\|_{\mathcal{L}(\mathcal{B}_1, \mathcal{B}_2)} \rightarrow 0$ when $j \rightarrow \infty$. Let us consider a sequence $(u_n)_{n \geq 1}$ in the unit ball of \mathcal{B}_1 . From the compactness of T_1 , we can extract a subsequence $(u_{\varphi_1(k)})_{k \geq 1}$ of (u_n) (that is, $\varphi_1 : \mathbb{N}^* \rightarrow \mathbb{N}^*$ is strictly growing), such that $T_1 u_{\varphi_1(k)}$ admits a limit $v_1 \in \mathcal{B}_2$ when $k \rightarrow \infty$.

Then, from the sequence $(u_{\varphi_1(k)})_{k \geq 1}$ we can further extract a subsequence $(u_{\varphi_2(k)})_{k \geq 1}$ such that $T_2 u_{\varphi_2(k)}$ converges to some $v_2 \in \mathcal{B}_2$. And so on: for each $j \geq 2$, there is a subsequence $(u_{\varphi_j(k)})_{k \geq 1}$ of $(u_{\varphi_{j-1}(k)})_{k \geq 1}$, such that $T_j u_{\varphi_j(k)} \rightarrow v_j$.

What can we do with this “sequence of thinner and thinner sequences” $(\varphi_j(k))_{k \geq 1}$? It does not make sense to consider the limit $j \rightarrow \infty$ of those sequences, because this limit could actually be empty. Instead, we invoke a *diagonal trick*, that is define the “diagonal sequence”

$$\tilde{\varphi}(n) \stackrel{\text{def}}{=} \varphi_n(n), \quad n \geq 1.$$

For each $j \geq 1$, the integers $(\tilde{\varphi}(n))_{n \geq j}$ are elements of the sequence $(\varphi_j(k))_{k \geq 1}$, therefore

$$T_j u_{\tilde{\varphi}(n)} \xrightarrow{n \rightarrow \infty} v_j.$$

We now use the assumption $\|T_j - T\| \rightarrow 0$, to show that

$$\|v_j - v_{j'}\| = \lim_{n \rightarrow \infty} \|T_j u_{\tilde{\varphi}(n)} - T_{j'} u_{\tilde{\varphi}(n)}\| \leq C \|T_j - T_{j'}\|,$$

where C is a global bound for the sequence (u_n) . The above expression converges to zero when $j, j' \rightarrow \infty$, showing that the (v_j) form a Cauchy sequence in \mathcal{B}_2 , and thus converge to some $v \in \mathcal{B}_2$. We easily check that the limit operator satisfies $T u_{\tilde{\varphi}(n)} \rightarrow v$. Hence, we have extracted a subsequence of (u_n) , such that $T u_{\tilde{\varphi}(n)}$ converges. This proves the compactness of T . \square

Below we will provide various characterizations of compact operators between Hilbert spaces. Those characterizations (in particular *i*)) are also valid on certain types of Banach spaces, namely the ones satisfying the Property of Approximation.

Theorem 5.1.5 (Characterizations of a compact operator on a Hilbert space) Let $\mathcal{H}_1, \mathcal{H}_2$ be two Hilbert spaces, and let $T : \mathcal{H}_1 \rightarrow \mathcal{H}_2$ be a continuous operator. Then the following statements are equivalent:

- i*) There exists a sequence $(T_n)_{n \in \mathbb{N}}$ of finite rank operators, such that $\|T_n - T\|_{\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)} \rightarrow 0$.
- ii*) T is compact.
- iii*) The image $T(\overline{B(0, 1)})$ is compact.
- iv*) For any sequence $(u_n)_n$ in \mathcal{H}_1 which weakly converges to $u \in \mathcal{H}_1$, then $(T u_n)_n$ strongly converges to $T u$ in \mathcal{H}_2 .
- v*) If $(e_n)_{n \in \mathbb{N}}$ forms an orthonormal family in \mathcal{H}_1 , then $\|T e_n\| \rightarrow 0$.

Proof.— $i) \rightarrow ii)$: for any $n \geq 0$, the image $T_n(B(0, 1))$ is contained in a ball in a finite dimensional subspace, it is therefore precompact. This shows that each T_n is a compact operator. Prop. 5.1.4 then ensures that the limit operator T is compact.

$ii) \rightarrow iii)$: Since $\overline{B(0, 1)} \subset B(0, 2)$, the image $T(\overline{B(0, 1)})$ is precompact. There remains to show that it is closed. Take a sequence $(u_n)_{n \geq 1}$ in $\overline{B(0, 1)}$. From the compactness of T , we may extract a subsequence $(u_{\varphi_0(k)})_{k \geq 1}$ such that $Tu_{\varphi_0(k)} \rightarrow v \in \mathcal{H}_2$. On the other hand, from Prop. 5.1.1 we can extract from the bounded sequence $(u_{\varphi_0(k)})_{k \geq 1}$ a subsequence $(u_{\varphi_1(k)})_{k \geq 1}$ which weakly converges to some $u \in \mathcal{H}_1$; one easily checks that this weak limit u belongs to $\overline{B(0, 1)}$ as well:

$$\|u\| \geq \|u\| \|u_{\varphi_1(k)}\| \geq |\langle u, u_{\varphi_1(k)} \rangle| \rightarrow \|u\|^2.$$

For any $w \in \mathcal{H}_2$, we have the limits:

$$\begin{aligned} \langle T^*w, u_{\varphi_1(k)} \rangle &\rightarrow \langle T^*w, u \rangle = \langle w, Tu \rangle, \\ \langle w, Tu_{\varphi_1(k)} \rangle &\rightarrow \langle w, v \rangle, \end{aligned}$$

which shows that $v = Tu \in T(\overline{B(0, 1)})$. This image is therefore closed, hence compact.

$iii) \rightarrow iv)$: without loss of generality, let us assume that a sequence $(u_n)_n \subset \mathcal{H}_1$ weakly converges to 0. From Prop. 5.1.1, the sequence $(u_n)_n$ is necessarily bounded: $\|u_n\| \leq C$. The assumption tells us that $(Tu_n)_n$ belongs to a compact set, hence it admits a limit point $v \in \mathcal{H}_2$, which can be reached by extracting a subsequence $(Tu_{\varphi(k)})_k$. As a result, for any $w \in \mathcal{H}_2$,

$$\langle w, Tu_{\varphi(k)} \rangle \rightarrow \langle w, v \rangle, \quad \text{while} \quad \langle T^*w, u_{\varphi(k)} \rangle \rightarrow \langle T^*w, 0 \rangle = 0.$$

We deduce that $v = 0$ is the only limit point; this means that the full sequence $(Tu_n)_n$ converges to 0, as stated.

$iv) \rightarrow v)$: for any orthonormal family $(e_n)_n$ of \mathcal{H}_1 , one has $e_n \rightarrow 0$, so the assumption $iv)$ implies that $Te_n \rightarrow 0$.

$v) \rightarrow i)$: a natural guess would be to use the restricted operators $T|_{\text{span}(e_1, \dots, e_n)}$ as approximants for T . Yet, the assumption $Te_n \rightarrow 0$ is not sufficient to produce a direct bound on $T|_{\text{span}(e_1, \dots, e_n)^\perp}$.

We instead reason *ab absurdo*. Namely, we assume that there exists $\epsilon > 0$ such that, for any finite rank operator R , $\|T - R\| \geq \epsilon$. In particular, this implies $\|T\| \geq \epsilon$, so there exists a normalized state $e_1 \in \mathcal{H}_1$ such that $\|Te_1\| \geq \epsilon$. Let us now iteratively construct an orthonormal family (e_1, e_2, \dots) , such that $\|Te_j\| \geq \epsilon$ for all e_j ; this will thus contradict the statement $v)$.

Let us assume we have constructed (e_1, \dots, e_n) with the above property. Call Π_n the orthogonal projector on $\text{span}(e_1, \dots, e_n)$. Then $\|T - T\Pi_n\| \geq \epsilon$ implies the existence of $u \neq 0$ such that

$$\|(T(I - \Pi_n)u)\| \geq \epsilon\|u\| \geq \epsilon\|(1 - \Pi_n)u\|,$$

where we used Pythagore's theorem for the last inequality. We then define the normalized vector

$$e_{n+1} \stackrel{\text{def}}{=} \frac{(1 - \Pi_n)u}{\|(1 - \Pi_n)u\|},$$

it is orthogonal to e_1, \dots, e_n , and satisfies $\|Te_{n+1}\| \geq \epsilon$. This constructs our infinite family (e_1, \dots) , and gives a contradiction with $v)$. \square

Remark 5.1.6 1. Using the weak compactness property of Prop. 5.1.1, the statement *iv*) shows that T is compact iff any bounded sequence $(u_n) \subset \mathcal{H}_1$ admits a subsequence (u_{n_k}) such that Tu_{n_k} converges (strongly) in \mathcal{H}_2 .

2. The statement *i*) induces the fact that if $A \in \mathcal{L}(\mathcal{B})$ is a continuous operator and $B \in \mathcal{K}(\mathcal{B})$ is a compact one, then the products AB and BA are compact operators. One says that the space $\mathcal{K}(\mathcal{B})$ forms a two-sided ideal of $\mathcal{L}(\mathcal{B})$.

Examples of compact operators

1. On $\ell^2(\mathbb{Z})$, consider the multiplication operator $T = M_f$ by a function $(f_n)_{n \in \mathbb{Z}}$ such that $f_n \rightarrow 0$ when $|n| \rightarrow \infty$. We already know that $\|M_f\| = \max_n |f_n|$. Let us define $T_N \stackrel{\text{def}}{=} T\Pi_N$, where Π_N is the orthogonal projector on $\text{span}(e_{-N}, \dots, e_N)$. We then check that

$$\|T - T_N\| = \max_{|n| > N} |f_n| \xrightarrow{N \rightarrow \infty} 0,$$

so the criterium *i*) in Thm 5.1.5 shows that T is compact.

2. Let us consider the space $L^2(\mathbb{T})$, for $\mathbb{T} = \mathbb{R}/\mathbb{Z}$ the 1-dimensional torus. Through the Fourier transform \mathcal{F} , $L^2(\mathbb{T})$ is unitarily identified with $\ell^2(\mathbb{Z})$. We have seen that this Fourier transform conjugates the operator $-\Delta_{\mathbb{T}}$ with the multiplication by the function $(f(n) = n^2)_{n \in \mathbb{Z}}$ on $\ell^2(\mathbb{Z})$. Taking any real $s > 0$, we define the operator $(1 - \Delta_{\mathbb{T}})^{-s/2}$ through the inverse Fourier conjugacy with the multiplication by the function $(f_s(n) = \frac{1}{(1+|n|^2)^s})_{n \in \mathbb{Z}}$ on $\ell^2(\mathbb{Z})$. Since $s > 0$ and since the Fourier conjugacy is unitary, the operator $(1 - \Delta_{\mathbb{T}})^{-s/2}$ is compact on $L^2(\mathbb{T})$. Such an operator $(1 - \Delta_{\mathbb{T}})^{-s/2}$ are said to be *regularizing*: it maps an L^2 function to a smoother function, belonging to some Sobolev space $H^s(\mathbb{T})$ with positive index s .

In the section 5.4 we will study various families of compact operators: Hilbert-Schmidt and trace-class operators.

5.2 The Fredholm alternative

We now describe the spectral properties of a holomorphic family of compact operators on a Hilbert space. This is part of the analytic Fredholm theory.

Theorem 5.2.1 (Analytic Fredholm theorem) Let $\Omega \subset \mathbb{C}$ a domain of the complex plane, and

$$z \in \Omega \mapsto T(z) \in \mathcal{K}(\mathcal{B})$$

a holomorphic family of compact operators. Then:

- (a) either $(I - T(z))^{-1}$ does not exist as bounded operator for any $z \in \Omega$;
- (b) or $(I - T(z))^{-1}$ exists in $\mathcal{L}(\mathcal{B})$ for $z \in \Omega \setminus S$, where S is a discrete set of Ω . $(I - T(z))^{-1}$

is then a meromorphic operator valued function in Ω , and the residue on each pole z_j is an operator of finite rank. Besides, for each $z_j \in S$ there exists $u_j \in \mathcal{B}$ s.t. $T(z_j)u_j = u_j$.

As an application, for $T \in \mathcal{K}(\mathcal{B})$ and $z \in \Omega = \mathbb{C}^*$, we take $T(z) = \frac{1}{z}T$. Since $(I - z^{-1}T)$ can be inverted for z large enough, we are necessarily in the second alternative.

Corollary 5.2.2 For $T \in \mathcal{K}(\mathcal{B})$ and $z_0 \in \mathbb{C}^*$, either $(z_0 - T) : \mathcal{B} \rightarrow \mathcal{B}$ is invertible with bounded inverse, or $\text{Ker}(z_0 - T) \neq \{0\}$, in which case this kernel has finite dimension.

Proof.— We will restrict here the proof to the Hilbert space setting, so that any compact operator T can be approached by a family of finite rank operators, as shown in Thm 5.1.5.

The idea of the proof is to “project” the spectral problem on finite dimensional subspaces, using the approximation of the compact operators by finite rank ones.

Let us assume that $(I - T(z))^{-1}$ exists at $z = z_0 \in \Omega$. For a given $\varepsilon > 0$, the compact operator $T(z_0)$ can be approximated by an operator T_N of rank N : $\|T(z_0) - T_N\| \leq \varepsilon$.

Besides, by continuity of $z \mapsto T(z)$, we know that for $|z - z_0| \leq r$ small enough (in particular, such that all such z lie in Ω), $\|T(z) - T(z_0)\| \leq \varepsilon$. As a result,

$$\forall z \in D(z_0, r), \quad \|T(z) - T_N\| \leq 2\varepsilon.$$

By Neumann series, if we had chosen $\varepsilon < 1/2$, we can invert $(I - (T(z) - T_N))$ in that disk, and call its inverse

$$R(z) \stackrel{\text{def}}{=} (I - (T(z) - T_N))^{-1}, \quad \text{holomorphic in } z \in D(z_0, r).$$

An easy factorization shows that

$$(I - T(z)) = (I - (T(z) - T_N)) (I - R(z)T_N),$$

which implies that $(I - T(z))$ is invertible iff $(I - R(z)T_N)$ is invertible, in which case we have

$$(I - T(z))^{-1} = (I - R(z)T_N)^{-1} R(z),$$

and this operator is holomorphic for $s \in D(z_0, r)$.

Through this algebraic manipulation, we have replaced the question of the invertibility of $(I - T(z))$ by the invertibility of $(I - R(z)T_N)$, which is a *finite rank* perturbation of the identity, locally holomorphic in z . Let us show that this second invertibility problem can be mapped to the one of some $N \times N$ matrix.

Since T_N has rank N , there exists (ψ_1, \dots, ψ_N) a basis for $\text{Ran}(T_N)$ and (ϕ_1, \dots, ϕ_N) a basis for $\text{Ker}(T_N)^\perp = \text{Ran}(T_N^*)$, such that

$$T_N u = \sum_{j=1}^N \langle \phi_j, u \rangle \psi_j.$$

Then the spectral equation $(I - T(z))u = 0$ is equivalent with $(I - R(z)T_N)u = 0$, which can be written:

$$u = \sum_{j=1}^N \langle \phi_j, u \rangle R(z)\psi_j.$$

If we write this vector as $u = \sum_j \alpha_j R(z)\psi_j$, the coefficients α_j satisfy

$$\forall j = 1, \dots, N, \quad \alpha_j = \sum_{k=1}^N \langle \phi_j, R(z)\psi_k \rangle \alpha_k,$$

or in matrix notation $\vec{\alpha} = M_N(z)\vec{\alpha}$, with the matrix $M_N(z)$ having entries $\langle \phi_j, R(z)\psi_k \rangle$, which depend holomorphically on z .

We have transformed our spectral problem into the problem of inverting $I_N - M_N(z)$; the non-invertibility of this square matrix is equivalent with the determinantal equation

$$d(z) \stackrel{\text{def}}{=} \det(I_N - M_N(z)) = 0.$$

The matrix $M_N(z)$ is sometimes called an *effective Hamiltonian* for the initial invertibility problem.

The function $d(z)$ is holomorphic in Ω , so it is either vanishing everywhere, or only on a discrete set $S \subset \Omega$.

On a point such that $d(z) = 0$, the eigenvector $\vec{\alpha} \in \mathbb{C}^N$ such that $(I_N - M_N(z))\vec{\alpha} = 0$ leads to an eigenvector $u \in \mathcal{B}$ such that $(I - T(z))u = 0$.

On the opposite, if $d(z) \neq 0$, for a given $f \in \mathcal{H}$ we may solve the equation $(I - T(z))u_z = f$ by the noticing that u_z also satisfies $(I - R(z)T_N)u_z = R(z)f$. The state $R(z)T_N u_z$ belongs to $\text{Ran } R(z)T_N$, so it can be decomposed in the basis $(\psi_j(z) = R(z)\psi_j)_{j=1, \dots, N}$ of that subspace: there exists a z -dependent vector $\vec{\beta}(z) = (\beta_1, \dots, \beta_N)$ s.t.

$$u_z = R(z)f + \sum_j \beta_j(z)\psi_j(z).$$

After a straightforward computation, we find that the vector $\vec{\beta}(z)$ is uniquely given by

$$\vec{\beta}(z) = (I_N - M_N(z))^{-1} (\langle \phi_j, R(z)f \rangle).$$

Putting together these expressions, we obtain:

$$(I - T(z))^{-1}f = R(z)f + {}^t(R(z)\vec{\psi}) (I_N - M_N(z))^{-1} \langle \vec{\phi}, R(z)f \rangle$$

This element is meromorphic in z , with poles of finite rank. Note that the residue at any pole z , is independent of the integer N , as long as the latter is large enough.

The codimension of $\text{Ran}(I - T(z))$ in \mathcal{H} is equal the codimension of $\text{Ran}(I_N - M_N(z))$ in \mathbb{C}^N . \square
The proof for a general Banach space does not use the approximation by finite rank operators.

5.3 Compact operators on a Hilbert space

We will henceforth concentrate on operators defined on a Hilbert space. We start with simple consequences of the characterizations of Thm. 5.1.5.

Proposition 5.3.1 Let T be a compact operator on a Hilbert space \mathcal{H} . Then its adjoint T^* is also compact.

Proof.— If T is approximated by a sequence (T_N) of finite rank operators, then T^* is similarly approximated by the finite rank operators T_N^* . We deduce that T^* is compact as well. \square

The next proposition shows that for $z \neq 0$, we can be more precise on the relative dimensions of $\text{Ker}(T - z)$ and $\text{Ran}(T - z)$.

Proposition 5.3.2 Let T be a compact operator on a Hilbert space \mathcal{H} . Then $\text{Ran}(I - T)$ is closed, of finite codimension. More precisely,

$$\text{codim Ran}(I - T) = \dim \text{Ker}(I - T^*) = \dim \text{Ker}(I - T).$$

These equalities indicate that $(I - T)$ is a Fredholm operator of index $\dim \text{Ker}(I - T) - \text{codim Ran}(I - T) = 0$.

Proof.— Let us show that the space $\text{Ran}(I - T)$ is closed. Assume that for some sequence (u_n) in $\text{Ker}(I - T)^\perp$, we have

$$v_n \stackrel{\text{def}}{=} (I - T)u_n \rightarrow v \in \mathcal{H}.$$

We claim that there exists $c > 0$ such that

$$\forall u \in \text{Ker}(I - T)^\perp, \quad \|(I - T)u\| \geq c\|u\|.$$

Before proving this claim, let us use it. The limit $(I - T)u_n \rightarrow v$ implies that $((I - T)u_n)_n$ is a Cauchy sequence; the claim shows that $(u_n)_n$ is itself a Cauchy sequence, hence it converges to some $u \in \mathcal{H}$. The continuity of $(I - T)$ implies that $(I - T)u = v$, hence $v \in \text{Ran}(I - T)$: this shows that this subspace is closed.

Let us now prove the claim, by reasoning *ab absurdo*. The inverse statement would imply the existence of a sequence $(u_n)_n$ of normalized vectors in $\text{Ker}(I - T)^\perp$, such that $\|(I - T)u_n\| \leq \frac{1}{n}$. Since the states are normalized, one can extract a weakly converging subsequence $u_{\varphi(k)} \rightharpoonup u_\infty$. The compactness of T implies that $Tu_{\varphi(k)} \rightarrow Tu_\infty$. On the other hand, we have assumed that $u_n - Tu_n \rightarrow 0$, hence the sequence $u_{\varphi(k)}$ strongly converges to Tu_∞ . Since the strong limit must be equal to the weak one, we deduce that $Tu_\infty = u_\infty$. This shows that $u_\infty \in \text{Ker}(I - T)$. On the other hand, since $u_{\varphi(k)} \in \text{Ker}(I - T)^\perp$, their limit $u_\infty \in \text{Ker}(I - T)^\perp$ as well. Both properties would imply that $u_\infty = 0$, which contradicts the normalization $\|u_n\| = 1$. This proves the claim.

We already have the general identity $\text{Ker}(I - T^*) = \text{Ran}(I - T)^\perp$. Taking the orthogonal spaces, we get

$$\text{Ker}(I - T^*)^\perp = (\text{Ran}(I - T)^\perp)^\perp = \overline{\text{Ran}(I - T)} = \text{Ran}(I - T).$$

We know that $\text{Ker}(I - T^*) \neq \{0\}$ iff $1 \in \text{spec}(T^*)$ iff $1 \in \text{spec}(T)$ iff $\text{Ker}(I - T) \neq \{0\}$, and this is equivalent with the fact that $(I - T)$ is not surjective.

There remains to show that $\text{Ker}(I - T)$ and $\text{Ker}(I - T^*)$ have the same dimensions. We already know that if one space is nontrivial, then so is the second one. Let us first show that $\dim \text{Ker}(I - T) \leq \dim \text{Ran}(I - T)^\perp$. To do this, let us split \mathcal{H} into the two orthogonal decompositions

$$\begin{aligned}\mathcal{H} &= \text{Ker}(I - T) \oplus \text{Ker}(I - T)^\perp, \\ \mathcal{H} &= \text{Ran}(I - T)^\perp \oplus \text{Ran}(I - T).\end{aligned}$$

Let us assume *ab absurdo* that $\dim \text{Ker}(I - T) > \dim \text{Ran}(I - T)^\perp$. In that case, there exists a surjective map $\varphi : \text{Ker}(I - T) \rightarrow \text{Ran}(I - T)^\perp$. From the inequality of dimensions, this map is not injective: there exists $u_0 \in \text{Ker}(I - T)$ such that $\varphi(u_0) = 0$.

Using the first decomposition, let us now define the linear map $\mathcal{T} : \mathcal{H} \rightarrow \mathcal{H}$ by

$$\mathcal{T}(u) = \begin{cases} u - \varphi(u), & \text{for } u \in \text{Ker}(I - T) \\ Tu, & \text{for } u \in \text{Ker}(I - T)^\perp, \end{cases}$$

completing by linearity. This linear map is the sum of a finite rank operator and a compact one, so it is compact. Besides, the above definition, and the surjectivity of φ show that $(I - \mathcal{T})$ is surjective. From the above equivalences, this would imply that $(I - \mathcal{T})$ is injective, which contradicts $(I - \mathcal{T})u_0 = \varphi(u_0) = 0$. We hence proved that $\text{Ker}(I - T) \leq \text{Ran}(I - T)^\perp = \text{Ker}(I - T^*)$. Exchanging T and T^* , we obtain the requested equality. \square In a sense, the Fredholm alternative shows

that the operators $(I - T)$, with T compact, behave like operators on finite dimensional spaces. We know that a linear operator A on a finite dimensional space is injective if and only if it is surjective, with $\dim \text{Ker}(A) = \dim \text{Ran}(A)^\perp$, and we see a similar feature in the case of $I - T$.

Using this Fredholm alternative, we are now ready to describe the spectrum of a compact operator on \mathcal{H} .

Theorem 5.3.3 (Spectrum of compact operator) Let \mathcal{H} be an infinite-dimensional Hilbert space and $T \in \mathcal{K}(\mathcal{H})$. Then

- (a) $0 \in \text{spec } T$;
- (b) $\text{spec } T \setminus \{0\}$ is composed of at most countably eigenvalues of T ; each eigenvalue is isolated from the rest of the spectrum, and of finite multiplicity: for any $n \geq 1$ the dimensions $\dim \text{Ker}(T - \lambda_j)^n$ are finite, and saturate after a certain power n_j .
- (c) If we order the eigenvalues by decreasing moduli $|\lambda_1| \geq |\lambda_2| \geq \dots$, we are in one and only one of the following situations:

- $\text{spec } T \setminus \{0\} = \emptyset$,
- $\text{spec } T \setminus \{0\}$ is a finite set of eigenvalues $\lambda_1, \dots, \lambda_N$,
- $\text{spec } T \setminus \{0\}$ is an infinite sequence $(\lambda_n)_{n \geq 1}$ converging to 0.

(d) On the opposite, $\{0\}$ makes up the essential spectrum of T .

These properties can be summarized by the fact that $\text{spec } T \setminus \{0\}$ is composed of discrete spectrum.

Proof.— (a) Assume that $0 \notin \text{spec } T$, then $T^{-1} \in \mathcal{L}(\mathcal{H})$, and the operator $I = T^{-1}T$ is compact. This is possible only if \mathcal{H} is finite-dimensional.

(b) If $\lambda \neq 0$ we have $T - \lambda = -\lambda(1 - T/\lambda)$, and by the Fredholm alternative the condition $\lambda \in \text{spec } T$ is equivalent to $\text{Ker}(1 - T/\lambda) = \text{Ker}(T - \lambda) \neq \{0\}$. A value $\lambda \neq 0$ satisfying this condition is thus an eigenvalue, of finite multiplicity, and it is isolated from the rest of the spectrum. This isolation property implies that the nontrivial spectrum is at most countable: indeed, this isolation shows that any annulus $\{\frac{1}{n+1} < |z| \leq \frac{1}{n}\}$ contains at most finitely many eigenvalues.

The point (c) is just a more detailed version of (b).

(d) if T has no or finitely many nonzero eigenvalues, 0 is an isolated spectral point, but it cannot be a finite multiplicity eigenvalue. Indeed, the sum of all the generalized eigenspaces associated with the $\lambda_j \neq 0$ and with $\lambda_{N+1} = 0$ would be finite dimensional. \square

Let us now specifically study the spectra of compact *selfadjoint* operators.

