

Spectral Theory

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Foreword

These notes are based on the semester project of Yann Péquignot, *Théorie spectrale et évolution en mécanique quantique*, which was supervised by Prof. Boris Buffoni and myself at EPFL (Lausanne) in 2008. I am especially indebted to Yann for the exceptional quality of his work, and his permission to use it as teaching material.

The goal of the course is to provide a straightforward but comprehensive proof of the spectral theorem for unbounded selfadjoint operators in Hilbert spaces, and some applications to elementary quantum mechanics. The main focus will be on the decomposition of a selfadjoint operator onto its family of spectral projections. Some elements of functional calculus will also be given.

We will start in Chapter 1 by some recalls about bounded operators in Hilbert spaces and their spectra, as well as important properties of projections and positive operators, which will play a crucial role in the main proofs. Chapter 2 will be devoted to the proof of the spectral theorem for bounded selfadjoint operators, while Chapter 3 will present the extension to the unbounded case. In Chapter 4 we will apply the spectral theorem to discuss Stone's theorem, which characterizes strongly continuous one-parameter groups of unitary transformations of the Hilbert space. After a brief exposition of the main concepts of quantum mechanics formulated in the Hilbert space framework, we will use Stone's theorem to define the operators representing the energy and the momentum of a quantum particle.

The original work, as well as the present version, are based on classic books which are listed in the Bibliography. However, considerable effort is made here to present a unified and self-contained theory. The student with basic knowledge of functional analysis in Hilbert spaces should be sufficiently equipped to read these notes. Of course, as always in mathematics, we can only recommend very active reading (doing the exercises, reproducing the proofs mentally and on paper, etc.) in order to get familiar with the theory.

As I am translating this work to English and adding extra material and exercises, I of course take full responsibility should there be any mistakes or imprecisions in the text.

Delft, February 2015

Terminology We shall speak of *unbounded operators* when referring to general, not necessarily bounded, operators. The price to pay for this abuse of terminology is that bounded operators become a special case of unbounded operators! But we prefer to live with this rather than repeatedly using the awkward phrase ‘general, not necessarily bounded, operators’.

The notion of selfadjointness for unbounded operators requires a careful definition (in particular the definition of the domain of the adjoint operator), while for a bounded operator A acting in a Hilbert space \mathcal{H} , it only amounts to requiring that A be symmetric, i.e. that $\langle Au, v \rangle = \langle u, Av \rangle$, for all $u, v \in \mathcal{H}$. If A is unbounded, it is also called symmetric provided the previous relation holds for all u, v in the domain of A . Throughout the course we shall reserve the term *selfadjoint* for unbounded operators, while bounded selfadjoint operators will merely be called *symmetric*.

Chapter 1

Preliminary notions

We start by recalling elements of the theory of linear operators acting in a Hilbert space \mathcal{H} . We present some basic results about bounded linear operators and some elementary properties of orthogonal projections.

1.1 Hilbert spaces

In these notes we will consider Hilbert spaces over the field \mathbb{C} of complex scalars. The definition of Hilbert space is as follows.

Definition 1.1.1 A **pre-Hilbert space** \mathcal{H} is a complex vector space endowed with an inner product $\langle \cdot, \cdot \rangle : \mathcal{H} \rightarrow \mathbb{C}$ satisfying

- (i) for all $u \in \mathcal{H}$, $\langle u, u \rangle \geq 0$, and $\langle u, u \rangle = 0$ if and only if $u = 0$;
- (ii) for all $u, v, w \in \mathcal{H}$, $\langle u + v, w \rangle = \langle u, w \rangle + \langle v, w \rangle$;
- (iii) for all $u, v \in \mathcal{H}$ and all $\lambda \in \mathbb{C}$, $\langle \lambda u, v \rangle = \lambda \langle u, v \rangle$;
- (iv) for all $u, v \in \mathcal{H}$, $\langle u, v \rangle = \overline{\langle v, u \rangle}$.

\mathcal{H} is called a **Hilbert space** if it is a Banach space for the norm $\|u\| := \sqrt{\langle u, u \rangle}$, i.e. if the metric space (\mathcal{H}, d) , with $d(u, v) := \|u - v\|$, is complete. ♦

We shall use the notations of Definition 1.1.1 throughout the text without further mention. We recall, without proof, the following fundamental property of the Hilbert norm.

Theorem 1.1.2 (Cauchy-Schwarz Inequality) *For all $u, v \in \mathcal{H}$, there holds*

$$|\langle u, v \rangle| \leq \|u\| \|v\|.$$

A typical example of Hilbert space is the following.

Example 1.1.3 (The Hilbert space $L^2[0, 1]$) Consider the set of functions $u : [0, 1] \rightarrow \mathbb{C}$ such that

$$\int_{[0,1]} |u(x)|^2 dx < \infty,$$

where the integral is taken with respect to the Lebesgue measure on $[0, 1]$. We define an equivalence relation by

$$u \sim v \quad \text{iff} \quad u = v \text{ almost everywhere.}$$

We denote by $L^2[0, 1]$ the set of equivalence classes obtained in this way. This is a (complex) Hilbert space for the following operations:

$$\begin{aligned} (\lambda u)(x) &= \lambda u(x), \quad (\lambda \in \mathbb{C}) \\ (u + v)(x) &= u(x) + v(x), \\ \langle u, v \rangle &= \int_{[0,1]} u(x) \overline{v(x)} dx, \end{aligned}$$

where u, v denote any elements of their respective equivalence classes.

The corresponding norm is given by

$$\|u\| = \left(\int_{[0,1]} |u(x)|^2 dx \right)^{1/2}$$

and the Cauchy-Schwarz inequality takes the form

$$\int_{[0,1]} u \bar{v} dx \leq \left(\int_{[0,1]} |u|^2 dx \right)^{1/2} \left(\int_{[0,1]} |v|^2 dx \right)^{1/2}. \quad \blacklozenge$$

In fact, Example 1.1.3 is generic, in the sense that all infinite-dimensional *separable* Hilbert spaces are isomorphic to $L^2[0, 1]$.

The Cartesian product $\mathcal{H} \times \mathcal{H}$ has a natural Hilbert space structure given by the following operations:

$$\begin{aligned} \lambda(u_1, v_1) &= (\lambda u_1, \lambda v_1), \\ (u_1, v_1) + (u_2, v_2) &= (u_1 + u_2, v_1 + v_2), \\ \langle (u_1, v_1), (u_2, v_2) \rangle &= \langle u_1, u_2 \rangle + \langle v_1, v_2 \rangle, \end{aligned}$$

for all $(u_1, v_1), (u_2, v_2) \in \mathcal{H} \times \mathcal{H}$ and all $\lambda \in \mathbb{C}$. The metric topology induced by the inner product of $\mathcal{H} \times \mathcal{H}$ coincides with the product topology inherited from \mathcal{H} .

1.2 Linear operators

In these notes we are interested in linear operators between Hilbert spaces \mathcal{H}_1 and \mathcal{H}_2 , that is, mappings $A : \mathcal{H}_1 \rightarrow \mathcal{H}_2$ which preserve the vector space structures of \mathcal{H}_1 and \mathcal{H}_2 . In the first part we will consider linear operators which are bounded, i.e. continuous, and so also preserve the topology. Then we will deal with general, unbounded, operators.

We start by recalling the basic notions of the theory of linear operators in the more general framework of operators $A : \mathcal{X}_1 \rightarrow \mathcal{X}_2$ acting between two Banach spaces \mathcal{X}_1 and \mathcal{X}_2 .

Definition 1.2.1 A **linear operator** A from \mathcal{X}_1 to \mathcal{X}_2 is a mapping $A : \mathcal{X}_1 \rightarrow \mathcal{X}_2$ such that:

- (i) for all $u, v \in \mathcal{X}_1$, $A(u + v) = A(u) + A(v)$;
- (ii) for all $\lambda \in \mathbb{C}$ and all $u \in \mathcal{X}_1$, $A(\lambda u) = \lambda A(u)$.

We shall merely write Au for the image $A(u)$ of the element $u \in \mathcal{X}_1$. The **range** of A is the subspace of \mathcal{X}_2 defined as

$$\text{rge } A = \{Au ; u \in \mathcal{X}_1\},$$

and the **kernel** of A is the subspace of \mathcal{X}_1 defined as

$$\ker A = \{u \in \mathcal{X}_1 ; Au = 0\}.$$

If there is a constant $C \geq 0$ such that

$$\|Au\|_{\mathcal{X}_2} \leq C \|u\|_{\mathcal{X}_1} \quad \text{for all } u \in \mathcal{X}_1, \quad (1.2.1)$$

we say that A is **bounded**. The norm of $A \in \mathcal{B}(\mathcal{X}_1, \mathcal{X}_2)$ is defined as the infimum of all $C \geq 0$ satisfying (1.2.1) and can be characterized as (Problem 1.2)

$$\|A\|_{\mathcal{B}(\mathcal{X}_1, \mathcal{X}_2)} = \sup_{\|u\|_{\mathcal{X}_1}=1} \|Au\|_{\mathcal{X}_2} = \sup_{\|u\|_{\mathcal{X}_1} \leq 1} \|Au\|_{\mathcal{X}_2}. \quad (1.2.2)$$

The set $\mathcal{B}(\mathcal{X}_1, \mathcal{X}_2)$ of bounded operators from \mathcal{X}_1 to \mathcal{X}_2 , endowed with the norm $\|\cdot\|_{\mathcal{B}(\mathcal{X}_1, \mathcal{X}_2)}$, is a Banach space for the operations:

$$\begin{aligned} (A + B)u &= Au + Bu & \text{for all } A, B \in \mathcal{B}(\mathcal{X}_1, \mathcal{X}_2), u \in \mathcal{X}_1; \\ (\lambda A)u &= \lambda Au & \text{for all } A \in \mathcal{B}(\mathcal{X}_1, \mathcal{X}_2), \lambda \in \mathbb{C}, u \in \mathcal{X}_1. \end{aligned}$$

We shall simply write $\|u\|$, $\|Au\|$, $\|A\|$ when there is no risk of confusion. ♦

- Remark 1.2.2** (a) The above definitions can be made when \mathcal{X}_1 and \mathcal{X}_2 are merely normed vector spaces. The space of bounded operators $\mathcal{B}(\mathcal{X}_1, \mathcal{X}_2)$ is a Banach space for the norm $\|\cdot\|_{\mathcal{B}(\mathcal{X}_1, \mathcal{X}_2)}$ defined as in (1.2.2), provided that the target space \mathcal{X}_2 is Banach. Note that the bounded linear operators from \mathcal{X}_1 to \mathcal{X}_2 are precisely those linear operators which are continuous with respect to the topologies of \mathcal{X}_1 and \mathcal{X}_2 , induced by the norms $\|\cdot\|_{\mathcal{X}_1}$ and $\|\cdot\|_{\mathcal{X}_2}$, respectively.
- (b) In these notes we shall be mainly concerned with Hilbert spaces, and especially the case where $\mathcal{H} := \mathcal{X}_1 = \mathcal{X}_2$. Then we shall simply write $\mathcal{B}(\mathcal{H})$ instead of $\mathcal{B}(\mathcal{H}, \mathcal{H})$. If $A, B \in \mathcal{B}(\mathcal{H})$, we then have $\|AB\| \leq \|A\| \|B\|$.

In the context of Banach spaces, we now recall a fundamental result due to Banach and Steinhaus. The proof can be found e.g. in [Fri82, Kre78, RSN90, Wei80].

Theorem 1.2.3 (Uniform Boundedness Principle) *Consider a sequence $(A_n)_{n \in \mathbb{N}}$ of bounded operators acting between Banach spaces $\mathcal{X}_1, \mathcal{X}_2$. If, for all $u \in \mathcal{X}_1$, we have*

$$\sup_{n \in \mathbb{N}} \|A_n u\|_{\mathcal{X}_2} < \infty,$$

then there holds

$$\sup_{n \in \mathbb{N}} \|A_n\|_{\mathcal{B}(\mathcal{X}_1, \mathcal{X}_2)} < \infty.$$

Remark 1.2.4 In Theorem 1.2.3, one can merely assume that \mathcal{X}_2 is a normed vector space; completeness is not needed in the proof.

Definition 1.2.5 Let $(A_n)_{n \in \mathbb{N}} \subset \mathcal{B}(\mathcal{X}_1, \mathcal{X}_2)$ be a sequence of bounded linear operators.

- (i) If there is an operator $A \in \mathcal{B}(\mathcal{X}_1, \mathcal{X}_2)$ such that $\lim_{n \rightarrow \infty} \|A_n - A\|_{\mathcal{B}(\mathcal{X}_1, \mathcal{X}_2)} = 0$, we say that the sequence $(A_n)_{n \in \mathbb{N}}$ **converges (in operator norm)** to A .
- (ii) If, for all $u \in \mathcal{X}_1$, the limit $\lim_{n \rightarrow \infty} A_n u$ exists in \mathcal{X}_2 , we say that the sequence $(A_n)_{n \in \mathbb{N}}$ is **strongly convergent**. The mapping $u \mapsto \lim_{n \rightarrow \infty} A_n u$ is then clearly a linear operator from \mathcal{X}_1 to \mathcal{X}_2 . ♦

Corollary 1.2.6 *Let $(A_n)_{n \in \mathbb{N}} \subset \mathcal{B}(\mathcal{X}_1, \mathcal{X}_2)$. Suppose $(A_n)_{n \in \mathbb{N}}$ is strongly convergent and let $A : \mathcal{X}_1 \rightarrow \mathcal{X}_2$ be the operator defined by $u \mapsto \lim_{n \rightarrow \infty} A_n u$. Then $A \in \mathcal{B}(\mathcal{X}_1, \mathcal{X}_2)$.*

Proof. For all $u \in \mathcal{X}_1$, it follows by continuity of the norm (Problem 1.1) that

$$\lim_{n \rightarrow \infty} \|A_n u\| = \|Au\| \quad \text{exists.}$$

Therefore the sequence $(\|A_n u\|)_{n \in \mathbb{N}}$ is bounded for all $u \in \mathcal{X}_1$. It then follows from the Uniform Boundedness Principle that $(\|A_n\|)_{n \in \mathbb{N}}$ is bounded by a constant $C \geq 0$. Thus, for all $u \in \mathcal{X}_1$,

$$\|Au\| = \lim_{n \rightarrow \infty} \|A_n u\| \leq C \|u\|,$$

and so A is bounded. □

We next recall another fundamental result in the context of two Banach spaces $\mathcal{X}_1, \mathcal{X}_2$. The **graph** of a linear operator $A : \mathcal{X}_1 \rightarrow \mathcal{X}_2$ is defined as the subspace

$$\mathbf{G}_A = \{(u, Au) ; u \in \mathcal{X}_1\} \subseteq \mathcal{X}_1 \times \mathcal{X}_2.$$

A natural norm on $\mathcal{X}_1 \times \mathcal{X}_2$ is given by

$$\|(u, v)\| = \|u\| + \|v\|.$$

Note, however, that all product norms ¹ are equivalent, so your favorite choice is good enough.

In Problem 1.3, we will prove the following theorem, which is a consequence of the bounded inverse theorem.

Theorem 1.2.7 (Closed Graph Theorem) *$A : \mathcal{X}_1 \rightarrow \mathcal{X}_2$ is bounded if and only if \mathbf{G}_A is a closed subset of $\mathcal{X}_1 \times \mathcal{X}_2$.*

A **(continuous) linear functional** on the Hilbert space \mathcal{H} is an element of the **dual space** of \mathcal{H} , $\mathcal{H}^* = \mathcal{B}(\mathcal{H}, \mathbb{C})$. The linear functionals on a Hilbert space are characterized by the following theorem due to F. Riesz, the proof of which can be found e.g. in [Fri82, p. 206] or [Kre78, p. 188].

