CHAPTER 1

Self-Adjoint Operators

We denote by $H, \langle\cdot,\cdot\rangle$ a separable complex Hilbert space,[1] by $\mathcal{D}$ a dense linear subspace of H, and by A an operator from $\mathcal{D}$ to H. The space $\mathcal{D}$ is called the domain of the operator A and is denoted $D(A)$. Unlike bounded operators,[2] in particular, operators on any finite dimensional Hilbert space, simple consideration of the symmetry of operators does not lead to a theorem of spectral decomposition. We will introduce directly the notion of self-adjointness by utilizing spectral conditions based on an exposé of P. Cartier at l'École Polytechnique.

1.1. Symmetric operators

***Definition* 1.1.1.** We say that the complex number λ is in the resolvent set $\rho(A)$ of A if $(\lambda\mathrm{Id}-A)$ is injective, its image $(\lambda\mathrm{Id}-A)\mathcal{D}$ is dense in $\mathcal{H}$, and if the inverse operator $(\lambda\,\mathrm{Id}-A)^{-1}$ is a bounded operator from $(\lambda\,\mathrm{Id}-A)\mathcal{D}$ to H. This operator is then uniquely extended to a bounded operator R_λ on H called the resolvent operator.

We often abbreviate $A-\lambda\,\mathrm{Id}$ by $A-\lambda$.

***Proposition* 1.1.2 (*Resolvent Equation*).** . *For all λ, $\mu\in\rho(A)$ we have:*

$$R_\lambda - R_\mu = (\lambda-\mu)R_\mu R_\lambda.$$

Note that the Resolvent Equation implies that $\{R_\lambda\}$ is a commutative family of operators.

***Definition* 1.1.3.** We say that A is closed if $\mathcal{D}$ is complete for the norm

$$\|\psi\|_A = \left(\|\psi\|^2 + \|A\psi\|^2\right)^{1/2}.$$

Consider the graph of A:

$$\mathcal{G}_A = \{(\psi, A\psi)\in H\times H \;:\; \psi\in\mathcal{D}\}.$$

It is obvious that the projection of the graph of A, with the usual product norm $H\times H$, onto $\mathcal{D}$, with the norm $|\cdot|_A$, is an isometry. Thus it is clear that A is closed if its graph $\mathcal{G}_A$ is closed in $H\times H$. For a closed operator A one can express the resolvent set $\rho(A)$ in a simpler way.

[1]The scalar product is left linear and right anti-linear.

[2]Recall that an operator B is bounded if there exists a constant M such that $\|B\|\le M\|x\|$ for all x in $\mathcal{D}$.

***Proposition* 1.1.4.** *Let A be a closed operator. In order for λ to be in $\rho(A)$, it is necessary and sufficient that one of the two following conditions hold:*

(1) *The mapping $(\lambda - A)$ is a bijection of $\mathcal{D}$ onto H.*
(2) *There exists a bounded operator R_λ of H such that:*

$$\begin{cases} R_\lambda \circ (\lambda - A) = \mathrm{Id}_{\mathcal{D}} \\ (\lambda - A) \circ R_\lambda = \mathrm{Id}_H \,. \end{cases} \tag{1.1.1}$$

PROOF. (1) In order to show the necessity of the condition, we need to show that if $\lambda \in \rho(A)$ then $\mathrm{Image}(\lambda - A) = H$. Since this image is dense, there exists for any $x \in H$ a sequence y_n of elements in $\mathcal{D}$ such that $x = \lim(\lambda y_n - A y_n)$. By applying the bounded operator R_λ, we can conclude that $y_n = R_\lambda(\lambda - A)y_n$ converges. Since both y_n and Ay_n converge, and $\mathcal{G}_A$ is closed, the limit y of y_n is in $\mathcal{D}$ and $\lim(Ay_n) = Ay$ from which we conclude that $\lambda y - Ay = x$. Since x is arbitrary, we see that $(\lambda - A)\mathcal{D} = H$.

Now suppose $\lambda - A$ is a bijection. It is a continuous mapping from the Hilbert space $(\mathcal{D}, \|\cdot\|_A)$ to the Hilbert space H. By Banach's open mapping theorem, the inverse mapping is continuous and obviously remains continuous if we equip $\mathcal{D}$ with the weaker norm $\|\cdot\|_H$.

(2) We see these conditions are equivalent to the initial definition if we take into account the fact that $\lambda - A$ is surjective if its image is dense. □

Self-adjoint operators are a special class of symmetric operators where by a symmetric operator A with a dense domain $\mathcal{D}$ in H we mean a linear operator $A : \mathcal{D} \longrightarrow H$ that satisfies:

$$\forall \varphi, \psi \in \mathcal{D} \quad \langle A\varphi, \psi\rangle = \langle \varphi, A\psi\rangle.$$

They are often defined on natural domains that are too small for the operator A to be closed. A basic example is the Laplacian Δ defined, say, on $\mathcal{D} = \mathcal{C}_c^\infty(\mathbb{R}^n)$, the space of infinitely differentiable functions on $\mathbb{R}^n$ with compact support. However these operators are easily seen to be closeable in the following sense:

***Proposition* 1.1.5.** *The closure of the graph of the symmetric operator A with domain $\mathcal{D}$ as a subset of $H \times H$ is the graph of an operator $\overline{A}$ defined on a domain $\mathcal{D}' \supset \mathcal{D}$. Moreover the resolvent sets and the resolvent operators are the same for both operators. ($\overline{A}$ is called the closure of A.)*

PROOF. We first show that $\overline{\mathcal{G}}_A$ is a graph of a function from H to H. We need to show that if $(\varphi, \psi) \in \overline{\mathcal{G}_A}$ and $(\varphi, \psi') \in \overline{\mathcal{G}_A}$ then $\psi = \psi'$. There exists a sequence $(\varphi_n, A\varphi_n)$ that converges to (φ, ψ) and similarly a sequence $(\varphi'_n, A\varphi'_n)$ that converges to (φ, ψ'). Let w be an arbitrary element of $\mathcal{D}$. Since

$$\langle w, \psi\rangle = \lim_{n\to\infty} \langle w, A\varphi_n\rangle = \lim_{n\to\infty} \langle Aw, \varphi_n\rangle = \langle Aw, \varphi\rangle,$$

and similarly since $\langle w, \psi'\rangle = \langle Aw, \varphi\rangle$ for all w in the dense space $\mathcal{D}$, one necessarily has $\psi = \psi'$.