Theorem 5.3.4 (Spectrum of compact self-adjoint operator) Let $T = T^* \in \mathcal{K}(\mathcal{H})$, then one can construct an orthonormal basis consisting of eigenvectors of T , and the corresponding eigenvalues form a real sequence converging to 0.

Proof.— Let $(\lambda_n)_{n \geq 1}$ be the distinct nonzero eigenvalues of T , ordered by decreasing moduli; this set can be empty, finite or infinite countable. Since T is self-adjoint, these eigenvalues are real. For $n \geq 1$, denote $E_n \stackrel{\text{def}}{=} \text{Ker}(T - \lambda_n)$ the corresponding finite dimensional eigenspace. We also call $E_0 \stackrel{\text{def}}{=} \text{Ker}(T)$, which can be trivial, finite dimensional or infinite dimensional. Due to selfadjointness, one can easily see that $E_n \perp E_m$ for any pair $n \neq m$. Denote by F the linear hull of $\cup_{n \geq 0} E_n$. We are going to show that F is dense in \mathcal{H} , equivalently that $F^\perp = \{0\}$.

Clearly, we have $T(F) \subset F$. Due to the selfadjointness of T we also have $T(F^\perp) \subset F^\perp$. Denote by \tilde{T} the restriction of T to F^\perp ; then \tilde{T} is compact, self-adjoint, and its spectrum equals $\{0\}$, so $\tilde{T} = 0$. But this means that $F^\perp \subset \text{Ker } T = E_0 \subset F$ which shows that $F^\perp = \{0\}$.

Taking an orthonormal basis in each subspace $(E_n)_{n \geq 0}$, we obtain an orthonormal basis in the whole space \mathcal{H} . We may relabel the nonzero eigenvalues by $(\mu_k)_{k \geq 1}$, with repetitions according to the multiplicities, and corresponding eigenstates ϕ_k . The operator T can then be represented by:

$$(5.3.1) \quad T = \sum_{k \geq 1} \mu_k \langle \phi_k, \cdot \rangle \phi_k.$$

This expansion is called the spectral decomposition of T . Notice that the sum may be empty, finite or countable, and that the basis states in $\text{Ker } T$ do not contribute. \square

Let us finish this section by defining the singular values of a general compact operator.

Theorem 5.3.5 For any operator $T \in \mathcal{K}(\mathcal{H})$, there exist two orthonormal bases $(\phi_j)_{j \geq 1}$ and $(\psi_j)_{j \geq 1}$, and a decreasing sequence of positive numbers $(s_j)_{j \geq 1}$, converging to zero, such that

$$(5.3.2) \quad T = \sum_{j \geq 1} s_j \langle \phi_j, \cdot \rangle \psi_j.$$

The $(s_j)_{j \geq 1}$ are called the *singular values* of the operator T .

The above representation, valid for any compact operator, is in general different from the representation (5.3.1) for selfadjoint compact operators. The two coincide only when T is positive.

Proof.— The operator T^*T is compact, selfadjoint and positive, so its spectral decomposition can be written:

$$\sum_{k=1}^N s_k^2 \langle \phi_k, \cdot \rangle \phi_k,$$

simply by defining $s_k = \sqrt{\mu_k} > 0$. Here N is either finite or infinite, according to the number of nonzero eigenvalues. The $(\phi_k)_{k=1, \dots, N}$ generate the sum of eigenspaces associated with nonzero eigenvalues. If necessary, we may then append an orthonormal basis of $\text{Ker } T$ to obtain an orthonormal basis $(\phi_j)_k$ of \mathcal{H} . We then also append the values $s_j = 0$ associated with these extra vectors.

For each $j = 1, \dots, N$, we define $\tilde{\psi}_j = T\phi_j$, and normalize it into $\psi_j = \frac{\tilde{\psi}_j}{\|\tilde{\psi}_j\|} = \frac{\tilde{\psi}_j}{s_j}$. One easily checks that $(\psi_j)_{j=1, \dots, N}$ forms an orthonormal family, which can be completed by an orthonormal basis of $\text{Ran}(T)^\perp = \text{Ker}(T^*)$ if necessary, to obtain an o.n.b. of all \mathcal{H} .

An easy computation shows that the action of T on the o.n.b. $(\phi_j)_k$ corresponds to the expansion (5.3.2). \square

5.4 An example of compact operators on \mathcal{H} : Hilbert-Schmidt operators

5.4.1 Integral operators

An important class of compact operators on L^p spaces is composed of integral operators, that is operators defined by an integral kernel enjoying certain properties. For simplicity we restrict our attention to the case $\mathcal{H} = L^2(\Omega, dx)$, where $\Omega \subset \mathbb{R}^d$ is an open set.

Let $K \in L^1_{\text{loc}}(\Omega \times \Omega)$. We consider the operator T_K acting on essentially bounded functions with compact support $u \in L^\infty_{\text{comp}}(\Omega)$ as follows:

$$(5.4.3) \quad T_K u(x) = \int_{\Omega} K(x, y) u(y) dy.$$

We would first like to find conditions under which the expression (5.4.3) defines a bounded operator on $\mathcal{H} = L^2(\Omega)$. A standard result in this direction is provided by the following important theorem.

Theorem 5.4.1 (Schur's test) Assume that

$$M_1 = \text{ess - sup}_{x \in \Omega} \int_{\Omega} |K(x, y)| dy < \infty \quad \text{and} \quad M_2 = \text{ess - sup}_{y \in \Omega} \int_{\Omega} |K(x, y)| dx < \infty.$$

Then the operator defined by (5.4.3) extends to a continuous linear operator $T_K : L^2 \rightarrow L^2$, and its norm satisfies the bound

$$\|T_K\|_{\mathcal{L}(L^2)} \leq \sqrt{M_1 M_2}.$$

Proof.— We have

$$\begin{aligned} |T_K u(x)|^2 &\leq \left(\int_{\Omega} \sqrt{|K(x, y)|} \sqrt{|K(x, y)|} |u(y)| dy \right)^2 \\ &\stackrel{C-S}{\leq} \int_{\Omega} |K(x, y)| dy \int_{\Omega} |K(x, y)| \cdot |u(y)|^2 dy \\ &\stackrel{x\text{-a.e.}}{\leq} M_1 \int_{\Omega} |K(x, y)| \cdot |u(y)|^2 dy. \end{aligned}$$

$$\text{integrating over } x, \text{ we get } \|T_K u\|^2 \leq M_1 \int_{\Omega} \int_{\Omega} |K(x, y)| |u(y)|^2 dy dx \stackrel{Fubini}{\leq} M_1 M_2 \|u\|^2.$$

□

Proposition 5.4.2 Another class of integral operators are bounded, namely those such that $K \in L^2(\Omega \times \Omega)$. One indeed has the bound

$$\|T_K\| \leq \|K\|_{L^2(\Omega \times \Omega)}.$$

Proof.— For any $u \in L^2(\Omega)$, we find

$$\begin{aligned} |T_K u(x)|^2 &= \left| \int K(x, y) u(y) dy \right|^2 \\ &\stackrel{C-S}{\leq} \int |K(x, y)|^2 dy \int |u(y)|^2 dy \\ \implies \|T_K u\|^2 &\leq \iint |K(x, y)|^2 dy dx \|u\|^2 = \|K\|_{L^2}^2 \|u\|^2 \end{aligned}$$

□

The next section will show that the operators associated with such L^2 kernels form an important class of compact operators.

5.4.2 Hilbert-Schmidt operators

To obtain a class of compact integral operators we introduce the following class of operators.

Definition 5.4.3 An operator $T \in \mathcal{L}(\mathcal{H})$ is said to be *Hilbert-Schmidt* if, for some orthonormal basis $(e_n)_{n \geq 1}$ of \mathcal{H} the sum

$$(5.4.4) \quad \|T\|_2^2 \stackrel{\text{def}}{=} \sum_{n \geq 1} \|T e_n\|^2 \quad \text{is finite.}$$

For any two Hilbert-Schmidt operators T, T' , one defines their Hilbert-Schmidt scalar product as follows:

$$\langle T, T' \rangle_{HS} = \sum_{n \geq 1} \langle e_n, T^* T' e_n \rangle.$$

(the Cauchy-Schwartz inequality ensures that the sum converges). One obviously has $\langle T, T \rangle_{HS} = \|T\|_2^2$. This explains why $\|T\|_2$ is called the Hilbert-Schmidt norm of T .

This definition could let believe that the choice of o.n.b. (e_n) matters. This is fortunately not the case.

Proposition 5.4.4 (Hilbert-Schmidt norm) For a Hilbert-Schmidt operator T , the quantity $\|T\|_2$ does not depend on the choice of the basis $(e_n)_n$.

In particular, another characterization of Hilbert-Schmidt operators consists in the following property of its singular values:

$$(5.4.5) \quad \sum_{j \geq 1} s_j^2 < \infty.$$

The operator norm satisfies

$$(5.4.6) \quad \|T\| \leq \|T\|_2.$$

Moreover, the adjoint operator T^* is also Hilbert-Schmidt with $\|T^*\|_2 = \|T\|_2$.

Proof.— Let $(e_n)_n$ and $(f_m)_m$ be two orthonormal bases. Using the resolution of identity associated with these two bases, we get

$$\sum_n \|Te_n\|^2 = \sum_n \left(\sum_m |\langle f_m, Te_n \rangle|^2 \right) = \sum_m \left(\sum_n |\langle T^* f_m, e_n \rangle|^2 \right) = \sum_m \|T^* f_m\|^2.$$

Note that the two sums could be switched since all terms are positive.

This equality shows that the expression (5.4.4) is independent of the choice of the basis. It also shows that $\|T^*\|_2 = \|T\|_2$. If we take for basis (e_n) the basis (ϕ_j) associated with the singular value decomposition (5.3.2), we see that

$$\|T\|_2^2 = \sum_{j \geq 1} s_j^2.$$

To show $\|T\| \leq \|T\|_2$, choose some o.n.b. $(e_n)_n$, and for any $u \in \mathcal{H}$, call the coefficients $u_n = \langle e_n, u \rangle$.

$$\|Tu\|^2 = \left\| \sum_n u_n Te_n \right\|^2 \leq \left(\sum_n |u_n| \|Te_n\| \right)^2 \stackrel{C-S}{\leq} \sum_n |u_n|^2 \sum_n \|Te_n\|^2 = \|T\|_2^2 \|u\|^2.$$

□

Due to the characterization (5.4.5) in terms of singular values, the space of Hilbert-Schmidt operators is often denoted by $S_2(\mathcal{H})$, the *second Schatten class* of the Hilbert space \mathcal{H} . This class forms a Hilbert space, when equipped with the H-S scalar product.

Remark 5.4.5 The compact operators T satisfying the property

$$\sum_j s_j < \infty$$

are also interesting. They are called *trace class* operators, and form the first Schatten class $S_1(\mathcal{H})$. We will not study them any further in these notes, but only mention that this class of operators admit a trace linear functional, which is defined, for any given o.n.b. $(e_n)_n$, by

$$\operatorname{tr} T = \sum_n \langle e_n, Te_n \rangle.$$

This trace extends the usual trace functional of finite rank operators.

These operators can be equipped with a so-called *trace norm*, defined by:

$$\|T\|_{tr} \stackrel{\text{def}}{=} \sum_j s_j.$$

This trace norm is equal to the trace of the operator

$$|T| \stackrel{\text{def}}{=} \sqrt{T^*T},$$

where the square root of the positive operator T^*T can be defined either by spectrally, replacing the positive eigenvalues μ_k by their square roots $s_k = \sqrt{\mu_k}$.

The crucial property of Hilbert-Schmidt operators is their compactness.

Proposition 5.4.6 Any Hilbert-Schmidt operator is compact. In other words, the class $S_2(\mathcal{H}) \subset \mathcal{K}(\mathcal{H})$. Besides, finite rank operators are dense in the Hilbert space $S_2(\mathcal{H})$.

Proof.— Let us choose an o.n.b. (e_n) . For any $u \in \mathcal{H}$, we have the expansion

$$Tu = \sum_{n=1}^{\infty} \langle e_n, u \rangle Te_n.$$

For $N \geq 1$, let us define the truncated operators

$$T_N u = \sum_{n=1}^N \langle e_n, u \rangle Te_n.$$

These operators are obviously of finite rank. Using the inequality (5.4.6), we find:

$$\|T - T_N\|^2 \leq \|T - T_N\|_2^2 = \sum_{n \geq N+1} \|Te_n\|^2 \xrightarrow{N \rightarrow \infty} 0.$$

This proves the compactness of T , norm-limit of the finite rank operators T_N . Incidentally, we also proved that T_N converges to T in the H-S norm. Hence finite rank operators are dense in the Hilbert space $S_2(\mathcal{H})$. \square

The following proposition gives a nice characterization of Hilbert-Schmidt operators as a particular class of integral operators.

Proposition 5.4.7 (Hilbert-Schmidt operators as integral operators) Let $\mathcal{H} = L^2(\Omega)$. An operator T in \mathcal{H} is Hilbert-Schmidt iff there exists an integral kernel $K \in L^2(\Omega \times \Omega)$ such that $T = T_K$, cf. Eq. (5.4.3).

In that case, we have the equality

$$\|T_K\|_2 = \|K\|_{L^2(\Omega \times \Omega)}.$$

We thus recover the norm inequality of Prop. 5.4.2.

Proof.— Let first $K \in L^2(\Omega \times \Omega)$. Let us show that the associated operator T_K is Hilbert-Schmidt. Let (e_n) be an orthonormal basis in \mathcal{H} , then the functions $e_{m,n}(x, y) = e_m(x)\overline{e_n(y)}$ forms an orthonormal basis in $\mathcal{H} \otimes \mathcal{H}^* \simeq L^2(\Omega \times \Omega)$. Again, by expanding the identity in the o.n.b. (e_n) , we find:

$$\begin{aligned} \sum_{n \geq 1} \|T_K e_n\|^2 &= \sum_{m, n \geq 1} |\langle e_m, T_K e_n \rangle|^2 = \sum_{m, n \geq 1} \left| \int_{\Omega} \overline{e_m(x)} \left(\int_{\Omega} K(x, y) e_n(y) dy \right) dx \right|^2 \\ &= \sum_{m, n \geq 1} \left| \int_{\Omega} \int_{\Omega} \overline{e_m(x)} e_n(y) K(x, y) dx dy \right|^2 = \sum_{m, n \geq 1} |\langle e_{m,n}, K \rangle|^2 = \|K\|_{L^2(\Omega \times \Omega)}^2. \end{aligned}$$

Conversely, let T be a Hilbert-Schmidt operator on \mathcal{H} . Let us choose an o.n.b. (e_n) , and let us use the same finite rank approximations T_N of T as in the proof of Prop. 5.4.6. We have, for any $u \in \mathcal{H}$ and with $u_n = \langle e_n, u \rangle$ as before:

$$T_N u = \sum_{n=1}^N \langle e_n, u \rangle T e_n = \sum_{n=1}^N \sum_{m \geq 1} \langle e_n, u \rangle \langle e_m, T e_n \rangle e_m.$$

If we take

$$K_N(x, y) \stackrel{\text{def}}{=} \sum_{n=1}^N \sum_{m \geq 1} \overline{e_n(y)} \langle e_m, T e_n \rangle e_m(x) = \sum_{n=1}^N \sum_{m \geq 1} \langle e_m, T e_n \rangle e_{m,n}(x, y),$$

we see that $T_N u(x) = \int K_N(x, y) u(y) dy$, which shows that T_N is equal to the integral operator T_{K_N} . In turn, the kernel K_N belongs to $L^2(\Omega \times \Omega)$:

$$\begin{aligned} \int |K_N(x, y)|^2 dx dy &= \int \left| \sum_{n=1}^N \sum_{m \geq 1} \langle e_m, T e_n \rangle e_{m,n}(x, y) \right|^2 dx dy \\ &= \sum_{n, n'=1}^N \sum_{m, m' \geq 1} \langle e_{m,n}, e_{m',n'} \rangle_{L^2(\Omega \times \Omega)} \overline{\langle e_m, T e_n \rangle} \langle e_{m'}, T e_{n'} \rangle \\ &= \sum_{n=1}^N \sum_{m \geq 1} |\langle e_m, T e_n \rangle|^2 \\ &= \sum_{n=1}^N \|T e_n\|^2 = \|T_N\|_2^2. \end{aligned}$$

The proof of Prop. 5.4.6 actually shows that $\|T_N - T\|_2 \rightarrow 0$. Hence, the kernels K_N form a Cauchy sequence in $L^2(\Omega \times \Omega)$, which converge to a kernel K , and we have $T = T_K$.

We have thus obtained a unitary equivalence between $S_2(\mathcal{H})$ (equipped with the H-S scalar product) and $L^2(\Omega \times \Omega)$. \square

One can easily see that the operator T_K is self-adjoint iff $K(x, y) = \overline{K(y, x)}$ for a.e. $(x, y) \in \Omega \times \Omega$. The characterization of H-S operators from their integral kernel (Proposition 5.4.7) often allows to

identify the H-S property rather easily. For this reason, it is often easier to prove that an operator is H-S, rather than trying to directly prove that it is compact.

If we now focus on self-adjoint compact operators, we see that a compact self-adjoint operator T is H-S iff its nonzero eigenvalues (μ_k) (counted with multiplicities) satisfy

$$\sum_{k \geq 1} \mu_k^2 = \|T\|_2^2 < \infty.$$

Moreover, by Proposition 5.4.7, for $T = T_K$ one has the exact equality (trace formula)

$$\sum_{k \geq 1} \mu_k^2 = \|K\|_{L^2(\Omega \times \Omega)}^2.$$

This expression may be used to estimate properties of the eigenvalues from the integral kernel.

5.5 Unbounded operators with compact resolvent

Now that we have analyzed the spectral properties of compact operators, we will apply these results to a particular family of operators, namely the resolvents of certain unbounded selfadjoint operators on a Hilbert space \mathcal{H} .

Proposition 5.5.1 (Operators with compact resolvent) Assume that $(T, D(T))$ is selfadjoint on \mathcal{H} , and that for some $z_0 \in \text{res}(T)$, the resolvent $(T - z_0)^{-1}$ is a compact operator.

Then the spectrum of T is purely discrete, it consists in isolated eigenvalues $(\lambda_n)_{n \geq 1}$ of finite multiplicities, with $|\lambda_n| \rightarrow \infty$, associated with an orthonormal basis $(\phi_n)_n$. Here the eigenvalues λ_n are not necessarily distinct from one another, each value appears as often as its multiplicity.

Such a $(T, D(T))$ is said to be an operator of compact resolvent.

Proof.— Through the resolvent identity, the compactness of $(T - z_0)^{-1}$ implies the compactness of all resolvents $(T - z)^{-1}$, $z \in \text{res}(T)$. We claim that this compactness implies that $\text{res}(T) \cap \mathbb{R} \neq \emptyset$. This will be shown later through the spectral theorem, see Example 6.3.15 below. Let us admit this fact for now: we may then assume that $z_0 \in \mathbb{R} \cap \text{res}(T)$. In this case, the resolvent $(T - z_0)^{-1}$ is compact and selfadjoint, it admits discrete nonzero eigenvalues $(\mu_n)_{n \geq 1}$, associated with an orthonormal family (ϕ_n) . I claim that $\text{Ker}(T - z_0)^{-1} = \{0\}$: indeed, the existence of a nontrivial eigenstate $(T - z_0)^{-1}\phi_0 = 0$ would imply

$$0 = (T - z_0)(T - z_0)^{-1}\phi_0 = \phi_0,$$

hence a contradiction. This implies that the family $(\phi_n)_{n \geq 1}$ generates all \mathcal{H} , in particular the sequence of nonzero eigenvalues $(\mu_n)_{n \geq 1}$ is infinite, and converges to 0.

For any such eigenvalue, we have

$$\begin{aligned} (T - z_0)^{-1}\phi_n &= \mu_n \phi_n \\ \implies \phi_n &= \mu_n (T - z_0) \phi_n \\ \implies T\phi_n &= (z_0 + \mu_n^{-1}) \phi_n. \end{aligned}$$

The o.n.b. (ϕ_n) thus forms a basis of eigenstates of T , associated with the eigenvalues $\lambda_n = (z_0 + \mu_n^{-1})$ (counted with multiplicities). Since $\mu_n \rightarrow 0$, the eigenvalues of T satisfy $|\lambda_n| \rightarrow \infty$. In particular, they have no accumulation point. The full spectrum of T is thus discrete. \square

For an example of such operators, we come back to the construction of selfadjoint operators associated with closed quadratic forms, see Section 3.

We recall the Theorem 3.1.5 and the more particular Prop. 3.1.7, which start from a symmetric (resp. closed) quadratic form q , such that the form domain $D(q) = \mathcal{V}$ is complete w.r.t. the form norm $\|\cdot\|_q = \|\cdot\|_{\mathcal{V}}$, and construct from there a selfadjoint (resp. selfadjoint and bounded below) operator $(T, D(T))$.

The proof of Theorem 3.1.5 starts from Thm 3.1.4, which describes properties of the operator T constructed from a quadratic form q elliptic on the Hilbert space $(\mathcal{V}, \|\cdot\|_{\mathcal{V}})$, a dense subspace of the ambient space \mathcal{H} . The latter theorem states that the inverse operator $T^{-1} : \mathcal{H} \rightarrow \mathcal{H}$ is continuous. One can actually strengthen the statement as follows:

Lemma 5.5.2 In the situation of Theorem 3.1.4, the operator T^{-1} maps \mathcal{H} to \mathcal{V} , and it is also continuous from $(\mathcal{H}, \|\cdot\|_{\mathcal{H}})$ to $(\mathcal{V}, \|\cdot\|_{\mathcal{V}})$: $T^{-1} \in \mathcal{L}(\mathcal{H}, \mathcal{V})$.

Proof.— For any $u \in D(T)$ we have:

$$\|u\|_{\mathcal{H}} \|Tu\|_{\mathcal{H}} \stackrel{C-S}{\geq} |\langle u, Tu \rangle_{\mathcal{H}}| = |q(u, u)| \stackrel{ellipt.}{\geq} \alpha \|u\|_{\mathcal{V}}^2 \geq C\alpha \|u\|_{\mathcal{V}} \|u\|_{\mathcal{H}},$$

i.e. $\|Tu\|_{\mathcal{H}} \geq C\alpha \|u\|_{\mathcal{V}}$ and $\|T^{-1}u\|_{\mathcal{V}} \leq (C\alpha)^{-1} \|u\|_{\mathcal{H}}$. \square

This improved control on T^{-1} leads to an important consequence:

Corollary 5.5.3 In the situation of Theorem 3.1.4, let us assume that the embedding $j : \mathcal{V} \rightarrow \mathcal{H}$ is compact. Then the operator $T^{-1} : \mathcal{H} \rightarrow \mathcal{H}$ is a compact operator.

This applies in particular to the situations of Theorem 3.1.5 Prop. 3.1.7, if $j : \mathcal{V} \rightarrow \mathcal{H}$ is compact.

Proof.— Indeed, the operator $T^{-1} : \mathcal{H} \rightarrow \mathcal{H}$ can be decomposed as $T^{-1} = j \circ L$, where L is the operator T^{-1} viewed as an operator from \mathcal{H} to \mathcal{V} , which is continuous according to Lemma 5.5.2. Hence T^{-1} is compact, as the composition of a bounded operator and a compact one. \square

The above can be applied to a variety of cases. To identify situations where the embedding $\mathcal{V} \hookrightarrow \mathcal{H}$ is compact, we may invoke the following compactness criterion for a subset in $L^2(\mathbb{R}^d)$.

Theorem 5.5.4 (Riesz-Kolmogorov Theorem) A subset $\mathcal{F} \subset L^2(\mathbb{R}^d)$ is precompact if and only if:

i) For any $\epsilon > 0$, there exists $R = R_\epsilon > 0$ such that

$$\forall u \in \mathcal{F}, \quad \int_{|x|>R} |u(x)|^2 dx \leq \epsilon.$$

This property is sometimes referred to as *equitightness* (roughly speaking, the elements of \mathcal{F} are essentially of uniform bounded support).

ii) For any $\epsilon > 0$, there exists $\eta = \eta_\epsilon$ such that

$$\forall h \in \mathbb{R}^d, |h| \leq \eta, \quad \forall u \in \mathcal{F}, \quad \|\tau_h u - u\|_{L^2(\mathbb{R}^d)} \leq \epsilon.$$

Here $\tau_h u(x) = u(x - h)$ is the translation of u by the vector h . This condition is a form of *equicontinuity*, it states that the oscillations of u are uniformly under control.

This second condition is equivalent with the equitightness of the Fourier transform \hat{u} :

ii') For any $\epsilon > 0$, there exists $\hat{R} > 0$ such that

$$\forall u \in \mathcal{F}, \quad \int_{|\xi|>\hat{R}} |\hat{u}(\xi)|^2 d\xi \leq \epsilon.$$

Remark 5.5.5 The first versions of the theorem were proved independently by M. Riesz and by A. Kolmogorov, complemented by Tamarkin. It contained the extra condition that \mathcal{F} must be bounded in $L^2(\mathbb{R}^d)$. However, this extra condition was later proved to be redundant by Sudakov. The theorem extends to all $L^p(\Omega)$ $p \in [1, \infty[$, and Ω an open subset of \mathbb{R}^d .

Dirichlet Laplacian on a bounded domain

The first example we provide is the Dirichlet Laplacian $T_0 = -\Delta_\Omega$ on an open set $\Omega \subset \mathbb{R}^d$, defined in Example 3.1.15. If Ω is bounded, then the embedding of $\mathcal{V} = H_0^1(\Omega)$ to $\mathcal{H} = L^2(\Omega)$ is compact.

This should be a well-known fact, but let us check it using the Riesz-Kolmogorov theorem. One needs to prove that the unit ball in $H_0^1(\Omega)$ is precompact in $L^2(\Omega)$. First, the equitightness property i) is obvious, due to the compact support. Any function $u \in H_0^1(\Omega)$ with $\|u\|_{H^1} \leq 1$ extends to $\underline{u} \in H^1(\mathbb{R}^d)$, so we may use the Fourier transform criterion ii'). The fact that $\|u\|_{H^1} \leq 1$ implies that

$$\int_{|\xi|>R} |\hat{u}(\xi)|^2 d\xi \leq \frac{1}{R^2} \int_{|\xi|>R} |\xi|^2 |\hat{u}(\xi)|^2 d\xi \leq \frac{1}{R^2} \|u\|_{H^1}^2 \leq \frac{1}{R^2}.$$

This directly proves the property ii'), hence the compactness of the embedding $H_0^1(\mathbb{R}^d) \hookrightarrow L^2(\mathbb{R}^d)$.