Theorem 1.2.8 (Riesz's Representation Theorem) *Let \mathcal{H} be a Hilbert space. For any $u_0 \in \mathcal{H}$, the formula*

$$f(u) = \langle u, u_0 \rangle \quad \forall u \in \mathcal{H}, \tag{1.2.3}$$

defines a linear functional on \mathcal{H} , with $\|f\| = \|u_0\|$. Conversely, for any linear functional f on \mathcal{H} , there exists a unique $u_0 \in \mathcal{H}$ such that (1.2.3) holds.

We complete this section by recalling some spectral properties of linear operators. The fundamental problem motivating the definition of the spectrum is the following. Let \mathcal{X} be a normed vector space and $A \in \mathcal{B}(\mathcal{X})$. For which values of $\lambda \in \mathbb{C}$ does the equation

$$(A - \lambda I)u = v \tag{1.2.4}$$

¹ $\|(\cdot, \cdot)\|$ is a product norm on $\mathcal{X}_1 \times \mathcal{X}_2$ iff $\|(u, 0)\| = \|u\|_{\mathcal{X}_1} \ \forall u \in \mathcal{X}_1$ and $\|(0, v)\| = \|v\|_{\mathcal{X}_2} \ \forall v \in \mathcal{X}_2$.

have a unique solution $u \in \mathcal{X}$, for any given $v \in \mathcal{X}$?

Firstly, the solution will be unique if $\ker(A - \lambda I) = \{0\}$, i.e. if λ is not an eigenvalue of A . Furthermore, there will be a solution for any $v \in \mathcal{X}$ provided $\text{rge}(A - \lambda I) = \mathcal{X}$. Relaxing slightly the latter condition (we only require that (1.2.4) can be solved for v in a dense subspace of \mathcal{X}), the solution to this problem can be stated by the introduction of the resolvent set of A .

Definition 1.2.9 Let $A \in \mathcal{B}(\mathcal{X})$ be a bounded linear operator acting in a complex normed vector space $\mathcal{X} \neq \{0\}$, and $I : \mathcal{X} \rightarrow \mathcal{X}$ be the identity. The **resolvent set** $\rho(A)$ of A is the set of all complex numbers λ such that $\ker(A - \lambda I) = \{0\}$, $\text{rge}(A - \lambda I)$ is dense in \mathcal{X} and the inverse operator $(A - \lambda I)^{-1} : \text{rge}(A - \lambda I) \rightarrow \mathcal{X}$ is bounded. The **spectrum** $\sigma(A)$ of A is defined as $\sigma(A) = \mathbb{C} \setminus \rho(A)$. It can be decomposed as

$$\sigma(A) = \sigma_p(A) \cup \sigma_c(A) \cup \sigma_r(A), \quad (1.2.5)$$

where the sets $\sigma_p(A), \sigma_c(A), \sigma_r(A)$ are pairwise disjoint subsets of \mathbb{C} defined as follows:

- (i) $\lambda \in \sigma_p(A)$ iff $\ker(A - \lambda I) \neq \{0\}$, i.e. λ is an eigenvalue of A ;
- (ii) $\lambda \in \sigma_c(A)$ iff $\ker(A - \lambda I) = \{0\}$ and $\text{rge}(A - \lambda I)$ is dense in \mathcal{X} but $(A - \lambda I)^{-1}$ is not bounded;
- (iii) $\lambda \in \sigma_r(A)$ iff $\ker(A - \lambda I) = \{0\}$ but $\text{rge}(A - \lambda I)$ is not dense in \mathcal{X} .

The sets $\sigma_p(A)$, $\sigma_c(A)$ and $\sigma_r(A)$ are respectively called the **point spectrum**, the **continuous spectrum** and the **residual spectrum**. ♦

Remark 1.2.10 (a) The requirement that $(A - \lambda I)^{-1}$ be bounded is to ensure that, if $\lambda \in \rho(A)$, the solution u of (1.2.4) depends continuously on the data v .

(b) We will see in problem 1.4 that, if \mathcal{X} is Banach, then $\lambda \in \rho(A)$ iff $(A - \lambda I)$ is a bijection.

We now collect without proof some important properties of the spectrum; see e.g. [Kre78].

Theorem 1.2.11 Let $A \in \mathcal{B}(\mathcal{X})$ with $\mathcal{X} \neq \{0\}$ a complex Banach space. Then the spectrum $\sigma(A)$ of A is a compact non-empty subset of \mathbb{C} . Furthermore,

$$\sigma(A) \subseteq \{\lambda \in \mathbb{C}; |\lambda| \leq \|A\|\}.$$

Definition 1.2.12 The number $r_\sigma(A) = \sup_{\lambda \in \sigma(A)} |\lambda|$ is called the **spectral radius** of A . ♦

Theorem 1.2.13 (Spectral Radius Theorem) Let $A \in \mathcal{B}(\mathcal{X})$ with $\mathcal{X} \neq \{0\}$ a complex Banach space. Then the limit $\lim_{n \rightarrow \infty} \|A^n\|^{1/n}$ exists and we have

$$r_\sigma(A) = \inf_{n \geq 1} \|A^n\|^{1/n} = \lim_{n \rightarrow \infty} \|A^n\|^{1/n}.$$

1.3 Orthogonal projections

An orthogonal projection is a bounded linear transformation of the Hilbert space \mathcal{H} that maps the whole space onto a closed linear subspace, parallelly to the directions orthogonal to this subspace. The essence of the Spectral Theorem is to decompose a selfadjoint operator as a linear combination of orthogonal projections, so these will play a prominent role throughout the course.

Definition 1.3.1 (a) Two elements $u, v \in \mathcal{H}$ are **orthogonal** if $\langle u, v \rangle = 0$.

(b) Given a subspace $M \subseteq \mathcal{H}$, an element $u \in \mathcal{H}$ is orthogonal to M if u is orthogonal to all elements of M .

(c) A subspace $N \subseteq \mathcal{H}$ is orthogonal to M if each element of N is orthogonal to M .

(d) The **orthogonal complement** M^\perp of M is the *closed* subspace

$$M^\perp = \{u \in \mathcal{H}; \langle u, v \rangle = 0 \text{ for all } v \in M\} \subseteq \mathcal{H}.$$

We shall sometimes write $u \perp v$, $u \perp M$ or $N \perp M$, to denote orthogonality.

The following theorem will allow us to define the notion of orthogonal projection. Its proof can be found e.g. in [Wei80, p. 31] or [Kre78, p. 146].

Theorem 1.3.2 *Let M be a closed subspace of the Hilbert space \mathcal{H} . For all $u \in \mathcal{H}$, there exists a unique $v \in M$ and a unique $w \in M^\perp$ such that $u = v + w$. That is,*

$$\mathcal{H} = M \oplus M^\perp.$$

Definition 1.3.3 If M is a closed subspace of the Hilbert space \mathcal{H} , the **orthogonal projection** or simply **projection** onto M is the bounded operator defined by $Pu = v$ for all $u \in \mathcal{H}$, where $u = v + w$ is the unique decomposition of u with $v \in M$ and $w \in M^\perp$. ♦

Note that it follows immediately from the definition that $M = \text{rge } P$, $M^\perp = \ker P$, and that $I - P$ is the projection onto M^\perp .

Proposition 1.3.4 *Let P be the orthogonal projection onto a closed subspace M of \mathcal{H} . Then:*

(a) $P^2 = P$;

(b) $\langle Pu, u \rangle \geq 0$ for all $u \in \mathcal{H}$, with equality if and only if $u \in M^\perp$;

(c) for all $u, v \in \mathcal{H}$, $\langle Pu, v \rangle = \langle u, Pv \rangle$;

(d) if $P \neq 0$ then $\|P\| = 1$.

Proof. We shall write $u = v + w$ as in Theorem 1.3.2 throughout the proof.

Then $Pu = v \in M$, and the decomposition of Pu according to Theorem 1.3.2 is simply $Pu = v$. That is, $PPu = v$, which proves (a).

To prove (b), observe that $\langle Pu, u \rangle = \langle v, v + w \rangle = \langle v, v \rangle = \|v\|^2$.

To prove (c), write $\langle Pu, u \rangle = \langle v, v + w \rangle = \langle v, v \rangle = \langle v + w, v \rangle = \langle u, Pu \rangle$.

To prove (d), note that $\|u\|^2 = \|v\|^2 + \|w\|^2$ implies $\|v\| \leq \|u\|$, hence $\|P\| \leq 1$. Furthermore, if $P \neq 0$ then $M \neq \{0\}$ and we can find $u_0 \in M$ with $\|u_0\| = 1$. Hence, $\|Pu_0\| = \|u_0\| = 1$ and $\|P\| = \sup_{\|u\|=1} \|Pu\| \geq \|Pu_0\| = 1$. \square

The following additional properties will be proved in the problems.

Theorem 1.3.5 *Let M and N be closed subspaces of the Hilbert space \mathcal{H} . Denote by P and Q the associated projections. Then one has:*

- (a) $M \subseteq N$ if and only if $PQ = QP = P$;
- (b) $M \subseteq N$ if and only if $\langle Pu, u \rangle \leq \langle Qu, u \rangle$ for all $u \in \mathcal{H}$;
- (c) $PQ = 0 \Leftrightarrow QP = 0 \Leftrightarrow M \perp N$.

1.4 Symmetric operators

Symmetric operators on the Hilbert space are bounded operators having a peculiar behaviour with respect to the inner product. They are often referred to as ‘selfadjoint’ in the literature. However we shall reserve the term selfadjoint for the extension of the notion of symmetric operator to unbounded operators, where the definition of the adjoint operator requires extra care.

Definition 1.4.1 Consider a bounded operator A on the Hilbert space \mathcal{H} . The **adjoint** $A^* \in \mathcal{B}(\mathcal{H})$ of A is defined by

$$\langle Au, v \rangle = \langle u, A^*v \rangle, \quad \text{for all } u, v \in \mathcal{H}. \quad (1.4.1)$$

The operator A is called **symmetric** if $A = A^*$. We shall merely call **symmetric operator** a bounded symmetric operator. \blacklozenge

We now verify that this definition makes sense.

Theorem 1.4.2 *The relation (1.4.1) defines a unique operator $A^* \in \mathcal{B}(\mathcal{H})$, satisfying $\|A^*\| = \|A\|$.*

Proof. Fix $v \in \mathcal{H}$ and define $f_v(u) = \langle Au, v \rangle$, $u \in \mathcal{H}$. Since A is bounded, $f_v \in \mathcal{H}^*$ with $\|f_v\| \leq \|A\| \|v\|$. Hence, by Theorem 1.2.8, there exists a unique $v^* \in \mathcal{H}$ such that $f_v(u) = \langle u, v^* \rangle$, for all $u \in \mathcal{H}$. Letting $A^*v := v^*$, we recover (1.4.1) and it is easy to check that this defines a linear operator $A^* : \mathcal{H} \rightarrow \mathcal{H}$. Furthermore, by Theorem 1.2.8,

$$\|A^*v\| = \|f_v\| \leq \|A\| \|v\|, \quad \forall v \in \mathcal{H},$$

showing that $A^* \in \mathcal{B}(\mathcal{H})$ and $\|A^*\| \leq \|A\|$. Conversely, using again Theorem 1.2.8,

$$\begin{aligned} \|A^*\| &= \sup_{v \neq 0} \frac{\|A^*v\|}{\|v\|} = \sup_{v \neq 0} \frac{\|f_v\|}{\|v\|} = \sup_{v \neq 0} \sup_{u \neq 0} \frac{|\langle Au, v \rangle|}{\|v\| \|u\|} = \sup_{u, v \neq 0} \frac{|\langle Au, v \rangle|}{\|u\| \|v\|} \\ &\geq \sup_{u, Au \neq 0} \frac{|\langle Au, Au \rangle|}{\|u\| \|Au\|} = \sup_{u, Au \neq 0} \frac{\|Au\|^2}{\|u\| \|Au\|} = \sup_{u \neq 0} \frac{\|Au\|}{\|u\|} = \|A\|. \end{aligned}$$

Hence, $\|A^*\| = \|A\|$. □

We now collect some basic properties of the adjoint operator. The proofs can be found e.g. in [Fri82] or [Kre78].

Proposition 1.4.3 *Consider two bounded linear operators $A, B : \mathcal{H} \rightarrow \mathcal{H}$ and any scalar $\lambda \in \mathbb{C}$. Then we have:*

- (a) $(A + B)^* = A^* + B^*$;
- (b) $(AB)^* = B^*A^*$;
- (c) $(\lambda A)^* = \bar{\lambda}A^*$;
- (d) $A^{**} = A$;
- (e) $0^* = 0$ and $I^* = I$;
- (f) $\|A^*A\| = \|AA^*\| = \|A\|^2$;
- (g) if $A^{-1} \in \mathcal{B}(\mathcal{H})$ then A^* is invertible, $(A^*)^{-1} \in \mathcal{B}(\mathcal{H})$ and $(A^*)^{-1} = (A^{-1})^*$.

The following lemma is a fundamental structural result about the adjoint operator.

Lemma 1.4.4 *Consider a bounded operator $A : \mathcal{H} \rightarrow \mathcal{H}$. Then*

$$\mathcal{H} = \ker A^* \oplus \overline{\text{rge } A}.$$

Proof. See Problem 1.12. □

The following characterization of the residual spectrum is often useful to study the spectrum of an operator (see Problem 1.16).

Proposition 1.4.5 *The residual spectrum $\sigma_r(T)$ of a bounded operator $T : \mathcal{H} \rightarrow \mathcal{H}$ can be characterized as*

$$\sigma_r(T) = \{\lambda \in \mathbb{C} ; \lambda \notin \sigma_p(T), \bar{\lambda} \in \sigma_p(T^*)\}.$$

Proof. We apply Lemma 1.4.4 with $A = T - \lambda I$. By definition of $\sigma_r(T)$ we have, using Proposition 1.4.3 (a) and (c),

$$\begin{aligned} \lambda \in \sigma_r(T) &\iff T - \lambda I \text{ is injective but } \overline{\text{rge}(T - \lambda I)} \subsetneq \mathcal{H} \\ &\iff \ker(T - \lambda I) = \{0\}, \ker(T^* - \bar{\lambda}I) \neq \{0\}, \end{aligned}$$

which proves the proposition. □

The **numerical range** of a bounded operator A is the set

$$\text{nr}(A) := \{\langle Au, u \rangle ; u \in \mathcal{H}, \|u\| = 1\} \subset \mathbb{C}.$$

For instance, the numerical range of 0 is $\{0\}$ and the numerical range of I is $\{1\}$. For general projections, we have the following result.

Proposition 1.4.6 *Let $P \notin \{0, I\}$ be an orthogonal projection. Then $\text{nr}(P) = [0, 1]$.*

Proof. Firstly, if $\|u\| = 1$,

$$0 \leq \langle Pu, u \rangle = \langle P^2u, u \rangle = \langle Pu, Pu \rangle = \|Pu\|^2 \leq \|u\|^2 = 1,$$

showing that $\text{nr}(P) \subset [0, 1]$.

Conversely, consider a number $t \in [0, 1]$. Let $v \in \text{rge } P, w \in \ker P$ with $\|v\| = \|w\| = 1$, and define $u_t := tv + \sqrt{1 - t^2}w$. Then,

$$\|u_t\| = 1 \quad \text{and} \quad \langle Pu_t, u_t \rangle = \langle tv, tv + \sqrt{1 - t^2}w \rangle = t^2,$$

showing that $t^2 \in \text{nr}(P)$. Hence, $[0, 1] \subset \text{nr}(P)$. □

Proposition 1.4.7 *An operator $A \in \mathcal{B}(\mathcal{H})$ is symmetric if and only if $\text{nr}(A) \subset \mathbb{R}$.*

Proof. If A is symmetric then $\langle Au, u \rangle = \langle u, Au \rangle = \overline{\langle Au, u \rangle}$ for all $u \in \mathcal{H}$. Conversely, if $\langle Au, u \rangle$ is real for all $u \in \mathcal{H}$, we have $\langle Au, u \rangle = \langle A^*u, u \rangle$ and so

$$\langle (A - A^*)u, u \rangle = 0 \quad \text{for all } u \in \mathcal{H}.$$

It now follows by Problem 1.13 that $A - A^* = 0$. \square

Remark 1.4.8 Note that it is essential for the ‘if’ part that \mathcal{H} be complex. Indeed, in a real Hilbert space, the numerical range of any operator is real. (See also in Problem 1.13 why the last part of the above argument fails when \mathcal{H} is real.)