It is immediate by passing to the limit that the operator associated to the graph $\overline{\mathcal{G}_A}$ remains symmetric and that it is closed. We establish that $\rho(A) \subset \rho(\overline{A})$ as follows: for $\lambda \in \rho(A)$ the only thing that needs to be justified is that $\lambda - \overline{A}$ is injective. In fact, if $\varphi \in \ker(\lambda - \overline{A})$, there exists a sequence φ_n that converges to φ and such that $\psi_n = \lambda\varphi_n - A\varphi_n$ converges to 0, from which we have: $\varphi = \lim \varphi_n = \lim R_\lambda \psi_n = 0$.

We now consider the inclusion in the other direction. By construction, $\mathcal{D}$ is dense in $\mathcal{D}'$ for the norm $\|\cdot\|_{\overline{A}}$ and A is continuous with respect to this norm. Using this, the property $\overline{(\lambda - A)\mathcal{D}} = H$ follows from the fact that $\overline{(\lambda - \overline{A})\mathcal{D}'} = H$. The other properties characterizing $\rho(A)$ follow immediately from the fact that it is contained in $\rho(\overline{A})$. □

The following lemma allows us to study *a priori* the resolvent set and the spectrum $\sigma(A) := \mathbb{C}\backslash\rho(A)$ of a symmetric operator A.

***Lemma* 1.1.6.** *Let A be a closed operator and let $|\cdot|$ be the uniform norm on bounded operators on H.*

1. *If $\lambda \in \rho(A)$, then the open disk $D(\lambda, \|R_\lambda\|^{-1})$ in $\mathbb{C}$ is contained in $\rho(A)$. In particular $\rho(A)$ is open.*
2. *If A is symmetric and $\lambda \in \rho(A)$, then the disk $D(\lambda, \Im(\lambda))$ is contained in $\rho(A)$.*

Proof. (1) If $|\mu-\lambda| < \|R_\lambda\|^{-1}$, the series $S = \sum\limits_{n=0}^{\infty} (\lambda-\mu)^n R_\lambda^n$ converges in the uniform norm on the algebra of bounded operators and $R_\lambda S$ is a bounded operator R_μ that satisfies the equations (1.1).

(2) If α and β are two real numbers, we have:

$$\alpha + i\beta \in \rho(A) \text{ and } \beta \neq 0 \Rightarrow \|R_\lambda\| \leqslant \beta^{-1}. \tag{1.1.2}$$

This follows from the coercivity inequality

$$\|(A - \alpha - i\beta)x\|^2 \geqslant \beta^2\|x\|^2, \tag{1.1.3}$$

which in turn follows from the calculation, for $x \in \mathcal{D}$,

$$\begin{aligned}\|(A - \alpha - i\beta)x\|^2 &= \langle (A-\alpha)x, (A-\alpha)x\rangle + \langle \beta x, \beta x\rangle \\ &\qquad + i\langle \beta x, (A-\alpha)x\rangle - i\langle (A-\alpha)x, \beta x\rangle \\ &= \|(A-\alpha)x\|^2 + \beta^2\|x\|^2.\end{aligned}$$

□

Let $\mathbb{C}^{\pm} := \{\lambda \in \mathbb{C} \;:\; \pm\Im(\lambda) \geq 0\}$. Then we have the following proposition, the proof of which is left as an exercise for the reader.

***Proposition* 1.1.7.** *There are only four mutually exclusive possibilities for the spectrum of a symmetric operator A: $\sigma(A)$ is equal to $\mathbb{C}^+$, $\mathbb{C}^-$, $\mathbb{C}$, or it is included in $\mathbb{R}$.*

***Definition* 1.1.8.** We say an operator $(A, \mathcal{D})$ is essentially self-adjoint if it is symmetric and if $\sigma(A) \subset \mathbb{R}$; if, in addition, it is closed we say it is self-adjoint. If A is self-adjoint, a *core* for A is any dense domain contained in the domain of A on which the restriction of A is essentially self-adjoint.

***Proposition* 1.1.9.** *Let A be a symmetric (resp. symmetric and closed) operator on $\mathcal{D}$. Then (1) below is a sufficient condition that A be essentially self-adjoint (resp. self-adjoint) and (2) and (3) are necessary and sufficient conditions that it be essentially self-adjoint (resp. self-adjoint).*

(1) *There exists a real number λ in $\rho(A)$.*
(2) *$\pm i$ are in $\rho(A)$.*
(3) *The images $(i - A)\mathcal{D}$ and $(i + A)\mathcal{D}$ are dense.*

PROOF. The first two conditions allow us to eliminate the first three possibilities in Proposition 1.1.7. Finally, condition (3) is equivalent to (2). Indeed, the conditions of injectivity and of the continuity of the inverse, which are part of the definition of R_i (or R_{-i}), are always satisfied in the symmetric case by applying the inequality (1.1.3). □

***Exercise* 1.1.10.** Verify that for A symmetric and λ real the necessary condition of injectivity for $\lambda \in \rho(A)$ is a consequence of the density condition.

***Exercise* 1.1.11.** Let $(W, \mathcal{F}, \mu)$ be a measure space and let χ be a real-valued measurable function on W.

Show that the possibly unbounded operator M_χ on $H = L^2(\mu)$ defined on $\mathcal{D} := \{\varphi \in H : \ \varphi\chi\} \in H$ by $M_\chi(\varphi) := \ \chi\varphi$ is self-adjoint and that the resolvent operator R_λ, when it exists, is multiplication by $(\lambda - \chi)^{-1}$.