From the Corollary 5.5.3, we deduce that the operator $L = (T_0 + 1)^{-1}$ is compact and self-adjoint. This shows that the Dirichlet Laplacian admits a discrete spectrum $(\lambda_n)_{n \geq 1}$. From Poincaré's inequality we already know that all eigenvalues of T_0 are strictly positive, hence the eigenvalues $\lambda_n \rightarrow +\infty$.

The eigenvalues λ_n are called the Dirichlet eigenvalues of the domain Ω . An important part of modern analysis, *spectral geometry*, study the relations between the geometric and topological properties of Ω , and the distribution of its Dirichlet eigenvalues.

Schrödinger operators with a confining potential

Let us discuss another class of operators with compact resolvents, namely the Schrödinger operators $T = -\Delta + V$, where the potential $V \in L^2_{\text{loc}}(\mathbb{R}^d)$ is positive, and diverges when $|x| \rightarrow \infty$:

$$w(r) \stackrel{\text{def}}{=} \inf_{|x| \geq r} V(x) \xrightarrow{r \rightarrow \infty} +\infty,$$

Remark 5.5.6 1. Such a potential is said to be *confining*, since in classical mechanics particles of total energy $E > 0$ are confined (trapped) in the region $\mathcal{A}_E = \{x \in \mathbb{R}^d, V(x) \leq E\}$, which is bounded in \mathbb{R}^d .

2. Actually, it suffices to ensure that $\text{ess-inf}_{|x| \geq r} V(x)$ diverges as $r \rightarrow \infty$, since negligible points x will not contribute to the operator of multiplication by V .

The operator $T = -\Delta + V$ can be properly defined through the Friedrichs extension of the differential operator $T_0 = -\Delta + V$ acting on $C_c^\infty(\mathbb{R}^d)$, as discussed in Example 3.2.6. We already know that T is self-adjoint and semibounded from below on $\mathcal{H} = L^2(\mathbb{R}^d)$. The following theorem shows that T has discrete spectrum.

Theorem 5.5.7 If the potential $V \in L^2_{\text{loc}}(\mathbb{R}^d)$ is confining, then the selfadjoint Schrödinger operator $T = -\Delta + V$ admits a compact resolvent. As a result, its spectrum is purely discrete, with finite multiplicity eigenvalues $\lambda_n \rightarrow +\infty$.

Proof.— As follows from Example 3.2.6, it is sufficient to show that the embedding of $\mathcal{V} = H^1_{\mathcal{V}}(\mathbb{R}^d) \hookrightarrow L^2(\mathbb{R}^d)$ is compact, where \mathcal{V} is equipped with the norm

$$\|u\|_{\mathcal{V}}^2 = \|u\|_{H^1}^2 + \|\sqrt{V}u\|_{L^2}^2.$$

Let B be the unit ball in \mathcal{V} . We will show that B is relatively compact in $L^2(\mathbb{R}^d)$ using the Riesz-Kolmogorov Theorem 5.5.4.

The equitightness condition *i*) follows from

$$\int_{|x| \geq R} |u(x)|^2 dx \leq \frac{1}{w(R)} \int_{|x| \geq R} V(x) |u(x)|^2 \leq \frac{1}{w(R)} \|\sqrt{V}u\|_{L^2}^2 \leq \frac{1}{w(R)} \|u\|_{\mathcal{V}}^2.$$

For the condition *ii*) we have:

$$\begin{aligned} \int_{\mathbb{R}^d} |u(x+h) - u(x)|^2 dx &= \int_{\mathbb{R}^d} \left| \int_0^1 \frac{d}{dt} u(x+th) dt \right|^2 dx \\ &= \int_{\mathbb{R}^d} \left| \int_0^1 h \cdot \nabla u(x+th) dt \right|^2 dx \leq h^2 \int_{\mathbb{R}^d} \int_0^1 |\nabla u(x+th)|^2 dt dx \\ &\leq h^2 \int_0^1 \int_{\mathbb{R}^d} |\nabla u(x+th)|^2 dx dt = h^2 \|\nabla u\|_{L^2}^2 \leq h^2 \|u\|_{\mathcal{V}}^2. \end{aligned}$$

□

The confining assumption of Theorem 5.5.7 is not necessary to ensure a discrete spectrum. For example, it is known that the Schrödinger operator on $L^2(\mathbb{R}^d)$ with potential $V(x_1, x_2) = x_1^2 x_2^2$ admits a compact resolvent, although that potential is not confining.

A rather simple necessary and sufficient condition is known in the case $d = 1$:

Proposition 5.5.8 (Molchanov criterium) The operator $T = -d^2/dx^2 + V$ has a compact resolvent iff

$$\forall \delta > 0, \quad \lim_{x \rightarrow \infty} \int_x^{x+\delta} V(s) ds = +\infty.$$

Necessary and sufficient conditions are also available for the multi-dimensional case, but their forms are more complicated. An advanced reader may refer to [10] for the discussion of such questions.

Chapter 6

The spectral theorem for selfadjoint operators

Some points in this section are just sketched to avoid technicalities. A more detailed presentation can be found in [4, Chapter 2] or in [12, Section 12.7].

Given a *selfadjoint* operator $(T, D(T))$ on a Hilbert space \mathcal{H} , the goal of the present chapter is to give a meaning to the operator $f(T)$, where f is a sufficiently general function on \mathbb{R} ; here \mathbb{R} represents the “spectral real line”, and we will use the parameter $\lambda \in \mathbb{R}$ to represent the corresponding variable. We have several interesting functions in mind:

- i)* for $z \in \mathbb{C} \setminus \mathbb{R}$, the function $f_z(\lambda) = \frac{1}{\lambda - z}$ will lead to the resolvent $f_z(T) = (T - z)^{-1}$. These functions will be a “benchmark” for our functional calculus.
- ii)* the characteristic functions on a Borel set on \mathbb{R} , e.g. an interval $I \subset \mathbb{R}$. Indeed, we will see later that $\mathbb{1}_I(T)$ is the associated spectral projector on the interval I . The functions $\mathbb{1}_I(T)$ are bounded, but unfortunately they are not smooth, so dealing with them will require some efforts.
- iii)* some functions will be issued from certain evolution equations. For instance, the function $\lambda \mapsto e^{-it\lambda}$ will lead to e^{-itT} , the propagator of the Schrödinger equation generated by the Hamiltonian T . This function is smooth and bounded.

6.1 The case of operators with compact resolvent

To prepare the ground, let us first consider $(T, D(T))$ to be a selfadjoint operator with a compact resolvent. As shown in the previous section, there exists then an orthonormal eigenbasis $(e_n)_{n \in \mathbb{N}}$ and associated (real) eigenvalues of finite multiplicities $(\lambda_n)_{n \in \mathbb{N}}$, such that

$$\forall u \in D(T), \quad Tu = \sum_{n \in \mathbb{N}} \lambda_n \langle e_n, u \rangle e_n,$$

and the domain $D(T)$ is the subspace of \mathcal{H} composed of the vectors $u \in \mathcal{H}$ such that

$$\sum_{n \in \mathbb{N}} \lambda_n^2 |\langle e_n, u \rangle|^2 < \infty.$$

For $f \in C_b(\mathbb{R})$ (the space of bounded continuous functions), one can define an operator $f(T) \in \mathcal{L}(\mathcal{H})$ by the expansion

$$f(T)u = \sum_{n \in \mathbb{N}} f(\lambda_n) \langle e_n, u \rangle e_n.$$

This expression is equivalent with the following procedure. Introduce the map $U : \mathcal{H} \rightarrow \ell^2(\mathbb{N})$ defined by $Uu = (u_n)_{n \in \mathbb{N}}$, where $u_n = \langle e_n, u \rangle$. This map is unitary, it is simply the expansion of u in the eigenbasis (e_n) of T . Through this diagonalization, the conjugated operator UTU^* is merely the selfadjoint multiplication operator $(u_n) \mapsto (\lambda_n u_n)$ on $\ell^2(\mathbb{N})$, cf. Example 4.2.18. Similarly, for any $f \in C_b(\mathbb{R})$, the conjugation of $f(T)$, $Uf(T)U^*$, is the (bounded) multiplication operator $(u_n) \mapsto (f(\lambda_n)u_n)$ on $\ell^2(\mathbb{N})$.

$f(T)$ is therefore unitarily conjugated to the multiplication operator $(u_n) \mapsto (f(\lambda_n)u_n)$ on $\ell^2(\mathbb{N})$. We will see below that this structure generalizes to arbitrary selfadjoint operators: $f(T)$ will be defined through a conjugation to a multiplication operator on some (more complicated) L^2 space.

Some properties of $f(T)$

At this stage, we can already observe some interesting properties of the operators $f(T)$, in this situation of operators with compact resolvent:

$$(fg)(T) = f(T)g(T), \quad \bar{f}(T) = f(T)^*, \quad 1(T) = Id.$$

These properties show that the family of operators $(f(T))$ form a commutative $*$ -algebra.

The expansion (6.1) shows that the basis (e_n) is also an eigenbasis of the operator $f(T)$, with eigenvalues $(f(\lambda_n))$. From this, we immediately deduce the formula:

$$\text{spec } f(T) = \overline{f(\text{spec } T)}.$$

The expression (6.1) also provides explicit expressions to solutions of certain differential equations involving the operator T . An example is the “ T -Schrödinger equation”, which is the evolution equation of the form:

$$iu'(t) = Tu(t), \quad u(0) = v \in D(T), \quad u : \mathbb{R} \rightarrow D(T).$$

Conjugating through the diagonalizing operator U , we obtain an infinite set of independent ordinary differential equations

$$u'_n(t) = \lambda_n u_n(t),$$

which are obvious to solve as $u_n(t) = v_n e^{-it\lambda_n}$. Conjugating back, we see that the solution to (6.1) can be written in the form $u(t) = f_t(T)v$, using the family of bounded functions $f_t(\lambda) = e^{-it\lambda}$.

6.2 Continuous functional calculus for general selfadjoint operators

In the preceding paragraph we have dealt with operator with a compact resolvent (the procedure actually applies to any selfadjoint operator admitting an orthonormal eigenbasis). The aim of the present section is to develop a theory for general selfadjoint operators.

6.2.1 A Cauchy formula

Notation 6.2.1 Let us recall that $C_0(\mathbb{R})$ denotes the class of the continuous functions $f : \mathbb{R} \rightarrow \mathbb{C}$ with $\lim_{|\lambda| \rightarrow +\infty} f(\lambda) = 0$, equipped with the sup-norm. This should not be confused with the space $C^0(\mathbb{R}) = C(\mathbb{R})$ of continuous functions on \mathbb{R} , or the space $C_c(\mathbb{R}) = C_c^0(\mathbb{R})$ of compactly supported continuous functions on \mathbb{R} .

We say that a function $f : \mathbb{C} \rightarrow \mathbb{C}$ belongs to $C^\infty(\mathbb{C})$ if the function of two real variables $\mathbb{R}^2 \ni (x, y) \mapsto f(x + iy) \in \mathbb{C}$ belongs to $C^\infty(\mathbb{R}^2)$. In the similar way one defines the classes $C_c^\infty(\mathbb{C})$, $C^k(\mathbb{C})$ etc. In what follows we always use the notation $\operatorname{Re} z =: x$, $\operatorname{Im} z =: y$ for $z \in \mathbb{C}$. Using $x = \frac{z + \bar{z}}{2}$ and $y = \frac{z - \bar{z}}{2i}$, for $f \in C^1(\mathbb{C})$ one defines the antiholomorphic derivative

$$\frac{\partial f}{\partial \bar{z}} := \frac{1}{2} \left(\frac{\partial f}{\partial x} + i \frac{\partial f}{\partial y} \right)$$

Clearly, $\partial f / \partial \bar{z} \equiv 0$ if f is a holomorphic function.

Here is a particular case of the *Stokes formula*: if $f \in C^\infty(\mathbb{C})$ and $\Omega \subset \mathbb{C}$ is a domain with a sufficiently regular boundary, then

$$\int_{\Omega} \frac{\partial f}{\partial \bar{z}} dx dy = \frac{1}{2i} \oint_{\partial \Omega} f dz.$$

This Stokes formula allows to recover the following Cauchy formula, presented in a slightly unusual form.

Lemma 6.2.2 (Cauchy integral formula) Let $f \in C_c^\infty(\mathbb{C})$, then for any $w \in \mathbb{C}$ we have

$$f(w) = \frac{1}{\pi} \int_{\mathbb{C}} \frac{\partial f}{\partial \bar{z}} \frac{1}{w - z} dx dy.$$

Proof.— We note first that the singularity $1/(w - z)$ is integrable in two dimensions, so the integral is well-defined. Let Ω be a large disk containing the support of f and the point w . For small $\epsilon > 0$ denote the small disk $B_\epsilon := \{z \in \mathbb{C} : |z - w| \leq \epsilon\}$, and set $\Omega_\epsilon := \Omega \setminus B_\epsilon$. Using the Stokes formula

we have:

$$\begin{aligned}
\frac{1}{\pi} \int_{\mathbb{C}} \frac{\partial f}{\partial \bar{z}} \frac{1}{w-z} dx dy &= \frac{1}{\pi} \int_{\Omega} \frac{\partial f}{\partial \bar{z}} \frac{1}{w-z} dx dy \\
&= \lim_{\epsilon \rightarrow 0} \frac{1}{\pi} \int_{\Omega_{\epsilon}} \frac{\partial f}{\partial \bar{z}} \frac{1}{w-z} dx dy = \lim_{\epsilon \rightarrow 0} \frac{1}{\pi} \int_{\Omega_{\epsilon}} \frac{\partial}{\partial \bar{z}} \left(f(z) \frac{1}{w-z} \right) dx dy \\
&= \lim_{\epsilon \rightarrow 0} \frac{1}{2\pi i} \oint_{\partial \Omega_{\epsilon}} f(z) \frac{1}{w-z} dz \\
&= \frac{1}{2\pi i} \oint_{\partial \Omega} f(z) \frac{1}{w-z} dz - \lim_{\epsilon \rightarrow 0} \frac{1}{2\pi i} \oint_{|z-w|=\epsilon} f(z) \frac{1}{w-z} dz.
\end{aligned}$$

The first term on the right-hand side is zero, because f vanishes on the boundary of Ω . The second term can be calculated explicitly:

$$\begin{aligned}
\lim_{\epsilon \rightarrow 0} \frac{1}{2\pi i} \oint_{|z-w|=\epsilon} f(z) \frac{1}{w-z} dz &= \lim_{\epsilon \rightarrow 0} \frac{1}{2\pi i} \int_0^{2\pi} f(w + \epsilon e^{it}) \frac{i\epsilon e^{it} dt}{w - (w + \epsilon e^{it})} \\
&= - \lim_{\epsilon \rightarrow 0} \frac{1}{2\pi} \int_0^{2\pi} f(w + \epsilon e^{it}) dt = -f(w),
\end{aligned}$$

which gives the result. \square

The main idea of the subsequent presentation is to define the operators $f(T)$, for a self-adjoint operator T , using an operator valued generalization of the Cauchy integral formula. Namely, taking $\tilde{f} \in C_c^{\infty}(\mathbb{C}, \mathbb{C})$, to define

$$(6.2.1) \quad \tilde{f}(T) \stackrel{\text{def}}{=} \frac{1}{\pi} \int_{\mathbb{C}} \frac{\partial \tilde{f}}{\partial \bar{z}} (T - z)^{-1} dx dy.$$

In view of the singularity of the resolvent $(T - z)^{-1}$ when z approaches the real line, it is not clear whether the above integral actually converges. Besides, the above formula starts from a function \tilde{f} defined on the complex plane, and returns an operator $\tilde{f}(T)$. On the opposite, in Section 6.1 we were constructing operators $f(T)$ associated with functions f defined over the real line. Can we connect the two formulations?

The strategy to address these two questions will be to start from a function defined on the real line, $f \in C_c^{\infty}(\mathbb{R}, \mathbb{C})$, and extend this function to a function \tilde{f} defined on the complex plane, in a way such as to ensure that the integral (6.2.1) is well-defined. This extension can be done in various ways, but all of them share the property to be *almost analytic*.

6.2.2 Almost analytic extensions

Let $f \in C^{\infty}(\mathbb{R})$. Pick $n \in \mathbb{N}$ and a smooth function $\tau : \mathbb{R} \rightarrow \mathbb{R}$ such that $\tau(s) = 1$ for $|s| < 1$ and $\tau(s) = 0$ for $|s| > 2$. For $x, y \in \mathbb{R}$ and set $\sigma(x, y) \stackrel{\text{def}}{=} \tau(y/\langle x \rangle)$. Define then the function $\tilde{f} \in C^{\infty}(\mathbb{C})$ by

$$(6.2.2) \quad \tilde{f}(z) = \left[\sum_{r=0}^n f^{(r)}(x) \frac{(iy)^r}{r!} \right] \sigma(x, y).$$

For $x \in \mathbb{R}$, we clearly have $\tilde{f}(x) = f(x)$, so \tilde{f} is an extension of f . Besides, if $\text{supp } f \subset [-a, a]$, one easily finds¹ that $\text{supp } \tilde{f} \subset [-a, a] \times [-2\langle a \rangle, 2\langle a \rangle]$. Let us now show that the function \tilde{f} is *almost analytic* when $y \rightarrow 0$. Let us remark that if g is holomorphic in some tubular neighbourhood of \mathbb{R} , then for any $x \in \mathbb{R}$ and $y \leq \varepsilon$, we have the power series expansion

$$g(x + iy) = \sum_{r \geq 0} g^{(r)}(x) \frac{(iy)^r}{r!}.$$

The expression (6.2.2) tries to mimick the following expression, in cases where f is only smooth on \mathbb{R} . Computing its anti-holomorphic derivative, we find

$$(6.2.3) \quad \frac{\partial \tilde{f}}{\partial \bar{z}} = \frac{1}{2} \left[\sum_{r=0}^n f^{(r)}(x) \frac{(iy)^r}{r!} \right] (\partial_x \sigma + i \partial_y \sigma) + \frac{1}{2} f^{(n+1)}(x) \frac{(iy)^n}{n!} \sigma.$$

The derivatives $\partial_x \sigma$, $\partial_y \sigma$ can be nonzero only in the region $\{|y| \geq \langle x \rangle \geq 1\}$, thus away from the real axis. As a result, in the strip $\{|y| \leq 1\}$ the above derivative satisfies

$$(6.2.4) \quad \left| \frac{\partial \tilde{f}}{\partial \bar{z}}(x, y) \right| \leq \frac{1}{2n!} |f^{(n+1)}(x)| |y|^n,$$

in particular it converges fast to zero when $y \rightarrow 0$. An extension \tilde{f} with this property is said to be *almost analytic* of order n . In the case f is compactly supported, the RHS of (6.2.4) is $\mathcal{O}(y^n)$ uniformly w.r.t. $x \in \mathbb{R}$.

In the next section, we will use such an extension \tilde{f} in the formula (6.2.1), in order to define the operator $f(T)$.

6.2.3 The Helffer-Sjöstrand formula

Now let T be a self-adjoint operator in a Hilbert space \mathcal{H} . For $f \in C_c^\infty(\mathbb{R})$, construct an almost analytic extension \tilde{f} of f of some order $n \in \mathbb{N}$ to be defined below, and define the operator $f(T)$ by

$$(6.2.5) \quad f(T) := \frac{1}{\pi} \int_{\mathbb{C}} \frac{\partial \tilde{f}}{\partial \bar{z}} (T - z)^{-1} dx dy.$$

This integral expression is called the *Helffer-Sjöstrand formula*. We need to show several points: that the integral is well-defined, that it does not depend in the choice of σ and n etc. This will be done in a series of lemmas.

Let us address the first question, namely the convergence of the integral (6.2.1). As shown in Proposition 4.3.2, the resolvent is bounded by $\|(T - z)^{-1}\| \leq 1/|\text{Im } z|$, while the estimate (6.2.4) shows that, if f is compactly supported, that $\tilde{\partial} f / \partial \bar{z}(x + iy) = \mathcal{O}(y^n)$ for any fixed x , so the integrand in (6.2.5) forms a continuous family of bounded operators; the integral is therefore well-defined, and produces a bounded operator.

Let us show that the resulting operator does not depend on the choice of almost analytic extension.

1. We recall the Japanese brackets notation $\langle \bullet \rangle = (1 + |\bullet|^2)^{1/2}$.

Lemma 6.2.3 If $F \in C_c^\infty(\mathbb{C})$ and $F(x + iy) = O(y^2)$ as $y \rightarrow 0$, then

$$A := \frac{1}{\pi} \iint_{\mathbb{C}} \frac{\partial F}{\partial \bar{z}} (T - z)^{-1} dx dy = 0.$$

Proof.— By choosing a sufficiently large $N > 0$ one may assume that the support of F is contained in $\Omega := \{z \in \mathbb{C} : |x| < N, |y| < N\}$. For small $\epsilon > 0$ define $\Omega_\epsilon := \{z \in \mathbb{C} : |x| < N, \epsilon < |y| < N\}$. Using the Stokes formula we have

$$A = \lim_{\epsilon \rightarrow 0} \frac{1}{\pi} \iint_{\Omega_\epsilon} \frac{\partial F}{\partial \bar{z}} (T - z)^{-1} dx dy = \lim_{\epsilon \rightarrow 0} \frac{1}{2\pi i} \oint_{\partial \Omega_\epsilon} F(z) (T - z)^{-1} dz.$$

The boundary $\partial \Omega_\epsilon$ consists of eight segments. The integral over the vertical segments and over the horizontal segments with $y = \pm N$ are equal to 0 because the function F vanishes on these segments. It remains to estimate the integrals over the segments with $y = \pm \epsilon$. Here we have $\|(T - z)^{-1}\| \leq \epsilon^{-1}$ and

$$\|A\| \leq \lim_{\epsilon \rightarrow 0} \frac{1}{2\pi} \int_{\mathbb{R}} (|F(x + i\epsilon)| + |F(x - i\epsilon)|) \epsilon^{-1} dx = \lim_{\epsilon \rightarrow 0} \mathcal{O}(\epsilon) = 0.$$

□

Corollary 6.2.4 For $f \in C_c^\infty(\mathbb{R})$, the integral (6.2.5) is independent of the choice of parameters $n \geq 1$ and σ defining the almost-analytic extension \tilde{f} .

Proof.— For $f \in C_c^\infty(\mathbb{C})$, let us consider two almost analytic extensions \tilde{f}_1, \tilde{f}_2 of f , constructed with order $n_1 \geq 1$ and cutoff σ_1 (resp. $n_2 \geq 1, \sigma_2$). Assuming $n_1 \leq n_2$, the equation (6.2.2) shows that

$$\tilde{f}_2 - \tilde{f}_1(z) = \left(\sum_{r=0}^{n_1} f^{(r)}(x) \frac{(iy)^r}{r!} \right) [\sigma_2(z) - \sigma_1(z)] + \mathcal{O}(y^{n_1+1}).$$

The definitions of σ_1, σ_2 show that these two functions are equal to unity in the strip $\{|y| \leq 1\}$. As a result, we have

$$\tilde{f}_2 - \tilde{f}_1(z) = \mathcal{O}(y^{n_1+1}), \quad x \in \text{supp } f, |y| \leq 1.$$

Applying Lemma 6.2.3 to $F := \tilde{f}_2 - \tilde{f}_1$, we get the result. □

Let us now study some basic properties of the operator $f(T)$.

Lemma 6.2.5 Let $f \in C_c^\infty(\mathbb{R})$ with $\text{supp } f \cap \text{spec } T = \emptyset$, then $f(T) = 0$.

Proof.— If $f \in C_c^\infty(\mathbb{R})$, then automatically $\tilde{f} \in C_c^\infty(\mathbb{C})$. One can find a finite family of closed curves γ_r which enclose a domain U containing $\text{supp } \tilde{f}$, but with no intersection with $\text{spec}(T)$. Using an

extension of the Stokes formula to operator valued functions, we get

$$\begin{aligned} f(T) &= \frac{1}{\pi} \iint_U \frac{\partial \tilde{f}}{\partial \bar{z}} (T - z)^{-1} dx dy \\ &= \frac{1}{\pi} \iint_U \frac{\partial}{\partial \bar{z}} \left(\tilde{f}(z)(T - z)^{-1} \right) dx dy \\ &\stackrel{Stokes}{=} \sum_r \frac{1}{2\pi i} \oint_{\gamma_r} \tilde{f}(z) (T - z)^{-1} dz. \end{aligned}$$

Since \tilde{f} vanishes on γ_r , all the terms in the sum vanish. □

6.2.4 An algebra of smooth decaying functions

We will now extend the above calculus to an algebra of functions $\mathcal{A} \supset C_c^\infty(\mathbb{R})$, which are not compactly supported, but decay fast enough when $|x| \rightarrow \infty$. This algebra will have the advantage to contain the functions $r_w(\lambda) = (\lambda - w)^{-1}$ for $w \in \mathbb{C} \setminus \mathbb{R}$, which will be important below.

For $\beta < 0$ we denote by \mathcal{S}_β the set of smooth functions $f : \mathbb{R} \rightarrow \mathbb{C}$ satisfying the following estimates:

$$\forall n \in \mathbb{N}, \exists c_n > 0, \forall x \in \mathbb{R}, \quad |f^{(n)}(x)| \leq c_n \langle x \rangle^{\beta-n}.$$

(the constants $c_n > 0$ may depend on the function f). This set obviously forms a vector space of smooth functions.

We now define the class

$$\mathcal{A} := \bigcup_{\beta < 0} \mathcal{S}_\beta.$$

Applying recursively the Leibniz formula, one can show that \mathcal{A} forms an algebra of smooth functions. Moreover, if $f = P/Q$, where P and Q are polynomials with $\deg P < \deg Q$ and $Q(x) \neq 0$ for $x \in \mathbb{R}$, then $f \in \mathcal{A}$.

For any $n \geq 1$ we introduce the following norm on \mathcal{A} :

$$\|f\|_n := \sum_{r=0}^n \int_{\mathbb{R}} |f^{(r)}(x)| \langle x \rangle^{r-1} dx.$$

The above norms induce continuous embeddings $\mathcal{A} \rightarrow C_0(\mathbb{R})$. Moreover, one can prove that the space $C_c^\infty(\mathbb{R})$ is dense in \mathcal{A} , with respect to any norm $\|\cdot\|_n$.