Theorem 1.4.9 Consider a symmetric operator S on the Hilbert space \mathcal{H} . Then

$$\|S\| = \sup_{\|u\|=1} |\langle Su, u \rangle|.$$

Proof. Let $s := \sup_{\|u\|=1} |\langle Su, u \rangle|$. If $\|u\| = 1$, then

$$|\langle Su, u \rangle| \leq \|Su\| \|u\| = \|Su\| \leq \|S\| \|u\| = \|S\|.$$

Hence, $s \leq \|S\|$.

To prove the converse inequality, take $v \in \mathcal{H}$ such that $Sv \neq 0$ (if no such v exists the result is trivial) and consider $u = \lambda^{-1}Sv$, where $\lambda = (\|Sv\| / \|v\|)^{1/2}$. Then, using the polarization identity,

$$\begin{aligned} \|Sv\|^2 &= \langle S(\lambda v), u \rangle = \frac{1}{4} (\langle S(\lambda v + u), \lambda v + u \rangle - \langle S(\lambda v - u), \lambda v - u \rangle) \\ &\leq \frac{s}{4} (\|\lambda v + u\|^2 + \|\lambda v - u\|^2) = \frac{s}{2} (\|\lambda v\|^2 + \|u\|^2) \\ &= \frac{s}{2} \left(\lambda^2 \|v\|^2 + \frac{1}{\lambda^2} \|Sv\|^2 \right) = s \|v\| \|Sv\|. \end{aligned}$$

Hence, $\|Sv\| \leq s \|v\|$ and it follows that $\|S\| \leq s$. \square

The following results will be proved in the problems.

Theorem 1.4.10 Let S be a symmetric operator on \mathcal{H} . Then $\sigma(S) \subset \mathbb{R}$.

Definition 1.4.11 Let S be a symmetric operator on \mathcal{H} . The **lower bound** and **upper bound** of S are respectively defined as

$$m = \inf_{\|u\|=1} \langle Su, u \rangle \quad \text{and} \quad M = \sup_{\|u\|=1} \langle Su, u \rangle.$$

Remark that, by Theorem 1.4.9, $\|S\| = \max\{|m|, |M|\}$. \blacklozenge

Theorem 1.4.12 *Let S be a symmetric operator on \mathcal{H} and let m, M be as in Definition 1.4.11. Then $\sigma(S)$ is real. In fact, we have*

$$\sigma(S) \subset [m, M] \quad \text{and} \quad m, M \in \sigma(S).$$

Corollary 1.4.13 *Let S be a symmetric operator on \mathcal{H} . The spectral radius of S , introduced in Definition 1.2.12, satisfies $r_\sigma(S) = \|S\|$.*

Corollary 1.4.14 *Let S be a symmetric operator on \mathcal{H} . Then $\sigma_r(S) = \emptyset$.*

Proof. This follows from Proposition 1.4.5 and the fact that $\sigma(S) \subset \mathbb{R}$. □

1.5 Positive operators

Our description of positive operators here essentially follows [Fri82].

Definition 1.5.1 A symmetric operator $S : \mathcal{H} \rightarrow \mathcal{H}$ is called **positive**, denoted $S \geq 0$, if

$$\langle Su, u \rangle \geq 0 \quad \text{for all } u \in \mathcal{H}.$$

We shall call **positive operator** a symmetric positive operator. For $S, T : \mathcal{H} \rightarrow \mathcal{H}$ symmetric, if $S - T \geq 0$ we say S is **larger** than T or T is **smaller** than S , and we write $S \geq T$ or $T \leq S$. ♦

It is an exercise to show that \leq defines a partial order on symmetric operators.

We shall now endeavour to define the square root of a positive operator. This requires several technical steps.

Lemma 1.5.2 *Let $P : \mathcal{H} \rightarrow \mathcal{H}$ be a positive operator. There exists a sequence $(P_n)_{n=1}^\infty$ of operators which are real polynomials² in P , such that the partial sums $(\sum_{k=1}^n P_k^2)_{n=1}^\infty$ strongly converge to P :*

$$Pu = \sum_{n=1}^{\infty} P_n^2 u, \quad u \in \mathcal{H}.$$

²A real polynomial is a polynomial with real coefficients.

Proof. If $P = 0$, the statement is trivial. Suppose $P \neq 0$ and define by induction the sequence of operators

$$B_1 = \frac{1}{\|P\|}P, \quad B_{n+1} = B_n - B_n^2, \quad n = 1, 2, \dots$$

Each B_n is a real polynomial in P and so is symmetric by Problem 1.8. We now prove by induction that

$$0 \leq B_n \leq I \quad \text{for all } n \geq 1. \quad (1.5.1)$$

For $n = 1$, it follows from the positivity of P that, for all $u \in \mathcal{H}$,

$$\langle B_1 u, u \rangle = \frac{1}{\|P\|} \langle Pu, u \rangle \geq 0,$$

and so $B_1 \geq 0$. Moreover, for all $u \in \mathcal{H}$,

$$\langle (I - B_1)u, u \rangle = \langle u, u \rangle - \langle B_1 u, u \rangle = \langle u, u \rangle - \frac{1}{\|P\|} \langle Pu, u \rangle \geq 0,$$

since $\langle Pu, u \rangle \leq \|P\| \|u\|^2$ by Cauchy-Schwarz. Suppose then that (1.5.1) holds for some $m \geq 1$ and let us show that it holds for $m + 1$. For all $u \in \mathcal{H}$, since $B_m \geq 0$ we have, on the one hand,

$$\langle B_m(I - B_m)^2 u, u \rangle = \langle B_m(I - B_m)u, (I - B_m)u \rangle \geq 0,$$

and on the other, since $B_m \leq I$,

$$\langle B_m^2(I - B_m)u, u \rangle = \langle (I - B_m)B_m u, B_m u \rangle \geq 0.$$

Hence $B_m(I - B_m)^2 \geq 0$ et $B_m^2(I - B_m) \geq 0$. Therefore,

$$\begin{aligned} B_{m+1} &= B_m - B_m^2 \\ &= B_m(I - B_m)^2 + B_m^2(I - B_m) \geq 0. \end{aligned}$$

Furthermore, since $B_m \leq I$, we have

$$I - B_{m+1} = (I - B_m) + B_m^2 \geq 0.$$

This conclude the proof of (1.5.1).

Let us now observe that

$$\sum_{k=1}^n B_k^2 = B_1 - B_{n+1}, \quad n \geq 1. \quad (1.5.2)$$

Together with (1.5.1), this implies

$$\sum_{k=1}^n B_k^2 \leq B_1, \quad n \geq 1.$$

Therefore, for all $u \in \mathcal{H}$,

$$\sum_{k=1}^n \langle B_k u, B_k u \rangle \leq \langle B_1 u, u \rangle, \quad n \geq 1.$$

It follows that $\sum_{n=1}^{\infty} \|B_n u\|^2 < \infty$ and so $\lim_{n \rightarrow \infty} \|B_n u\| = 0$. Hence, by (1.5.2),

$$\lim_{n \rightarrow \infty} \left\| B_1 u - \sum_{k=1}^n B_k^2 u \right\| = \lim_{n \rightarrow \infty} \|B_{n+1} u\| = 0.$$

On setting $P_n := \sqrt{\|P\|} B_n$, $n \geq 1$, the sequence $(P_n)_{n=1}^{\infty}$ does the job. \square

Corollary 1.5.3 *Let P and Q be positive operators. If $PQ = QP$ then PQ is positive.*

Proof. Consider the sequence $(P_n)_{n=1}^{\infty}$ given by Lemma 1.5.2 for P . As each P_n is a polynomial in P , we have $P_n Q = Q P_n$ for all $n \geq 1$. Thus, for all $u \in \mathcal{H}$, it follows from the continuity of the inner product that

$$\langle PQ u, u \rangle = \sum_{n=1}^{\infty} \langle P_n^2 Q u, u \rangle = \sum_{n=1}^{\infty} \langle P_n Q P_n u, u \rangle = \sum_{n=1}^{\infty} \langle Q P_n u, P_n u \rangle \geq 0,$$

by positivity of Q . \square

Corollary 1.5.4 *Consider a sequence of symmetric operators $(S_n)_{n=1}^{\infty}$ and suppose there is a symmetric operator T such that:*

- (i) *if $1 \leq m \leq n$ then $S_m \leq S_n$ (increasing sequence);*
- (ii) *for all $m, n \geq 1$, $S_m S_n = S_n S_m$;*
- (iii) *for all $n \geq 1$, $T S_n = S_n T$;*
- (iv) *for all $n \geq 1$, $S_n \leq T$ (upper bound).*

Then $(S_n)_{n=1}^{\infty}$ converges strongly to a symmetric operator S .

Proof. Consider the operators $P_n = T - S_n$. Each P_n is positive by (iv) and the sequence $(P_n)_{n=1}^\infty$ is decreasing by (i). Indeed, if $1 \leq m \leq n$ then $P_m - P_n = S_n - S_m \geq 0$. Moreover, by (ii) and (iii), $P_n P_m = P_m P_n$ for all $m, n \geq 1$. Hence, Corollary 1.5.3 ensures that, if $1 \leq m \leq n$ then

$$P_m(P_m - P_n) \geq 0 \quad \text{and} \quad (P_m - P_n)P_n \geq 0.$$

We deduce that

$$\langle P_m^2 u, u \rangle \geq \langle P_m P_n u, u \rangle \geq \langle P_n^2 u, u \rangle \geq 0, \quad 1 \leq m \leq n, \quad u \in \mathcal{H}. \quad (1.5.3)$$

Therefore, $(\langle P_n^2 u, u \rangle)_{n=1}^\infty$ is a decreasing sequence of non-negative numbers. Let $\alpha \in \mathbb{R}_+$ be its limit. By (1.5.3) we have, for all $1 \leq m \leq n$:

$$0 \leq \langle P_m P_n u, u \rangle - \alpha \leq \langle P_m^2 u, u \rangle - \alpha, \quad u \in \mathcal{H}.$$

It follows from the above identities that

$$\lim_{n, m \rightarrow \infty} \langle P_m P_n u, u \rangle = \lim_{m \rightarrow \infty} \langle P_m^2 u, u \rangle, \quad u \in \mathcal{H}.$$

Hence, for all $u \in \mathcal{H}$:

$$\begin{aligned} \|S_n u - S_m u\|^2 &= \|P_m u - P_n u\|^2 \\ &= \langle (P_m - P_n)^2 u, u \rangle \\ &= \langle P_m^2 u, u \rangle + \langle P_n^2 u, u \rangle - 2 \langle P_m P_n u, u \rangle \xrightarrow{m, n \rightarrow \infty} 0. \end{aligned}$$

It follows that, for all $u \in \mathcal{H}$, $(S_n u)_{n=1}^\infty$ is a Cauchy sequence in \mathcal{H} . It therefore has a limit, which we denote by $Su \in \mathcal{H}$. This defines a linear operator S , which is bounded by Corollary 1.2.6. Furthermore, S is symmetric. Indeed, by continuity of the inner product (Problem 1.1),

$$\langle Su, v \rangle = \left\langle \lim_{n \rightarrow \infty} S_n u, v \right\rangle = \lim_{n \rightarrow \infty} \langle S_n u, v \rangle = \lim_{n \rightarrow \infty} \langle u, S_n v \rangle = \left\langle u, \lim_{n \rightarrow \infty} S_n v \right\rangle = \langle u, Sv \rangle, \quad u, v \in \mathcal{H}.$$

The proof is complete. \square

We now introduce the important notion of the square root of a positive operator.

Definition 1.5.5 Let P be a positive operator. A **square root** of P is a symmetric operator R such that $R^2 = P$. \blacklozenge

Theorem 1.5.6 Let P be a positive operator. There exists a unique positive square root R of P . Furthermore, R commutes with any bounded operator which commutes with P .

Proof. The proof is in two steps.

1. Existence. We need only show that all positive operator P such that $P \leq I$ has a positive square root. The general case can be deduced from this one by considering $\tilde{P} = \varepsilon P$, with $\varepsilon > 0$ such that $\varepsilon \|P\| \leq 1$. So suppose that $P \leq I$ and define by induction the sequence of operators

$$\begin{aligned} R_0 &= 0 \\ R_{n+1} &= R_n + \frac{1}{2}(P - R_n^2) \quad n = 1, 2, \dots \end{aligned} \tag{1.5.4}$$

Each R_n is a real polynomial in P . Therefore, by Problem 1.8, R_n is symmetric and commutes with any bounded operator which commutes with P . It follows from the identity

$$I - R_{n+1} = \frac{1}{2}(I - R_n)^2 + \frac{1}{2}(I - P) \tag{1.5.5}$$

that $R_n \leq I$ for all $n \geq 0$. It then follows by subtraction that

$$\begin{aligned} R_{n+1} - R_n &= \frac{1}{2}(I - R_{n-1})^2 - \frac{1}{2}(I - R_n)^2 \\ &= \frac{1}{2}(R_{n-1}^2 - 2R_{n-1} + 2R_n - R_n^2) \\ &= \frac{1}{2}[(I - R_{n-1}) + (I - R_n)](R_n - R_{n-1}). \end{aligned}$$

Thanks to Corollary 1.5.3, this last identity allows one to show by induction that $R_{n+1} \geq R_n$ for all $n \geq 0$. In particular, since $R_0 = 0$, each R_n is positive. We can then apply Corollary 1.5.4 to the sequence $(R_n)_{n=0}^\infty$: there exists a symmetric operator R such that $\lim_{n \rightarrow \infty} R_n u = Ru$ for all $u \in \mathcal{H}$. On the other hand, the Uniform Boundedness Principle 1.2.3 yields a constant $C \geq 0$ such that $\|R_n\| \leq C$ for all $n \geq 1$, and so

$$\begin{aligned} \|R_n^2 u - R^2 u\| &= \|R_n^2 u - R_n R u + R_n R u - R^2 u\| \\ &\leq C \|R_n u - R u\| + \|R_n(R u) - R(R u)\| \xrightarrow{n \rightarrow \infty} 0. \end{aligned}$$

It follows that $\lim_{n \rightarrow \infty} R_n^2 u = R^2 u$ for all $u \in \mathcal{H}$. Therefore, letting $n \rightarrow \infty$ in (1.5.4), we have

$$R u = R u + \frac{1}{2}(P - R^2)u \quad \text{for all } u \in \mathcal{H}.$$

That is, $R^2 = P$. Since each R_n is positive, so is R by continuity of the inner product. Furthermore, since each R_n commutes with any bounded operator which commutes with P , this also holds for their limit R .