Deduce from this that the spectrum of M_χ is "the essential image" of χ, i.e., the support of the measure $\chi(\mu)$. By the support of a measure ν on $\mathbb{R}$, we mean the closed complement of the union of all open sets of ν-measure zero.

***Exercise* 1.1.12.** Let A and B be two self-adjoint operators such that A extends B, that is to say, $\mathcal{D}_A \supset \mathcal{D}_B$ and B is the restriction of A to $\mathcal{D}_B$. Show that $A = B$.

***Exercise* 1.1.13.** Consider $H = L^2([0,1])$ and let

$$\mathcal{D}_0 := \{f \in \mathcal{C}^1([0,1]) \ : \ f(0) = f(1) = 0\}.$$

For $f \in \mathcal{D}_0$, we set $Af = if'$.

Verify that the operator A is symmetric on $\mathcal{D}_0$. Verify that $(i - A)\mathcal{D}_0 \perp u$, where $u(x) = e^{-x}$, and deduce from this that $(A, \mathcal{D}_0)$ is not essentially self-adjoint. Show that any distribution u that is the solution of the equation $u' = ku$ is equal to the function $c\,e^{kx}$.

Let α be a fixed complex number of modulus 1. Let B be the operator defined by the same formula as A but on the domain: $\mathcal{D} = \{f \in \mathcal{C}^1([0,1]) \ : f(1) = \alpha f(0)\}$. Show that B is essentially self-adjoint.

A particularly useful application of Proposition 1.1.9 is to symmetric operators that are bounded below. We say a symmetric operator A is *positive* when:

$$\forall x \in \mathcal{D}(A) \qquad \langle Ax, x\rangle \geqslant 0,$$

and we say that A is bounded below if there exists a constant m such that $A - m\,\mathrm{Id}$ is positive. In this case we also say that A is bounded below by m, i.e.,

$$\exists m \; \forall x \qquad \langle Ax, x\rangle \geqslant m\|x\|^2.$$

***Proposition* 1.1.14.** *Let A be a symmetric operator that is bounded below by m and $\lambda < m$. Then in order for $\lambda \in \rho(A)$, it is necessary and sufficient that $(\lambda - A)\mathcal{D}$ is dense. Thus if $(\lambda - A)\mathcal{D}$ is dense, A is essentially self-adjoint on $\mathcal{D}$.*

PROOF. Since $\langle x, (A-\lambda)x\rangle \geqslant (m-\lambda)\|x\|^2$, we see right away that the condition of injectivity and the condition of continuity of R_λ are satisfied. Thus by the definition of $\rho(A)$, $\lambda \in \rho(A)$ if and only if $(\lambda - A)\mathcal{D}$ is dense. By Proposition 1.1.9(1), $\lambda \in \rho(A)$ implies A is essentially self-adjoint. □

***Proposition* 1.1.15.** *As an operator on the domain $\mathcal{D} = \mathcal{C}_c^\infty(\mathbb{R}^n)$ in the Hilbert space $L^2(\mathbb{R}^n)$, the operator Δ is essentially self-adjoint.*

PROOF. It obviously is sufficient to show that $-\Delta$ is essentially self-adjoint on this domain. We first see that $-\Delta$ is symmetric and positive from Green's formula:

$$\langle -\Delta\varphi, \psi\rangle = \int_{\mathbb{R}^n} \nabla\varphi \nabla\overline{\psi}\, dx.$$

To show that it is essentially self-adjoint it is sufficient by Proposition 1.1.14 to show that $(\mathrm{Id} - \Delta)\mathcal{D}$ is dense. Indeed if this were not the case, there would exist a function $f \neq 0$ in L^2 such that $\langle f, \varphi - \Delta\varphi\rangle = 0$, for all $\varphi \in \mathcal{D}$. Utilizing the Fourier transform on $L^2(\mathbb{R}^n)$, which is an isometry, we would have $\langle \widehat{f}(p), (p^2+1)\widehat{\varphi}(p)\rangle = 0$. This in turn would imply that $\widehat{f} = 0$ since the subspace of functions

$$T = \{(p^2+1)\widehat{\varphi}(p) \;:\; \varphi \in \mathcal{D}\}$$

is dense in $L^2(\mathbb{R}^n)$. This contradicts the assumption that $f \neq 0$.

Here we recall a proof that T is dense. Consider a function $\psi \in \mathcal{S}$ where $\mathcal{S}$ is the Schwartz space of rapidly decreasing functions on $\mathbb{R}$. One can find a sequence of functions φ_n of $\mathcal{C}_c^\infty$, such that for each order α the derivative φ_n^α tends to ψ^α in L^2. For example, $\varphi_n(x) = \varphi(x/n)\psi(x)$ where $\varphi \in \mathcal{C}_c^\infty$ is equal to 1 in a neighborhood of 0. Thus $-\Delta\varphi_n + \varphi_n$ converges to $-\Delta\psi + \psi$ in L^2. Since the Fourier transform is an isometry on L^2, we see that $(p^2+1)\widehat{\psi}$ is in the closure of T. But any function in $\mathcal{S}$ can be written in the preceding form. Hence $\overline{T}$ contains $\overline{\mathcal{S}} = L^2$. □

***Corollary* 1.1.16.** *The self-adjoint operator A defined by the above theorem coincides with the Laplacian operator Δ defined in the sense of distributions on the following domain:*

$$\mathcal{D} := \{u \in L^2(\mathbb{R}^n) \,:\, \Delta u \in L^2(\mathbb{R}^n)\}.$$