Proposition 6.2.6 The functional calculus presented above for compactly supported smooth functions continuously extends to functions $f \in \mathcal{A}$. The operator $f(T)$ can then be defined by the same formula (6.2.5), and is independent of the choice of almost analytic extension \tilde{f} of f .

Proof.— For any function $f \in C_c^\infty(\mathbb{R})$ and an almost analytic extension \tilde{f} of order $n \geq 1$, an explicit computation using (6.2.3) and the support properties of σ and $\bar{\partial}\sigma$ leads to the bound

$$\begin{aligned} \|f(T)\| &\leq C \sum_{r=0}^n \int |f^{(r)}(x)| \left(\int_{\langle x \rangle \leq |y| \leq 2\langle x \rangle} \frac{|y|^{r-2}}{r!} dy \right) dx \\ &\quad + \int |f^{(n+1)}(x)| \left(\int_{|y| \leq 2\langle x \rangle} \frac{|y|^{n-1}}{n!} dy \right) dx \\ (6.2.6) \quad &\leq C \|f\|_{n+1}, \end{aligned}$$

with a constant $C > 0$ independent of the support of f , but depending on τ and n . Hence, for a family (f_j) of functions $f_j \in C_c^\infty$ converging to a function $f \in \mathcal{A}$ (in the sense that all the norms $\|f - f_j\|_k \xrightarrow{j \rightarrow \infty} 0$), we see that taking almost analytic extensions \tilde{f}_j of some common order $n \geq 1$, we find that the sequence of operators $(f_j(T))_{j \geq 1}$ is Cauchy in $\mathcal{L}(\mathcal{H})$. As a result, it converges to some bounded operator, which we call $f(T)$. An easy verification shows that $f(T)$ does not depend on the choice of approximating sequence (f_j) , and that this operator can be obtained by the integral (6.2.1), with \tilde{f} the analytic extension of f .

The direct inspection of the integrals defining $f_j(T)$ show that they converge to the same integral involving the function \tilde{f} , the latter integral being well defined. \square

Let us continue to study the operators $f(T)$ for $f \in \mathcal{A}$, making use of the fact that this space is an algebra.

Proposition 6.2.7 For $f, g \in \mathcal{A}$ one has $(fg)(T) = f(T)g(T)$.

Proof.— By the density argument, it is sufficient to consider the case $f, g \in C_c^\infty(\mathbb{R})$. Let K and L be large balls containing the supports of \tilde{f} and \tilde{g} respectively. Using the notation $w = u + iv$, $u, v \in \mathbb{R}$, one can write:

$$f(T)g(T) = \frac{1}{\pi^2} \int_{K \times L} \frac{\partial \tilde{f}}{\partial \bar{z}} \frac{\partial \tilde{g}}{\partial \bar{w}} (T - z)^{-1} (T - w)^{-1} dx dy du dv.$$

Using the resolvent identity

$$(T - z)^{-1} (T - w)^{-1} = \frac{1}{w - z} (T - w)^{-1} - \frac{1}{w - z} (T - z)^{-1}$$

we rewrite the preceding integral in the form

$$\begin{aligned} f(T)g(T) &= \frac{1}{\pi^2} \int_L \frac{\partial \tilde{g}}{\partial \bar{w}} (T - w)^{-1} \left(\int_K \frac{\partial \tilde{f}}{\partial \bar{z}} \frac{1}{w - z} dx dy \right) du dv \\ &\quad - \frac{1}{\pi^2} \int_K \frac{\partial \tilde{f}}{\partial \bar{z}} (T - z)^{-1} \left(\int_L \frac{\partial \tilde{g}}{\partial \bar{w}} \frac{1}{w - z} du dv \right) dx dy. \end{aligned}$$

By Lemma 6.2.2, we have

$$\int_K \frac{\partial \tilde{f}}{\partial \bar{z}} \frac{1}{w - z} dx dy = \pi f(w), \quad \int_L \frac{\partial \tilde{g}}{\partial \bar{w}} \frac{1}{w - z} du dv = -\pi g(z),$$

and we get

$$\begin{aligned}
f(T)g(T) &= \frac{1}{\pi} \int_L \tilde{f}(w) \frac{\partial \tilde{g}}{\partial \bar{w}} (T - w)^{-1} du dv + \frac{1}{\pi} \int_K \tilde{g}(z) \frac{\partial \tilde{f}}{\partial \bar{z}} (T - z)^{-1} dx dy \\
&= \frac{1}{\pi} \int_{K \cup L} \frac{\partial(\tilde{f}\tilde{g})}{\partial \bar{z}} (T - z)^{-1} dx dy \\
&= \frac{1}{\pi} \int_{\mathbb{C}} \frac{\partial(\widetilde{fg})}{\partial \bar{z}} (T - z)^{-1} dx dy + \frac{1}{\pi} \int_{\mathbb{C}} \frac{\partial(\tilde{f}\tilde{g} - \widetilde{fg})}{\partial \bar{z}} (T - z)^{-1} dx dy \\
&= (fg)(T) + \frac{1}{\pi} \int_{\mathbb{C}} \frac{\partial(\tilde{f}\tilde{g} - \widetilde{fg})}{\partial \bar{z}} (T - z)^{-1} dx dy.
\end{aligned}$$

By a direct calculation, one can see that $(\tilde{f}\tilde{g} - \widetilde{fg})(z) = O(y^2)$ for small y , so Lemma 6.2.3 shows that the second integral vanishes. \square

The following Lemma will allow to relate the operators $f(T)$ constructed above, to the most natural bounded operators we had already associated with T , namely its resolvent.

Lemma 6.2.8 Take any $w \in \mathbb{C} \setminus \mathbb{R}$. The the function $\lambda \in \mathbb{R} \mapsto r_w(\lambda) = (\lambda - w)^{-1}$ belongs to \mathcal{A} , and the corresponding quantization satisfies $r_w(T) = (T - w)^{-1}$.

Proof.— The fact that $r_w \in \mathcal{A}$ follows from our above remark on rational functions P/Q .

There remains to show that the operator $r_w(T)$ constructed from the HS formula actually coincides with the resolvent $(T - w)^{-1}$. We only provide the main line of the proof without technical details. Use first the independence of n and σ . We take $n = 1$ and put $\sigma(z) = \tau(My/\langle x \rangle)$ where $M > 0$ is sufficiently large, so that $w \notin \text{supp } \sigma$. Without loss of generality we assume $\text{Im } w > 0$. For large $m > 0$ consider the region

$$\Omega_m := \{z \in \mathbb{C} : |x| < m, \frac{\langle x \rangle}{m} < y < 2m\}.$$

Using the definition and the Stokes formula (since $(T - z)^{-1}$ is holomorphic on Ω_m), we have

$$r_w(T) = \lim_{m \rightarrow \infty} \frac{1}{\pi} \int_{\Omega_m} \frac{\partial \tilde{r}_w}{\partial \bar{z}} (T - z)^{-1} dx dy = \lim_{m \rightarrow \infty} \frac{1}{2\pi i} \oint_{\partial \Omega_m} \tilde{r}_w(z) (T - z)^{-1} dz.$$

Next, we want to estimate the difference

$$\oint_{\partial \Omega_m} \left(\tilde{r}_w(z) - r_w(z) \right) (T - z)^{-1} dz,$$

for large values of m . Let us first write down the explicit expression for $\tilde{r}_w(z)$:

$$\tilde{r}_w(z) = \frac{1 - \left(\frac{-iy}{x-w}\right)^{n+1}}{z - w} \sigma(x, y),$$

We see that for $m > 2M$, the integral on the bottom side of $\partial\Omega_m$ lies in region where $\sigma = 1$, so it can be bounded by:

$$\int_{-m}^m \frac{1}{|z-w|} \left(\frac{\langle x \rangle / m}{|x-w|} \right)^{n+1} \frac{m}{\langle x \rangle} \leq C_w \int_{-m}^m \frac{1}{\langle x \rangle} \left(\frac{\langle x \rangle / m}{\langle x \rangle} \right)^{n+1} \frac{m}{\langle x \rangle} \leq C_w C m^{-n}.$$

The integrals on the two vertical segments of $\partial\Omega_m$ are estimated by

$$\int_1^m \frac{1}{|m+iy-w|} \frac{1}{y} dy \leq C \frac{\log m}{m}.$$

Finally, the integral on the top side of $\partial\Omega_m$ is easily bounded by $\mathcal{O}(1/m)$. These estimates show that

$$\lim_{m \rightarrow \infty} \oint_{\partial\Omega_m} \left(\tilde{r}_w(z) - r_w(z) \right) (T-z)^{-1} dz = 0,$$

so we arrive at

$$r_w(T) = \frac{1}{2\pi i} \lim_{m \rightarrow \infty} \oint_{\partial\Omega_m} \frac{1}{z-w} (T-z)^{-1} dz.$$

For sufficiently large m one has the inclusion $w \in \Omega_m$. Since $z \mapsto (T-z)^{-1}$ is holomorphic in Ω_m , the Cauchy formula² implies that the above integral provides the value of $(T-z)^{-1}$ at the point $z = w$, namely $r_w(T) = (T-w)^{-1}$. \square

Let us now study the action of complex conjugation on $f \in \mathcal{A}$.

Lemma 6.2.9 For any $f \in \mathcal{A}$ we have:

- (a) $\bar{f}(T) = f(T)^*$,
- (b) $\|f(T)\| \leq \|f\|_\infty$.

Proof.— The item (a) follows directly from the equalities

$$\left((T-z)^{-1} \right)^* = (T-\bar{z})^{-1}, \quad \overline{\tilde{f}(z)} = \tilde{f}(\bar{z}).$$

To show the bound (b), take an arbitrary $c > \|f\|_\infty$ and define $g(s) := c - \sqrt{c^2 - |f(s)|^2}$. One can show that $g \in \mathcal{A}$. There holds $\bar{f}f - 2cg + g^2 = 0$, and using the preceding lemmas we obtain $f(T)^*f(T) - cg(T) - cg(T)^* + g(T)^*g(T) = 0$, therefore

$$f(T)^*f(T) + (c-g(T))^*(c-g(T)) = c^2.$$

Let $u \in \mathcal{H}$. Using the preceding equality we have:

$$\begin{aligned} \|f(T)u\|^2 &\leq \|f(T)u\|^2 + \|(c-g(T))u\|^2 \\ &= \langle u, f(T)^*f(T)u \rangle + \langle u, (c-g(T))^*(c-g(T))u \rangle \\ &= c^2\|u\|^2. \end{aligned}$$

2. To verify that the Cauchy formula holds as well for operator valued functions, one may compute, for any $u, v \in \mathcal{H}$, the bracket $\langle u, r_w(T)v \rangle$.

As $c > \|f\|_\infty$ was arbitrary, this concludes the proof. \square

Notice how the estimate (b) strengthens the norm estimates (6.2.6) we had obtained above: the higher derivatives $f^{(r)}$ entering in the norms $\|f\|_n$ are actually irrelevant to bound $\|f(T)\|$, which only depends on the sup-norm of f . This remark will allow us to extend the calculus from the algebra \mathcal{A} to the space $C_0(\mathbb{R})$ of *continuous* functions decaying to zero at infinity.

Theorem 6.2.10 (Continuous functional calculus) Let T be a self-adjoint operator in a Hilbert space \mathcal{H} . There exists a unique linear map

$$C_0(\mathbb{R}) \ni f \mapsto f(T) \in \mathcal{L}(\mathcal{H})$$

with the following properties:

- $f \mapsto f(T)$ is an algebra homomorphism,
- $\overline{f}(T) = f(T)^*$,
- $\|f(T)\| \leq \|f\|_\infty$,
- if $w \notin \mathbb{R}$ and $r_w(s) = (s - w)^{-1}$, then $r_w(T) = (T - w)^{-1}$,
- if $\text{supp } f$ does not meet $\text{spec } T$, then $f(T) = 0$.

Proof.— Existence. If one replaces C_0 by \mathcal{A} , everything is already proved. But \mathcal{A} is dense in $C_0(\mathbb{R})$ w.r.t. the sup-norm, because $C_c^\infty(\mathbb{R}) \subset \mathcal{A}$, so the same type of density argument as in the proof of Prop. 6.2.6 leads to the construction of $f(T)$ for $f \in C_0(\mathbb{R})$.

Uniqueness. If we have two such maps, they coincide on the functions f which are linear combinations of r_w , $w \in \mathbb{C} \setminus \mathbb{R}$. But such functions are dense in C_0 by the Stone-Weierstrass theorem, so, again using the density argument, both maps coincide on C_0 . \square

Remark 6.2.11 ▪ One may wonder why to introduce the class of functions \mathcal{A} : one could just start by C_c^∞ which is also dense in C_0 . The reason is that, if $f \in C_c^\infty$, we have no operator of reference to compare with $f(T)$. On the other hand, it is naturally expected that for $r_w(\lambda) = (\lambda - w)^{-1}$ we should have $r_w(T) = (T - w)^{-1}$. So it is important to have an explicit formula for a sufficiently large class of functions containing all such r_w .

- The approach based on the Helffer-Sjöstrand formula, which is presented here, allows one to consider bounded and unbounded selfadjoint operators at once. The same results can be obtained by other methods, starting e.g. with polynomial functions of bounded operators instead of resolvents, see for example, Sections VII.1 and VIII.3 in the book [7].

6.3 Borelian functional calculus and L^2 representation

Now we would like to extend the functional calculus to more general functions, not necessarily continuous and not necessarily vanishing at infinity. To do this, we will invoke a duality argument.

Definition 6.3.1 (Invariant and cyclic subspaces) Let \mathcal{H} be a Hilbert space, L be a closed linear subspace of \mathcal{H} , and T be a self-adjoint linear operator in \mathcal{H} .

Assume T to be bounded. We say that L is an *invariant subspace* of T (or just T -invariant) if $T(L) \subset L$. We say that L is a *cyclic subspace* of T with cyclic vector v if L coincides with the closed linear hull of all vectors $p(T)v$, where p are polynomials.

Let now T be general, possibly unbounded. We say that L is an *invariant subspace* of T (or just T -invariant) if $(T - z)^{-1}(L) \subset L$ for all $z \notin \mathbb{R}$. We say that L is a *cyclic subspace* of T with cyclic vector v if L coincides with the closed linear space of all vectors $(T - z)^{-1}v$ with $z \notin \mathbb{R}$.

From the selfadjointness of T , if L is T -invariant, then L^\perp is also T -invariant.

Proposition 6.3.2 Both definitions of an invariant/cyclic subspace are equivalent for bounded selfadjoint operators.

Proof.— Let $T = T^* \in \mathcal{L}(\mathcal{H})$. We note first that $\text{res } T$ is a connected set.

Let a closed subspace L be T -invariant in the sense of the definition for bounded operators. If $z \in \mathbb{C}$ and $|z| > \|T\|$, then $z \notin \text{spec } T$ and

$$(T - z)^{-1} = -z \left(1 - \frac{T}{z}\right)^{-1} = -\sum_{n=0}^{\infty} z^{-n-1} T^n.$$

If $u \in L$, then $T^n u \in L$ for any n . As the series on the right hand side converges in the operator norm sense and as L is closed, $(T - z)^{-1}u$ belongs to L .

Let us denote $W = \{z \in \text{res } T : (T - z)^{-1}(L) \subset L\}$. As just shown, W is non-empty. On the other hand, W is closed in $\text{res } T$ in the relative topology: if $u \in L$, $z_n \in W$ and z_n converge to $z \in \text{res}(T)$, then $(T - z_n)^{-1}u \in L$ and $(T - z_n)^{-1}u$ converge to $(T - z)^{-1}u$, so the latter belongs to L ; as a result, $z \in W$. On the other hand, W is open: if $z_0 \in W$ and $|z - z_0|$ is sufficiently small, then

$$(T - z)^{-1} = \sum_{n=0}^{\infty} (z - z_0)^n (T - z_0)^{-n-1},$$

see (4.1.4), and $(T - z)^{-1}L \subset L$. Therefore, $W = \text{res } T$, which shows that L is T -invariant in the sense of the definition for general operators.

Now let $T = T^* \in \mathcal{L}(\mathcal{H})$, and assume that L is T -invariant in the sense of the definition for general operators, i.e. $(T - z)^{-1}(L) \subset L$ for any $z \notin \mathbb{R}$. Pick any $z \notin \mathbb{R}$ and any $u \in L$. We can represent $Tu = v_L + v_\perp$, where $v_L \in L$ and $v_\perp \in L^\perp$ are uniquely defined vectors. As L^\perp is T -invariant, $(T - z)^{-1}v_\perp \in L^\perp$. On the other hand

$$\begin{aligned} (T - z)^{-1}v_\perp &= (T - z)^{-1}(Tu - v_L) \\ &= (T - z)^{-1}((T - z)u + zu - v_L) \\ &= u + (T - z)^{-1}(zu - v_L). \end{aligned}$$

As $zu - v_\perp \in L$, both vectors on the right-hand side are in L . Therefore, $(T - z)^{-1}v_\perp \in L$, so that $(T - z)^{-1}v_\perp = 0$ and finally $v_\perp = 0$, which shows that $Tu = v_L \in L$. The equivalence of the two definitions of an invariant subspace is proved.

On the other hand, for both definitions, L is T -cyclic with cyclic vector v iff L is the smallest T -invariant subspace containing v . Therefore, both definitions of a cyclic subspace also coincide for bounded selfadjoint operators. \square

6.3.1 Spectral representation, cyclic case

Theorem 6.3.3 (Representation by a multiplication operator (cyclic case)) Let T be a self-adjoint linear operator in \mathcal{H} and let $S := \text{spec}(T)$. Assume that \mathcal{H} is a cyclic subspace for T with a cyclic vector v .

Then there exists a finite measure μ on S with $\mu(S) \leq \|v\|^2$ and a unitary map $U : \mathcal{H} \rightarrow L^2(S, d\mu)$ with the following properties:

- a vector $x \in \mathcal{H}$ is in $D(T)$ iff $hUx \in L^2(S, d\mu)$, where h is the function on S given by $h(s) = s$,
- for any $\psi \in U(D(T))$, there holds $UTU^{-1}\psi = h\psi$.

In other words, T is unitarily equivalent to the operator M_h of the multiplication by h in $L^2(S, d\mu)$.

Proof.— Step 1. We recall that we know how to construct the operator $f(T)$ for functions $f \in C_0(\mathbb{R})$. Consider the map $\phi : C_0(\mathbb{R}) \rightarrow \mathbb{C}$ defined by $\phi(f) = \langle v, f(T)v \rangle$, where v is our cyclic vector. Let us list the properties of this map:

- ϕ is linear,
- $\phi(\bar{f}) = \overline{\phi(f)}$,

- if $f \geq 0$, then $\phi(f) \geq 0$. This follows from

$$\phi(f) = \langle v, f(T)v \rangle = \langle v, \sqrt{f}(T)\sqrt{f}(T)v \rangle = \|\sqrt{f}(T)v\|^2.$$

- $|\phi(f)| \leq \|f\|_\infty \|v\|^2$.

By the Riesz representation theorem there exists a unique regular Borel measure μ on \mathbb{R} such that

$$\phi(f) = \int_{\mathbb{R}} f d\mu \quad \text{for all } f \in C_0(\mathbb{R}).$$

Moreover, for $\text{supp } f \cap S = \emptyset$ we have $f(T) = 0$ hence $\phi(f) = 0$, which implies that $\text{supp } \mu \subset S$. We can thus write

$$(6.3.7) \quad \langle v, f(T)v \rangle = \int_S f d\mu \quad \text{for all } f \in C_0(\mathbb{R}).$$

Step 2. For any function $f \in C_0(\mathbb{R})$, its restriction to S identifies to an element of $L^2(S, d\mu)$. We then have

$$\begin{aligned} \langle f|_S, g|_S \rangle_{L^2(S, \mu)} &= \int_S \bar{f}g d\mu = \phi(\bar{f}g) \\ &= \langle v, f(T)^*g(T)v \rangle_{\mathcal{H}} = \langle f(T)v, g(T)v \rangle_{\mathcal{H}}. \end{aligned}$$

Denote the space $\mathcal{M} := \{f(T)v : f \in C_0(\mathbb{R})\} \subset \mathcal{H}$, then the preceding equality means that the map

$$U^* : C_0(\mathbb{R}) \subset L^2(S, d\mu) \mapsto \mathcal{M} \subset \mathcal{H}, \quad U^*f|_S = f(T)v$$

is isometric, hence injective. By definition of \mathcal{M} , it is also surjective. Moreover, \mathcal{M} is dense in \mathcal{H} , because v is a cyclic vector. Furthermore, since μ is regular, $C_0(\mathbb{R})$ is a dense subspace of $L^2(S, d\mu)$. Therefore, U^* can be uniquely extended to a unitary map from $L^2(S, d\mu)$ to \mathcal{H} . We keep denoting this extension by the same symbol U^* , and call its inverse $U : \mathcal{H} \rightarrow L^2(S, \mu)$, which is also unitary.

Step 3. Let $f, f_j \in C_0(\mathbb{R})$ and $\psi_j := f_j(T)v$, $j = 1, 2$. There holds

$$\begin{aligned} \langle \psi_1, f(T)\psi_2 \rangle &= \langle f_1(T)v, f(T)f_2(T)v \rangle \\ &= \langle v, (\bar{f}_1 f f_2)(T)v \rangle \\ &= \int_S \bar{f}_1 f f_2 d\mu \\ &= \langle U\psi_1, M_f U\psi_2 \rangle, \end{aligned}$$

where M_f is the operator of the multiplication by f in $L^2(S, d\mu)$. In particular, for any $w \notin \mathbb{R}$ and $r_w(s) = (s - w)^{-1}$ we obtain

$$U r_w(T) U^* \xi = M_{r_w} \xi \quad \text{for all } \xi \in L^2(S, d\mu).$$

The operator U maps the set $\text{Ran } r_w(T) \equiv D(T)$ to the range of M_{r_w} . In other words, U is a bijection from $D(T)$ to

$$\text{Ran } M_{r_w} = \{\phi \in L^2(S, d\mu) : h\phi \in L^2(S, d\mu)\} = D(M_h).$$

Therefore, if $\xi \in L^2(S, d\mu)$, then $\psi := r_w \xi \in D(M_h)$,

$$Tr_w(T)U^*\xi = (T - w)r_w(T)U^*\xi + wr_w(T)U^*\xi = U^*\xi + wr_w(T)U^*\xi$$

and, finally,

$$UTU^*\psi = UTU^*r_w\xi = UTTr_w(T)U^*\xi = U(U^*\xi + wr_w(T)U^*\xi) = \xi + wr_w\xi = h\psi.$$

□

6.3.2 Spectral representation, general case

We may now get rid of the assumption that \mathcal{H} admits a cyclic vector.

Theorem 6.3.4 (L^2 representation, noncyclic case) Let T be a self-adjoint operator on a Hilbert space \mathcal{H} with $\text{spec } T =: S$. Then there exists $N \subset \mathbb{N}$, a finite measure μ on $S \times N$ and a unitary operator $U : \mathcal{H} \rightarrow L^2(S \times N, d\mu)$ with the following properties.

- Let $h : S \times N \rightarrow \mathbb{R}$ be given by $h(s, n) = s$ for each $n \in N$. A vector $u \in \mathcal{H}$ belongs to $D(T)$ iff $hUu \in L^2(S \times N, d\mu)$,
- for any $\xi \in U(D(T))$ there holds $UTU^*\xi = M_h\xi$.

$S \times N$ can be viewed as the union of $\#N$ copies of S . The set N can be taken to be an interval $\{1, \dots, n_0\}$ for $n_0 \in \mathbb{N}^* \cup \infty$. **Proof.**— Using an induction argument, one can find a finite or countable subset $N \subset \mathbb{N}$ and nonempty closed mutually orthogonal subspaces $\mathcal{H}_n \subset \mathcal{H}$ with the following properties:

- $\mathcal{H} = \bigoplus_{n \in N} \mathcal{H}_n$,
- each \mathcal{H}_n is a cyclic subspace of T with cyclic vector v_n satisfying $\|v_n\| \leq 2^{-n}$.

The restriction T_n of T to \mathcal{H}_n is a self-adjoint operator on \mathcal{H}_n , and one can apply to all these operators the preceding Thm 6.3.3, which gives associated measures μ_n on the n -th copy of S , with $\mu_n(S) \leq 4^{-n}$, and unitary maps $U_n : \mathcal{H}_n \rightarrow L^2(S, d\mu_n)$. Now one can define a global measure μ on $S \times N$ by $\mu(\Omega \times \{n\}) = \mu_n(\Omega)$, and a unitary map

$$U : \mathcal{H} \equiv \bigoplus_{n \in N} \mathcal{H}_n \rightarrow L^2(S \times N, d\mu) \equiv \bigoplus_{n \in N} L^2(S, d\mu_n)$$

by $U(\psi_n) = (U_n\psi_n)$. One can easily check that all the required properties are verified. □

Remark 6.3.5 ▪ The previous theorem shows that any self-adjoint operator is unitarily equivalent to a multiplication operator on some L^2 space. This multiplication operator is sometimes called a *spectral representation* of T . This representation is not unique, because the decomposition of \mathcal{H} into cyclic subspaces is not unique.

- The cardinality of the set N is not unique either. The minimal cardinality among all possible N is called the *spectral multiplicity* of T , and it generalizes the notion of multiplicity for eigenvalues. Calculating the spectral multiplicity for a selfadjoint operator T is not easy.

The last Thm 6.3.4 can be used to generalize the functional calculus of Thm 6.2.10, from function $f \in C_0(\mathbb{R})$ to a more general class of functions. In the rest of the section we use the function h and the measure μ from Theorem 6.3.4 without further specification.

Definition 6.3.6 (Bounded Borelian functions) Let \mathcal{B}_∞ be the space of bounded Borelian functions $f : \mathbb{R} \rightarrow \mathbb{C}$. We equip this space with the following topology: we say that a sequence $(f_n \in \mathcal{B}_\infty)_{n \in \mathbb{N}}$ converges to $f \in \mathcal{B}_\infty$, and write $f_n \xrightarrow{\mathcal{B}_\infty} f$, if the two following conditions hold:

- there exists a uniform $C > 0$ such that for any $n \in \mathbb{N}$, $\sup_s |f_n(s)| \leq C$;
- $f_n(s) \rightarrow f(s)$ for all $s \in \mathbb{R}$ (simple convergence).