2. Uniqueness. Suppose that S is also a positive square root of P . Since $P = S^2$, S commutes with P and so with R . Pick any $u \in \mathcal{H}$ and let $v = (R - S)u$. Then

$$\langle Rv, v \rangle + \langle Sv, v \rangle = \langle (R + S)(R - S)u, v \rangle = \langle (R^2 - S^2)u, v \rangle = 0.$$

Since $\langle Rv, v \rangle \geq 0$ and $\langle Sv, v \rangle \geq 0$, it follows that $\langle Rv, v \rangle = \langle Sv, v \rangle = 0$. Now consider a positive square root T of R . By symmetry of T we have

$$\|Tv\|^2 = \langle T^2v, v \rangle = \langle Rv, v \rangle = 0.$$

Hence $Tv = 0$ and we conclude that $Rv = T(Tv) = 0$. By the same argument we get $Sv = 0$. Finally,

$$\|Ru - Su\|^2 = \langle (R - S)^2u, u \rangle = \langle (R - S)v, u \rangle = 0,$$

that is $Ru = Su$. Since u is arbitrary, we conclude that $R = S$. \square

Lemma 1.5.7 *Let S and T be symmetric operators such that $ST = TS$ and $S^2 = T^2$. Denote by P the projection onto $L = \ker(S - T)$. We then have the following properties.*

- (a) *Any bounded operator which commutes with $S - T$ commutes with P .*
- (b) *If $Su = 0$ then $Pu = u$.*
- (c) *$P(S + T) = S + T$ and $P(S - T) = 0$.*

Proof. Let B be a bounded operator which commutes with $S - T$. We observe that, if $v \in L$ then $Bv \in L$ since $(S - T)Bv = B(S - T)v = 0$. Hence $BPu \in L$ for all $u \in \mathcal{H}$. Therefore, $PBPu = BPu$ for all $u \in \mathcal{H}$, in other words $PBP = BP$. By Problem 1.10, the adjoint B^* also commutes with $S - T$. Hence $B^*P = PB^*P$, and it follows that

$$PB = (B^*P)^* = (PB^*P)^* = PBP = BP.$$

This proves (a).

Now suppose that $Su = 0$ for some $u \in \mathcal{H}$. Then

$$\|Tu\|^2 = \langle T^2u, u \rangle = \langle S^2u, u \rangle = \|Su\|^2 = 0,$$

and so $Tu = 0$. Therefore, $(S - T)u = 0$ as well and $u \in L$. It follows that $Pu = u$, proving (b).

To prove (c), observe that, since S and T commute we have, for all $u \in \mathcal{H}$,

$$(S - T)(S + T)u = (S^2 - T^2)u = 0.$$

Hence $(S+T)u \in L$, and so $P(S+T) = S+T$. To prove the last statement, observe that $(S-T)P = 0$ by definition of P and that S and T commute with P by part (a). This concludes the proof. \square

We are now in a position to prove the following lemma, which will play a crucial role in the spectral decomposition of bounded symmetric operators.

Definition 1.5.8 For a symmetric operator S , we denote by $|S|$ the unique positive square root of S^2 . We shall call it the **absolute value** of S . Note that one has $|S|S = S|S|$ and $|S| \geq 0$, for any symmetric operator S . \blacklozenge

Lemma 1.5.9 *Let S be a symmetric operator. The projection E_+ onto $\ker(S - |S|)$ has the following properties.*

- (a) *Every bounded operator which commutes with S commutes with E_+ .*
- (b) *If $Su = 0$ then $E_+u = u$.*
- (c) *$SE_+ \geq 0$ and $S(I - E_+) \leq 0$.*

Proof. Let C be bounded operator which commutes with S . Since $CS^2 = SC S = S^2C$, C also commutes with S^2 . Then, by Theorem 1.5.6, C commutes with $|S|$ and so commutes with $S - |S|$. Hence, by Lemma 1.5.7 (a), C commutes with E_+ . This proves (a).

Part (b) follows directly from Lemma 1.5.7 (b).

We now prove (c). By Lemma 1.5.7 (c) and the fact that S and $|S|$ commute with E_+ , we have

$$SE_+ = |S|E_+. \quad (1.5.6)$$

We then deduce from Corollary 1.5.3 that $SE_+ \geq 0$. On the other hand, by Lemma 1.5.7 (c),

$$SE_+ + |S|E_+ = S + |S|.$$

Together with (1.5.6), this yields

$$S(I - E_+) = -(I - E_+)|S|. \quad (1.5.7)$$

But $|S|$ also commutes with $I - E_+$ and so again by Corollary 1.5.3 we have $S(I - E_+) \leq 0$. The proof is complete. \square

A good mental picture of Lemma 1.5.9 is obtained from the following definition.

Definition 1.5.10 Let S be a symmetric operator and E_+ be the projection onto $\ker(S - |S|)$. The operator $S_+ = SE_+$ is called the **positive part** of S , while $S_- = S(I - E_+)$ is called the **negative part** of S . ♦

As S and $|S|$ commute with $S - |S|$, Lemma 1.5.7 (a) ensures that both commute with E_+ as well. It therefore follows from (1.5.6) that

$$E_+S = SE_+ = |S|E_+ = E_+|S|.$$

Then, using (1.5.7), one obtains

$$S_+ = \frac{1}{2}(S + |S|) \quad \text{and} \quad S_- = S - S_+ = \frac{1}{2}(S - |S|).$$

Problems

1. Show that the inner product of a Hilbert space is continuous in each variable, and that the norm is a continuous function.
2. Show that the norm $\|A\|_{\mathcal{B}(\mathcal{X}_1, \mathcal{X}_2)}$ of an operator $A \in \mathcal{B}(\mathcal{X}_1, \mathcal{X}_2)$ can be defined equivalently by (1.2.2).
3. Prove that a linear operator $A : \mathcal{X}_1 \rightarrow \mathcal{X}_2$ is bounded if and only if its graph \mathbf{G}_A is a closed subset of $\mathcal{X}_1 \times \mathcal{X}_2$, where $\mathcal{X}_1, \mathcal{X}_2$ are Banach spaces.
4. Let $A \in \mathcal{B}(\mathcal{X})$ and $\lambda \in \mathbb{C}$, as in Definition 1.2.9. Show that, if \mathcal{X} is a Banach space and $\lambda \in \rho(A)$, then $(A - \lambda I)^{-1}$ is defined on the whole space \mathcal{X} .
Hint: Use the result proved in Problem 1.3.
5. Prove Theorem 1.3.5.
6. Show that a bounded operator $P : \mathcal{H} \rightarrow \mathcal{H}$ is a projection if and only if it is symmetric and idempotent (i.e. $P^2 = P$).
7. Prove Proposition 1.4.6.
8. Prove that, if S is a symmetric operator on \mathcal{H} , then any real polynomial in S is also symmetric.
9. Let S be a symmetric operator on \mathcal{H} , and B a bounded operator on \mathcal{H} . Show that $T = B^*SB$ is symmetric.

10. Let S be a symmetric operator on \mathcal{H} , B a bounded operator on \mathcal{H} . First suppose that $SB = BS$ and show that $SB^* = B^*S$. Then, if both S and B are symmetric, show that SB is symmetric if and only if $SB = BS$.
11. Consider a sequence $(S_n)_{n \geq 1}$ of symmetric operators, such that $S_n \rightarrow S$ in $\mathcal{B}(\mathcal{H})$ as $n \rightarrow \infty$. Show that S is symmetric.
Hint: Apply the triangle inequality to $\|S - S^*\|$.

12. Prove Lemma 1.4.4.
Hint: (Prove and) use the fact that $\mathcal{X}^{\perp\perp} = \overline{\mathcal{X}}$ for any subspace $\mathcal{X} \subset \mathcal{H}$.

13. For $T \in \mathcal{B}(\mathcal{H})$, prove that

$$\langle Tu, u \rangle = 0 \quad \forall u \in \mathcal{H} \implies T = 0.$$

Note that it is essential here that \mathcal{H} be complex. Find a counterexample in the real case.

Hint: Write $u = v + \lambda w$ and use special values of $\lambda \in \mathbb{C}$.

14. On ℓ^2 , let A be the multiplication operator defined by $(Au)_n = \theta_n u_n$, where $(\theta_n)_{n \geq 1} \subset \mathbb{C}$ is a given bounded sequence. Show that A is bounded, $\sigma_p(A) = (\theta_n)$ and $\sigma(A) = \overline{(\theta_n)}$. Determine under which condition A is symmetric.
Recall: ℓ^2 is the Hilbert space of all complex sequences (u_1, u_2, \dots) such that $\sum_{n \geq 1} |u_n|^2 < \infty$, endowed with the inner product $\langle u, v \rangle = \sum_{n \geq 1} u_n \overline{v_n}$.
15. Find an operator $T : C[0, 1] \rightarrow C[0, 1]$ such that $\sigma(T) = [a, b]$, with $a < b$ given.
16. We define two operators $S, T : \ell^2 \rightarrow \ell^2$ by

$$(Su)_n = u_{n+1}, \quad n \geq 1 \quad (\text{left shift}); \quad (Tu)_1 = 0, \quad (Tu)_n = u_{n-1}, \quad n \geq 2 \quad (\text{right shift}).$$

- (a) Show that S and T are bounded. Compute $\|S\|$ and $\|T\|$.
- (b) Find S^* and T^* .
- (c) Find $\sigma_p(S)$, $\sigma_r(S)$ and $\sigma_c(S)$.
17. Find a Hilbert space \mathcal{H} and a sequence of operators $(A_n)_{n \in \mathbb{N}} \subset \mathcal{B}(\mathcal{H})$ which converges strongly but not in operator norm.
18. Show that the multiplication operator $X : L^2[0, 1] \rightarrow L^2[0, 1]$ defined by

$$(Xu)(x) = xu(x), \quad x \in [0, 1],$$

is a bounded symmetric operator without eigenvalues. Find the spectrum of X .

19. Let $S : \mathcal{H} \rightarrow \mathcal{H}$ be bounded and symmetric. Prove that all the eigenvalues (if any) of S are real. Show that eigenvectors of S corresponding to distinct eigenvalues are orthogonal.
20. Deduce Corollary 1.4.13 from Theorem 1.2.13.
21. Show that the relation \geq introduced in Definition 1.5.1 defines a partial order among the symmetric operators on \mathcal{H} .
Recall: A partial order is a binary relation which is reflexive, transitive and antisymmetric.
Hint: Use Theorem 1.4.9.
22. Let $A : \ell^2 \rightarrow \ell^2$ be defined by $(u_1, u_2, \dots) \mapsto (0, 0, u_1, u_2, \dots)$. Show that A is bounded and compute its norm. Is A symmetric? Find $B : \ell^2 \rightarrow \ell^2$ such that $A = B^2$.
23. Consider the operator $A : L^2[0, 1] \rightarrow L^2[0, 1]$ defined by

$$(Au)(x) = a(x)u(x), \quad x \in [0, 1],$$

where $a \in L^\infty[0, 1]$. Show that:

- (a) $\sigma_p(A) = \{\lambda \in \mathbb{C} ; |\{x \in [0, 1] ; a(x) = \lambda\}| > 0\}$;
- (b) $\sigma_r(A) = \emptyset$;
- (c) $\sigma(A) = \text{essrge}(a)$.

Here, $|E|$ is the Lebesgue measure of a Borel set $E \subset [0, 1]$, and $\text{essrge}(a)$ is the *essential range* of a , defined as

$$\text{essrge}(a) = \{\lambda \in \mathbb{C} ; \text{for all } \epsilon > 0 : |\{x \in [0, 1] ; |a(x) - \lambda| < \epsilon\}| > 0\}.$$

Find a condition on a for A to be positive and, in this case, find the square root of A .

Chapter 2

The spectral decomposition of symmetric bounded operators

The goal of this chapter is to present the proof of the spectral theorem for (bounded) symmetric operators. The main idea is that a symmetric operator A can always be represented as a sum of projections, indexed by a real parameter running through $\sigma(A)$. In general, due to the presence of continuous spectrum, this representation involves a continuous sum, viz. a Riemann-Stieltjes integral. The projections are uniquely determined by A in the form of a spectral family. In the first part of the chapter we define the integral with respect to a general spectral family. Then we prove the spectral theorem, following [Fri82].

2.1 Integration with respect to a spectral family

We start with the definition of a spectral family.

Definition 2.1.1 A **spectral family** on \mathcal{H} is a mapping $E : \mathbb{R} \rightarrow \mathcal{B}(\mathcal{H})$, denoted $(E_\lambda)_{\lambda \in \mathbb{R}}$ and satisfying the following properties.

- (i) E_λ is a projection for all $\lambda \in \mathbb{R}$.
- (ii) If $\lambda < \mu$, then $E_\lambda \leq E_\mu$.
- (iii) The family $(E_\lambda)_{\lambda \in \mathbb{R}}$ is **strongly left-continuous**, i.e.

$$\lim_{\lambda \nearrow \mu} E_\lambda u = E_\mu u, \quad \text{for all } \mu \in \mathbb{R}, u \in \mathcal{H}.$$

- (iv) There exist $m, M \in \mathbb{R}$ such that $E_\lambda = 0$ for all $\lambda < m$ and $E_\lambda = I$ for all $\lambda > M$.

Two numbers $m, M \in \mathbb{R}$ satisfying (iv) are respectively called a **lower bound** and an **upper bound** of the spectral family. ♦

We consider a spectral family $(E_\lambda)_{\lambda \in \mathbb{R}}$ with bounds $m, M \in \mathbb{R}$. Let f be a continuous real-valued function defined on $[m, M]$. We now fix $0 < \varepsilon < 1$ and extend f continuously to $[m, M + \varepsilon]$. We denote this extension by f . Let Π be an arbitrary partition of $[m, M + \varepsilon]$, i.e. a finite sequence of numbers $(\lambda_k)_{k=0}^n$ such that

$$m = \lambda_0 < \lambda_1 < \cdots < \lambda_{n-1} < \lambda_n = M + \varepsilon.$$

We call **size** of the partition Π the number $|\Pi|$ defined as

$$|\Pi| = \max_{k=1, \dots, n} \lambda_k - \lambda_{k-1}.$$

We then choose real numbers μ_1, \dots, μ_k such that

$$\mu_k \in [\lambda_{k-1}, \lambda_k] \quad \text{for each } k = 1, \dots, n,$$

and form the sum

$$S_\Pi = \sum_{k=1}^n f(\mu_k)(E_{\lambda_k} - E_{\lambda_{k-1}}).$$

The following lemma ensures that S_Π converges in $\mathcal{B}(\mathcal{H})$ as $|\Pi| \rightarrow 0$, for any partition Π of $[m, M + \varepsilon]$.

Lemma 2.1.2 *Consider $(E_\lambda)_{\lambda \in \mathbb{R}}$ a spectral family with bounds $m, M \in \mathbb{R}$, and $f : [m, M] \rightarrow \mathbb{R}$ a continuous function. Let $0 < \varepsilon < 1$ and $f : [m, M + \varepsilon] \rightarrow \mathbb{R}$ a continuous extension of f . There is a unique bounded operator S such that, for all $\eta > 0$ there exists $\delta > 0$ such that for any partition Π of $[m, M + \varepsilon]$ satisfying $|\Pi| \leq \delta$, one has*

$$\|S_\Pi - S\| \leq \eta.$$

Furthermore, the operator S is independent of the extension chosen for f , of the choice of ε , and of the choice of the μ_k s.

Proof. Fix $\eta > 0$ arbitrary. Since f is uniformly continuous on the compact interval $[m, M + \varepsilon]$, there exists $\delta_\eta > 0$ such that

$$\text{for all } \lambda, \lambda' \in [m, M + \varepsilon], \quad |\lambda - \lambda'| \leq \delta_\eta \implies |f(\lambda) - f(\lambda')| \leq \frac{\eta}{2}. \quad (2.1.1)$$

Part 1. We start by showing that, for any partitions Π and Π' of $[m, M + \varepsilon]$,

$$|\Pi|, |\Pi'| \leq \delta_\eta \implies \|S_\Pi - S_{\Pi'}\| \leq \eta, \quad (2.1.2)$$

independently of the points μ_k chosen to construct the sums S_Π and $S_{\Pi'}$.

Let us write $\Pi = (\lambda_k)_{k=0}^n$ and fix μ_1, \dots, μ_n with $\mu_i \in [\lambda_{i-1}, \lambda_i]$ for all $i = 1, \dots, n$. We form a partition $\bar{\Pi} = (\bar{\lambda}_j)_{j=0}^{\bar{n}}$ as the union of Π and Π' . We denote by $0 = k_0 < k_1 < \dots < k_j < k_n = \bar{n}$ the subsequence of indices satisfying $\bar{\lambda}_{k_i} = \lambda_i$ for $i = 0, \dots, n$.