PROOF. Let $u \in \mathcal{D}$. We define the element v of L^2 by $v := -\Delta u + u$ in the sense of distributions and consider the resolvent operator R_1 at the point 1 of A. Let $\check{T} := \{\varphi - \Delta\varphi \,:\, \varphi \in \mathcal{C}_c^\infty\}$. The Fourier transform of the elements of $\check{T}$ are exactly the elements of the set T considered above, and thus $\check{T}$ is dense in L^2. Since $A\varphi$ and $\Delta\varphi$ coincide on C_c^∞, and upon letting $\psi := \varphi - \Delta\varphi$, we have:

$$\begin{aligned}\langle R_1 v, \psi\rangle = \langle v, R_1\psi\rangle = \langle v, \varphi\rangle = \langle \widehat{v}, \widehat{\varphi}\rangle \\ = \Big\langle \widehat{v}, \frac{1}{p^2+1}\widehat{\psi}\Big\rangle = \Big\langle \frac{1}{p^2+1}\widehat{v}, \widehat{\psi}\Big\rangle = \langle u, \psi\rangle.\end{aligned}$$

Since ψ is an arbitrary element in the dense subspace $\check{T}$, we have $u = R_1 v$, thus u is in the domain of A. In addition $u - Au = v = u - \Delta u$. The reader can easily check that $(\Delta, \mathcal{D})$ is closed and thus that $D(A)$ does not properly contain $\mathcal{D}$. $\square$

Taking into account the preceding corollary, we continue to denote the self-adjoint operator defined in Proposition 1.1.15 by Δ.

The most celebrated self-adjoint operators in $L^2(dx)$ are the Schrödinger operators $-\Delta + V$, where V designates multiplication by the function V. Here is a case where the precise definition of the operators is easy:

***Theorem* 1.1.17.** *Let $V \in L^2_{\mathrm{loc}}(\mathbb{R}^n)$ satisfy $V \geqslant 0$, almost everywhere. Then $-\Delta + V$ is essentially self-adjoint on $\mathcal{D} = \mathcal{C}_c^\infty(\mathbb{R}^n)$.*

PROOF. Recall Kato's Lemma (see, for example, Reed & Simon [**RS72**]) which says if u is a real function in $L^1_{\mathrm{loc}}(\mathbb{R}^n)$ such that $\Delta u \in L^1_{\mathrm{loc}}(\mathbb{R}^n)$, then one has, in the sense of distributions, that

$$\Delta|u| \geqslant \operatorname{sgn}(u)\Delta u.$$

We argue by contradiction. Suppose that $\mathcal{R} := (-\Delta + V + 1)\mathcal{D}$ is not dense in L^2; then we can find a non-zero function u in L^2 such that $\langle u, \varphi\rangle = 0$ for all functions φ in $\mathcal{R}$. Since $\mathcal{D}$ is stable under complex conjugation, it is easy to see that we can assume that u is real. We have that $(-\Delta + V + 1)u = 0$ in the sense of distributions. It follows immediately that $\Delta u \in L^1_{\mathrm{loc}}(\mathbb{R}^n)$, which allows us to apply Kato's Lemma:

$$\Delta|u| \geqslant \operatorname{sgn}(u)\Delta u = (V+1)|u| \geqslant |u|. \tag{1.1.4}$$

We regularize $|u|$, with the aid of an infinitely differentiable positive function e, with compact support and integral equal to 1, as follows. Let $e_\delta(x) :=$

$\delta^{-n}e(x/\delta)$ and $w_\delta := |u| * e_\delta$. The regularized function w_δ is an infinitely differentiable square integrable function and, applying (1.1.4), we have:

$$\Delta w_\delta = \Delta|u| * e_\delta \geqslant |u| * e_\delta = w_\delta,$$

$$\langle \Delta w_\delta, w_\delta\rangle \geqslant \|w_\delta\|^2. \tag{1.1.5}$$

On the other hand, $\Delta w_\delta = w * \Delta e_\delta \in L^2$, which by utilizing Corollary 1.1.16, implies that the function w_δ is in the domain of the negative self-adjoint operator Δ, thus $\langle w_\delta, \Delta w_\delta\rangle \leqslant 0$. Combining this with (1.1.5) we see that $w_\delta = 0$ for all δ. Since $w_\delta \to |u|$ in L^2 when $\delta \to 0$ we get $u = 0$, which is a contradiction. □

Up to this point we have not explained why our notion of "self-adjoint" is the same as the more traditional one. This we do now.

***Definition* 1.1.18.** The adjoint operator of A^* of $(\mathcal{D}, A)$ is the operator defined on the space $\mathcal{D}^*$ of vectors g such that the linear form $f \mapsto \langle g, Af\rangle$ is continuous and where $A^*(g)$ is defined by

$$\forall f \in \mathcal{D} \qquad \langle g, Af\rangle = \langle A^*g, f\rangle.$$

***Remark* 1.1.19.** The existence of a unique $A^*(g)$ satisfying the above equation follows from the Riesz Representation Theorem.

***Proposition* 1.1.20.** *Let $(\mathcal{D}, A)$ be a symmetric operator in H. The operator A is self-adjoint if and only if $\mathcal{D}$ coincides with the set of vectors g such that there exists a constant $c(g)$ satisfying*

$$\forall f \in \mathcal{D} \qquad |\langle g, Af\rangle| \leqslant c(g)\|f\|_H. \tag{1.1.6}$$

In other words, A is self-adjoint if and only if $A = A^*$.

Proof. We first suppose that A is self-adjoint. If $g \in \mathcal{D}$, then we have, for all $f \in \mathcal{D}$, the relation $\langle Af, g\rangle = \langle f, Ag\rangle$, which shows the continuity $f \mapsto \langle Af, g\rangle$ on H as a function of f. Conversely the condition (1.1.6) implies the continuity of $f \mapsto \langle g, if - Af\rangle$ and thus the existence of a vector $\psi \in H$ such that $\langle g, if - Af\rangle = \langle \psi, f\rangle$. In particular we set $f = R_i\varphi$ in the preceding relation. We then have $\langle g, \varphi\rangle = \langle \psi, R_i\varphi\rangle = \langle R_{-i}\psi, \varphi\rangle$. Since φ is arbitrary, we have $g = R_{-i}\psi$, which is an element of $\mathcal{D}$.