This topology on \mathcal{B}_∞ will be the “symbolic version” of the following topology on the space of bounded operators.

Definition 6.3.7 (Strong convergence) We say that a sequence $A_n \in \mathcal{L}(\mathcal{H})$ *strongly converges* to $A \in \mathcal{L}(\mathcal{H})$, and write $A = s - \lim_{n \rightarrow \infty} A_n$, if $Au = \lim_{n \rightarrow \infty} A_n u$ for any $u \in \mathcal{H}$. In general, this notion of convergence is weaker than the convergence in the topology of $\mathcal{L}(\mathcal{H})$.

We are now in position to construct a functional calculus of our selfadjoint operator T for functions $f \in \mathcal{B}_\infty$.

Theorem 6.3.8 (Borel functional calculus) (a) Let T be a selfadjoint operator on a Hilbert space \mathcal{H} . There exists a map $\mathcal{B}_\infty \ni f \mapsto f(T) \in \mathcal{L}(\mathcal{H})$ extending the map from Theorem 6.2.10, and satisfying the same properties, except that the estimate $\|f(T)\| \leq \|f\|_\infty$ can be improved to $\|f(T)\| \leq \sup_{s \in S} |f(s)|$ (we recall that $S = \text{spec}(T)$).

- (b) This extension is unique if we further assume the property that $f_n \xrightarrow{\mathcal{B}_\infty} f$ implies $f(T) = s - \lim f_n(T)$.

Proof.— Consider the unitary map U from Theorem 6.2.10. For $f \in \mathcal{B}_\infty$, let us define

$$f(T) := U^* M_{f \circ h} U.$$

One easily checks that all the properties stated in Theorem 6.2.10 hold, so this extension satisfies (a).

To prove (b) we remark that the map just defined satisfies the requested condition: if $\xi \in L^2(S, d\mu)$ and $f_n \xrightarrow{\mathcal{B}_\infty} f$, then the theorem of dominated convergence shows that $f_n \circ h\xi$ converges to $f \circ h\xi$ in $L^2(S \times N, d\mu)$. Through the conjugacy by U , this exactly means that $f(T) = s\text{-}\lim_{n \rightarrow \infty} f_n(T)$.

On the other hand, $C_0(\mathbb{R})$ is dense in \mathcal{B}_∞ , so any $f(T)$ can also be defined as the strong limit of operators $f_n(T)$ with $f_n \in C_0(\mathbb{R})$; this makes the extension unique. \square The unitary conjugacy of T with a multiplication operator leads us to straightforward, yet important corollaries. Their proofs are elementary modifications of the constructions given for the multiplication operator in Example 4.2.14.

Corollary 6.3.9 \blacksquare $\text{spec } T = \text{ess}_\mu \text{Ran } h$.

- \blacksquare for any $f \in \mathcal{B}_\infty$ one has $\text{spec } f(T) = \text{ess}_\mu \text{Ran } f \circ h$,
- \blacksquare in particular, $\|f(T)\| = \text{ess}_\mu \sup |f \circ h|$.

Remark 6.3.10 One can also define operators $f(T)$ with *unbounded*, locally bounded Borel functions f by $\varphi(T) = U^* M_{f \circ h} U$. These operators may be unbounded (depending on the measure μ), but they are selfadjoint for real valued f : this follows from the selfadjointness of the multiplication operator $M_{f \circ h}$, on its natural domain.

Example 6.3.11 The usual Fourier transform on \mathbb{R} is a classical example of a spectral representation. For example, Take $\mathcal{H} = L^2(\mathbb{R}, dx)$ and $T_0 = -id/dx$ with the natural domain $D(T_0) = H^1(\mathbb{R}, dx)$. If \mathcal{F} is the Fourier transform, then $\mathcal{F}T_0\mathcal{F}^*$ is exactly the operator of multiplication M_x on $L^2(\mathbb{R}, dx)$, hence $S = \text{spec } T_0 = \text{spec } M_x = \mathbb{R}$. So \mathcal{F} is a unitary operator which maps T_0 to a multiplication operator.

For bounded Borel functions $f : \mathbb{R} \rightarrow \mathbb{C}$, one can define the operator $f(T_0)$ by $f(T_0) = \mathcal{F}^* M_f \mathcal{F}$, where M_f is the operator of multiplication by f . Such operator $f(T_0)$ is called a *Fourier multiplier*, it is a particular case of a pseudodifferential operator.

Let us look at some particular examples. Consider the translation operator A on \mathcal{H} which is defined by $Au(x) = u(x+1)$. It is a bounded operator, and for any $v \in \mathcal{S}(\mathbb{R})$ we have $\mathcal{F}A\mathcal{F}^*v(p) = e^{ip}v(p)$. This means that $A = e^{iT_0}$, and this gives the relation $\text{spec } A = \{z : |z| = 1\}$.

One may also look at the operator B defined by

$$Bu(x) = \int_{x-1}^{x+1} u(t) dt.$$

Using the Fourier transform one can show that $B = f(T_0)$, where $f(x) = 2 \sin x/x$. As a consequence, $\text{spec } B = \overline{f(\mathbb{R})} = [2 \frac{\sin x_1}{x_1}, 2]$, where $x_1 \in]\pi, 2\pi[$ is the first nontrivial root of the equation $\tan x = x$.

6.3.3 Generalized spectral representation

For practical computations, one does not need the canonical representation from Thm 6.3.4 to construct the Borel functional calculus. It is sufficient to represent T as $T = U^*M_\varphi U$, where $U : \mathcal{H} \rightarrow L^2(X, d\mu)$ for *some* topological space X , μ a regular finite measure on X , M_h the multiplication operator by *some* function $h : X \rightarrow \mathbb{R}$. Then for any bounded Borel function f on \mathbb{R} , one can define $f(T) = U^*M_{f \circ h}U$.

Example 6.3.12 For example, for the free Laplacian $T = -\Delta$ on $\mathcal{H} = L^2(\mathbb{R}^d)$ the above is realized with $X = \mathbb{R}^d$, U being the d -dimensional Fourier transform, and $h(p) = p^2$ for all momenta $p \in \mathbb{R}^d$. This means that the operators $f(T)$ act by

$$f(T)u(x) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} f(p^2) \hat{u}(p) e^{ipx} dx,$$

namely they are Fourier multipliers with symbol $p \mapsto f(p^2)$. For example, the operator

$$\sqrt{-\Delta + 1}u(x) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \sqrt{1 + p^2} \hat{u}(p) e^{ipx} dx.$$

From this expression, one can easily show that $D(\sqrt{-\Delta + 1}) = H^1(\mathbb{R}^d)$.

Example 6.3.13 Another classical example is provided by the Fourier series. Take $\mathcal{H} = \ell^2(\mathbb{Z}^d)$ and let a function $t : \mathbb{Z}^d \rightarrow \mathbb{R}$ satisfy $t(-m) = t(m)$ and $|t(m)| \leq c_1 e^{-c_2|m|}$ with some $c_1, c_2 > 0$. Define T by

$$Tu(m) = \sum_{n \in \mathbb{Z}^d} t(m - n)u(n).$$

One can easily see that T is bounded. If one introduces the unitary map $\Phi : \mathcal{H} \rightarrow L^2(\mathbb{T}^d)$, $\mathbb{T} := \mathbb{R}/\mathbb{Z}$,

$$\Phi u(x) = \sum_{m \in \mathbb{Z}^d} e^{2\pi i m \cdot x} u(m), \quad \text{where } m \cdot x := m_1 x_1 + \cdots + m_d x_d,$$

then $T = \Phi^* M_h \Phi$ where

$$h(x) = \sum_{m \in \mathbb{Z}^d} t(m) e^{2\pi i m x}$$

is the Fourier series with coefficients $(t(m))_{m \in \mathbb{Z}^d}$.

Example 6.3.14 A less obvious example is given by the Neumann Laplacian T_N on the half-line, defined in Example 3.1.12.

Let T be the free Laplacian on $L^2(\mathbb{R})$, with domain $D(T) = H^2(\mathbb{R})$. Denote by $\mathcal{G} := L^2_e(\mathbb{R})$ the subspace of $L^2(\mathbb{R})$ consisting of the even functions. Clearly, \mathcal{G} is an invariant subspace for $(T, D(T))$ (the second derivative of an even function is also an even function), and the restriction of T to \mathcal{G} , with domain $\mathcal{G} \cap D(T)$, is a self-adjoint operator. Let us denote this restriction by $(A, D(A))$. Introduce now the a map $\Phi : L^2(\mathbb{R}_+) \rightarrow \mathcal{G}$ by $\Phi u(x) = 2^{-1/2} u(|x|)$. One easily checks that Φ is unitary, and that $D(A) = \Phi(D(T_N))$.

We notice that the space \mathcal{G} is also invariant through the Fourier transform \mathcal{F} (the Fourier transform of an even function is also an even function). So we have the two conjugacies $T_N = \Phi^* A \Phi$ and $A = \mathcal{F}^* \tilde{M}_\varphi \mathcal{F}$, where \tilde{M}_φ is the multiplication by the function $h(p) = p^2$ on \mathcal{G} . Finally, $\tilde{M}_h = \Phi M_h \Phi^*$, where M_h is the multiplication by h on $L^2(\mathbb{R}_+)$.

Finally, we obtain $T_N = U^* M_h U$ with $U = \Phi^* \mathcal{F} \Phi$, and U is unitary as composition of three unitary operators. By a direct calculation, for $u \in L^2(\mathbb{R}_+) \cap L^1(\mathbb{R}_+)$ one has

$$Uu(p) = \sqrt{\frac{2}{\pi}} \int_0^\infty \cos(px) u(x) dx.$$

This transform U is sometimes called the cosine transform. Roughly speaking, U is the Fourier transform restricted to the even functions, together with some identifications.

An interested reader may adapt the preceding constructions to the Dirichlet Laplacian T_D on the half-line, see Example 3.1.13.

Example 6.3.15 [Operators with compact resolvents] Let us fill the gap which was left open in section 5.5. Namely let us show that if a selfadjoint operator T has a compact resolvent, then $\text{spec } T \neq \mathbb{R}$.

Assume *ab absurdo* that $\text{spec } T = \mathbb{R}$ and consider the function g given by $g(x) = (x - i)^{-1}$. Then $g(T) = (T - i)^{-1}$ is a compact operator, and its spectrum has at one accumulation point, namely the origin.

On the other hand, using Corollary 6.3.9 and the continuity of g , one gets the equality $\text{spec } g(T) = \overline{g(\text{spec } T)} = \overline{g(\mathbb{R})}$; this set is a continuous curve in \mathbb{C} , which has infinitely many accumulation points. Therefore we get a contradiction

6.4 Some applications of the spectral theorem

In this chapter we discuss some direct applications of the spectral theorem to the estimates of the spectra of self-adjoint operators. We still use without special notification the measure μ and the function h from Theorem 6.3.4, or from the generalization of subsection 6.3.3. An important fact is that we will not need a precise description of the spectral measure μ to obtain the following applications: we will just use the fact that our selfadjoint operator is conjugate to some multiplication operator on some L^2 space.

Theorem 6.4.1 (Distance to spectrum) Let T be a self-adjoint operator in a Hilbert space \mathcal{H} , and $0 \neq u \in D(T)$, then for any $z \in \mathbb{C}$ one has the estimate

$$\text{dist}(z, \text{spec } T) \leq \frac{\|(T - z)u\|}{\|u\|}.$$

More precisely, if $z \notin \text{spec } T$, one has the equality

$$\|(T - z)^{-1}\| = \frac{1}{\text{dist}(z, \text{spec } T)}.$$

We notice that this equality improves the estimate $\|(T - z)^{-1}\| \leq \frac{1}{|\operatorname{Im} z|}$ for $z \in \mathbb{C} \setminus \mathbb{R}$. **Proof.**— If $z \in \operatorname{spec} T$, then the left-hand side is zero, and the inequality is obvious. Assume now that $z \notin \operatorname{spec} T$. By Corollary 6.3.9, one has, with $r_z(\lambda) = (\lambda - z)^{-1}$:

$$\|(T - z)^{-1}\| = \operatorname{ess}_\mu \sup |r_z \circ h| = \frac{1}{\operatorname{ess}_\mu \inf |\lambda - z|} = \frac{1}{\operatorname{dist}(z, \operatorname{spec} T)},$$

which gives for any $u \in \mathcal{H}$:

$$\|u\| = \|(T - z)^{-1}(T - z)u\| \leq \frac{1}{\operatorname{dist}(z, \operatorname{spec} T)} \|(T - z)u\|.$$

□

Remark 6.4.2 The previous theorem is one of the basic tools to approximately identify the spectrum of a selfadjoint operator. It is important to understand that the resolvent estimate obtained in Theorem 6.4.1 uses in an essential way the selfadjointness of the operator T . For nonself-adjoint operators the estimate fails even in the finite-dimensional case. For example, take $\mathcal{H} = \mathbb{C}^2$ and

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

then $\operatorname{spec} T = \{0\}$, and for $z \neq 0$ we have

$$(T - z)^{-1} = -\frac{1}{z^2} \begin{pmatrix} z & 1 \\ 0 & z \end{pmatrix}.$$

For the vectors $e_1 = (1, 0)$ and $e_2 = (0, 1)$ one has $\langle e_1, (T - z)^{-1}e_2 \rangle = -z^{-2}$. This shows that $\|(T - z)^{-1}\| \geq |z|^{-2}$, which is larger than $|z|^{-1}$ when $|z| < 1$.

In the infinite dimensional case, one can construct examples with $\|(T - z)^{-1}\| \sim \operatorname{dist}(z, \operatorname{spec} T)^{-n}$ for any power n .

6.4.1 Spectral projectors of selfadjoint operators

We now consider the main application of the Borelian functional calculus, namely the construction of spectral projectors of general selfadjoint operators. These projectors will provide an intrinsic spectral representation of T , independent of the choices of cyclic vectors we had to do in Thm 6.3.4, generalizing the spectral decomposition

$$T = \sum_{j \geq 1} \lambda_j \Pi_{\lambda_j}$$

for a selfadjoint operator with purely discrete spectrum $(\lambda_j)_{j \geq 1}$.

Definition 6.4.3 (Spectral projectors) Let T be a self-adjoint operator on a Hilbert space \mathcal{H} and $\Omega \subset \mathbb{R}$ be a Borel subset. The *spectral projector* of T on Ω is the operator $\Pi_\Omega := \mathbb{1}_\Omega(T)$, where $\mathbb{1}_\Omega$ is the characteristic function on Ω (this function obviously belongs to \mathcal{B}_∞).

The following proposition summarizes the most important properties of the spectral projectors.

Proposition 6.4.4 The spectral projectors $(\Pi_\Omega)_\Omega$ associated with a selfadjoint operator satisfy the following properties:

- i) for any Borel subset $\Omega \subset \mathbb{R}$, the associated spectral projection Π_Ω is an orthogonal projector commuting with T . In particular, $\Pi_\Omega D(T) \subset D(T)$.
- ii) $\Pi_{(a,b)} = 0$ if and only if $\text{spec } T \cap (a, b) = \emptyset$.
- iii) for any $\lambda \in \mathbb{R}$ there holds $\text{Ran } \Pi_{\{\lambda\}} = \text{Ker}(T - \lambda)$, and $u \in \text{Ker}(T - \lambda)$ iff $u = \Pi_{\{\lambda\}}u$.
- iv) $\text{spec } T = \{\lambda \in \mathbb{R} : \Pi_{(\lambda-\epsilon, \lambda+\epsilon)} \neq 0 \text{ for all } \epsilon > 0\}$.

Proof.— The proof uses the unitary conjugacy of T with the multiplication by h on $L^2(X, \mu)$, and the simultaneous conjugacy of Π_Ω with the multiplication by $\mathbb{1}_\Omega \circ h$.

To prove (1) we remark that $\mathbb{1}_\Omega^2 = \mathbb{1}_\Omega$ and $\mathbb{1}_\Omega = \overline{\mathbb{1}_\Omega}$, which yields $\Pi_\Omega^2 = \Pi_\Omega$ and $\Pi_\Omega = \Pi_\Omega^*$: this shows that Π_Ω is an orthogonal projector. The commutativity with T is a general property of all operators $f(T)$ for any $f \in \mathcal{B}_\infty$. After conjugacy by U , we remember that $D(T)$ corresponds to $D(M_h) \subset L^2(X, \mu)$. Now, $\xi \in D(M_h)$ iff $h\xi \in L^2$, and from the boundedness of f , we then also have

$$h(f \circ h)\xi = (f \circ h)h\xi \in L^2(X, \mu),$$

showing that $M_{f \circ h}$ preserves $D(M_h)$, and that it commutes with M_h .

To prove (2) we note that the condition $\Pi_{(a,b)} = 0$ is, by definition, equivalent to $\mathbb{1}_{(a,b)} \circ h = 0$ μ -a.e., which in turn means that $(a, b) \cap \text{ess}_\mu \text{Ran } h = \emptyset$. It remains to recall that $\text{ess}_\mu \text{Ran } h = \text{spec } T$, see Corollary 6.3.9.

The items (3) and (4) are drawn from the characterization of the point spectrum, resp. spectrum, of a multiplication operator, see Prop. 4.2.14. □

The spectral projectors were defined after we constructed the full \mathcal{B}_∞ functional calculus. For elementary subsets $\Omega \subset \mathbb{R}$, one can obtain more direct expressions of Π_Ω using our ubiquitous resolvent operators.

Proposition 6.4.5 (Spectral projection to a singleton) For any $\lambda \in \mathbb{R}$, the spectral projector to the singleton $\{\lambda\}$ (namely, the eigenspace of T for the value λ) can be computed as the following limit:

$$\Pi_{\{\lambda\}} = \text{s-}\lim_{\epsilon \rightarrow 0^+} -i\epsilon(T - \lambda - i\epsilon)^{-1}.$$

Proof.— For $\epsilon > 0$ consider the function $f_\epsilon : \mathbb{R} \rightarrow \mathbb{C}$

$$f_\epsilon(x) := -\frac{i\epsilon}{x - \lambda - i\epsilon} = -i\epsilon r_{\lambda+i\epsilon}$$

It satisfies the following properties:

- $|f_\epsilon| \leq 1$,
- $f_\epsilon(\lambda) = 1$,
- if $x \neq \lambda$, then $f_\epsilon(x) \xrightarrow[\epsilon \searrow 0]{0}$.

Altogether, this means that $f_\epsilon \xrightarrow{\mathcal{B}_\infty} \mathbb{1}_{\{\lambda\}}$. By Thm 6.3.8, $\Pi_{\{\lambda\}} = \text{s-}\lim_{\epsilon \searrow 0} f_\epsilon(T)$, and it remains to note that $f_\epsilon(T) = -i\epsilon(T - \lambda - i\epsilon)^{-1}$ by Theorem 6.2.10. \square

Proposition 6.4.6 (Stone's formula) For $a < b$ one has:

$$\Pi_{(a,b)} + \frac{1}{2}\Pi_{\{a,b\}} = \text{Im} \frac{1}{\pi} \text{s-}\lim_{\epsilon \searrow 0} \int_a^b (T - \lambda - i\epsilon)^{-1} d\lambda = \frac{1}{\pi} \text{s-}\lim_{\epsilon \searrow 0} \int_a^b \text{Im} (T - \lambda - i\epsilon)^{-1} d\lambda$$

where we recall the notation for bounded operators $\text{Im} A = \frac{1}{2i}(A - A^*)$.

The left hand side means that the contribution of the boundary points $\{a, b\}$ to the projector is halved. **Proof.**— For $\epsilon > 0$, consider the function

$$f_\epsilon(x) = \frac{1}{\pi} \int_a^b \text{Im} \frac{1}{x - \lambda - i\epsilon} d\lambda.$$

By direct computation, we find

$$f_\epsilon(x) = \frac{1}{\pi} \int_a^b \frac{\epsilon}{(\lambda - x)^2 + \epsilon^2} d\lambda = \frac{1}{\pi} \left(\arctan \frac{b-x}{\epsilon} - \arctan \frac{a-x}{\epsilon} \right).$$

Therefore, $|f_\epsilon| \leq 1$, and

$$\lim_{\epsilon \rightarrow 0^+} f_\epsilon(x) = \begin{cases} 0, & x \notin [a, b], \\ 1, & x \in (a, b), \\ \frac{1}{2}, & x \in \{a, b\}, \end{cases} = \mathbb{1}_{(a,b)}(x) + \frac{1}{2}\mathbb{1}_{\{a,b\}}(x).$$

The rest follows as in the previous proposition. \square

The following formula can be useful for the computation of spectral projections on isolated components of the spectrum.

Proposition 6.4.7 (Spectral projection on isolated part of spectrum) Let $\omega \subset \mathbb{C}$ be a connected open set containing an isolated part of the spectrum of T , meaning that $\Gamma \stackrel{\text{def}}{=} \partial\omega$ does not intersect $\text{spec } T$. Call $\Omega = \omega \cap \mathbb{R}$. Then the spectral projector on Ω is given by

$$\Pi_\Omega = \frac{1}{2\pi i} \oint_\Gamma (z - T)^{-1} dz,$$

where the contour Γ is oriented anticlockwise.

Proof.— If s is an intersection point of Γ with \mathbb{R} , then, by assumption $s \notin \text{spec } T$, so $s \notin \text{ess}_\mu \text{Ran } h$. On the other hand, for $s \in \mathbb{R} \setminus \Gamma$ we find, using the Cauchy formula,

$$\frac{1}{2\pi i} \oint_\Gamma (z - s)^{-1} dz = \begin{cases} 1, & s \text{ is inside } \Gamma, \\ 0, & s \text{ is outside } \Gamma. \end{cases}$$

Therefore, for μ -a.e. $x \in X$, one has

$$\frac{1}{2\pi i} \oint_\Gamma (z - h(x))^{-1} dz = \mathbb{1}_\Omega \circ h(x).$$

One can finally replace $h(x)$ by T using the $L^2(X, \mu)$ representation of Theorem 6.3.8. \square

6.4.2 Spectral projectors as a projector valued measure

Below we group some properties satisfied by the spectral projectors (Π_Ω) .

Proposition 6.4.8 The family of spectral projectors $(\Pi_\Omega)_{\Omega \in \mathcal{B}(\mathbb{R})}$ satisfies the following properties:

- (a) Each Π_Ω is an orthogonal projector;
- (b) $\Pi_\emptyset = 0$ and $\Pi_{\mathbb{R}} = Id_{\mathcal{H}}$;
- (c) For any disjoint union $\Omega = \bigsqcup_{n \in \mathbb{N}} \Omega_n$, we have $\Pi_\Omega = s - \lim_{N \rightarrow \infty} \sum_{n=0}^N \Pi_{\Omega_n}$;
- (d) For any pair of Borel sets Ω_1, Ω_2 , $\Pi_{\Omega_1} \Pi_{\Omega_2} = \Pi_{\Omega_1 \cap \Omega_2}$.

From these properties, one easily checks that for any state $\phi \in \mathcal{H}$, the map

$$(6.4.8) \quad \Omega \in \mathcal{B}(\mathbb{R}) \mapsto \mu_\phi(\Omega) \stackrel{\text{def}}{=} \langle \phi, \Pi_\Omega \phi \rangle$$

defines a finite Borel measure on \mathbb{R} .

Any family of projectors $(\Pi_\Omega)_{\Omega \in \mathcal{B}(\mathbb{R})}$ satisfying the properties in Prop. 6.4.8 is said to define a *projection valued measure* (PVM).

Theorem 6.4.9 Let a family of projectors $(\Pi_\Omega)_{\Omega \in \mathcal{B}(\mathbb{R})}$ define a projection valued measure. Let $f : \mathbb{R} \rightarrow \mathbb{C}$ be a bounded Borel function.

Then we may define a unique operator in $\mathcal{L}(\mathcal{H})$ as follows. We define its diagonal components:

$$\forall \phi \in \mathcal{H}, \quad \langle \phi, B\phi \rangle \stackrel{\text{def}}{=} \int_{\mathbb{R}} f(\lambda) d\mu_\phi(\lambda),$$

and then complete the definition by polarization.

From this expression and the definition (6.4.8) of the measure μ_ϕ , it is natural to denote this operator by:

$$B = \int_{\mathbb{R}} f(\lambda) d\Pi_\lambda.$$

Remark 6.4.10 We may extend the definition to any unbounded Borel function $g : \mathbb{R} \rightarrow \mathbb{C}$. The operator

$$\int g(\lambda) d\Pi_\lambda \quad \text{is well-defined on the domain } D_g \stackrel{\text{def}}{=} \{\phi \in \mathcal{H} : \int |g(\lambda)|^2 d\mu_\phi < \infty\}.$$

Example 6.4.11 Let $(T, D(T))$ be selfadjoint on \mathcal{H} . Then the associated spectral projectors $(\Pi_\Omega(T))$ form a PVM. For any $f \in \mathcal{B}_\infty$, we recover this way the operator

$$f(T) = \int_{\mathbb{R}} f(\lambda) d\Pi_\lambda.$$

By taking $g(\lambda) = \lambda$, we also recover a representation of the operator T itself:

$$(6.4.9) \quad T = \int_{\mathbb{R}} \lambda d\Pi_\lambda, \quad \text{defined on the domain } D(T) = \{\phi \in \mathcal{H} : \int \lambda^2 d\mu_\phi < \infty\}.$$

Theorem 6.4.12 (Spectral theorem, PVM representation) There is a 1-to-1 correspondence between selfadjoint operators $(T, D(T))$ on \mathcal{H} and PVM $(\Pi_\Omega)_{\Omega \in \mathcal{B}(\mathbb{R})}$. The correspondence is given by the expression (6.4.9).

6.5 Application of the spectral theorem to Schrödinger propagators

The functional calculus allows one to easily define the propagator for the Schrödinger equation generated by a selfadjoint operator (the Hamiltonian of the system).

Theorem 6.5.1 (Schrödinger propagator) Let $(T, D(T))$ be a selfadjoint operator on \mathcal{H} . The propagator for the Schrödinger equation generated by T

$$i \frac{d}{dt} \psi(t) = T \psi(t), \quad \psi(0) = \psi_0 \in \mathcal{H},$$

is the family of operators $(U(t))_{t \in \mathbb{R}}$ which solves the above equation through $\psi(t) = U(t)\psi_0$.