We then pick up numbers

$$\bar{\mu}_i \in [\bar{\lambda}_{i-1}, \bar{\lambda}_i] \quad i = 1, \dots, k_n.$$

The sum associated with $\bar{\Pi}$ and the $\bar{\mu}_j$ s is given by

$$S_{\bar{\Pi}} = \sum_{i=1}^n \sum_{j=k_{i-1}+1}^{k_i} f(\bar{\mu}_j)(E_{\bar{\lambda}_j} - E_{\bar{\lambda}_{j-1}}).$$

Since, for all $i = 1, \dots, n$,

$$\sum_{j=k_{i-1}+1}^{k_i} E_{\bar{\lambda}_j} - E_{\bar{\lambda}_{j-1}} = E_{\bar{\lambda}_{k_i}} - E_{\bar{\lambda}_{k_{i-1}}} = E_{\lambda_i} - E_{\lambda_{i-1}},$$

we can write S_Π as

$$S_\Pi = \sum_{i=1}^n \sum_{j=k_{i-1}+1}^{k_i} f(\mu_i)(E_{\bar{\lambda}_j} - E_{\bar{\lambda}_{j-1}}).$$

Since $|\Pi| < \delta_\eta$, it now follows from (2.1.1) that, for all $i = 1, \dots, n$ and all $j = k_{i-1} + 1, \dots, k_i$,

$$|\mu_i - \bar{\mu}_j| \leq \lambda_i - \lambda_{i-1} \leq \delta_\eta \implies |f(\mu_i) - f(\bar{\mu}_j)| \leq \frac{\eta}{2}.$$

Moreover, since $E_m = 0$ and $E_{M+\varepsilon} = I$ we have, for all $u \in \mathcal{H}$ such that $\|u\| = 1$:

$$\begin{aligned} |\langle (S_\Pi - S_{\bar{\Pi}})u, u \rangle| &= \left| \sum_{i=1}^n \sum_{j=k_{i-1}+1}^{k_i} [f(\mu_i) - f(\bar{\mu}_j)] \langle (E_{\bar{\lambda}_j} - E_{\bar{\lambda}_{j-1}})u, u \rangle \right| \\ &\leq \sum_{i=1}^n \sum_{j=k_{i-1}+1}^{k_i} |f(\mu_i) - f(\bar{\mu}_j)| \langle (E_{\bar{\lambda}_j} - E_{\bar{\lambda}_{j-1}})u, u \rangle \\ &\leq \frac{\eta}{2} \left\langle \sum_{i=1}^n \sum_{j=k_{i-1}+1}^{k_i} (E_{\bar{\lambda}_j} - E_{\bar{\lambda}_{j-1}})u, u \right\rangle \\ &= \frac{\eta}{2} \langle (E_{M+\varepsilon} - E_m)u, u \rangle = \frac{\eta}{2} \|u\|^2 = \frac{\eta}{2}. \end{aligned}$$

Since f is real-valued, S_Π and $S_{\bar{\Pi}}$ are symmetric operators. Hence, by Theorem 1.4.9, $\|S_\Pi - S_{\bar{\Pi}}\| \leq \frac{\eta}{2}$. Similarly we have $\|S_{\Pi'} - S_{\bar{\Pi}}\| \leq \frac{\eta}{2}$ and so

$$\|S_\Pi - S_{\Pi'}\| \leq \|S_\Pi - S_{\bar{\Pi}}\| + \|S_{\bar{\Pi}} - S_{\Pi'}\| \leq \eta,$$

as advertised.

Part 2. Let us now consider a sequence $(\Pi_n)_{n=1}^\infty$ of partitions of $[m, M+\varepsilon]$ such that $\lim_{n \rightarrow \infty} |\Pi_n| = 0$. The operators $(S_{\Pi_n})_{n=1}^\infty$ then form a Cauchy sequence in $\mathcal{B}(\mathcal{H})$. Indeed, there is an $N \geq 1$ such that $|\Pi_n| \leq \delta_\eta$ for all $n \geq N$. Hence, by (2.1.2), for all $n, n' \geq N$ there holds $\|S_{\Pi_n} - S_{\Pi_{n'}}\| \leq \eta$. Since $\mathcal{B}(\mathcal{H})$ is complete, the sequence $(S_{\Pi_n})_{n=1}^\infty$ has a limit $S \in \mathcal{B}(\mathcal{H})$. In particular, there exists $N_\eta \geq 1$ such that $|\Pi_{N_\eta}| \leq \delta_{\frac{\eta}{2}}$ and $\|S_{\Pi_{N_\eta}} - S\| \leq \frac{\eta}{2}$. Therefore, in view of (2.1.2), any partition Π smaller than $\delta_{\frac{\eta}{2}}$ satisfies

$$\|S_\Pi - S\| \leq \|S_\Pi - S_{\Pi_{N_\eta}}\| + \|S_{\Pi_{N_\eta}} - S\| \leq \eta.$$

The limit S does not depend on the extension of f , neither on ε , for $E_\lambda - E_\mu = 0$ for all $M < \mu < \lambda$. Furthermore, it is clear from Part 1 that the limit does not depend on the choice of the points μ_k . \square

Thanks to Lemma 2.1.2, we can now make the following definition.

Definition 2.1.3 Consider a spectral family $(E_\lambda)_{\lambda \in \mathbb{R}}$ with bounds $m, M \in \mathbb{R}$ and $f : [m, M] \rightarrow \mathbb{R}$ continuous. The limit operator $S \in \mathcal{B}(\mathcal{H})$ obtained from Lemma 2.1.2 is called the **integral of f with respect to the spectral family $(E_\lambda)_{\lambda \in \mathbb{R}}$** . It is written

$$S = \int_m^{M^+} f(\lambda) dE_\lambda.$$

For a continuous $f : [m, M] \rightarrow \mathbb{C}$, we define the integral of f with respect to $(E_\lambda)_{\lambda \in \mathbb{R}}$ by

$$\int_m^{M^+} f(\lambda) dE_\lambda = \int_m^{M^+} \Re f(\lambda) dE_\lambda + i \int_m^{M^+} \Im f(\lambda) dE_\lambda. \blacklozenge$$

Observe that, for any spectral family $(E_\lambda)_{\lambda \in \mathbb{R}}$, one has

$$\int_m^{M^+} dE_\lambda = E_{M^+} - E_m = I.$$

2.2 The spectral theorem for symmetric operators

We are now ready to prove the spectral theorem for bounded symmetric operators.

Theorem 2.2.1 (Spectral Theorem I) *Let S be a bounded symmetric operator. There exists a unique spectral family $(E_\lambda)_{\lambda \in \mathbb{R}}$ with the following properties.*

(a) *Every bounded operator which commutes with S commutes with E_λ , for all $\lambda \in \mathbb{R}$.*

(b) *For all $u \in \mathcal{H}$ there exists*

$$E_{\mu+}u = \lim_{\lambda \searrow \mu} E_\lambda u.$$

(c) *The lower and upper bounds m, M of S are respectively lower and upper bounds for $(E_\lambda)_{\lambda \in \mathbb{R}}$.*

(d) *The operator S has the representation*

$$S = \int_m^{M+} \lambda dE_\lambda.$$

*The family $(E_\lambda)_{\lambda \in \mathbb{R}}$ is called **the spectral family of S** .*

Proof. For all $\lambda \in \mathbb{R}$, let $E_+(\lambda)$ be the projection onto $\ker[(S - \lambda I) - |S - \lambda I|]$, which was studied in Lemma 1.5.9. Observe that $E_+(\lambda)$ is uniquely determined in this way. We will show that the projections $E_\lambda = I - E_+(\lambda)$ form a spectral family satisfying (a)–(d).

Since $E_+(\lambda)$ commutes with all bounded operators which commute with S , this is also true for E_λ . Hence, (a) is readily satisfied. In particular, $E_\mu E_\lambda = E_\lambda E_\mu$ for all $\mu, \lambda \in \mathbb{R}$.

Let us now show that, if $\lambda < \mu$ then $E_\lambda \leq E_\mu$, i.e. part (ii) of Definition 2.1.1 holds. Suppose $\lambda < \mu$ and let $P = E_\lambda(I - E_\mu)$. We will show that $P = 0$. Firstly, we have

$$E_\lambda P = P, \quad (I - E_\mu)P = P. \quad (2.2.1)$$

Moreover, by definition of E_λ and E_μ , Lemma 1.5.9 implies that

$$(S - \lambda I)E_\lambda = (S - \lambda I)(I - E_+(\lambda)) \leq 0, \quad (S - \mu I)(I - E_\mu) = (S - \mu I)E_+(\mu) \geq 0. \quad (2.2.2)$$

Choosing $u \in \mathcal{H}$ and letting $v = Pu$, it follows from (2.2.1) that

$$E_\lambda v = E_\lambda Pu = Pu = v.$$

Similarly, $(I - E_\mu)v = v$. Therefore, by (2.2.2),

$$\begin{aligned}\langle (S - \lambda I)v, v \rangle &= \langle (S - \lambda I)E_\lambda v, v \rangle \leq 0, \\ \langle (S - \mu I)v, v \rangle &= \langle (S - \mu I)(I - E_\mu)v, v \rangle \geq 0.\end{aligned}$$

We deduce that

$$(\mu - \lambda) \langle v, v \rangle = \langle (S - \lambda I)v, v \rangle - \langle (S - \mu I)v, v \rangle \leq 0.$$

However, since $\mu > \lambda$, we must have $Pu = v = 0$. Since u is arbitrary, we have shown that $P = 0$. By definition of P , this means that $E_\lambda = E_\lambda E_\mu$ which, by Theorem 1.3.5, is equivalent to $E_\lambda \leq E_\mu$. The family $(E_\lambda)_{\lambda \in \mathbb{R}}$ therefore satisfies condition (ii) of Definition 2.1.1.

We now show that $(E_\lambda)_{\lambda \in \mathbb{R}}$ satisfies (b). Let $u \in \mathcal{H}$. Since $E_\lambda \leq E_\mu$ for $\lambda < \mu$, $\langle E_\lambda u, u \rangle$ is a positive non-decreasing function of λ . Therefore, for all $\mu \in \mathbb{R}$, it has a limit from the left:

$$\lim_{\lambda \nearrow \mu} \langle E_\lambda u, u \rangle = \sup_{\lambda < \mu} \langle E_\lambda u, u \rangle = l_\mu.$$

Hence, for all $\eta > 0$ there exists $\delta > 0$ such that $0 < \mu - \lambda < \delta$ implies $l_\mu - \langle E_\lambda u, u \rangle < \frac{1}{2}\eta$. It follows that, for $\mu - \delta < \lambda < \nu < \mu$, $E_\lambda E_\nu = E_\lambda \implies$

$$\|E_\nu u - E_\lambda u\|^2 = \langle (E_\nu - E_\lambda)^2 u, u \rangle = \langle (E_\nu - E_\lambda)u, u \rangle \leq |\langle E_\nu u, u \rangle - l_\mu| + |l_\mu - \langle E_\lambda u, u \rangle| < \eta.$$

Therefore, since \mathcal{H} is complete, an argument similar to Part 1 in the proof of Lemma 2.1.2 shows that

$$\lim_{\lambda \nearrow \mu} E_\lambda u = E_{\mu-} u \quad \text{exists for all } u \in \mathcal{H}.$$

Similarly, for all $u \in \mathcal{H}$, the limit

$$\lim_{\lambda \searrow \mu} E_\lambda u = E_{\mu+} u$$

exists as well. This proves (b) and half of part (iii) of Definition 2.1.1.

We now complete the proof of part (iii) of Definition 2.1.1, i.e. we show that $(E_\lambda)_{\lambda \in \mathbb{R}}$ is strongly left-continuous. If $\lambda < \mu$, we write $E_\Delta = E_\mu - E_\lambda$ and we have

$$E_\mu E_\Delta = E_\Delta \quad \text{et} \quad (I - E_\lambda)E_\Delta = E_\mu - E_\lambda - E_\lambda E_\mu + E_\lambda^2 = E_\Delta. \quad (2.2.3)$$

Using (2.2.2), $E_\Delta \geq 0$, and the fact that a composition of commuting positive operators is positive (Corollary 1.5.3),

$$\begin{aligned}(S - \mu I)E_\Delta &= (S - \mu I)E_\mu E_\Delta \leq 0, \\ (S - \lambda I)E_\Delta &= (S - \lambda I)(I - E_\lambda)E_\Delta \geq 0.\end{aligned}$$

In consequence, we have the following inequalities

$$\lambda E_\Delta \leqslant S E_\Delta \leqslant \mu E_\Delta \quad \text{if } \lambda < \mu. \quad (2.2.4)$$

Consider now the operator $E_{\Delta_0} = E_\mu - E_{\mu^-}$. We want to show that $E_{\Delta_0} = 0$. Observe that, for all $u \in \mathcal{H}$,

$$\lim_{\lambda \nearrow \mu} E_\Delta u = E_{\Delta_0} u.$$

Thus, letting $\lambda \nearrow \mu$ in (2.2.4), we get

$$\mu E_{\Delta_0} \leqslant S E_{\Delta_0} \leqslant \mu E_{\Delta_0}.$$

It follows by antisymmetry of \leqslant that

$$(S - \mu I) E_{\Delta_0} = 0.$$

Let us now fix $u \in \mathcal{H}$ and set $v = E_{\Delta_0} u$, so that $(S - \mu I)v = 0$ and, by part (c) of Lemma 1.5.9, we have

$$E_\mu E_{\Delta_0} u = E_\mu v = (I - E_+(\mu))v = 0.$$

Finally, it follows from (2.2.3) that

$$E_{\Delta_0} u = \lim_{\lambda \nearrow \mu} E_\Delta u = \lim_{\lambda \nearrow \mu} E_\mu E_\Delta u = E_\mu E_{\Delta_0} u = 0.$$

Since $u \in \mathcal{H}$ is arbitrary, we have indeed shown that $E_{\Delta_0} = 0$.

Let us now prove part (c), thereby showing that $(E_\lambda)_{\lambda \in \mathbb{R}}$ satisfies condition (iv) of Definition 2.1.1. Suppose by contradiction that $\lambda < m$ and $E_\lambda \neq 0$. Then there exists $u \in \mathcal{H}$ such that $E_\lambda u \neq 0$ and we let $v = E_\lambda u$. We can suppose that $\|v\| = 1$, and we obtain from (2.2.2) that

$$\langle S v, v \rangle - \lambda = \langle (S - \lambda I) v, v \rangle = \langle (S - \lambda I) E_\lambda u, u \rangle \leqslant 0.$$

Therefore, by definition of the lower bound of S ,

$$m \leqslant \langle S v, v \rangle \leqslant \lambda,$$

a contradiction. Hence $E_\lambda = 0$ for all $\lambda < m$. Suppose now by contradiction that $\lambda > M$ and $E_\lambda \neq I$. Then there is $u \in \mathcal{H}$ such that $w = (I - E_\lambda)u \neq 0$. We can again suppose that $\|w\| = 1$. Hence, by (2.2.2),

$$\langle S w, w \rangle - \lambda = \langle (S - \lambda I) w, w \rangle = \langle (S - \lambda I)(I - E_\lambda)u, u \rangle \geqslant 0.$$

Therefore, by definition of the upper bound of S ,

$$\lambda \leqslant \langle S w, w \rangle \leqslant M,$$

a contradiction. Hence $E_\lambda = I$ for all $\lambda > M$.