Conversely, suppose that $\mathcal{D}$ is characterized by the property (1.1.6). We will argue by contradiction to show that A is self-adjoint. First of all, A is closed. In fact, if $g_n \to g$ and $Ag_n \to h$ in H, then for $f \in D$, we have:

$$|\langle g, Af\rangle| = \lim_{n\to\infty} |\langle g_n, Af\rangle| = \lim_{n\to\infty} |\langle Ag_n, f\rangle| = |\langle h, f\rangle| \leqslant \|h\|\|f\|,$$

which implies $g \in \mathcal{D}$. Now suppose that $(i - A)\mathcal{D}$ is not dense. Then there exists a non-zero vector $\psi \in H$ such that $\langle \psi, (i - A)\varphi\rangle = 0$, for all $\varphi \in \mathcal{D}$. Since the zero linear form is continuous, the condition (1.1.6) shows that $\psi \in \mathcal{D}$, and by symmetry we have $\langle(-i - A)\psi, \varphi\rangle = 0$ for all φ, which would imply that $i\psi + A\psi = 0$, which by (1.1.3) leads to the contradiction $\psi = 0$. Therefore $(i - A)\mathcal{D}$ is dense in H. The same argument works for $-i$, thus by Proposition 1.1.9 the operator A is self-adjoint on $\mathcal{D}$. □

***Corollary* 1.1.21.** *The closure of the domain $\mathcal{D}$ of an essentially self-adjoint operator $(\mathcal{D}_0, A)$ is the set of vectors g in H such that $\langle g, Af\rangle$ is a continuous function of f from H to $\mathbb{C}$.*

***Exercise* 1.1.22 (*the Dirichlet Laplacian*). .** Let G be an open subset of $\mathbb{R}^d$ and $\mathcal{D}_0$ the space $\mathcal{C}_c^\infty(G)$ of $\mathcal{C}^\infty$ functions with compact support in G. We equip $\mathcal{D}_0$ with the norm

$$\|u\|_1 = \Big(\int_G |\nabla u|^2 + |u|^2\, dx\Big)^{1/2}$$

and the corresponding scalar product $\langle \cdot\,, \cdot\rangle_1$. The completion $\mathcal{D}_1$ of $\mathcal{D}_0$ with respect to this norm is injected into $H = L^2(G)$. Since any element w of $\mathcal{D}_1$ is the limit of a sequence w_n of elements in $\mathcal{D}_0$, it is sufficient to prove that if w_n converges to 0 in L^2 then $w = 0$. To show this let $\varphi \in \mathcal{D}_0$. Since

$$\langle w, \varphi\rangle_1 = \lim_{n\to\infty} \langle w_n, \varphi\rangle_1 = \langle w_n, -\Delta\varphi + \varphi\rangle_{L^2} = 0$$

and φ is arbitrary, we have $w = 0$. We denote by $\mathcal{D}$ the set of functions u in $\mathcal{D}_1$ such that the linear form $\varphi \mapsto \langle \varphi, u\rangle_1$ on $\mathcal{D}_0$ is continuous with respect to the norm L^2. With the aid of the Riesz Representation Theorem, this linear form can be written in a unique manner as $\langle \varphi, Au\rangle_{L^2(g)}$. Define $\Delta_{\mathrm{d}} := -A + \mathrm{Id}$. The operator Δ_{d} defined on $\mathcal{D}$ is called the Laplacian on G with Dirichlet boundary conditions. It follows from Proposition 1.1.20 that it is self-adjoint.

***Remark* 1.1.23 (*the Friedrichs extension*). .** Note that in the preceding example we did not use the special properties of differential operators. The method extends immediately to the case of a positive operator B_0 defined on a domain $\mathcal{D}_0$ in H. One just uses the norm $(\|u\|_1)^2 = \langle u, B_0 u\rangle + \|u\|_H^2$ in place of the Dirichlet norm in the above example and argue just as before.

1.2. Spectral decomposition of self-adjoint operators

We fix a self-adjoint operator $(A, \mathcal{D})$ on H. The spectral measure of A associated with a vector ψ of norm 1 is a probability measure characterized mathematically by the formula (1.2.1) below. It is of fundamental importance in physics because it governs the quantum mechanical uncertainty when one measures the observable defined by A in the state ψ. See, for example, [**LLB83**].

1.2.1. Construction of spectral measures. We denote by $C \subset \mathbb{C}(X)$ the space of rational functions on $\mathbb{C}$ with no real poles and bounded at infinity. The elements of C are exactly those that can be written:

$$F(z) = \alpha_0 + \sum_{k=1}^{p} \sum_{m=1}^{n_k} \frac{\alpha_{k,m}}{(\lambda_k - z)^m} \quad \text{with } \lambda_k \notin \mathbb{R},$$

and this representation is unique. We refer to the elements of C as fractions. For $F \in C$, we define a bounded operator by:

$$F(A) = \alpha_0 \operatorname{Id} + \sum_{k=1}^{p} \sum_{m=1}^{n_k} \alpha_{k,m} \left(R_{\lambda_k}\right)^m .$$

We say that $F \geqslant 0$ if for all $z \in \mathbb{R}$ we have $F(z) \geqslant 0$. We define the fraction F^* from the fraction F by changing α_k into $\overline{\alpha_k}$ and λ_k into $\overline{\lambda_k}$. In other words $F^*(z) = \overline{F}(\overline{z})$.