These operators can be constructed through functional calculus: if we call $e_t : \mathbb{R} \rightarrow \mathbb{C}$ the function defined by $e_t(\lambda) = e^{-it\lambda}$, then

$$U(t) = e_t(T).$$

By an abuse of notation, one sometimes notes $U(t) = e^{-itT}$.

Applying the spectral theorem to T allows to easily show the above theorem, as well as the following properties:

- (a) $(U(t))_{t \in \mathbb{R}}$ forms a strongly continuous unitary group. Namely, $U(t_1)U(t_2) = U(t_1 + t_2)$, and $s - \lim_{t \rightarrow 0} U(t) = Id$.
- (b) For any $\psi \in D(T)$, $\lim_{t \rightarrow 0} \frac{U(t)\psi - \psi}{t} = -iT\psi$.
- (c) Conversely, for $\psi \in \mathcal{H}$, if $\lim_{t \rightarrow 0} \frac{U(t)\psi - \psi}{t} = \varphi \in \mathcal{H}$, then $\psi \in D(T)$ and $\varphi = -iT\psi$.

The following theorem is a converse for the preceding one:

Theorem 6.5.2 (Stone's theorem) If $(U(t))_{t \in \mathbb{R}}$ forms a strongly continuous unitary group on \mathcal{H} , then there exists $(T, D(T))$ a selfadjoint operator with dense domain, such that $U(t) = e^{-itT}$ is the group generated by T .

The operator T is called the infinitesimal generator of the group $(U(t))_{t \in \mathbb{R}}$.

We won't give the proof of this theorem, which is a particular case of the more general analysis of contractive strongly continuous semigroups. See for instance [13, Chap. 5.1].

6.6 Spectral decomposition of Tensor products

Tensor products of Hilbert spaces naturally appear when considering differential operators acting in several dimensions: $L^2(\mathbb{R}^{d_1+d_2}) = L^2(\mathbb{R}^{d_1}) \otimes L^2(\mathbb{R}^{d_2})$. If a selfadjoint differential operator T acts *separately* on the d_1 first variables and on the d_2 last ones, in the form

$$T = T_1 + T_2,$$

where T_i acts on the d_i first (resp. last) variables, then the spectral analysis of T can often be reduced to the spectral analyses of T_1 and T_2 . This reduction of dimension can be very helpful in practice.

In this section we will present a general theorem, and then apply it to particular Schrödinger type operators. A more detailed discussion of tensor products can be found e.g. in [7, Sections II.4 and VIII.10] or in [13, Sections 1.4 and 4.5].

We will present a more general situation than the above L^2 spaces framework. Let $(T_j, D(T_j))$ be selfadjoint operators on Hilbert spaces \mathcal{H}_j , $j = 1, \dots, n$. To any monomial $\lambda_1^{m_1} \cdot \dots \cdot \lambda_n^{m_n}$, $m_j \in \mathbb{N}$, one can associate the operator $T_1^{m_1} \otimes \dots \otimes T_n^{m_n}$ acting on the tensor product space $\mathcal{H} := \mathcal{H}_1 \otimes \dots \otimes \mathcal{H}_n$ as follows: we first define it on tensor product states $\Psi = \psi_1 \otimes \dots \otimes \psi_n$:

$$(T_1^{m_1} \otimes \dots \otimes T_n^{m_n})(\psi_1 \otimes \dots \otimes \psi_n) = T_1^{m_1}\psi_1 \otimes \dots \otimes T_n^{m_n}\psi_n, \quad \text{where each } \psi_j \in D(T_j^{m_j}),$$

and then extend it by linearity on $\Psi \in \bigotimes_{j=1}^n D(T_j)$. Here the zero power T_j^0 equals the identity operator on \mathcal{H}_j .

Remark 6.6.1 For an operator $(T, D(T))$ acting on a Hilbert space \mathcal{H} , the domains of its powers $D(T^n)$ are usually defined in a recursive way:

$$D(T^0) = \mathcal{H}, \quad D(T^n) = \{u \in D(T) : Tu \in D(T^{n-1})\} \text{ for } n \in \mathbb{N}.$$

Exercise 6.6.2 Show that for a selfadjoint operator $(T, D(T))$, one has $D(T^n) = \text{Ran } R_T(z)^n$, for any $z \in \text{res } T$, and that $D(T^n)$ is dense in \mathcal{H} for any n .

Using the above construction, one can associate with any real valued polynomial P on \mathbb{R}^n of degree $N > 0$, a linear operator $P(T_1, \dots, T_n)$ on \mathcal{H} defined on the subspace of \mathcal{H} consisting of the linear combinations of the vectors of the form $\psi_1 \otimes \dots \otimes \psi_n$ with $\psi_j \in D(T_j^N)$, namely on

$$\bigotimes_{j=1}^n D(T_j^N).$$

Theorem 6.6.3 (Spectrum of a tensor product operator) Denote by B the closure of the above operator $P(T_1, \dots, T_n)$. Then B is selfadjoint, and

$$\text{spec } B = \overline{\{P(\lambda_1, \dots, \lambda_n) : \lambda_j \in \text{spec } T_j, j = 1, \dots, n\}}.$$

Proof.—[Sketch of the proof] The complete proof involves a number of technicalities, see e.g. [7, Section III.10], but the main idea is rather simple. By the spectral theorem, it is sufficient to consider the case when T_j is the multiplication by a function h_j on $\mathcal{H}_j := L^2(X_j, d\mu_j)$. Then

$$\mathcal{H} = L^2(X, d\mu), \quad X = X_1 \times \dots \times X_n, \quad \mu = \mu_1 \otimes \dots \otimes \mu_n \text{ the product measure,}$$

and $P(T_1, \dots, T_n)$ acts on \mathcal{H} through the multiplication by the function

$$p(x_1, \dots, x_n) = P(h_1(x_1), \dots, h_n(x_n));$$

Its domain includes the linear combinations of functions $\Psi = \psi_1 \otimes \dots \otimes \psi_n$, where $\psi_j \in L^2(X_j, d\mu_j)$ with compact supports, so that h_j is bounded when restricted to $\text{supp } \psi_j$; as a result, Ψ belongs to the domain of the multiplication operator M_p . There remains to show that the closure of this operator is the multiplication operator M_p on $L^2(X, \mu)$, which is selfadjoint since p is real valued. The spectrum

$$\text{spec } M_p = \text{ess}_\mu - \text{Ran } p = \text{ess}_\mu - \text{Ran } P(h_1(\bullet), h_2(\bullet), \dots, h_n(\bullet))$$

There remains to show that the right hand side is equal to the closure of $P(\text{spec } T_1, \dots, \text{spec } T_n)$.

For $P(\lambda_1, \dots, \lambda_n) = \lambda$, the continuity of P shows that, for any $\epsilon > 0$,

$$h_1^{-1}(\lambda_1 \pm \eta) \times \dots \times h_n^{-1}(\lambda_n \pm \eta) \subset p^{-1}((\lambda \pm \epsilon))$$

for some $\eta > 0$ which can go to zero when $\epsilon \rightarrow 0$. Hence, $\mu p^{-1}((\lambda \pm \epsilon))$ is bounded from below by

$$\mu_1(h_1^{-1}(\lambda_1 \pm \eta)) \times \dots \times \mu_n(h_n^{-1}(\lambda_n \pm \eta)).$$

If $(\lambda_1, \dots, \lambda_n)$ belongs to $\text{spec } T_1 \times \dots \times \text{spec } T_n$, then the above left hand side is positive for any $\eta > 0$, so that the right hand side is positive as well, showing that $\lambda \in \text{spec } T$. This shows that

$$P(\text{spec } T_1 \times \dots \times \text{spec } T_n) \subset \overline{P(\text{spec } T_1 \times \dots \times \text{spec } T_n)} \subset \text{spec } T.$$

On the opposite, if $\lambda \notin \overline{P(\text{spec } T_1 \times \dots \times \text{spec } T_n)}$, then

$$|P(\lambda_1, \dots, \lambda_n) - \lambda| \geq \epsilon \quad \text{for all } (\lambda_1, \dots, \lambda_n) \in \text{spec } T_1 \times \dots \times \text{spec } T_n,$$

hence

$$|p(x_1, \dots, x_n) - \lambda| \geq \epsilon \quad \text{for } \mu\text{-almost every } (x_1, \dots, x_n),$$

which shows that $\lambda \notin \text{spec } T$. □

Let us now present an example of *separable* differential operator, to which the above theorem applies.

Example 6.6.4 (Laplacian on a rectangular domain) Let $a, b > 0$ and $\Omega = (0, a) \times (0, b) \subset \mathbb{R}^2$, $\mathcal{H} = L^2(\Omega)$, and T_D be the Dirichlet Laplacian on Ω .

One can show that T_D can be obtained using the above procedure, using the representation

$$T = L_a \otimes 1 + 1 \otimes L_b,$$

where by L_1 we denote the Dirichlet Laplacian on $\mathcal{H}_1 := L_x^2((0, a))$, i.e.

$$L_1 f = -f'', \quad D(L_1) = H^2((0, a)) \cap H_0^1((0, a)),$$

and similarly L_2 is the Dirichlet Laplacian on $\mathcal{H}_2 = L_y^2((0, b))$. Here we labeled the two L^2 spaces with the names of their respective variables.

It is known (from the exercises) that the spectrum of L_1 is discrete, made of the simple eigenvalues $\{(\pi n/a)^2, n \in \mathbb{N}^*\}$, with the normalized eigenfunctions $e_n^{(a)} = \sqrt{2/a} \sin(\pi n \bullet /a)$. According to the above theorem, the spectrum of T consists of the (discrete) set

$$\{\lambda_{m,n}^{(a,b)} = \left(\frac{\pi m}{a}\right)^2 + \left(\frac{\pi n}{b}\right)^2, \quad m, n \in \mathbb{N}^*\}.$$

The orthonormal basis $(e_m^{(a)} \otimes e_n^{(b)})_{m,n \in \mathbb{N}^*}$ is made of eigenfunctions associated with $\lambda_{m,n}^{(a,b)}$, so the spectrum of T is also purely discrete. The multiplicity of each eigenvalue λ is given by the number of pairs $(m, n) \in \mathbb{N}^{*2}$ for which $\lambda = \lambda_{m,n}^{(a,b)}$.

The same construction holds for the Neumann Laplacian on the rectangle, one obtains the same formula for the eigenvalues but now with $m, n \in \mathbb{N}$.

Exercise 6.6.5 Describe the spectrum of the Dirichlet Laplacian on the half-strip $\Omega = \mathbb{R}_+^* \times (0, b)$.

Chapter 7

Perturbation theory

Perturbation theory aims at describing qualitatively or quantitatively the spectrum of an operator of the form

$$T = T_0 + B,$$

where T_0 is a “well-known” operator, and B , its perturbation, is “smaller” than T_0 . The strategy is to use our knowledge of T_0 to say something nontrivial about the perturbed operator T , in particular about its spectrum. In this chapter, we will state several conditions of “smallness” for B relative to T_0 , which will ensure various properties of T .

7.1 Perturbations of selfadjoint operators

We recall (see Def. 2.2.10) that a linear operator $(T, D(T))$ on \mathcal{H} is essentially selfadjoint if it is closable, and its closure \overline{T} is selfadjoint.

Proposition 7.1.1 An essentially selfadjoint operator admits a unique selfadjoint extension.

Proof.— Let $(T, D(T))$ be essentially selfadjoint operator, and let $(S, D(S))$ be a selfadjoint extension of T . Since S is closed, the inclusion $T \subset S$ implies $\overline{T} \subset S$. On the other hand, $S = S^* \subset (\overline{T})^* = \overline{T}$ (because \overline{T} is self-adjoint). Hence $S = \overline{T}$. \square

Let us recall the criteria of Prop. 2.2.16 for the (essential) selfadjointness of a symmetric operator $(T, D(T))$.

Remark 7.1.2 Those criteria were using the operators $(T \pm i)$ and $(T^* \pm i)$. This proposition can be modified in several ways. For example, it still holds if one replaces $(T \pm i)$ by $(T \pm i\lambda)$ for any $\lambda \in \mathbb{R} \setminus \{0\}$.

If T is also semibounded below, we have the following alternative version:

Proposition 7.1.3 (Self-adjointness criterion for semibounded operators) Let $(T, D(T))$ be a symmetric operator on a Hilbert space \mathcal{H} , such that $T \geq 0$. Then, for any $a > 0$, the following three assertions are equivalent.

- i) $(T, D(T))$ is essentially selfadjoint (selfadjoint);
- ii) $\text{Ker}(T^* + a) = \{0\}$ (and furthermore $(T, D(T))$ is closed);
- iii) $\text{Ran}(T + a)$ is dense in \mathcal{H} (is equal to \mathcal{H}).

The proof, which mimics that of Prop. 2.2.16, is left as an exercise.

7.1.1 The Kato-Rellich theorem

Now we would like to apply the above criteria to show that, starting from a selfadjoint operator $(T_0, D(T_0))$, under a certain condition on the perturbations B , the perturbed operator $T = T_0 + B$ is still selfadjoint for the same domain $D(T_0)$. We have already proved this property in the Exercises when B is bounded and symmetric. We want to generalize the setup by considering unbounded perturbations B as well. However, B still needs to be “smaller than T_0 ”, in a precise sense, which we now introduce.

Definition 7.1.4 (Relative boundedness) Let $(A, D(A))$ be a self-adjoint operator on a Hilbert space \mathcal{H} and $(B, D(B))$ be a linear operator such that:

- i) $D(A) \subset D(B)$;
- ii) there exist real numbers $a, b \geq 0$ such that

$$\|Bu\| \leq a\|Au\| + b\|u\| \quad \text{for all } u \in D(A).$$

We then say that B is *relatively bounded* with respect to A or, for short, *A-bounded*.

The infimum a_{inf} of all possible values $a \geq 0$ for which such a bound holds (where b can be taken arbitrary large, depending on a) is called the *relative bound* of B with respect to A .

If the relative bound is equal to 0, then B is said to be *infinitesimally small* with respect to A .

Notice that if B is a bounded operator, then one can take $a = 0$ in the above bound.

The following theorem

Theorem 7.1.5 (Kato-Rellich) Let $(T_0, D(T_0))$ be (essentially) selfadjoint on \mathcal{H} , and let B be a symmetric operator on \mathcal{H} , which is T_0 -bounded with a relative bound $a_{inf} < 1$.

Then the operator $T = T_0 + B$ with the domain $D(T) = D(T_0)$ is (essentially) selfadjoint.

Proof.— We will give the proof for the case T_0 is selfadjoint.

By assumption, one can find $a \in (0, 1)$ and $b > 0$ such that

$$(7.1.1) \quad \|Bu\| \leq a\|T_0u\| + b\|u\|, \quad \text{for all } u \in D(T_0).$$

Step 1. For any $\lambda > 0$ one has the Pythagore's splitting between symmetric and skew-symmetric parts of the operators $(T_0 + B \pm i\lambda)$:

$$\forall u \in D(T_0), \quad \|(T_0 + B \pm i\lambda)u\|^2 = \|(T_0 + B)u\|^2 + \lambda^2\|u\|^2.$$

Therefore, for all $u \in D(T_0)$ one can estimate

$$(7.1.2) \quad \begin{aligned} \sqrt{2}\|(T_0 + B \pm i\lambda)u\| &\geq \|(T_0 + B)u\| + \lambda\|u\| \\ &\geq \|T_0u\| - \|Bu\| + \lambda\|u\| \\ &\geq (1 - a)\|T_0u\| + (\lambda - b)\|u\|. \end{aligned}$$

Let us choose $\lambda > b$.

Step 2. Let us show that $T = T_0 + B$, with the domain $D(T_0)$, is a closed operator. Let a sequence $(u_n)_n \subset D(T_0)$ and $v_n := (T_0 + B)u_n$ be such that both u_n and v_n converge in \mathcal{H} respectively to u and v .

We see that $((T_0 + B)u_n)$ is a Cauchy sequence. By (7.1.2), T_0u_n is also a Cauchy sequence. Since T_0 is closed, the limit $u = \lim_n u_n$ belongs to $D(T_0)$, and T_0u_n converge to $\tilde{v} = T_0u$. By (7.1.1), Bu_n is a Cauchy sequence and is hence convergent to some $w \in \mathcal{H}$. Let us check that this limit satisfies $w = Bu$. For this, take any $h \in D(T_0)$; then the symmetry of B implies that

$$\langle w, h \rangle = \lim_n \langle Bu_n, h \rangle = \lim_n \langle u_n, Bh \rangle = \langle u, Bh \rangle = \langle Bu, h \rangle.$$

Summing the two limits, we get that $(T_0 + B)u_n$ converges to $\tilde{v} + w = (T_0 + B)u$. This shows that $T_0 + B$ is closed.

Step 3. Let us show that the operators $T_0 + B \pm i\lambda : D(T_0) \rightarrow \mathcal{H}$ are bijective, at least provided $\lambda > 0$ is chosen large enough. From Pythagore's splitting

$$\|(T_0 \pm i\lambda)u\|^2 = \|T_0u\|^2 + \lambda^2\|u\|^2,$$

one draws the obvious inequalities:

$$\|(T_0 \pm i\lambda)u\| \geq \|T_0u\|, \quad \|(T_0 \pm i\lambda)u\| \geq \lambda\|u\|.$$

Then, starting from the relative boundedness of B , we obtain:

$$\begin{aligned}
 \|Bu\| &\leq a\|T_0u\| + b\|u\| \\
 &\leq a\|(T_0 \pm i\lambda)u\| + \frac{b}{\lambda}\|(T_0 \pm i\lambda)u\| \\
 (7.1.3) \quad &\leq \left(a + \frac{b}{\lambda}\right)\|(T_0 \pm i\lambda)u\|.
 \end{aligned}$$

Since $a \in (0, 1)$, we can choose λ sufficiently large to have $a + \frac{b}{\lambda} < 1$.

Since T_0 is selfadjoint, the operators $T_0 \pm i\lambda : D(T_0) \rightarrow \mathcal{H}$ are bijections. We may thus factorize

$$T_0 + B \pm i\lambda = \left(I + B(T_0 \pm i\lambda)^{-1}\right)(T_0 \pm i\lambda),$$

and the above inequality shows that

$$\|B(T_0 \pm i\lambda)^{-1}\| \leq a + \frac{b}{\lambda} < 1.$$

As a result, $I + B(T_0 \pm i\lambda)^{-1}$ is a bijection from \mathcal{H} to itself. Finally, $T \pm i\lambda$ are bijective, in particular, $\text{Ran}(T \pm i\lambda) = \mathcal{H}$. By Prop. 2.2.16 and Remark 7.1.2, $(T, D(T_0))$ is self-adjoint.

The part concerning the essential selfadjointness is a simple exercise along the lines of Step 2 above. \square

Remark 7.1.6 The condition $a_{inf} < 1$ is necessary. For instance, taking $(T_0, D(T_0))$ and unbounded operator, and $B = -T_0$ would give $T = 0$, which is not selfadjoint on the domain $D(T_0)$.

7.1.2 Application: selfadjointness of Schrödinger operators

The Kato-Rellich theorem allows to construct a large family of selfadjoint Schrödinger operators, obtained e.g. by perturbing the free Laplacian on \mathbb{R}^d .

Theorem 7.1.7 Let $V \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ be a real valued potential, with $p = 2$ if $d \leq 3$ and $p > d/2$ if $d > 3$. We say that these potentials are in the *Kato-Rellich class*.

Then the operator $T = -\Delta + V$, with domain $D(T) = H^2(\mathbb{R}^d)$, is selfadjoint on $L^2(\mathbb{R}^d)$, and its restriction to $C_c^\infty(\mathbb{R}^d)$ is essentially selfadjoint.

Proof.— We give the proof here only for the dimensions $d \leq 3$. For all $f \in \mathcal{S}(\mathbb{R}^d)$ and $\lambda > 0$ we

have the representation

$$\begin{aligned}
 (7.1.4) \quad f(x) &= \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} e^{i\xi \cdot x} \hat{f}(\xi) d\xi \\
 &= \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \frac{1}{\xi^2 + \lambda} (\xi^2 + \lambda) \hat{f}(\xi) d\xi \\
 &\stackrel{C-S}{\leq} \frac{1}{(2\pi)^{d/2}} \left\| \frac{1}{\xi^2 + \lambda} \right\| \cdot \left\| (\xi^2 + \lambda) \hat{f}(\xi) \right\| \\
 &\leq \frac{1}{(2\pi)^{d/2}} \left\| \frac{1}{\xi^2 + \lambda} \right\| \cdot \left(\|\xi^2 \hat{f}(\xi)\| + \lambda \|\hat{f}\| \right) \\
 &\leq a_\lambda \|\Delta f\| + b_\lambda \|f\|,
 \end{aligned}$$

where

$$a_\lambda = \frac{1}{(2\pi)^{d/2}} \left\| \frac{1}{\xi^2 + \lambda} \right\|, \quad b_\lambda = \frac{\lambda}{(2\pi)^{d/2}} \left\| \frac{1}{\xi^2 + \lambda} \right\|.$$

This bound can be recast into the quantitative Sobolev embedding:

$$(7.1.5) \quad \forall f \in H^2(\mathbb{R}^d), \quad \|f\|_\infty \leq a_\lambda \|\Delta f\| + b_\lambda \|f\|.$$

By density, for all $f \in H^2(\mathbb{R}^d)$ and all $\lambda > 0$ we have

$$\|f\|_\infty \leq a_\lambda \|\Delta f\| + b_\lambda \|f\|.$$

Notice that $\xi \mapsto \frac{1}{\xi^2 + \lambda}$ belongs to $L^2(\mathbb{R}^d)$ since we are in dimension $d \leq 3$.

By assumption on our potential V , we can represent it as

$$V = V_1 + V_2, \quad \text{with } V_1 \in L^2(\mathbb{R}^d) \text{ and } V_2 \in L^\infty(\mathbb{R}^d).$$

Using the Sobolev estimate (7.1.5), we obtain

$$\begin{aligned}
 \forall f \in H^2(\mathbb{R}^d), \quad \|Vf\| &\leq \|V_1 f\| + \|V_2 f\| \\
 &\leq \|V_1\|_2 \|f\|_\infty + \|V_2\|_\infty \|f\| \\
 &\leq \tilde{a}_\lambda \|\Delta f\| + \tilde{b}_\lambda \|f\|,
 \end{aligned}$$

with $\tilde{a}_\lambda = \|V_1\|_2 a_\lambda$ and $\tilde{b}_\lambda = \|V_1\|_2 b_\lambda + \|V_2\|_\infty$. One easily checks that a_λ can be made arbitrary small by taking λ large, so the above estimate shows that the multiplication operator M_V is infinitesimally small with respect to the free Laplacian. We may thus apply the Kato-Rellich theorem to $T = -\Delta + V$.

The essential selfadjointness of the operator restricted to $C_c^\infty(\mathbb{R}^3)$ comes from the essential selfadjointness of the Laplacian restricted to that space.

In dimension $d > 3$, the function $\xi \mapsto (\xi^2 + \lambda)^{-1}$ does not belong to $L^2(\mathbb{R}^d)$. The Cauchy-Schwarz bound in (7.1.4) should be replaced by a suitable Hölder inequality, leading to some Sobolev embedding theorem involving some L^p space, in place of the bound (7.1.5). \square

Example 7.1.8 (Coulomb potential) Consider the three-dimensional Coulomb potential $V(x) = \alpha/|x|$, $\alpha \in \mathbb{R}$, describing the electrostatic interaction between two charged particles.

For any bounded open set Ω containing the origin, one has $V_1 \stackrel{\text{def}}{=} \mathbb{1}_\Omega V \in L^2(\mathbb{R}^3)$ and $V_2 \stackrel{\text{def}}{=} (1 - \mathbb{1}_\Omega)V \in L^\infty(\mathbb{R}^3)$, so that $V = V_1 + V_2 \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. From the previous theorem, this implies that the operator $T = -\Delta + \alpha/|x|$ is selfadjoint on the domain $D(T) = H^2(\mathbb{R}^d)$. Notice that this fact is independent on the sign of α (repulsive, vs. attractive interaction).

We have thus proved that the Schrödinger operator with Coulomb potential $T = -\Delta + \frac{\alpha}{|x|}$, with domain $H^2(\mathbb{R}^3)$, is selfadjoint on $L^2(\mathbb{R}^3)$.

Notice that we had already proved, in Section 3.2, that this operator, restricted to $C_c^\infty(\mathbb{R}^3)$, is bounded from below, and therefore admits a selfadjoint Friedrichs extension. The present proof provides a precise information on the domain of this selfadjoint operator.

Below we show that an assumption of boundedness from below of a Schrödinger operator implies its essential selfadjointness. In a way, we recover here the construction of the Friedrichs extension of T , by a direct “hands-on” computation. Notice that the potential has stronger regularity than in Corollary 3.2.9, where the potential was assumed to be in $L_{\text{loc}}^2(\mathbb{R}^d)$ (and bounded from below by $-\frac{(d-2)^2}{4|x|^2}$).

Theorem 7.1.9 Let $\mathcal{H} = L^2(\mathbb{R}^d)$ and let $V \in C^0(\mathbb{R}^d)$ be real valued, such that, for some $c \in \mathbb{R}$, one has the inequality

$$\langle u, (-\Delta + V)u \rangle \geq c\|u\|^2$$

for all $u \in C_c^\infty(\mathbb{R}^d)$.

Then the operator $T = -\Delta + V$ with domain $C_c^\infty(\mathbb{R}^d)$ is essentially selfadjoint.

Proof.— By adding a constant to the potential V one can assume that $T \geq 1$. In other words, using integration by parts:

$$(7.1.6) \quad \int_{\mathbb{R}^d} |\nabla u(x)|^2 dx + \int_{\mathbb{R}^d} V(x)|u(x)|^2 dx \geq \int_{\mathbb{R}^d} |u(x)|^2 dx$$

for all $u \in C_c^\infty(\mathbb{R}^d)$. This inequality extends by density to all $u \in H_{\text{comp}}^1(\mathbb{R}^d)$.

By Prop. 7.1.3, it is sufficient to show that the range of T is dense in $L^2(\mathbb{R}^d)$. To show this density, let $f \in L^2(\mathbb{R}^d)$ such that $\langle f, (-\Delta + V)u \rangle = 0$ for all $u \in C_c^\infty(\mathbb{R}^d)$. Note that T preserve the real valuedness, and we can suppose without loss of generality that f is real valued.