We finally prove part (d). For a small $\varepsilon > 0$, consider a sequence of partitions $(\Pi_j)_{j=1}^\infty$, denoted as

$$\Pi_j : \quad m = \lambda_0^j < \lambda_1^j < \cdots < \lambda_{n_j-1}^j < \lambda_{n_j}^j = M + \varepsilon,$$

and satisfying $\lim_{j \rightarrow \infty} |\Pi_j| = 0$. For all $j \geq 1$ and all $k = 1, \dots, n_j$, writing $E_{\Delta_k^j} = E_{\lambda_k^j} - E_{\lambda_{k-1}^j}$, it follows from (2.2.4) that

$$\lambda_{k-1}^j E_{\Delta_k^j} \leq S E_{\Delta_k^j} \leq \lambda_k^j E_{\Delta_k^j}.$$

Hence, for fixed $j \geq 1$, since $\sum_{k=1}^{n_j} E_{\Delta_k^j} = I$, summation over $k = 1, \dots, n_j$ yields

$$S_{\Pi_j} \leq S \leq \tilde{S}_{\Pi_j},$$

where the sum S_{Π_j} is taken over the partition Π_j , with the function $f(\lambda) = \lambda$ and the choice of $\mu_k^j = \lambda_{k-1}^j$, while \tilde{S}_{Π_j} is computed with $\tilde{\mu}_k^j = \lambda_k^j$. Hence, letting $j \rightarrow \infty$, Lemma 2.1.2 gives

$$\int_m^{M^+} \lambda \, dE_\lambda \leq S \leq \int_m^{M^+} \lambda \, dE_\lambda \implies S = \int_m^{M^+} \lambda \, dE_\lambda.$$

It remains to prove the uniqueness of the spectral family of S . This will be done in the problems using the following lemma. \square

Lemma 2.2.2 *Consider a symmetric operator S and let $(E_\lambda)_{\lambda \in \mathbb{R}}$ be a corresponding spectral family satisfying parts (a) to (d) of the theorem. For any real polynomial p , there holds*

$$p(S) = \int_m^{M^+} p(\lambda) \, dE_\lambda.$$

Proof. We need only show that the conclusion holds for any monomial $p(\lambda) = \lambda^l$ with $l \geq 0$. We already know that this is true for $l = 0$, and the theorem gives the result for $l = 1$. We prove the result by induction, assuming it holds for $p(\lambda) = \lambda^l$ and inferring it holds for $p(\lambda) = \lambda^{l+1}$. Fix $0 < \eta < 1$ arbitrary. Using the theorem and the induction hypothesis, there exists $\delta > 0$ such that, for any partition $\Pi = (\lambda_k)_{k=0}^n$ satisfying $|\Pi| \leq \delta$, there holds

$$\|S - \sum_{k=1}^n \lambda_k E_{\Delta_k}\| \leq \eta \quad \text{and} \quad \|S^l - \sum_{k=1}^n \lambda_k^l E_{\Delta_k}\| \leq \eta,$$

where $E_{\Delta_k} = E_{\lambda_k} - E_{\lambda_{k-1}}$. Let us write $T = \sum_{k=1}^n \lambda_k E_{\Delta_k}$ and $T^{(l)} = \sum_{k=1}^n \lambda_k^l E_{\Delta_k}$. For all k ,

$$E_{\Delta_k}^2 = E_{\lambda_k}^2 - 2E_{\lambda_k} E_{\lambda_{k-1}} + E_{\lambda_{k-1}}^2 = E_{\Delta_k},$$

while for all $i \neq j$,

$$E_{\Delta_i} E_{\Delta_j} = E_{\lambda_i} E_{\lambda_j} - E_{\lambda_i} E_{\lambda_{j-1}} - E_{\lambda_{i-1}} E_{\lambda_j} + E_{\lambda_{i-1}} E_{\lambda_{j-1}} = 0.$$

It follows that $T^{(l)}T = \sum_{k=1}^n \lambda_k^{l+1} E_{\Delta_k} = T^{(l+1)}$. Using

$$\|S^l T - S^{l+1}\| \leq \|S^l\| \|T - S\| \leq \|S\|^l \eta,$$

$$\|S T^{(l)} - S^{l+1}\| \leq \|S\| \|T^{(l)} - S^l\| \leq \|S\| \eta,$$

and

$$\begin{aligned} \|S^{l+1} - S^l T - T^{(l)} S + T^{(l)} T\| &= \|(S^l - T^{(l)})(S - T)\| \\ &\leq \|S^l - T^{(l)}\| \|S - T\| \leq \eta^2, \end{aligned}$$

we deduce that

$$\begin{aligned} \|T^{(l+1)} - S^{l+1}\| &= \|(S^{l+1} - S^l T - T^{(l)} S + T^{(l)} T) + (S^l T - S^{l+1}) + (S T^{(l)} - S^{l+1})\| \\ &\leq \eta^2 + \|S\|^l \eta + \|S\| \eta. \end{aligned}$$

Hence, by Lemma 2.1.2,

$$S^{l+1} = \int_m^{M^+} \lambda^{l+1} dE_\lambda,$$

which concludes the proof. \square

Corollary 2.2.3 *Let S be a symmetric operator and $(E_\lambda)_{\lambda \in \mathbb{R}}$ a corresponding spectral family satisfying parts (a) to (d) of the theorem. For all $u, v \in \mathcal{H}$ and all real polynomial p , we have*

$$\langle p(S)u, v \rangle = \int_m^{M+\varepsilon} p(\lambda) d\langle E_\lambda u, v \rangle \quad \forall \varepsilon > 0. \quad (2.2.5)$$

Proof. See Problem 2.1. \square

The right-hand side of (2.2.5) is a Riemann-Stieltjes integral (cf. Appendix A). For all $u \in \mathcal{H}$ the function $\lambda \mapsto \langle E_\lambda u, u \rangle$ is non-decreasing and so, in particular, of bounded variations in $[m, M + \varepsilon]$. Its total variation in $[m, M + \varepsilon]$ is equal to $\|u\|^2$. Furthermore, the value of the right-hand side does not depend on ε . This follows again from the fact that, for $\lambda > \mu > M$, $E_\lambda - E_\mu = 0$.

2.3 Further properties of the spectral family

We conclude this chapter by discussing the relation between the spectral family of a symmetric operator S and the two components of its spectrum, $\sigma_p(S)$ and $\sigma_c(S)$. Notice that, by Corollary 1.4.14, $\sigma_r(S) = \emptyset$ for any symmetric operator S .

Theorem 2.3.1 *Let S be a symmetric operator and $(E_\lambda)_{\lambda \in \mathbb{R}}$ the corresponding spectral family. The real number λ_0 is an eigenvalue of S if and only if the mapping $\lambda \mapsto E_\lambda$ is discontinuous at $\lambda = \lambda_0$ (i.e. $E_{\lambda_0} \neq E_{\lambda_0^+}$). In this case,*

$$\ker(S - \lambda_0 I) = \text{rge}(E_{\lambda_0^+} - E_{\lambda_0}). \quad (2.3.1)$$

Proof. See Problem 2.6. □

The next result completes our discussion by a remarkable characterization of the resolvent set.

Theorem 2.3.2 *Let S be a symmetric operator and $(E_\lambda)_{\lambda \in \mathbb{R}}$ the corresponding spectral family. Then a real number λ_0 belongs to the resolvent set $\rho(S)$ of S if and only if there exists $\epsilon > 0$ such that the mapping $\lambda \mapsto E_\lambda$ is constant on the interval $[\lambda_0 - \epsilon, \lambda_0 + \epsilon]$. We call such a λ_0 a point of constancy of $(E_\lambda)_{\lambda \in \mathbb{R}}$.*

Our final result follows immediately from the two previous theorems, and Corollary 1.4.14

Corollary 2.3.3 *Let S be a symmetric operator and $(E_\lambda)_{\lambda \in \mathbb{R}}$ the corresponding spectral family. A real number λ_0 belongs to the continuous spectrum $\sigma_c(S)$ of S if and only if λ_0 is neither a point of constancy, nor a point of discontinuity of $(E_\lambda)_{\lambda \in \mathbb{R}}$.*

Problems

1. Prove Corollary 2.2.3.
Hint: Use Lemma 2.2.2 and Theorem A.2.1.
2. Prove the uniqueness of the spectral family in Theorem 2.2.1.
Hint: Use the Weierstrass approximation theorem, Corollary 2.2.3 and Theorems A.3.3 and A.3.4.

3. We consider again the operator $X : L^2(0, 1) \rightarrow L^2(0, 1)$, $(Xu)(x) = xu(x)$. In Problem 1.18 we showed that $\sigma(X) = \sigma_c(X) = [0, 1]$. Prove that the spectral family $(E_\lambda)_{\lambda \in \mathbb{R}}$ of X is given by

$$E_\lambda u = \begin{cases} 0 & \text{if } \lambda \leq 0, \\ \chi_{[0, \lambda]} u & \text{if } \lambda \in (0, 1], \\ u & \text{if } \lambda > 1, \end{cases}$$

where $\chi_{[0, \lambda]}$ is the characteristic function of the interval $[0, \lambda]$.

Hint: Start by showing that $|X - \lambda I|$ is the operator $T_\lambda : L^2(0, 1) \rightarrow L^2(0, 1)$ defined by $(T_\lambda u)(x) = |x - \lambda|u(x)$, $x \in [0, 1]$. Then find the corresponding projection $E_+(\lambda)$ appearing in the proof of Theorem 2.2.1.

4. From Theorems 2.2.1, 2.3.1 and 2.3.2, deduce the structure of the spectral family and the spectral decomposition (a) of a (finite-dimensional) Hermitian matrix, (b) of a compact operator having infinitely many eigenvalues.
5. Verify that the spectral family obtained in Problem 2.3 satisfies the conclusions of Theorems 2.3.1 and 2.3.2.
6. The goal of this problem is to prove Theorem 2.3.1. First, the whole proof can be reduced to checking (2.3.1). Explain why. Then, to prove (2.3.1), one can proceed as follows.
- (a) To prove that $\ker(S - \lambda_0 I) \supset \text{rge}(E_{\lambda_0^+} - E_{\lambda_0})$, use inequality (2.2.4).
- (b) The other inclusion is more involved. We need to show that, if $u \in \ker(S - \lambda_0 I)$ then $F_0 u = u$, where we have put $F_0 = E_{\lambda_0^+} - E_{\lambda_0}$ — explain why this is enough. To do this, use Corollary 2.2.3 with $p(\lambda) = (\lambda - \lambda_0)^2$ to prove that $\langle E_{\lambda_0 - \varepsilon} u, u \rangle = \langle u - E_{\lambda_0 + \varepsilon} u, u \rangle = 0$, for any $\varepsilon > 0$.
7. In this problem we shall prove Theorem 2.3.2. We will use the fact that $\lambda_0 \in \rho(S)$ if and only if there exists $\gamma > 0$ such that

$$\|(S - \lambda_0 I)u\| \geq \gamma \|u\|, \quad u \in \mathcal{H}. \quad (2.3.2)$$

- (a) To prove that the constancy condition implies $\lambda_0 \in \rho(S)$, use Corollary 2.2.3 with $p(\lambda) = (\lambda - \lambda_0)^2$, and (2.3.2).
- (b) To show that λ_0 is a point of constancy if it is in the resolvent set, proceed by contradiction using again (2.3.2) and Corollary 2.2.3, with $p(\lambda) = (\lambda - \lambda_0)^2$ and a suitably chosen u .
Hint: The identities $E_\lambda E_\mu = E_\mu E_\lambda = E_\lambda$, $\lambda \leq \mu$, can be useful here.

Chapter 3

The spectral decomposition of selfadjoint operators

In this chapter we will extend the spectral theorem to general (unbounded) selfadjoint operators. We start by introducing the properties of unbounded operators that will be relevant to our analysis.

3.1 Unbounded linear operators

Some natural operators in a Hilbert space \mathcal{H} fail to be bounded. Those are typically only defined on a subspace of \mathcal{H} , called their *domain*.

Definition 3.1.1 Let \mathcal{H} be a Hilbert space. A **linear operator** (or simply **operator**) in \mathcal{H} is a mapping $T : \mathfrak{D}_T \subseteq \mathcal{H} \rightarrow \mathcal{H}$ satisfying:

- (i) \mathfrak{D}_T is a subspace of \mathcal{H} called the **domain** of T ;
- (ii) for all $u, v \in \mathfrak{D}_T$,
$$T(u + v) = Tu + Tv;$$
- (iii) for all $\lambda \in \mathbb{C}$ and all $u \in \mathfrak{D}_T$,
$$T(\lambda u) = \lambda Tu. \blacklozenge$$

We also adapt in the obvious way the notions of range and kernel. Let T be a linear operator acting in \mathcal{H} . Its **range** is defined as

$$\text{rge}(T) = \{Tu; u \in \mathfrak{D}_T\},$$

and its **kernel** as

$$\ker(T) = \{u \in \mathfrak{D}_T; Tu = 0\}.$$

Note that, unlike the kernel of a bounded operator, this is not a closed subspace in general.

We say that $T : \mathfrak{D}_T \subseteq \mathcal{H} \rightarrow \mathcal{H}$ is bounded (on \mathfrak{D}_T) if there is a constant $C \geq 0$ such that, for all $u \in \mathfrak{D}_T$,

$$\|Tu\| \leq C \|u\|. \quad (3.1.1)$$

Consider two operators T and T' in \mathcal{H} , with respective domains \mathfrak{D}_T and $\mathfrak{D}_{T'}$. If

$$\mathfrak{D}_T \subseteq \mathfrak{D}_{T'} \quad \text{and} \quad Tu = T'u \quad \text{for all } u \in \mathfrak{D}_T,$$

we say that T' is an **extension** of T , and we write

$$T \subseteq T' \text{ or } T' \supseteq T.$$

This is easily seen to define a partial order on the operators of \mathcal{H} . In particular, two operators are equal ($T = T'$, i.e. $T \subseteq T'$ and $T \supseteq T'$) if and only if $\mathfrak{D}_T = \mathfrak{D}_{T'}$ and $Tu = T'u$ for all $u \in \mathfrak{D}_T$.

Proposition 3.1.2 *Consider an operator $T : \mathfrak{D}_T \subseteq \mathcal{H} \rightarrow \mathcal{H}$ satisfying (3.1.1) on \mathfrak{D}_T . Then there exists a unique linear extension of T to $\overline{\mathfrak{D}_T}$, still denoted $T : \overline{\mathfrak{D}_T} \rightarrow \mathcal{H}$. Furthermore, this extension satisfies (3.1.1) on $\overline{\mathfrak{D}_T}$.*

Proof. Suppose T satisfies (3.1.1) on \mathfrak{D}_T , let $u \in \overline{\mathfrak{D}_T}$ and consider a sequence $(u_n) \subset \mathfrak{D}_T$ such that $u_n \rightarrow u$. Since

$$\|Tu_n - Tu_m\| = \|T(u_n - u_m)\| \leq C \|u_n - u_m\| \rightarrow 0, \quad n, m \rightarrow \infty,$$

the sequence (Tu_n) is Cauchy in \mathcal{H} . Let us denote by Tu its limit. This defines a linear extension of T to $\overline{\mathfrak{D}_T}$ (still denoted T). It is clear that the extension is unique by uniqueness of the limit. Furthermore, since u_n satisfies (3.1.1) for all $n \in \mathbb{N}$, passing to the limit yields (3.1.1) on $\overline{\mathfrak{D}_T}$. \square

Remark 3.1.3 By the same argument, one shows that a linear functional that is bounded on a subspace can be extended uniquely to a bounded linear functional on the closure of this subspace.

If \mathfrak{D}_T is dense in \mathcal{H} , we say that T is **densely defined**. Proposition 3.1.2 implies that any bounded densely defined operator can be extended to an operator in $\mathcal{B}(\mathcal{H})$.