***Lemma* 1.2.1.** *The fraction $F \in C$ is positive if and only if it can be factored in the form $G\,G^*$ with $G \in C$.*

Proof. If we have this factorization, we have for $x \in \mathbb{R}$ that $F(x) = G(x)\overline{G}(x) \geqslant 0$. Conversely, since F is real on the real axis, we have for all real x that $\overline{F}(x) = F^*(x) = F(x)$, and thus by analyticity $F = F^*$ everywhere and formally in $\mathbb{C}(X)$. We deduce from this that F is the quotient $\dfrac{P(x)}{Q(x)}$ of two real polynomials. The denominator does not vanish on the real axis and can be supposed positive. Hence P and Q are positive and thus they can be written $P_0 P_0^*$ and $Q_0 Q_0^*$. □

We denote by C_{r} the set of fractions such that $F = F^*$. We have just seen that this means that F is real valued on the real numbers. We will now make explicit the properties of the "functional calculus" $F \mapsto F(A)$. We define a norm on C by

$$\|F\|_\infty = \sup_{x \in \mathbb{R}} |F|(x).$$

(1) For $F \in C$ the operator $F(A)$ is bounded.
(2) $(F \cdot G)(A) = F(A)G(A)$ or more precisely the functional calculus is a homomorphism of the algebra C into the algebra of bounded operators.
(3) $F(A)^* = F^*(A)$, where "$*$" in the left member denotes the adjoint of a bounded operator. In particular, $F(A)$ is symmetric if $F \in C_{\mathrm{r}}$.
(4) $F \geqslant 0$ implies that $F(A) \geqslant 0$, in the sense of order on symmetric operators.
(5) The linear mapping $F \mapsto F(A)$ is continuous from C to the space of bounded operators with respect to the usual operator norm.

Proof. The first assertion follows from the definition of the resolvent operators.

The second is proved with the aid of the resolvent equation. By linearity, we are reduced to considering the simple cases

$$F(z) = \frac{1}{(a-z)^k}, \qquad G(z) = \frac{1}{(b-z)^h}, \quad h, k \geqslant 0,$$

where we can suppose that $b \neq a$, the case of equality being trivial. In order to argue by induction on $k+h$ we note that:

$$(b-a)FG(z) = (a-z)^{1-k}(b-z)^{1-h}\Big(\frac{1}{a-z} - \frac{1}{b-z}\Big).$$

Thus utilizing the induction hypothesis and the resolvent equation we have:

$$\begin{aligned}(b-a)FG(A) &= R_a^k R_b^{h-1} - R_a^{k-1} R_b^h = R_a^{k-1} R_b^{h-1}(R_a - R_b)\\ &= (b-a) R_a^k R_b^h.\end{aligned}$$

The third assertion is proved by checking that $R_\lambda = R^*_{\overline{\lambda}}$ for all symmetric operators when $\lambda \in \rho(A)$ and $\overline{\lambda} \in \rho(A)$. The fourth follows from Lemma 1.2.1. In fact, if $F \geqslant 0$ we are able by the lemma to write $F = G^*G$ and thus

$$\langle F(A)x, x\rangle = \langle G(A)x, G(A)x\rangle \geqslant 0.$$

It is sufficient to establish the last assertion for all $F \in C_{\mathrm{r}}$ because we can write any $H \in C$ as a linear combination of elements in C_{r}:

$$H = \frac{H + H^*}{2} + i\frac{H - H^*}{2i}.$$

We next note that for all $t \in \mathbb{R}$ we have $-\|F\| \leqslant F(t) \leqslant \|F\|$, which by (4) above implies that for $M := \|F\|$,

$$0 \leqslant F(A) + M\,\mathrm{Id} \leqslant 2M\,\mathrm{Id}\,.$$

In other words for all $x \in H$ we have the inequality:

$$0 \leqslant q(x) \leqslant 2M\|x\|^2 \quad \text{where } q(x) = \big\langle x, (F(A) + M\,\mathrm{Id})x\big\rangle.$$

By applying the Schwarz inequality to the quadratic form q, we obtain:

$$|\langle y, (F(A) + M\,\mathrm{Id})x\rangle| \leqslant 2M\|x\|\,\|y\|.$$

Finally, since x and y are arbitrary we have that: $\big\|F(A) + M\,\mathrm{Id}\big\| \leqslant 2M$ or $\|F(A)\| \leqslant 3\|F\|$. In fact, the inequality without the factor 3 is still true and can be proved using the spectral theorem. $\square$

We consider the compact space $\underline{\mathbb{R}} := \mathbb{R} \cup \{\infty\}$, which is obtained by adding a point at infinity to $\mathbb{R}$.[3] Since the functions of C_{r} have the same limit for $x \to \pm\infty$ they can be extended to functions on $\underline{\mathbb{R}}$ and by the Stone-Weierstrass Theorem we see that they form a dense subspace of $\mathcal{C}(\underline{\mathbb{R}}, \mathbb{R})$. Let φ be a vector in H. The linear form defined on C_{r} by $F \mapsto \langle F(A)\varphi, \varphi\rangle$ is continuous by the last part of the preceding lemma and thus extends to a linear form on $\mathcal{C}(\underline{\mathbb{R}}, \mathbb{R})$. This positive linear form is a bounded positive measure on $\underline{\mathbb{R}}$ and is denoted by μ_φ. By linearity we extend the definition to functions in C:

$$\forall F \in C \qquad \langle F(A)\varphi, \varphi\rangle = \int F(x)\,\mu_\varphi(dx). \tag{1.2.1}$$

[3]For example, we can identify a circle minus a point with $\mathbb{R}$ by $\theta \mapsto \mathrm{tg}(\theta/2)$.