The above property means that $(-\Delta + V)f = 0$ in the sense of $\mathcal{D}'(\mathbb{R}^d)$, or equivalently $\Delta f = Vf$. Since V is locally bounded, the function Vf is in $L_{\text{loc}}^2(\mathbb{R}^d)$; the elliptic regularity then shows that $f \in H_{\text{loc}}^2(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$.

Let us pick a real valued cutoff function $\chi \in C_c^\infty(\mathbb{R}^d, [0, 1])$ such that $\chi(x) = 1$ for $|x| \leq 1$, $\varphi(x) = 0$ for $|x| \geq 2$. For $n \in \mathbb{N}^*$, rescale this cutoff into $\chi_n(x) := \chi(x/n)$.

For any $u \in C_c^\infty(\mathbb{R}^d)$ we have, by a standard computation:

$$(7.1.7) \quad \int_{\mathbb{R}^d} \nabla(\chi_n f) \nabla(\chi_n u) dx + \int_{\mathbb{R}^d} V \chi_n f \chi_n u dx \\ = \int_{\mathbb{R}^d} |\nabla \chi_n|^2 f u dx + \int_{\mathbb{R}^d} \chi_n (f \nabla u - u \nabla f) \cdot \nabla \chi_n dx + \langle f, T \chi_n^2 u \rangle.$$

Since $\chi_n^2 u \in C_c^\infty(\mathbb{R}^d)$, the last term vanishes. Since the resulting integrals only involve first derivatives of u , and all functions are truncated in $B(0, 2n)$, we may extend them to $u \in H_{\text{loc}}^1$. In particular, we may take $u = f \in H_{\text{loc}}^2$. Then the second term in the above expression vanishes as well. Applying the inequality (7.1.6) to the state $\chi_n f \in H_{\text{comp}}^1$, we obtain:

$$\int_{\mathbb{R}^d} |\nabla \chi_n|^2 f^2 dx \geq \int_{\mathbb{R}^d} \chi_n^2 f^2 dx.$$

When n tends to infinity, the left hand side goes to 0 since $\nabla \chi_n$ is supported outside of $\{|x| \leq n\}$ and is uniformly bounded. On the other hand, the RHS converges to $\|f\|^2$ when $n \rightarrow \infty$. We thus deduce that $f = 0$: this shows that the range of T is dense. \square

7.2 Stability of the essential spectrum

In Def. 4.2.11 we introduced the splitting of $\text{spec } T$ between discrete spectrum and essential spectrum. This splitting will be useful when considering perturbations.

We recall that the discrete spectrum $\text{spec}_{\text{disc}} T$ consists in the eigenvalues of finite multiplicity, which are isolated from the rest of the spectrum (since we will be dealing with selfadjoint operators, the algebraic and geometric multiplicities are identical).

Proposition 7.2.1 Let T be a selfadjoint operator in a Hilbert space \mathcal{H} . Its discrete spectrum $\text{spec}_{\text{disc}} T$ can be characterized in terms of the spectral projectors Π_Ω of T :

$$(7.2.8) \quad \text{spec}_{\text{disc}} T = \left\{ \lambda \in \text{spec } T : \exists \epsilon > 0 \text{ such that } 0 < \dim \text{Ran } \Pi_{(\lambda-\epsilon, \lambda+\epsilon)} < \infty \right\}.$$

Proof.— Let λ belong to the set on the RHS of (7.2.8). Since the range of $\Pi_{(\lambda-\epsilon, \lambda+\epsilon)}$ can only decrease when $\epsilon \searrow 0$, the dimension of this range must stabilize at some value $d_\lambda > 0$ when $\epsilon \searrow 0$, and hence the range itself: there exists $\epsilon_0 > 0$ such that the operators $\Pi_{(\lambda-\epsilon, \lambda+\epsilon)}$ do not depend on ϵ if $\epsilon \in (0, \epsilon_0)$, and are nontrivial. This implies that

$$\Pi_{\{\lambda\}} = \text{s-}\lim_{\epsilon \rightarrow 0^+} \Pi_{(\lambda-\epsilon, \lambda+\epsilon)} \neq 0,$$

hence that $\lambda \in \text{spec}_p T$ by Prop. 6.4.4(3). At the same time, $\Pi_{(\lambda-\epsilon_0, \lambda)} = \Pi_{(\lambda, \lambda+\epsilon_0)} = 0$, and Prop. 6.4.4(2) shows that λ is an isolated eigenvalue of finite multiplicity in the spectrum, hence an element in the discrete spectrum.

Conversely, let λ be an isolated eigenvalue of finite multiplicity of T . Then there exists $\epsilon_0 > 0$ such that $\Pi_{(\lambda-\epsilon_0, \lambda)} = \Pi_{(\lambda, \lambda+\epsilon_0)} = 0$, and $\dim \Pi_{\{\lambda\}} = \dim \text{Ker}(T - \lambda) < \infty$. Therefore,

$$\dim \text{Ran } \Pi_{(\lambda-\epsilon_0, \lambda+\epsilon_0)} = \dim \text{Ran } \Pi_{(\lambda-\epsilon_0, \lambda)} + \dim \text{Ran } \Pi_{(\lambda, \lambda+\epsilon_0)} + \dim \text{Ran } \Pi_{\{\lambda\}} < \infty.$$

□

On the opposite, the essential spectrum of T can be characterized by the following properties.

Proposition 7.2.2 A value $\lambda \in \text{spec } T$ belongs to the essential spectrum iff at least one of the following three conditions holds:

- $\lambda \notin \text{spec}_p T$;
- λ is an accumulation point of $\text{spec}_p T$;
- $\dim \text{Ker}(T - \lambda) = \infty$.

Furthermore, the essential spectrum is a closed set.

Proof.— Each of the three conditions describes the points of the spectrum which are not isolated eigenvalues of finite multiplicity.

For last statement, we note that $\text{spec}_{\text{ess}} T$ is obtained from the closed set $\text{spec } T$ by removing finitely or countably many isolated points. Removing from $\text{spec } T$ an isolated point $\{\lambda\}$ amounts to remove some neighbourhood $(\lambda - \epsilon, \lambda + \epsilon)$. Removing an open set leaves our set closed, so $\text{spec}_{\text{ess}} T$ is a closed set. □

Let us list some examples.

Proposition 7.2.3 (Essential spectrum of compact operators) Let T be a compact self-adjoint operator in an infinite-dimensional space \mathcal{H} , then $\text{spec}_{\text{ess}} T = \{0\}$.

Proposition 7.2.4 (Essential spectrum of operators with compact resolvents) The essential spectrum of a selfadjoint operator T is empty iff the operator has a compact resolvent.

Sometimes one uses the following terminology:

Definition 7.2.5 (Purely discrete spectrum) We say that a selfadjoint operator T has a *purely discrete spectrum in some interval* (a, b) if $\text{spec}_{\text{ess}} T \cap (a, b) = \emptyset$.

If $\text{spec}_{\text{ess}} T = \emptyset$, then we say that the spectrum of T is *purely discrete*.

Example 7.2.6 The free Laplacian in $L^2(\mathbb{R}^d)$ admits the spectrum $[0, +\infty)$. This set has no isolated points, so this operator has no discrete spectrum.

The main difference between the discrete and the essential spectra comes from their behavior with respect to perturbations. This will be discussed in the following sections.

7.2.1 Weyl criterion and relatively compact perturbations

The main goal of this section will be to show that, starting from a selfadjoint operator $(T_0, D(T_0))$, if we add a “sufficiently small” perturbation B to T_0 (in particular, such that $T_0 + B$ remains selfadjoint), then the operator $T_0 + B$ has the same essential spectrum as T_0 . We refer to this property as the stability of the essential spectrum.

The “smallness” necessary for this stability phenomenon is more restrictive than the one used in the Kato-Rellich theorem.

The following proposition transforms an isolated eigenvalue

Proposition 7.2.7 Let T be a selfadjoint operator on \mathcal{H} , and λ_0 an isolated eigenvalue of T . Then there exists $c > 0$ such that $\|(T - \lambda_0)u\| \geq c\|u\|$ for all $u \in D(T)$ such that $u \perp \text{Ker}(T - \lambda_0)$.

Proof.— Without loss of generality, let us take $\lambda_0 = 0$. Since 0 is an isolated eigenvalue of T , the distance $c := \text{dist}(0, \text{spec} T \setminus \{0\})$ is strictly positive. We have $\text{spec} T \cap (-c, c) = \{0\}$, so that $\Pi_{\{0\}} = \Pi_{(-c, c)}$.

So, our state u satisfies

$$\begin{aligned} u \perp \text{Ker}(T) &\iff u \perp \text{Ran } \Pi_{\{0\}} = \Pi_{(-c, c)} \\ &\iff u = \Pi_{\mathbb{R} \setminus (-c, c)} u. \end{aligned}$$

We may split the state u in two orthogonal pieces:

$$u = u_- + u_+, \quad u_- = \Pi_{(-\infty, -c]} u, \quad u_+ = \Pi_{[c, \infty)} u.$$

Using the spectral representation of T , the state Tu_+ reads

$$Tu_+ = \int_{\mathbb{R}} \lambda d\Pi_{\lambda} u_+ = \int_{[c, \infty)} \lambda d\Pi_{\lambda} u_+ = \int_{\mathbb{R}} f_+(\lambda) d\Pi_{\lambda} u_+,$$

where $f_+(\lambda) = \lambda$ on $[c, \infty)$, and can be chosen arbitrarily on $(-\infty, c)$, since for any function f , one has $\int_{(-\infty, c)} f(\lambda) d\Pi_\lambda \Pi_{[c, \infty)} = 0$. Let us choose $f_+(\lambda) = \max(\lambda, c)$ for all $\lambda \in \mathbb{R}$. We thus have

$$Tu_+ = f_+(T)u_+, \quad \text{and similarly} \quad Tu_- = f_-(T)u_-,$$

where $f_-(\lambda) = \min(\lambda, -c)$. The functions f_\pm are bounded away from zero, and so are the corresponding selfadjoint operators:

$$f_-(T) \leq -c, \quad f_+(T) \geq c.$$

These bounds entail the norm bounds:

$$\|Tu_-\| = \|f_-(T)u_-\| \geq c\|u_-\|, \quad \|Tu_+\| = \|f_+(T)u_+\| \geq c\|u_+\|.$$

On the other hand, the spaces u_-, u_+ (resp. $f_-(T)u_-, f_+(T)u_+$) are orthogonal to each other, so Pythagore's theorem gives

$$\|Tu\|^2 = \|Tu_-\|^2 + \|Tu_+\|^2 \geq c^2(\|u_-\|^2 + \|u_+\|^2) = c^2\|u\|^2.$$

□ The following theorem is important in practice: it provides a characterization of the essential spectrum through the construction of *Weyl singular sequences*, which are often quite easy to exhibit.

Theorem 7.2.8 (Weyl criterion for the essential spectrum) The condition $\lambda \in \text{spec}_{\text{ess}} T$ is equivalent to the existence of a sequence $(u_n)_{n \in \mathbb{N}} \subset D(T)$ satisfying the following three conditions:

- i) $\|u_n\| \geq 1$ for all $n \in \mathbb{N}$;
- ii) u_n weakly converges to 0 in \mathcal{H} ;
- iii) $(T - \lambda)u_n$ converges to 0 in \mathcal{H} .

Such a sequence will be called a *singular Weyl sequence* for λ . Moreover, as will be shown in the proof, one can replace the conditions (1) and (2) by:

- 1'. $(u_n)_{n \in \mathbb{N}}$ forms an orthonormal family in \mathcal{H} .

Notice the difference with the characterization of $\lambda \in \text{spec } T$: the latter only needs a sequence $(v_n)_n$ satisfying the conditions (1) and (3). The specificity of belonging to the essential spectrum is thus due to the condition (2), $u_n \rightharpoonup 0$.

Proof.— Denote by $W(T)$ the set of all real numbers λ to which one can associate a singular Weyl sequence.

1. Let us first show the inclusion $W(T) \subset \text{spec}_{\text{ess}} T$. Let $\lambda \in W(T)$ and let $(u_n)_n$ be an associated singular Weyl sequence. As noticed above, the conditions (1) and (3) imply that $\lambda \in \text{spec } T$. Assume

by contradiction that $\lambda \in \text{spec}_{\text{disc}} T$ and denote by $\Pi = \Pi_{\{\lambda\}}$ the orthogonal projector to $\text{Ker}(T - \lambda)$. Since Π has finite rank operator, it is compact, so the assumption (2) implies that the sequence Πu_n converges (strongly) to 0. Therefore, the norms of the vectors $w_n := (1 - \Pi)u_n$ satisfy $\|w_n\| \geq 1/2$ for n large enough. On the other hand, the vectors $(T - \lambda)w_n = (1 - \Pi)(T - \lambda)u_n$ converge to 0; because $w_n \perp \text{Ker}(T - \lambda)$, Proposition 7.2.7 implies that $\|w_n\| \leq C\|(T - \lambda)w_n\| \rightarrow 0$, which is a contradiction

2. Conversely, if $\lambda \in \text{spec}_{\text{ess}} T$, then $\dim \text{Ran } \Pi_{(\lambda - \epsilon, \lambda + \epsilon)} = \infty$ for all $\epsilon > 0$. We have to consider two cases: *i*). Assume that $\text{Ran } \Pi_{\{\lambda\}} = \infty$. Then we can consider an orthonormal family $(u_n)_{n \geq 0}$ in $\text{Ker}(T - \lambda)$. This sequence is obviously a Weyl sequence for λ .

ii) Assume now that $\dim \text{Ran } \Pi_{(\lambda - \epsilon, \lambda + \epsilon)} < \infty$. Then we have, for any $\epsilon > 0$, $\dim \text{Ran } \Pi_{(\lambda - \epsilon, \lambda)} = \infty$ or $\dim \text{Ran } \Pi_{(\lambda, \lambda + \epsilon)} = \infty$. Since these quantities decay when $\epsilon \rightarrow 0$, one of the two operators must have infinite rank for all $\epsilon > 0$. Without loss of generality, let us assume that

$$\forall \epsilon > 0, \quad \text{Ran } \Pi_{(\lambda, \lambda + \epsilon)} = \infty.$$

Since $(\lambda, \lambda + 1) = \bigcap_{\epsilon > 0} (\lambda + \epsilon, \lambda + 1)$, there exists $\epsilon_1 \in (0, 1)$ such that $\Pi_{[\lambda + \epsilon_1, \lambda + 1]} \neq 0$. Similarly, there exists $\epsilon_2 \in (0, \epsilon_1)$ such that $\Pi_{[\lambda + \epsilon_2, \lambda + \epsilon_1]} \neq 0$. Iteratively, we construct a strictly decreasing sequence $\epsilon_n \searrow 0$ such that $\Pi_{[\lambda + \epsilon_{n+1}, \lambda + \epsilon_n]} \neq 0$ for all n . Now let us choose $u_n \in \text{Ran } \Pi_{[\lambda + \epsilon_{n+1}, \lambda + \epsilon_n]}$ with $\|u_n\| = 1$. These vectors form an orthonormal sequence, in particular, converge weakly to 0. On the other hand,

$$\|(T - \lambda)u_n\| = \|(T - \lambda)\Pi_{[\lambda + \epsilon_{n+1}, \lambda + \epsilon_n]}u_n\| \leq \epsilon_n \|u_n\| = \epsilon_n,$$

which shows that the vectors $\|(T - \lambda)u_n\| \rightarrow 0$. Therefore, $(u_n)_n$ forms a singular Weyl sequence, therefore $\text{spec}_{\text{ess}} T \subset W(T)$. \square

The following theorem provides a starting point to the study of perturbations of selfadjoint operators.

Theorem 7.2.9 (Stability of the essential spectrum) Let $(A, D(A))$ and $(B, D(B))$ be self-adjoint operators such that, for some $z \in \text{res } A \cap \text{res } B$ the difference of their resolvents $K(z) := (A - z)^{-1} - (B - z)^{-1}$ is a compact operator.

Then $\text{spec}_{\text{ess}} A = \text{spec}_{\text{ess}} B$.

Proof.— Using the resolvent identities (Prop. 4.1.8), one sees that if $K(z)$ is compact for some $z \in \text{res } A \cap \text{res } B$, then it is compact for all $z \in \text{res } A \cap \text{res } B$.

Let $\lambda \in \text{spec}_{\text{ess}} A$ and let $(u_n)_n$ be an associated singular Weyl sequence. Without loss of generality we assume that $\|u_n\| = 1$ for all n . We have, for any $z \in \text{res } A \cap \text{res } B$:

$$(7.2.9) \quad \lim \left((A - z)^{-1} - \frac{1}{\lambda - z} \right) u_n = \lim \frac{1}{z - \lambda} (A - z)^{-1} (A - \lambda) u_n = 0.$$

This shows that (u_n) is a singular Weyl sequence for the operator $(A - z)^{-1}$. Note that if $z \notin \mathbb{R}$, this operator is not selfadjoint, however it is normal (commutes with its adjoint), and the definition and characterization of the essential spectrum is identical with the selfadjoint case.

On the other hand, $K(z)$ is compact, so the sequence $K(z)u_n$ strongly converges to 0. We thus deduce:

$$(7.2.10) \quad \begin{aligned} \lim \frac{1}{z - \lambda} (B - \lambda)(B - z)^{-1} u_n &= \lim \left((B - z)^{-1} - \frac{1}{\lambda - z} \right) u_n \\ &= \lim \left((A - z)^{-1} - \frac{1}{\lambda - z} \right) u_n - \lim K(z) u_n = 0. \end{aligned}$$

This shows that (u_n) is also a singular Weyl sequence for the operator $(B - z)^{-1}$, associated to the spectral value $(\lambda - z)^{-1}$. From there, we want to exhibit a singular Weyl sequence for the operator B and the spectral value λ .

Let us denote $v_n := (B - z)^{-1} u_n$. First, the assumption $u_n \rightarrow 0$ easily implies that $v_n \rightarrow 0$. Second, the equalities (7.2.10) show that $(B - \lambda)v_n$ converges to 0. Third, it also follows from (7.2.10) that $\lim \|v_n\| = |\lambda - z|^{-1} > 0$. As a consequence, (v_n) is a singular Weyl sequence for B , associated with the value λ , hence $\lambda \in \text{spec}_{\text{ess}} B$.

So we have shown the inclusion $\text{spec}_{\text{ess}} A \subset \text{spec}_{\text{ess}} B$. Since the roles of A and B can be exchanged, we have also $\text{spec}_{\text{ess}} A \supset \text{spec}_{\text{ess}} B$, hence the equality between the two essential spectra. \square

Let us define a class of perturbations to which we may apply the preceding theorem.

Definition 7.2.10 (Relatively compact operators) Let $(T_0, D(T_0))$ be a selfadjoint operator on a Hilbert space \mathcal{H} , and let B be a closable linear operator on \mathcal{H} with $D(T_0) \subset D(B)$. We say that B is *compact with respect to T_0* (or simply *A -compact*) if $B(T_0 - z)^{-1}$ is compact for at least one $z \in \text{res } T_0$. (It follows from the resolvent identities that this holds then for all $z \in \text{res } T_0$.)

The following proposition shows that the assumption of T_0 -relative compactness is stronger than the T_0 -boundedness we used in the previous section.

Proposition 7.2.11 Let B be T_0 -compact, then B is infinitesimally small with respect to T_0 .

Proof.— Let us first show that if B is T_0 -compact, we have:

$$(7.2.11) \quad \lim_{\lambda \rightarrow +\infty} \|B(T_0 - i\lambda)^{-1}\| = 0$$

We will proceed *ab absurdo*, that is assume that this limit is false. Then one can find a constant $\alpha > 0$, nonzero vectors u_n and a sequence $(\lambda_n > 0)$ with $\lim \lambda_n = +\infty$, such that $\|B(T_0 - i\lambda)^{-1} u_n\| > \alpha \|u_n\|$ for all n . Set $v_n := (T_0 - i\lambda)^{-1} u_n$. Using Pythagore's identity

$$\|u_n\|^2 = \|(T_0 - i\lambda_n)v_n\|^2 = \|T_0 v_n\|^2 + \lambda_n^2 \|v_n\|^2,$$

we obtain

$$\|Bv_n\|^2 > \alpha^2\|T_0v_n\|^2 + \alpha^2\lambda_n^2\|v_n\|^2.$$

Without loss of generality one may assume the normalization $\|Bv_n\| = 1$, then the sequence T_0v_n is bounded and v_n converge to 0. Let $z \in \text{res } T_0$, then $(T_0 - z)v_n$ is also bounded, so one can extract a weakly convergent subsequence $((T_0 - z)v_{n_k})_k$. Due to the compactness of $B(T_0 - z)^{-1}$, the vectors $B(T_0 - z)^{-1}(T_0 - z)v_{n_k} = Bv_{n_k}$ converge to some $w \in \mathcal{H}$ with $\|w\| = 1$. On the other hand, as shown above, v_{n_k} converge to 0, and the closability of B imposes that $w = 0$. This contradiction shows that (7.2.11) must hold.

As a consequence, for any $a > 0$ one can find $\lambda > 0$ such that $\|B(T_0 - i\lambda)^{-1}u\| \leq a\|u\|$ for any $u \in \mathcal{H}$. Denoting $v := (T_0 - i\lambda)^{-1}u$ and remembering that $(T_0 - i\lambda)^{-1}$ is a bijection between \mathcal{H} and $D(T_0)$ we deduce from the above estimate that

$$\forall v \in D(T_0), \quad \|Bv\| \leq a\|(T_0 - i\lambda)v\| \leq a\|T_0v\| + a\lambda\|v\|$$

Since $a > 0$ is arbitrary, this proves our result. \square

So a combination of the preceding assertions leads us to the main theorem of this section:

Theorem 7.2.12 (Relatively compact perturbations) Let $(T_0, D(T_0))$ be a selfadjoint operator in a Hilbert space \mathcal{H} , and let $(B, D(B))$ be symmetric and T_0 -compact.

Then the operator $T = T_0 + B$, with domain $D(T) = D(T_0)$, is self-adjoint, and the essential spectra of T and T_0 coincide.

Proof.— The selfadjointness of T follows from the Kato-Rellich theorem. It remains to show that the difference of the resolvents of T and T_0 is compact. This follows directly from the obvious identity

$$(T_0 - z)^{-1} - (T_0 + B - z)^{-1} = (T_0 + B - z)^{-1}B(T_0 - z)^{-1},$$

which holds for all $z \notin \mathbb{R}$. \square

As an easy exercise, one can show the following assertion, which can be useful in some situations.

Proposition 7.2.13 Let T_0 be selfadjoint, B be symmetric and T_0 -bounded with a relative bound $a_{inf} < 1$, and C be T_0 -compact.

Then C is also $(T_0 + B)$ -compact.

7.2.2 Essential spectra of Schrödinger operators

The following class of potentials is a restriction of the Kato-Rellich class introduced in Thm 7.1.7.

Definition 7.2.14 (Kato class potential) We say that a measurable function $V : \mathbb{R}^d \rightarrow \mathbb{R}$ belongs to the Kato class if, for any $\epsilon > 0$, one can find real valued $V_\epsilon \in L^p(\mathbb{R}^d)$ and $V_{\infty,\epsilon} \in L^\infty(\mathbb{R}^d)$ such that $\|V_{\infty,\epsilon}\|_\infty < \epsilon$ and $V = V_\epsilon + V_{\infty,\epsilon}$.

Here the index $p = 2$ for $d \leq 3$ and $p > d/2$ for $d \geq 4$, like for the Kato-Rellich classes.

Theorem 7.2.15 If a potential $V : \mathbb{R}^d \rightarrow \mathbb{R}$ belongs to the Kato class, then M_V is compact with respect to the free Laplacian $T_0 = -\Delta$ on $L^2(\mathbb{R}^d)$. As a result, the essential spectrum of the operator $T = -\Delta + V$, with domain $D(T) = H^2(\mathbb{R}^d)$, is equal to $[0, \infty)$.

Proof.— As in Thm. 7.1.7, we only give the proof for $d \leq 3$. Let \mathcal{F} denote the Fourier transform on \mathbb{R}^d . Then, for any $f \in \mathcal{S}(\mathbb{R}^d)$ and $z \in \text{res } T_0$ we have

$$\forall \xi \in \mathbb{R}^d, \quad (\mathcal{F}(T_0 - z)^{-1}f)(p) = (\xi^2 - z)^{-1}\mathcal{F}f(\xi).$$

In other words, $(T_0 - z)^{-1}$ is a Fourier multiplier for the symbol $(\xi^2 - z)^{-1}$. Since a Fourier multiplier corresponds to a convolution operator, we have

$$(T - z)^{-1}f(x) = g_z \star f(x) = \int_{\mathbb{R}^d} g_z(x - y)f(y)dy, \quad \text{where } g_z = \mathcal{F}_{\xi \rightarrow x}^{-1}(\xi^2 - z)^{-1}.$$

Let $\epsilon > 0$ and let the decomposition $V = V_\epsilon + V_{\infty,\epsilon}$ be as in Definition 7.2.14. The operator $V_\epsilon(T - z)^{-1}$ admits the integral kernel $K(x, y) = V_\epsilon(x)g_z(x - y)$. Let us compute the L^2 norm of this kernel:

$$\begin{aligned} \int_{\mathbb{R}^d \times \mathbb{R}^d} |K(x, y)|^2 dx dy &= \int_{\mathbb{R}^d} |V_\epsilon(x)|^2 dx \int_{\mathbb{R}^d} |g_z(y)|^2 dy \\ &= \|V_\epsilon\|_2^2 \|g_z\|^2 < \infty. \end{aligned}$$

This means that $V_\epsilon(T - z)^{-1}$ is a Hilbert-Schmidt operator, therefore is compact, see Section 5.4. At the same time we have the easy estimate

$$\|V_{\infty,\epsilon}(T - z)^{-1}\| \leq \epsilon \|(T - z)^{-1}\|,$$

so the norm of this operator goes to zero when $\epsilon \rightarrow 0$. Finally, the bounded operator $V(T - z)^{-1}$ can be represented as the limit in $\mathcal{L}(L^2)$ of the compact operators $V_\epsilon(T - z)^{-1}$, when ϵ tends to 0. Since compact operators form a closed subspace in $\mathcal{L}(L^2)$, the limit operator $V(T - z)^{-1}$ is compact as well. \square

Example 7.2.16 (Coulomb potential) The previous theorem easily applies to the Schrödinger operators with Coulomb potential we have mentioned in the previous section, $T = -\Delta + \alpha/|x|$. It is sufficient to represent

$$\frac{1}{|x|} = \frac{\mathbb{1}_R(x)}{|x|} + \frac{1 - \mathbb{1}_R(x)}{|x|},$$

where $\mathbb{1}_R$ is the characteristic function of the ball of radius $R > 0$ and centered at the origin. When R is large, the second part $V_{\infty, \epsilon}(x) = \frac{1 - \mathbb{1}_R(x)}{|x|}$ is smaller than ϵ provided $R > \epsilon^{-1}$. So the essential spectrum of $-\Delta + \alpha/|x|$ is always the same as for the free Laplacian, i.e. $[0, +\infty)$.