Similarly to the bounded case, we define the **graph** of an operator $T : \mathfrak{D}_T \subseteq \mathcal{H} \rightarrow \mathcal{H}$ as

$$\mathbf{G}_T = \{(x, Tx) ; x \in \mathfrak{D}_T\} \subset \mathcal{H} \times \mathcal{H},$$

and we equip the product Hilbert space $\mathcal{H} \times \mathcal{H}$ with the natural inner product inherited from \mathcal{H} :

$$\langle (u, v), (u', v') \rangle := \langle u, u' \rangle + \langle v, v' \rangle, \quad (u, v), (u', v') \in \mathcal{H}.$$

If T_1 and T_2 are linear operators, then obviously $T_1 \subseteq T_2$ is equivalent to $\mathbf{G}_{T_1} \subseteq \mathbf{G}_{T_2}$.

Definition 3.1.4 We say that T is **closed** if its graph is a closed subset of $\mathcal{H} \times \mathcal{H}$. ♦

Consider two linear operators $T_1 : \mathfrak{D}_{T_1} \subseteq \mathcal{H} \rightarrow \mathcal{H}$ and $T_2 : \mathfrak{D}_{T_2} \subseteq \mathcal{H} \rightarrow \mathcal{H}$, and a scalar $\lambda \in \mathbb{C}$. The sum of T_1 and T_2 is defined as:

$$\begin{aligned} T_1 + T_2 : \mathfrak{D}_{T_1} \cap \mathfrak{D}_{T_2} &\longrightarrow \mathcal{H} \\ u &\longmapsto T_1 u + T_2 u. \end{aligned}$$

The multiplication of T_1 by λ is defined by:

$$\begin{aligned} \lambda T_1 : \mathfrak{D}_{T_1} &\longrightarrow \mathcal{H} \\ u &\longmapsto \lambda T_1 u. \end{aligned}$$

Finally, the composition (or product) of T_1 and T_2 is the operator defined as:

$$\begin{aligned} T_1 T_2 : \{u \in \mathfrak{D}_{T_2} ; T_2 u \in \mathfrak{D}_{T_1}\} &\longrightarrow \mathcal{H} \\ u &\longmapsto T_1(T_2 u). \end{aligned}$$

We also introduce the notion of inverse for unbounded operators. If an operator $T : \mathfrak{D}_T \rightarrow \mathcal{H}$ is one-to-one, we call **inverse** of T the mapping T^{-1} defined by:

$$\begin{aligned} T^{-1} : \text{rge}(T) &\longrightarrow \mathcal{H} \\ Tu &\longmapsto u. \end{aligned}$$

Observe that $\text{rge}(T^{-1}) = \mathfrak{D}_T$. Furthermore, if T is one-to-one, there holds

$$TT^{-1} \subseteq I \quad \text{and} \quad T^{-1}T \subseteq I.$$

Definition 3.1.5 We define the **resolvent set** $\rho(T)$ of T as the set of all complex numbers λ such that $T - \lambda I$ is a bijection from \mathfrak{D}_T onto \mathcal{H} , with a bounded inverse. The (point/continuous/residual) **spectrum** is then defined exactly as in the bounded case; see Definition 1.2.9. ♦

Note that for a complex number λ to belong to $\rho(T)$ several conditions must be met, which in some cases are not independent. For instance, if T is closed it follows from the Closed Graph Theorem that, if $T - \lambda I$ is a bijection from \mathfrak{D}_T onto \mathcal{H} then its inverse is automatically bounded. For other relations, see Problem 3.2.

3.2 The adjoint operator

We shall now extend the notion of an adjoint operator to unbounded operators having a dense domain. In the case of a bounded T , recall that the adjoint T^* of T was merely defined by

$$\langle Tu, v \rangle = \langle u, T^*v \rangle \text{ for all } u, v \in \mathcal{H}. \quad (3.2.1)$$

This definition relies on the fact that, for all $v \in \mathcal{H}$, the mapping

$$u \mapsto \langle Tu, v \rangle \quad (3.2.2)$$

is a continuous linear functional on \mathcal{H} . Then the Riesz Representation Theorem 1.2.8 yields a unique $v^* \in \mathcal{H}$ such that $\langle Tu, v \rangle = \langle u, v^* \rangle$, for all $u \in \mathcal{H}$.

In case T is not bounded, the definition of the adjoint is less straightforward. Indeed, the mapping (3.2.2) can *a priori* be defined only on \mathfrak{D}_T . Then, in general, it will not be bounded on \mathfrak{D}_T for all $v \in \mathcal{H}$. Furthermore, even if (3.2.2) is bounded for some v , then if \mathfrak{D}_T is not dense there will be several possible continuous extensions to \mathcal{H} and so, by Riesz, several points $v^* \in \mathcal{H}$ satisfying

$$\langle Tu, v \rangle = \langle u, v^* \rangle \text{ for all } u \in \mathfrak{D}_T.$$

These considerations lead naturally to the following definition.

Definition 3.2.1 Consider a densely defined operator $T : \mathfrak{D}_T \subseteq \mathcal{H} \rightarrow \mathcal{H}$. The domain of the **adjoint** T^* of T is defined as

$$\mathfrak{D}_{T^*} = \{v \in \mathcal{H}; \text{ there exists } C \geq 0 \text{ s.t. } |\langle Tu, v \rangle| \leq C \|u\| \text{ for all } u \in \mathfrak{D}_T\}.$$

Now for all $v \in \mathfrak{D}_{T^*}$, since \mathfrak{D}_T is dense in \mathcal{H} , Remark 3.1.3 yields a unique continuous extension to \mathcal{H} of the functional $u \mapsto \langle Tu, v \rangle$. Then, for all $v \in \mathfrak{D}_{T^*}$, the Riesz Representation Theorem 1.2.8 allows us to define T^*v as the unique element of \mathcal{H} satisfying

$$\langle Tu, v \rangle = \langle u, T^*v \rangle \text{ for all } u \in \mathfrak{D}_T. \blacklozenge$$

We now show that \mathfrak{D}_{T^*} is a subspace and T^* is linear. Let $u_1, u_2 \in \mathfrak{D}_{T^*}$ and $\lambda_1, \lambda_2 \in \mathbb{C}$. Then indeed, for all $u \in \mathfrak{D}_T$, we have

$$\begin{aligned} \langle Tu, \lambda_1 u_1 + \lambda_2 u_2 \rangle &= \overline{\lambda_1} \langle Tu, u_1 \rangle + \overline{\lambda_2} \langle Tu, u_2 \rangle \\ &= \overline{\lambda_1} \langle u, T^*u_1 \rangle + \overline{\lambda_2} \langle u, T^*u_2 \rangle \\ &= \langle u, \lambda_1 T^*u_1 + \lambda_2 T^*u_2 \rangle. \end{aligned}$$

It follows that $\lambda_1 u_1 + \lambda_2 u_2 \in \mathfrak{D}_{T^*}$ and

$$T^*(\lambda_1 u_1 + \lambda_2 u_2) = \lambda_1 T^* u_1 + \lambda_2 T^* u_2.$$

Note that, at this stage, we do not know whether \mathfrak{D}_{T^*} is trivial or not. The next lemma ensures that $\mathfrak{D}_{T^*} \neq \{0\}$ if $\text{rge}(T)$ is not dense in \mathcal{H} .

By definition, a densely defined operator T satisfies the fundamental relation

$$\langle Tu, v \rangle = \langle u, T^*v \rangle \text{ for all } u \in \mathfrak{D}_T \text{ and all } v \in \mathfrak{D}_{T^*}. \quad (3.2.3)$$

The following result extends Lemma 1.4.4 to unbounded operators.

Lemma 3.2.2 *Let $T : \mathfrak{D}_T \subseteq \mathcal{H} \rightarrow \mathcal{H}$ be densely defined. Then*

$$\mathcal{H} = \ker(T^*) \oplus \overline{\text{rge}(T)}.$$

Proof. We will prove that $\text{rge}(T)^\perp = \ker(T^*)$. In particular, $\ker(T^*)$ is closed. Then the result follows, as in the bounded case, from the identity $M^{\perp\perp} = \overline{M}$, satisfied by any subspace $M \subseteq \mathcal{H}$.

Let $v \in \ker(T^*)$. By (3.2.3), it follows that $v \in \mathfrak{D}_{T^*}$ and $\langle Tu, v \rangle = 0$ for all $u \in \mathfrak{D}_T$. Hence, $v \in \text{rge}(T)^\perp$. Conversely, let $v \in \text{rge}(T)^\perp$. Then $\langle Tu, v \rangle = 0$ for all $u \in \mathfrak{D}_T$. We deduce that $v \in \mathfrak{D}_{T^*}$ and

$$\langle u, T^*v \rangle = 0 \text{ for all } u \in \mathfrak{D}_T. \quad (3.2.4)$$

Now let $u \in \mathcal{H}$. Since \mathfrak{D}_T is dense, there exists a sequence $(u_n)_{n=1}^\infty \subset \mathfrak{D}_T$ such that $u_n \rightarrow u$. Hence, by (3.2.4), we have

$$\langle u, T^*v \rangle = \lim_{n \rightarrow \infty} \langle u_n, T^*v \rangle = 0.$$

We conclude that $\langle u, T^*v \rangle = 0$ for all $u \in \mathcal{H}$. Thus, $v \in \ker(T^*)$. □

The following proposition gives a fundamental property of the adjoint.

Proposition 3.2.3 *Let $T : \mathfrak{D}_T \subseteq \mathcal{H} \rightarrow \mathcal{H}$ be densely defined. Then T^* is closed.*

Proof. Consider a sequence $(u_n, T^*u_n)_{n=1}^\infty$ in the graph of T^* which converges to a point $(u, v) \in \mathcal{H} \times \mathcal{H}$. Let us show that $u \in \mathfrak{D}_{T^*}$ and $v = T^*u$. It follows from

$$\begin{aligned} \|(u_n, T^*u_n) - (u, v)\|_{\mathcal{H} \times \mathcal{H}}^2 &= \langle u_n - u, u_n - u \rangle + \langle T^*u_n - v, T^*u_n - v \rangle \\ &= \|u_n - u\|^2 + \|T^*u_n - v\|^2 \end{aligned}$$

that $u_n \rightarrow u$ and $T^*u_n \rightarrow v$ as $n \rightarrow \infty$. Then, by the continuity of the inner product, for all $w \in \mathfrak{D}_T$:

$$\langle Tw, u \rangle = \lim_{n \rightarrow \infty} \langle Tw, u_n \rangle = \lim_{n \rightarrow \infty} \langle w, T^*u_n \rangle = \langle w, v \rangle.$$

Hence, $w \mapsto \langle Tw, u \rangle$ is bounded on \mathfrak{D}_T , $u \in \mathfrak{D}_{T^*}$ and $\langle w, T^*u \rangle = \langle Tw, u \rangle = \langle w, v \rangle$. Since \mathfrak{D}_T is dense and $\langle w, T^*u - v \rangle = 0$ for any $w \in \mathfrak{D}_T$, we conclude that $T^*u = v$. \square

The adjoint operator also enjoys the following elementary properties.

Properties 3.2.4 Consider two densely defined operators $T_1 : \mathfrak{D}_{T_1} \rightarrow \mathcal{H}$, $T_2 : \mathfrak{D}_{T_2} \rightarrow \mathcal{H}$, and $\lambda \in \mathbb{C}$. Then:

- (a) $(\lambda T)^* = \bar{\lambda} T^*$;
- (b) if $\mathfrak{D}_{T_1+T_2}$ is dense, then $T_1^* + T_2^* \subseteq (T_1 + T_2)^*$;
- (c) if $\mathfrak{D}_{T_2 T_1}$ is dense, then $T_1^* T_2^* \subseteq (T_2 T_1)^*$;
- (d) if $T_1 \subseteq T_2$, then $T_1^* \supseteq T_2^*$.

3.3 Commutativity and reduction

We define here what it means for a bounded operator to commute with an unbounded operator.

Definition 3.3.1 Consider a bounded operator B and an operator $A : \mathfrak{D}_A \subset \mathcal{H} \rightarrow \mathcal{H}$. We say that B commutes with A , and we write $B \subseteq A$, if

$$BA \subseteq AB.$$

Explicitly, $BA \subseteq AB$ means that $\mathfrak{D}_A \subseteq \{u \in \mathcal{H} ; Bu \in \mathfrak{D}_A\}$ and $BAu = ABu$ for all $u \in \mathfrak{D}_A$. \blacklozenge

More generally, the commutativity between two unbounded *selfadjoint* operators will be defined later through the commutativity of their respective spectral families. This is the notion of commutativity which is required by quantum mechanics.

Lemma 3.3.2 Let P be a projection, $Q = I - P$ the projection onto the orthogonal complement of $\text{rge } P$, and A be any operator acting in \mathcal{H} . If $P \subseteq A$, then the closed subspaces $\text{rge } P$ and $\text{rge } Q$ reduce the operator A in the sense that, on the one hand,

$$PAP = AP \quad \text{and} \quad QAQ = AQ,$$

and, on the other hand,

$$A = AP + AQ.$$

Proof. Since $P \subseteq A$, i.e. $PA \subseteq AP$, we have

$$PAP = (PA)P \subseteq (AP)P = AP,$$

and since the operators PAP and AP have same domain,

$$PAP = AP.$$

Furthermore, since

$$QA = (I - P)A = A - PA \subseteq A - AP = A(I - P),$$

i.e. $Q \subseteq A$, we obtain similarly that $QAQ = AQ$. On the other hand, we have

$$A = (P + Q)A = PA + QA \subseteq AP + AQ \subseteq A(P + Q) = A,$$

and so

$$A = AP + AQ.$$

□

3.4 More on operator graphs

We define two linear operators $\mathbf{U}, \mathbf{V} : \mathcal{H} \times \mathcal{H} \rightarrow \mathcal{H} \times \mathcal{H}$ by

$$\mathbf{U}(u, v) = (v, u) \quad \text{and} \quad \mathbf{V}(u, v) = (v, -u), \quad (u, v) \in \mathcal{H} \times \mathcal{H}.$$

They are Hilbert space automorphisms of $\mathcal{H} \times \mathcal{H}$ (i.e. they are bijective and preserve the inner product). Furthermore, they satisfy the following identities, where \mathbf{I} denotes the identity on $\mathcal{H} \times \mathcal{H}$:

$$\mathbf{UV} = -\mathbf{VU} \quad \text{and} \quad -\mathbf{V}^2 = \mathbf{U}^2 = \mathbf{I}.$$

The following observation will be useful.

Lemma 3.4.1 *Let T be a densely defined operator in \mathcal{H} . The graphs of T and T^* satisfy*

$$\mathbf{G}_{T^*} = (\mathbf{V}\overline{\mathbf{G}_T})^\perp \text{ or, equivalently, } \mathbf{V}\overline{\mathbf{G}_T} = (\mathbf{G}_{T^*})^\perp.$$

Proof. For all $u \in \mathfrak{D}_T$ and all $v \in \mathfrak{D}_{T^*}$ we have

$$\langle Tu, v \rangle = \langle u, T^*v \rangle,$$

which can be written as

$$\langle \mathbf{V}(u, Tu), (v, T^*v) \rangle = 0. \quad (3.4.1)$$

Hence, we already remark that any element of \mathbf{G}_{T^*} is orthogonal to $\mathbf{V}\mathbf{G}_T$. Now the proof is in two steps.

$\mathbf{G}_{T^*} \subseteq (\overline{\mathbf{V}\mathbf{G}_T})^\perp$. Consider $(w, T^*w) \in \mathbf{G}_{T^*}$ and a sequence $(u_n, v_n)_{n=1}^\infty \subset \mathbf{V}\mathbf{G}_T$ which converges to $(u, v) \in \overline{\mathbf{V}\mathbf{G}_T} = \mathbf{V}\overline{\mathbf{G}_T}$. It then follows from (3.4.1) that

$$\langle (u, v), (w, T^*w) \rangle = \lim_{n \rightarrow \infty} \langle (u_n, v_n), (w, T^*w) \rangle = 0.$$

Hence, $(w, T^*w) \in (\mathbf{V} \overline{\mathbf{G}_T})^\perp$.