***Lemma* 1.2.2.** *If $\Re(\lambda)$ remains bounded and $\Im(\lambda)$ tends to infinity, λR_λ tends strongly to* Id.

Proof. From the formula (1.1.2), we have $\|\lambda R_\lambda\| \leqslant |\lambda|\,|\Im(\lambda)|^{-1}$; thus the operators $\lambda R_\lambda - \mathrm{Id}$ remain uniformly bounded. Because $\mathcal{D}$ is dense it is sufficient to show the convergence of $\lambda R_\lambda \psi$ to ψ for all $\psi \in \mathcal{D}$. The latter results from:

$$\|(\lambda R_\lambda - \mathrm{Id})\psi\| = \|R_\lambda A\psi\| \leqslant |\Im(\lambda)|^{-1}\|A\psi\|.$$

□

***Proposition* 1.2.3.** *For any $\varphi \in H$ there exists a unique positive measure μ_φ on $\mathbb{R}$ satisfying (1.2.1). This measure has mass $\|\varphi\|^2$.*

Proof. The total mass formula follows by setting F equal to 1 in (1.2.1). It remains to show that the measure μ_φ is supported by $\mathbb{R} = \underline{\mathbb{R}}/\{\infty\}$. To show this we note that the function $F_\alpha(t) = \dfrac{\alpha^2}{t^2+\alpha^2}$ converges to 1 when $\alpha \to +\infty$, except for $t = \infty$. Consequently the dominated convergence theorem implies

$$\mu_\varphi(\mathbb{R}) = \lim_{\alpha\to\infty} \int F_\alpha \, d\mu_\varphi = \lim \langle F_\alpha(A)\varphi, \varphi\rangle.$$

But since $F_\alpha(A) = \frac{1}{2}(\alpha i R_{\alpha i} - \alpha i R_{-\alpha i})$, the preceding lemma implies:

$$\lim_{\alpha\to\infty} F_\alpha(A) = \mathrm{Id}\,.$$

Thus we have $\mu_\varphi(\mathbb{R}) = \|\varphi\|^2$ which in turn implies μ_φ is supported by $\mathbb{R}$. □

1.2.2. Functional calculus. The simplest example of a self-adjoint operator is multiplication by a real-valued function on the space L^2. In fact, any self-adjoint operator A on a Hilbert space H is unitarily equivalent to this model:

***Theorem* 1.2.4 (*spectral decomposition*).** . *There exists a σ-finite measure space $(W, \mathcal{F}, \mu)$, a measurable real-valued function χ on W, and a unitary operator U from H to $L^2(\mu)$ that transforms A into the multiplication operator by χ :*

$$\varphi \in D(A) \Leftrightarrow \chi U(\varphi) \in L^2(\mu) \quad \text{and} \quad A\varphi = U^{-1}\big(\chi U(\varphi)\big). \tag{1.2.2}$$

More precisely, we can realize W as a countable union of spaces $\mathbb{R}_k$ that are disjoint images of $\mathbb{R}$ by bijections b_k, the measure μ as a sum of copies of spectral measures, i.e., $\mu = \sum_k b_k(\mu_{\psi_k})$, and χ as the identity function $\chi(x) = x$ on each $\mathbb{R}_k$.

Proof. We begin by considering the case where there exists a cyclic vector ψ_1, that is to say, the "orbit" of ψ_1 defined by $\Omega = \{F(A)\psi_1 \,:\, F \in C\}$ is dense in H. Note that any element of the orbit can be written in an essentially unique way in the form $F(A)\psi_1$.

In fact, if $F(A)\psi_1 = 0$ we also have: $0 = G(A)F(A)\psi_1 = F(A)G(A)\psi_1$ for all $G \in C$ and since the $G(A)\psi_1$ are dense we obtain $F(A) = 0_{\mathrm{op}}$. This in turn implies that:

$$0 = \langle F(A)\psi_1, F(A)\psi_1\rangle = \langle \psi_1, F^*(A)F(A)\psi_1\rangle.$$

Finally using (1.2.1) we see that $|F|(x) = 0$ for μ_{ψ_1}-almost all $x \in \mathbb{R}$. Conversely, if $F = H$ μ_{ψ_1}-almost everywhere analogous calculations show that $F(A)\psi_1 = H(A)\psi_1$.

Taking $\mu = \mu_{\psi_1}$ we can define U on Ω by

$$U[F(A)\psi_1] := F.$$

The mapping U is an isometry with dense image because:

$$\begin{aligned}\|F(A)\psi_1\|^2 &= \langle F(A)\psi_1, F(A)\psi_1\rangle \\ &= \langle \psi_1, F^*(A)F(A)\psi_1\rangle = \int_{\mathbb{R}} \overline{F}(x)F(x)\, d\mu_{\psi_1}.\end{aligned}$$

Thus it can be extended into an isometry H onto $L^2(\mu)$. It is clear by construction that any operator $G(A)$ is transformed by this isometry into the multiplication operator by G.

In order to find the transform of A under this isometry, we write $A = \lim_{\lambda\to+\infty} G_\lambda(A)$ where $G_\lambda(x) = \dfrac{\lambda x}{\lambda - x}$. Since $G_\lambda(A) = \lambda R_\lambda A$, Lemma 1.2.2 implies that for all $\varphi \in D(A)$ the vector $[G_\lambda A](\varphi)$ converges to $A\varphi$, when $\Re(\lambda)$ remains bounded and $\Im(\lambda)$ tends to infinity. It follows from this that $U\big(G_\lambda(A)\varphi\big) = G_\lambda \cdot U(\varphi)$ converges to $U(A\varphi)$. But the limit of $G_\lambda \cdot U(\varphi)$ in L^2 is determined directly by looking at a subsequence which converges almost everywhere: $G_\lambda(x)$ tends to x and we get $x\,U\varphi(x)$ as we claimed above.

We also have the inclusion $U(\mathcal{D}) \subset \{f \in L^2(\mu) \,:\, \chi f \in L^2(\mu)\}$ where $\chi(x) = x$ and $U(\mathcal{D})$ contains all of the functions $F \in C_{\mathrm{c}}$. Since $U(A)$ is self-adjoint, and thus closed, it is easy to see that we have equality.

In the case where there is a cyclic vector we have established the theorem with a single copy of $\mathbb{R}$ and a simple spectrum. In the general case, we begin by choosing a non-zero vector ψ_1 in $D(A)$ and forming the orbit Ω_1 generated as above using ψ_1. If ψ_1 is not cyclic we choose a non-zero vector $\psi_2 \in D(A) \cap \Omega_1^\perp$ and form the orbit Ω_2 generated by ψ_2. In this way we construct by recurrence a (possibly denumerable) sequence of vectors (ψ_n) which leads, since H is separable, to the Hilbertian direct sum:

$$H = \bigoplus_n \overline{\{F(A)\psi_n \,:\, F \in C\}}.$$

We then repeat the preceding construction for each orbit. □

***Exercise* 1.2.5.** Show that the support of μ_ψ is contained in $\sigma(A)$ and that $\sigma(A) = \overline{\bigcup_n \mathrm{supp}(\mu_{\psi_n})}$.