Another typical application of the Weyl criterion concerns “partially confining” bounded potentials.

Theorem 7.2.17 Let $V \in L^\infty(\mathbb{R}^d)$ be real valued. Assume that there exists $\alpha \in \mathbb{R}$ such that the set $\Omega := \{x \in \mathbb{R}^d : V(x) < \alpha\}$ has a finite Lebesgue measure. Then $-\Delta + V$ has a purely discrete spectrum in $(-\infty, \alpha)$.

Proof.— Let $\mathbb{1}_\Omega$ be the characteristic function of Ω . Call $U := (V - \alpha)\mathbb{1}_\Omega$ and $W := V - U$. Then $U \in L^p(\mathbb{R}^d)$ for any $p \geq 1$ (since U is bounded and supported on a set of finite measure), in particular, U is of Kato class. At the same time, $W \in L^\infty(\mathbb{R}^d)$ and $W \geq \alpha$. By Proposition 7.2.13, U is $(-\Delta + W)$ -compact. As a result,

$$\text{spec}_{\text{ess}}(-\Delta + V) = \text{spec}_{\text{ess}}(-\Delta + W + U) = \text{spec}_{\text{ess}}(-\Delta + W).$$

On the other hand, $\text{spec}_{\text{ess}}(-\Delta + W) \subset \text{spec}(-\Delta + W) \subset [\alpha, +\infty)$.

Notice that we have no problem with the domains: all the operators $-\Delta + V$ and $-\Delta + W$ are defined on the same domain $H^2(\mathbb{R}^d)$, due to the boundedness of the potentials. \square

Remark 7.2.18 In the physics literature, the situation of Theorem 7.2.17 is referred to as a *potential well* below the energy α . The same result holds without assumptions on V outside Ω (i.e. for unbounded potentials), but the proof would then require a slightly different machinery, and the operator domains may be different.

Chapter 8

Variational methods

8.1 Max-min vs. min-max principles

Throughout the subsection, we denote by $(T, D(T))$ a self-adjoint operator in an *infinite-dimensional* Hilbert space \mathcal{H} , and we assume that T is semibounded from below.

By “variational methods”, we have in mind the min-max and max-min principles, which provide, in a somewhat dual manner, explicit variational expressions for the discrete eigenvalues at the bottom of the spectrum (if any). This method is very powerful, and allows to obtain quantitative estimates of eigenvalues for various types of Schrödinger operators, including ones with many particles. This method is specific to selfadjoint operators bounded from below, and the discrete spectrum at the bottom of the spectrum.

We define the bottom of the essential spectrum of T :

$$\Sigma := \begin{cases} \inf \operatorname{spec}_{\text{ess}} T, & \text{if } \operatorname{spec}_{\text{ess}} \neq \emptyset, \\ +\infty, & \text{otherwise.} \end{cases}$$

8.1.1 The max-min theorem

Let us now state our first variational expression for the low lying eigenvalues.

Theorem 8.1.1 (Max-min principle) For $n \in \mathbb{N}$, we introduce the following numbers:

$$\mu_n = \mu_n(T) := \sup_{\psi_1, \dots, \psi_{n-1} \in \mathcal{H}} \inf_{\substack{0 \neq \varphi \in D(T), \\ \varphi \perp \psi_j, j=1, \dots, n-1}} \frac{\langle \varphi, T\varphi \rangle}{\langle \varphi, \varphi \rangle}.$$

Then we are in either of the following situations:

- (a) μ_n is the n th eigenvalue of T (when ordering all the eigenvalues in increasing order, counting their multiplicities), and T has a purely discrete spectrum in $(-\infty, \mu_n]$.

(b) $\mu_n = \Sigma$, and $\mu_j = \mu_n$ for all $j \geq n$.

The numbers μ_n can also be expressed as follows:

$$(8.1.1) \quad \mu_n(T) := \sup_{\substack{H_{n-1} \subset \mathcal{H} \\ \dim H_{n-1} = n-1}} \inf_{\varphi \in D(T) \cap H_{n-1}^\perp, \|\varphi\|=1} \frac{\langle \varphi, T\varphi \rangle}{\|\varphi\|^2}.$$

Proof.— Step 1. Let us first prove two preliminary assertions.

Lemma 8.1.2 Define the numbers $(\mu_n)_{n \geq 1}$ as above, and consider some real number a .

$$(8.1.2) \quad \text{rk } \Pi_{(-\infty, a)} < n \text{ if } a < \mu_n,$$

$$(8.1.3) \quad \text{rk } \Pi_{(-\infty, a)} \geq n \text{ if } a > \mu_n.$$

Proof.— Assume that the assertion (8.1.2) is false. Then, for some $a < \mu_n$ we have $\text{rk } \Pi_{(-\infty, a)} \geq n$, so there exists an n -dimensional subspace $V \subset \text{Ran } \Pi_{(-\infty, a)}$. Since T is semibounded below, $V \subset D(T)$. By dimensional consideration, for any $(n-1)$ -dimensional subspace $H_{n-1} \subset \mathcal{H}$, there exists a normalized vector $\varphi \in V$ orthogonal to H_{n-1} . The inclusion $\varphi \in \text{Ran } \Pi_{(-\infty, a)}$ implies that $\langle \varphi, T\varphi \rangle \leq a$. Therefore, whatever the subspace H_{n-1} , the infimum in the definition of μ_n is $\leq a$, which gives the inequality $\mu_n \leq a$: this contradicts our assumption, hence Eq. (8.1.2) holds.

Similarly, assume by contradiction that the assertion (8.1.3) is false. Then, for some $a > \mu_n$ we have $\text{rk } \Pi_{(-\infty, a)} \leq n-1$. Let $\psi_1, \dots, \psi_{n-1}$ be some vectors spanning $\text{Ran } \Pi_{(-\infty, a)}$. Due to the equality $\Pi_{(-\infty, a)} + \Pi_{[a, +\infty)} = Id$, for every normalized $\varphi \in D(T)$ with $\varphi \perp \text{span}(\{\psi_j, j = 1, \dots, n-1\})$, one has $\varphi = \Pi_{[a, +\infty)}\varphi$, hence $\langle \varphi, T\varphi \rangle \geq a$. This implies that $\mu_n \geq a$, which contradicts our assumption. This proves Eq. (8.1.3). \square

Let us now prove that $\mu_n < +\infty$ for any $n \geq 1$ (remark that $\mu_n > -\infty$ follows from the semiboundedness of T). Assume by contradiction that $\mu_n = +\infty$. Then, by (8.1.2), one has $\text{rk } \Pi_{(-\infty, a)} < n$ for any $a \in \mathbb{R}$. By taking the limit $a \rightarrow \infty$, we find eventually $\dim \text{Ran } \Pi_{(-\infty, \infty)} = \dim \mathcal{H} \leq n$, which contradicts the fact that \mathcal{H} is infinite dimensional.

The Lemma 8.1.2 shows that the rank of $\Pi_{(-\infty, a)}$ has a jump when a crosses μ_n : so there is spectrum of T at the point μ_n . The situation splits into two cases:

Case 1: $\text{rk } \Pi_{(-\infty, \mu_n + \epsilon)} = \infty$ for all $\epsilon > 0$;

Case 2: $n \leq \text{rk } \Pi_{(-\infty, \mu_n + \epsilon)} < \infty$ for small enough $\epsilon > 0$.

Let us consider Case 1. We are going to show that it corresponds to the case (b) of the theorem. Due to (8.1.2), one has $\text{rk } \Pi_{(\mu_n - \epsilon, \mu_n + \epsilon)} = \infty$ for all $\epsilon > 0$, so that $\mu_n \in \text{spec}_{\text{ess}} T$. On the other hand, again by (8.1.2), $\text{spec}_{\text{ess}} T \cap (-\infty, \mu_n - \epsilon) = \emptyset$ for all $\epsilon > 0$, which proves that $\mu_n = \Sigma$. It remains to show that $\mu_j = \mu_n$ for all $j \geq n$. Assume on the opposite that $\mu_j > \mu_n$ for some $j > n$; then, by

(8.1.2), for any $\epsilon < \mu_j - \mu_n$ we have $\text{rk } \Pi_{(-\infty, \mu_n + \epsilon)} \leq j$, which contradicts the assumption of Case 1. So $\mu_j = \mu_n$.

Consider now the Case 2, namely $\text{rk } \Pi_{(-\infty, \mu_n + \epsilon)} < \infty$ for some $\epsilon > 0$. It follows directly that the spectrum of T is purely discrete in $(-\infty, \mu_n + \epsilon)$. Moreover, one can find $\epsilon_1 > 0$ such that $\Pi_{(-\infty, \mu_n]} = \Pi_{(-\infty, \mu_n + \epsilon_1)}$. As $\text{rk } \Pi_{(-\infty, \mu_n + \epsilon_1)} \geq n$ by (8.1.2), we have $\text{rk } \Pi_{(-\infty, \mu_n]} \geq n$, which means that T has at least n eigenvalues $\lambda_1 \leq \dots \leq \lambda_n$ (counted with multiplicities) in $(-\infty, \mu_n]$. If $\lambda_n < \mu_n$, then $\text{rk } \Pi_{(-\infty, \lambda_n]} \geq n$, which contradicts to (8.1.2). This proves the equality $\mu_n = \lambda_n$. \square

An important fact is that the infimum over $\varphi \in D(T) \cap H_{n-1}^\perp$ can be replaced by the infimum over the larger space $\varphi \in D(T) \cap H_{n-1}^\perp$, where $Q(T)$ is the form domain of the operator T , namely the domain of the closure of the quadratic form q_T induced by T .

Proposition 8.1.3 One may replace the above definition of the numbers μ_n by

$$(8.1.4) \quad \mu_n = \sup_{H_{n-1} \subset \mathcal{H}} \inf_{\varphi \in Q(T) \cap H_{n-1}^\perp} \frac{\overline{q_T}(\varphi)}{\|\varphi\|^2}.$$

Proof.— For any $\varphi \in D(T)$ one has $\overline{q_T}(\varphi) = \langle \varphi, T\varphi \rangle$, so the infimum in (8.1.4) is a priori lower than the one in (8.1.1). However, $D(T)$ is dense in the Hilbert space $Q(T)$ (see Thm 3.1.5 and the subsequent discussion), so the infimum of $q_T(u)/\|u\|^2$ over $D(T)$ is equal to the infimum over $Q(T)$. This shows that both formulas are equal in the case of μ_1 . Let us check that this argument works as well for the higher values μ_n . Namely, the subspace $D(T) \cap H_{n-1}^\perp$ is also dense in the space $Q(T) \cap H_{n-1}^\perp$. The space H_{n-1}^\perp is defined by $n - 1$ continuous linear forms on \mathcal{H} , of the form $\ell_i(u) = \langle \psi_i, u \rangle$. Each such form, when restricted to the dense subspace $Q(T) \subset \mathcal{H}$, remains a continuous 1-form on the Hilbert space $Q(T)$:

$$\forall u \in Q(T), \quad |\ell_i(u)| \leq \|\ell_i\|_{\mathcal{H}^*} \|u\|_{\mathcal{H}} \leq \|\tilde{\ell}_i\|_{\mathcal{H}^* C} \|u\|_{Q(T)}.$$

Each such restriction is in 1-to-1 correspondence with a state $\tilde{\psi} \in Q(T)$:

$$\forall u \in Q(T), \quad \ell_i(u) = \langle \tilde{\psi}_i, u \rangle_{Q(T)}$$

As a result, $Q(T) \cap H_{n-1}^\perp$ is the codimension- $(n-1)$ subspace of $Q(T)$ defined by all vectors $u \in Q(T)$ orthogonal to $\{\tilde{\psi}_i, i = 1, \dots, n-1\}$ (for the scalar product on $Q(T)$). This space $Q(T) \cap H_{n-1}^\perp$ is also of codimension $(n-1)$ in \mathcal{H} , so it is dense in H_{n-1}^\perp .

Similarly, inside $Q(T) \cap H_{n-1}^\perp$, the subspace $D(T) \cap H_{n-1}^\perp$ is dense inside $Q(T) \cap H_{n-1}^\perp$.

As a result, the infimum of $q_T(u)/\|u\|^2$ over $D(T) \cap H_{n-1}^\perp$ is identical to the infimum over $Q(T) \cap H_{n-1}^\perp$. \square

Here is a simple consequence of the min-max principle, and of the above proposition.

Corollary 8.1.4 Assume there exists a nontrivial state $\varphi \in Q(T)$ such that

$$\frac{\langle \varphi, T\varphi \rangle}{\|\varphi\|^2} < \Sigma.$$

Then T has at least one isolated eigenvalue of finite multiplicity in $(-\infty, \Sigma)$, which satisfies

$$\mu_1 \leq \frac{\langle \varphi, T\varphi \rangle}{\|\varphi\|^2}.$$

Indeed, in this case one has $\mu_1 < \Sigma$, which means that μ_1 is in the discrete spectrum. This corollary is important in practice: many physically relevant Schrödinger operators admit discrete spectrum below some essential spectrum. To show the existence of this discrete spectrum, it is not necessary to identify the eigenvectors or eigenvalues, but just to construct a “good enough” trial function (or variational function) ϕ , which will contain a large enough component in the range of the discrete spectrum, $\text{Ran } \Pi_{(-\infty, \Sigma)}$, such as to satisfy the above inequality.

8.1.2 The min-max theorem

Let us now state a dual variational formula for the low-lying eigenvalues. In some sense, this statement is more natural than the max-min formula above.

Theorem 8.1.5 (Min-max principle) All the assertions of Theorem 8.1.1 hold if we replace the formulas for μ_n by:

$$(8.1.5) \quad \mu_n = \inf_{\substack{L_n \subset D(T) \\ \dim L=n}} \sup_{0 \neq \varphi \in L_n} \frac{\langle \varphi, T\varphi \rangle}{\langle \varphi, \varphi \rangle}$$

$$(8.1.6) \quad = \inf_{\substack{L_n \subset Q(T) \\ \dim L=n}} \sup_{0 \neq \varphi \in L_n} \frac{\overline{q_T}(\varphi)}{\langle \varphi, \varphi \rangle}.$$

Proof.— We only need to prove the two statements of Lemma 8.1.2 from the equations for μ_n given in (8.1.5), the rest of the proof being identical to that of Thm 8.1.1.

To prove the statement (8.1.2), we prove its contraposal. Namely, let us assume that $\text{rk } \Pi_{(-\infty, a)} \geq n$. There exists a subspace of dimension n $L_n \subset \text{Ran } \Pi_{(-\infty, a)}$. For this subspace, we see that any normalized nontrivial state $\varphi \in L_n$ will satisfy $\langle \varphi, T\varphi \rangle < a$, so that

$$\sup_{\substack{\varphi \in L_n \\ \|\varphi\|=1}} \langle \varphi, T\varphi \rangle = \max_{\substack{\varphi \in L_n \\ \|\varphi\|=1}} \langle \varphi, T\varphi \rangle < a.$$

Since this inequality holds for this specific L_n , it holds as well when minimizing over all L_n , so $\mu_n < a$. We have proved that $\text{rk } \Pi_{(-\infty, a)} \geq n$ implies $\mu_n < a$. The contraposal states that if $a \leq \mu_n$, then $\text{rk } \Pi_{(-\infty, a)} < n$, a statement slightly stronger than (8.1.2).

We then also show (8.1.3) by contraposal. Let us assume that $\text{rk } \Pi_{(-\infty, a)} \leq n - 1$, so that $(\text{Ran } \Pi_{(-\infty, a)})^\perp = \text{Ran } \Pi_{[a, \infty)}$ has codimension $\leq n - 1$ in \mathcal{H} . Linear algebra tells us that for any

n -dimensional subspace $L_n \subset \mathcal{H}$, the intersection $L_n \cap \text{Ran } \Pi_{[a, \infty)} \neq 0$, in particular there exists a normalized state φ in this intersection, satisfying $\langle \varphi, T\varphi \rangle \geq a$. In particular,

$$\sup_{\substack{\varphi \in L_n \\ \|\varphi\|=1}} \langle \varphi, T\varphi \rangle \geq a.$$

Taking the infimum over all L_n , we find $\mu_n \geq a$. The contraposal is exactly (8.1.3). \square

The max-min and min-max principles are powerful tools to analyze of the behavior of the eigenvalues with respect to various parameters. As a basic example, we mention the following situation, which will be applied later to some specific operators:

Definition 8.1.6 Let $(A, D(A))$ and $(B, D(B))$ be two selfadjoint operators on a Hilbert space \mathcal{H} , both semibounded from below. We write $A \leq B$ if the form domains $Q(A) \supset Q(B)$, and if $q_A(u) \leq q_B(u)$ for all $u \in Q(B)$.

As a direct corollary of the max-min principle we obtain the following “pointwise ordering” between the spectra of two operators A and B which are ordered.

Corollary 8.1.7 Let $(A, D(A))$ and $(B, D(B))$ be selfadjoint semibounded below, with $A \leq B$. In addition, assume that A and B have compact resolvents. If $(\lambda_j(A))_{j \geq 1}$ and $(\lambda_j(B))_{j \geq 1}$, denote their respective eigenvalues, enumerated in increasing order and with their multiplicities, then

$$\lambda_j(A) \leq \lambda_j(B) \quad \text{for all } j \geq 1.$$

Another practical application of the min-max theorem concerns the use of finite dimensional variational subspaces of \mathcal{H} , namely using trial functions in a subspace of finite dimension.

Corollary 8.1.8 (Rayleigh-Ritz method) Let $(T, D(T))$ be a selfadjoint operator on \mathcal{H} . Consider a subspace $\mathcal{V} = \mathcal{V}_n \subset D(T)$ of dimension n , and denote by

$$T_{\mathcal{V}} := \Pi_{\mathcal{V}} T \Pi_{\mathcal{V}} \quad \text{the restriction of } T \text{ on } \mathcal{V}.$$

(note that $T_{\mathcal{V}}$ is selfadjoint too). Denote by $(\hat{\mu}_j)_{j=1, \dots, n}$ the ordered eigenvalues of $T_{\mathcal{V}}$, counted with multiplicities.

Then,

$$\forall \leq n, \quad \mu_j(T) \leq \hat{\mu}_j.$$

This Corollary shows that one can try to approach the low-lying spectrum of T by restricting T to a finite rank operator. By choosing an orthonormal eigenbasis of \mathcal{V} , the operator $T_{\mathcal{V}}$ just takes the form of a Hermitian $n \times n$ matrix, which is easy to diagonalize numerically.

8.2 Negative eigenvalues of Schrödinger operators

As seen above in Thm 7.2.15, if V is a Kato class potential in \mathbb{R}^d , then the associated Schrödinger operator $T = -\Delta + V$ acting in $\mathcal{H} = L^2(\mathbb{R}^d)$ has the same essential spectrum as the free Laplacian, i.e. $\text{spec}_{\text{ess}} T = [0, \infty)$, with infimum $\Sigma = 0$. In the present section we will address the question on the existence of negative discrete eigenvalues for the operator T .

We will prove a rather a simple sufficient condition for the existence of such eigenvalues, in the 1 and 2-dimensional cases.

Theorem 8.2.1 Let $d \in \{1, 2\}$ and $V \in L^\infty(\mathbb{R}^d) \cap L^1(\mathbb{R}^d)$ be real valued such that

$$V_0 := \int_{\mathbb{R}^d} V(x) dx < 0,$$

then the associated Schrödinger operator $T = -\Delta + V$ has at least one negative eigenvalue.

Proof.— We assumed the boundedness of the potential just to avoid additional technical issues concerning the domains. The assumption $V \in L^1 \cap L^\infty$ implies by interpolation $V \in L^2(\mathbb{R}^d)$, so that V is in the Kato class, hence $\text{spec}_{\text{ess}} T = [0, +\infty)$ in virtue of Theorem 7.2.15. The domain $D(T) = H^2(\mathbb{R}^d)$, and its form domain $Q(T) = H^1(\mathbb{R}^d)$.

By Corollary 8.1.4, to identify a negative eigenvalue it is sufficient to construct a nonzero state $\varphi \in H^1(\mathbb{R}^d)$ satisfying

$$q_T(\varphi) := \int_{\mathbb{R}^d} |\nabla \varphi(x)|^2 dx + \int_{\mathbb{R}^d} V(x) |\varphi(x)|^2 dx < 0.$$

Consider first the case $d = 1$. Take a small $\epsilon > 0$, and consider a slowly decaying trial function $\varphi_\epsilon(x) := e^{-\epsilon|x|/2}$. Clearly, $\varphi_\epsilon \in H^1(\mathbb{R})$ for any $\epsilon > 0$. A simple computation shows that

$$(8.2.7) \quad \int_{\mathbb{R}} |\varphi'_\epsilon(x)|^2 dx = \frac{\epsilon}{2}, \quad \text{while} \quad \lim_{\epsilon \rightarrow 0^+} \int_{\mathbb{R}} V(x) |\varphi_\epsilon(x)|^2 dx = V_0 < 0.$$

Therefore, for sufficiently small $\epsilon > 0$, the second integral dominates the first one, and one obtains $q_T(\varphi_\epsilon) < 0$.

Now consider the case $d = 2$. As opposed to the 1-dimensional case, the trial function $\varphi_\epsilon(x) = e^{-\epsilon|x|/2}$ will not “do the job”, because $\|\nabla \varphi_\epsilon\|^2 > 0$ is independent of ϵ , so it cannot be made small when $\epsilon \rightarrow 0$. We instead consider the function $\psi_\epsilon(x) = e^{-|x|^\epsilon/2}$, which decays much slower than the

previous one. We have

$$\begin{aligned}\nabla\psi_\epsilon(x) &= -\frac{\epsilon x|x|^{\epsilon-2}}{2} e^{-|x|^\epsilon/2}, \\ \int_{\mathbb{R}^2} |\nabla\psi_\epsilon(x)|^2 dx &= \frac{\epsilon^2}{4} \int_{\mathbb{R}^2} |x|^{2\epsilon-2} e^{-|x|^\epsilon} dx \\ &= \frac{\pi\epsilon^2}{2} \int_0^\infty r^{2\epsilon-1} e^{-r^\epsilon} dr \\ &= \frac{\pi\epsilon}{2} \int_0^\infty u e^{-u} du = \frac{\pi\epsilon}{2},\end{aligned}$$

and, as previously,

$$\lim_{\epsilon \rightarrow 0^+} \int_{\mathbb{R}^d} V(x) |\psi_\epsilon(x)|^2 dx = V_0 < 0.$$

As a result, for sufficiently small ϵ we have again $q_T(\psi_\epsilon) < 0$. \square

We see already in the above proof that finding suitable test functions for proving the existence of eigenvalues may become tricky and depending on various parameters. One have seen that the trial function φ_ϵ works in $d = 1$, but not in $d = 2$; the opposite is actually true for ψ_ϵ , which does not work in $d = 1$, the gradient $\nabla\psi_\epsilon$ having a too strong singularity at $x = 0$ to be in L^2 . It is a remarkable fact that the analog of Theorem 8.2.1 does not hold in higher dimension. In particular, we have the following

Proposition 8.2.2 Let $d \geq 3$ and let $V : \mathbb{R}^d \rightarrow \mathbb{R}$ be bounded with compact support. For $\lambda \in \mathbb{R}$, consider the Schrödinger operators $T_\lambda := -\Delta + \lambda V$.

Then there exists $\lambda_0 > 0$ (depending on V) such that $\text{spec } T_\lambda = [0, +\infty)$ for all $\lambda \in (-\lambda_0, \lambda_0)$.

Notice that we did not make any sign assumption on V , which can have both positive and negative values. **Proof.**— Due to the compactness of $\text{supp } V$ one can find $\lambda_0 > 0$ in such a way that

$$\lambda_0 |V(x)| \leq \frac{(d-2)^2}{4|x|^2} \text{ for all } x \in \mathbb{R}^d.$$

Using the Hardy inequality (see Prop. 3.2.7), for any $u \in C_c^\infty(\mathbb{R}^d)$ and any $|\lambda| < \lambda_0$, we have

$$\begin{aligned}\langle u, T_\lambda u \rangle &= \int_{\mathbb{R}^d} |\nabla u(x)|^2 dx + \lambda \int_{\mathbb{R}^d} V(x) |u(x)|^2 dx \\ &\geq \int_{\mathbb{R}^d} |\nabla u(x)|^2 dx - \lambda_0 \int_{\mathbb{R}^d} |V(x)| \cdot |u(x)|^2 dx \\ &\geq \int_{\mathbb{R}^d} |\nabla u(x)|^2 dx - \frac{(d-2)^2}{4} \int_{\mathbb{R}^d} \frac{|u(x)|^2}{|x|^2} dx \geq 0.\end{aligned}$$

Since T_λ is essentially selfadjoint on $C_c^\infty(\mathbb{R}^d)$, see Thm 7.1.7, this inequality extends to all $u \in D(T_\lambda) = H^2(\mathbb{R}^d)$, and we obtain $T_\lambda \geq 0$, which implies that $\text{spec } T_\lambda \subset [0, +\infty)$. On the other hand, $\text{spec}_{\text{ess}} T_\lambda = [0, +\infty)$, since λV is of Kato class (see Thm 7.2.15). \square

The precise ordering between the spectra of two operators satisfying the ordering $A \leq B$ (see Def. 8.1.6) allows to obtain a monotonicity of the eigenvalues of a perturbed operator, provided the perturbation is a negative operator.

Proposition 8.2.3 Let $(T_0, D(T_0))$ be selfadjoint on \mathcal{H} , and let $(B, D(B))$ be a T_0 -compact and symmetric operator. We also assume that $\text{spec}_{\text{ess}}(T_0) = \mathbb{R}_+$, and that $B \leq 0$. For $\beta \in \mathbb{R}_+$, we consider the perturbed operators $T_\beta = T_0 + \beta B$.

Then the discrete eigenvalues $(\mu_j(\beta))$ of T_β are monotone decreasing w.r.t. β .