***Exercise* 1.2.6.** In the case where $H = \mathbb{C}^d$ with the usual scalar product and A is given by a Hermitian matrix describe the relation between the spectral theorem and ordinary diagonalization.

***Exercise* 1.2.7.** Prove that a bounded symmetric operator is self-adjoint and that its norm is equal to its spectral radius, i.e.,

$$\|A\| = \sup_{\lambda \in \sigma(A)} |\lambda|.$$

Show that if A is self-adjoint and bounded below the best lower bound for the operator A is $m = \inf(\sigma(A))$.

***Exercise* 1.2.8.** Let (a, a') and (b, b') be two fixed non-zero elements of $\mathbb{R}^2$. Let $\mathcal{D}$ be the space of $\mathcal{C}^2$ functions f on $[0,1]$ satisfying $af'(0) - a'f(0) = bf'(1) - b'f(1) = 0$. Set $Af := -f''$ for $f \in \mathcal{D}$.

Show that A is symmetric and bounded below. For the bounded below property first prove the following inequality: for any $\delta > 0$

$$\big|\|f\|_{L^2([0,\delta])} - \sqrt{\delta} f(0)\big| \leqslant \frac{\delta}{\sqrt{2}} \Big(\int_0^\delta |f'(t)|^2 \, dt\Big)^{1/2}.$$

Prove that A is essentially self-adjoint. One will show the following elementary hypoellipticity property: any distribution solution of $u'' + \lambda u = 0$ on $]0,1[$ is a $\mathcal{C}^\infty$ function on $]0,1[$ and, in fact, on $[0,1]$.

Suppose from now on that $a = b = 0$ and $a' = b' = 1$, i.e., the Dirichlet boundary conditions hold. By letting $f(t) = \sin(\pi t) g(t)$, prove Wirtinger's inequality: if $f \in \mathcal{C}^1([0,1])$ with $f(0) = f(1) = 0$:

$$\int_0^1 f'^2(t) \, dt \geqslant \pi^2 \int_0^1 f^2(t).$$

Deduce from this the lower bound on the spectrum of A. Prove that the sequence of functions $\frac{1}{\sqrt{2}} \sin(n\pi x)$ with $n \in \mathbb{N}^*$ is an orthonormal basis for the Hilbert space $L^2([0,1])$ and reproduce the preceding result.

The definition of an arbitrary Borel measurable real-valued function of a self-adjoint operator A is now very simple. Given such a function f on $\mathbb{R}$, we define the self-adjoint operator $f(A)$ as follows: begin by utilizing the unitary operator U of the spectral decomposition of A to transform A into an operator $\widetilde{A}$ of multiplication by χ on the space $L^2(\mu)$. Then define $f(\widetilde{A})$ as the operator of multiplication by $f(\chi)$ on the domain $\{\varphi \in L^2 : \varphi f(\chi) \in L^2\}$ and transform it back using U^{-1}. One can show that this definition does not depend on this choice of U. See Exercise 1.2.10.

***Remark* 1.2.9.** There also exists another functional calculus in a different setting; see [**DS63**]. Let A be a bounded operator on a Banach space E and f a holomorphic function on an open set G containing $\sigma(A)$. We then define $f(A)$ using an extension of the Cauchy formula for a contour $\mathcal{C}$

contained in G and surrounding $\sigma(A)$ as follows:

$$f(A) = \frac{1}{2i\pi} \int_{\mathcal{C}} f(z) R_z \, dz.$$

***Exercise* 1.2.10.** Establish the following properties of the functional calculus $f \mapsto f(B)$ where B is the operator of multiplication by χ on the space $L^2(\mu)$ and f is a real-valued Borel-measurable function. If one restricts oneself to bounded functions then the mapping $f \to f(B)$ is continuous from L^∞ into the space of bounded operators on $L^2(\mu)$ with the usual operator norm. If f_n is a sequence of Borel measurable functions that converge to f, then for all $\lambda \in \mathbb{C} \setminus \mathbb{R}$ and all $\psi \in L^2(\mu)$, there is convergence of the resolvents, i.e.,

$$\lim_{n\to\infty} R\big(\lambda, f_n(B)\big)\psi = R\big(\lambda, f(B)\big)\psi.$$

Deduce from this that if a self-adjoint A on H is transformed into two multiplication operators χ and χ' on $L^2(W, \mu)$ and $L^2(W', \mu')$ respectively, then the operators $f(A)$ and $\big(f(A)\big)'$ defined by using the two spectral decompositions are the same. Carry out the proof in the following steps. Begin with the case where $f \in C_{\mathrm{r}}$, then where f is continuous and tends to 0 at infinity, then for f that are indicator functions for open sets, and finally utilize the monotone convergence theorem on monotone sequences of the preceding class of functions.

***Exercise* 1.2.11.** Let A be a positive self-adjoint operator that is invertible in H. Prove the inequality: $\|A + w\|^{-1} \leqslant w^{-1}$ for $w > 0$. Prove the following formula for all $\psi \in D(A^{-1/2})$:

$$A^{-1/2}(\psi) = \frac{1}{\pi} \int_0^{+\infty} w^{-\frac{1}{2}} (A + w)^{-1} \psi \, dw,$$

where the integral is the Bochner integral for functions with values in H.

***Exercise* 1.2.12.** Go back to the construction in Remark 1.1.23 of the Friedrichs' extension of a positive operator B. Show that $\mathcal{D}_1$ is the domain of the self-adjoint operator $B^{1/2} + \mathrm{Id}$.