$(\overline{\mathbf{V}\mathbf{G}_T})^\perp \subseteq \mathbf{G}_{T^*}$. Let $(u, v) \in (\overline{\mathbf{V}\mathbf{G}_T})^\perp$. Then, in particular, for all $w \in \mathfrak{D}_T$,

$$0 = \langle \mathbf{V}(w, Tw), (u, v) \rangle = \langle Tw, u \rangle - \langle w, v \rangle. \quad (3.4.2)$$

Therefore, the mapping $w \mapsto \langle Tw, u \rangle$ coincides on \mathfrak{D}_T with the linear functional $w \mapsto \langle w, v \rangle$, which is bounded on \mathcal{H} . Hence, $u \in \mathfrak{D}_{T^*}$ and $T^*u = v$, i.e. $(u, v) \in \mathbf{G}_{T^*}$. \square

For closed operators, the previous lemma has the following important consequence.

Theorem 3.4.2 *Let T be a closed operator with dense domain. Then the domain of T^* is also dense in \mathcal{H} , and so $T^{**} = (T^*)^*$ does exist. Furthermore, $T^{**} = T$.*

Proof. Let

$$h \in (\overline{\mathfrak{D}_{T^*}})^\perp. \quad (3.4.3)$$

We will prove that $h = 0$. Since \mathbf{V} is unitary, it follows from Lemma 3.4.1 that

$$\mathbf{G}_T = \overline{\mathbf{G}_T} = \mathbf{V}^2 \overline{\mathbf{G}_T} = \mathbf{V}(\mathbf{G}_{T^*})^\perp = (\mathbf{V}\mathbf{G}_{T^*})^\perp. \quad (3.4.4)$$

Hence,

$$\mathcal{H} \times \mathcal{H} = \mathbf{G}_T \oplus \mathbf{V}\mathbf{G}_{T^*},$$

so there is a unique $u_h \in \mathfrak{D}_T$ and a unique $v_h \in \mathfrak{D}_{T^*}$ such that

$$(0, h) = (u_h, Tu_h) + (T^*v_h, -v_h),$$

that is,

$$0 = u_h + T^*v_h, \quad h = Tu_h - v_h.$$

Combining these equations, we obtain

$$\|v_h\|^2 = \langle v_h, v_h \rangle = \langle v_h, Tu_h \rangle = \langle T^*v_h, u_h \rangle = -\langle T^*v_h, T^*v_h \rangle = -\|T^*v_h\|^2,$$

so that $v_h = 0$. Returning to the above equations, we deduce that $u_h = 0$ and $h = Tu_h = 0$. Hence, \mathfrak{D}_{T^*} is dense in \mathcal{H} , and T^{**} exists.

Now, applying Lemma 3.4.1 to T^* instead of T , (3.4.4) yields

$$\mathbf{G}_{T^{**}} = (\mathbf{V}\mathbf{G}_{T^*})^\perp = \mathbf{G}_T. \quad (3.4.5)$$

Hence, $T^{**} = T$. □

The next theorem will play an important role in the proof of the spectral theorem for selfadjoint operators.

Theorem 3.4.3 *Let T be a closed operator with dense domain. The operators*

$$\mathbf{B} = (I + T^*T)^{-1} \quad \text{and} \quad \mathbf{C} = T(I + T^*T)^{-1}$$

are defined and bounded on \mathcal{H} , with

$$\|\mathbf{B}\| \leq 1 \quad \text{and} \quad \|\mathbf{C}\| \leq 1.$$

Furthermore, \mathbf{B} is symmetric and positive.

Proof. Since T is closed and densely defined, it follows from (3.4.4) that \mathbf{G}_T and $\mathbf{V}\mathbf{G}_{T^*}$ are orthogonal complements in $\mathcal{H} \times \mathcal{H}$. Hence, for all $h \in \mathcal{H}$, there is a unique $u_h \in \mathfrak{D}_T$ and a unique $v_h \in \mathfrak{D}_{T^*}$ such that

$$(h, 0) = (u_h, Tu_h) + (T^*v_h, -v_h), \quad (3.4.6)$$

or, by components,

$$\begin{cases} h = u_h + T^*v_h, \\ 0 = Tu_h - v_h. \end{cases}$$

This first observation allows us to define two linear maps \mathbf{B} and \mathbf{C} by

$$\mathbf{B}h = u_h \quad \text{and} \quad \mathbf{C}h = v_h.$$

These operators are defined on \mathcal{H} , and satisfy

$$\begin{cases} I = B + T^*C, \\ 0 = TB - C, \end{cases}$$

from which we deduce that

$$C = TB \quad \text{and} \quad I = B + T^*TB = (I + T^*T)B. \quad (3.4.7)$$

Furthermore, the two terms in the right-hand side of (3.4.6) are orthogonal, so

$$\begin{aligned} \|h\|^2 &= \|(h, 0)\|_{\mathcal{H} \times \mathcal{H}}^2 = \|(u_h, Tu_h)\|_{\mathcal{H} \times \mathcal{H}}^2 + \|(T^*v_h, -v_h)\|_{\mathcal{H} \times \mathcal{H}}^2 \\ &= \|u_h\|^2 + \|Tu_h\|^2 + \|T^*v_h\|^2 + \|v_h\|^2. \end{aligned}$$

Therefore,

$$\|Bh\|^2 + \|Ch\|^2 = \|u_h\|^2 + \|v_h\|^2 \leq \|h\|^2,$$

and it follows that

$$\|B\| \leq 1 \quad \text{and} \quad \|C\| \leq 1.$$

We now observe that, for any u in the domain of T^*T ,

$$\langle (I + T^*T)u, u \rangle = \langle u, u \rangle + \langle Tu, Tu \rangle \geq \langle u, u \rangle = \|u\|^2 \geq 0.$$

Hence, if $(I + T^*T)u = 0$ then $u = 0$. This shows that $I + T^*T$ is one-to-one and so has an inverse $(I + T^*T)^{-1}$. But now the right identity in (3.4.7) implies that $\text{rge}(I + T^*T) = \mathcal{H}$, and it follows that

$$B = (I + T^*T)^{-1}.$$

Finally, B is symmetric and positive. Indeed, for all $u, v \in \mathcal{H}$,

$$\begin{aligned} \langle Bu, v \rangle &= \langle Bu, (I + T^*T)Bv \rangle = \langle Bu, Bv \rangle + \langle Bu, T^*TBv \rangle \\ &= \langle Bu, Bv \rangle + \langle T^*TBu, Bv \rangle = \langle (I + T^*T)Bu, Bv \rangle = \langle u, Bv \rangle. \end{aligned}$$

Furthermore, for all $u \in \mathcal{H}$,

$$\langle Bu, u \rangle = \langle Bu, (I + T^*T)Bu \rangle = \langle Bu, Bu \rangle + \langle TBu, TBu \rangle = \|Bu\|^2 + \|TBu\|^2 \geq 0.$$

This concludes the proof. □

A useful corollary of Theorem 3.4.3 will be stated in the next section.

3.5 Symmetric and selfadjoint operators

We will now introduce the terms *symmetric* and *selfadjoint* in the framework of unbounded operators. The two notions coincide for bounded operators.

Definition 3.5.1 We call **symmetric** an operator $T : \mathfrak{D}_T \subseteq \mathcal{H} \rightarrow \mathcal{H}$ such that \mathfrak{D}_T is dense in \mathcal{H} and

$$T \subseteq T^*. \blacklozenge$$

Proposition 3.5.2 An operator $T : \mathfrak{D}_T \subseteq \mathcal{H} \rightarrow \mathcal{H}$ is symmetric if and only if \mathfrak{D}_T is dense and

$$\langle Tu, v \rangle = \langle u, Tv \rangle \quad \text{for all } u, v \in \mathfrak{D}_T. \quad (3.5.1)$$

Proof. If T is symmetric then \mathfrak{D}_T is dense, $\mathfrak{D}_T \subset \mathfrak{D}_{T^*}$ and $T^*v = Tv$ for all $u \in \mathfrak{D}_T$. Since, $\langle Tu, v \rangle = \langle u, T^*v \rangle$ for all $u \in \mathfrak{D}_T$ and $v \in \mathfrak{D}_{T^*}$, in particular (3.5.1) holds.

Conversely, suppose that \mathfrak{D}_T is dense and (3.5.1) holds. Let $v \in \mathfrak{D}_T$. Then (3.5.1) implies that the linear functional $u \mapsto \langle Tu, v \rangle$ is bounded on \mathfrak{D}_T , hence $v \in \mathfrak{D}_{T^*}$. Thus, $\mathfrak{D}_T \subseteq \mathfrak{D}_{T^*}$. Furthermore, by definition of T^* , we deduce from (3.5.1) that $\langle u, T^*v - Tv \rangle = 0$ for all $u \in \mathfrak{D}_T$. Since \mathfrak{D}_T is dense, it follows that $T^*v - Tv = 0$. This shows that T^* indeed coincides with T on \mathfrak{D}_T . \square

Definition 3.5.3 An operator T is said to be **closable** provided the closure of its graph is the graph of an operator. This operator is then called the **closure** of T , denoted \overline{T} :

$$\overline{\mathbf{G}_T} = \mathbf{G}_{\overline{T}}. \blacklozenge$$

Remark 3.5.4 Let T be a symmetric operator. Then the domain of T^* is dense in \mathcal{H} . Indeed,

$$\mathcal{H} = \overline{\mathfrak{D}_T} \subseteq \overline{\mathfrak{D}_{T^*}} \subseteq \mathcal{H}.$$

Hence, T^{**} is well defined. The operator T^{**} is a closed extension of T since, by Lemma 3.4.1,

$$\mathbf{G}_{T^{**}} = (\mathbf{V}\mathbf{G}_{T^*})^\perp = \mathbf{V}^2\overline{\mathbf{G}_T} = \overline{\mathbf{G}_T} \supseteq \mathbf{G}_T. \quad (3.5.2)$$

Thus, T is closable, with $\overline{T} = T^{**}$. (As will be seen in Problem 3.4, this relation between closure and adjoint also holds for non-symmetric operators, whenever T^* is densely defined.)

Furthermore, T^{**} is symmetric. Indeed, $T \subseteq T^{**}$ implies that $\mathfrak{D}_{T^{**}}$ is dense. Moreover, since $T \subseteq T^*$, it follows by Theorem 3.4.2 that

$$T^{**} \subseteq T^* = (T^*)^{**} = (T^{**})^*.$$

If $B \in \mathcal{B}(\mathcal{H})$ is symmetric in the sense of Definition 3.5.1, then it is symmetric in the sense of bounded operators, i.e. $B^* = B$. However, for a general densely defined operator T , being symmetric does not imply $T^* = T$.

Definition 3.5.5 An operator $T : \mathfrak{D}_T \subseteq \mathcal{H} \rightarrow \mathcal{H}$ is called **selfadjoint** if \mathfrak{D}_T is dense in \mathcal{H} and

$$T = T^*. \blacklozenge$$

It follows immediately from Proposition 3.2.3 that a selfadjoint operator is closed. Remark 3.5.4 shows that any symmetric operator has closed symmetric extensions. However, a symmetric operator T (even closed) does not necessarily possess a selfadjoint extension. If it does, the inclusions

$$T \subseteq A = A^* \subseteq T^*$$

indicate where a selfadjoint extension is to be found.

A symmetric operator T is called **maximal symmetric** if it has no proper symmetric extension, i.e. if there is no symmetric operator S such that $T \subseteq S$ and $T \neq S$. Observe that any selfadjoint A is maximal symmetric. Indeed,

$$A \subseteq T \quad \text{and} \quad T \subseteq T^*$$

implies

$$A \subseteq T \subseteq T^* \subseteq A^* = A,$$

and so $T = A$.

We say that a symmetric operator A is **essentially selfadjoint** if \overline{A} is selfadjoint. The proof of the next theorem can be found in [Wei80, p. 108].

Theorem 3.5.6 *A symmetric operator A is essentially selfadjoint if and only if the subspaces $\text{rge}(A \pm iI)$ are dense in \mathcal{H} .*

We conclude this section with the following corollary of Theorem 3.4.3.

Corollary 3.5.7 *If A is selfadjoint, then the operators $B = (I + A^2)^{-1}$ and $C = AB$ given by Theorem 3.4.3 have the following additional properties:*

- (a) $B(\mathfrak{D}_A) = \mathfrak{D}_{A^3}$;
- (b) $B \restriction A$, i.e. $BA \subseteq AB$;
- (c) $CB = BC$;
- (d) any operator $T \in \mathcal{B}(\mathcal{H})$ such that $T \restriction A$ satisfies $TB = BT$.

Proof. Let us first prove that $B(\mathfrak{D}_A) = \mathfrak{D}_{A^3}$. Since $(I + A^2)B = I$ and $\mathfrak{D}_{A-C} = \mathfrak{D}_A$,

$$\begin{aligned} u \in \mathfrak{D}_A &\implies (A - C)u = Au - ABu \\ &= A(I - B)u \\ &= A((I + A^2)B - B)u \\ &= A^3Bu. \end{aligned}$$

Hence, $B(\mathfrak{D}_A) \subseteq \mathfrak{D}_{A^3}$. Conversely, if $v \in \mathfrak{D}_{A^3} \subseteq \mathfrak{D}_{A^2} = \mathfrak{D}_{B^{-1}}$, then

$$u = B^{-1}v = (I + A^2)v \in \mathfrak{D}_A.$$

This shows that $v \in B(\mathfrak{D}_A)$. Hence, $\mathfrak{D}_{A^3} \subseteq B(\mathfrak{D}_A)$.

We now show that $BA \subseteq AB$. Let $u \in \mathfrak{D}_A$. Then $Bu \in \mathfrak{D}_{A^3}$, $ABu \in \mathfrak{D}_{A^2}$ and we have

$$ABu = B(I + A^2)ABu = BA(I + A^2)Bu = BAu.$$

It follows that

$$BC = (BA)B \subseteq (AB)B = CB,$$

and, since BC is defined everywhere, $BC = CB$.

Finally, for $T \in \mathcal{H}$ such that $T \lrcorner A$, we have in particular that

$$TA^2 \subseteq ATA \subseteq A^2T, \tag{3.5.3}$$

and so

$$TB^{-1} = T(I + A^2) \subseteq (I + A^2)T = B^{-1}T. \tag{3.5.4}$$

It also follows from (3.5.3) that, if $u \in \mathfrak{D}_{A^2}$ then $TA^2u = A^2Tu$, and so $Tu \in \mathfrak{D}_{A^2}$. Consider $u \in \mathfrak{D}_A$ arbitrary. By part (a), $Bu \in \mathfrak{D}_{A^3} \subseteq \mathfrak{D}_{A^2}$ and so $TBu \in \mathfrak{D}_{A^2} = \mathfrak{D}_{B^{-1}}$. It then follows by (3.5.4) that

$$TBu = BB^{-1}TBu = BTB^{-1}Bu = BTu.$$

Since \mathfrak{D}_A is dense in \mathcal{H} and since TB and BT are continuous, it follows that $TB = BT$. \square

3.6 Integration with respect to a spectral family

In this section we extend the notion of spectral family in a natural way to deal with unbounded operators and, using Lebesgue integration, we define the integral with respect to a spectral family for a large class of functions.

Definition 3.6.1 A **spectral family** on \mathcal{H} is a mapping $E : \mathbb{R} \rightarrow \mathcal{B}(\mathcal{H})$, denoted $(E_\lambda)_{\lambda \in \mathbb{R}}$ which satisfies (i)–(iii) of Definition 2.1.1 and, instead of property (iv) of Definition 2.1.1,

(iv)' for all $u \in \mathcal{H}$:

$$\lim_{\lambda \rightarrow -\infty} E_\lambda u = 0 \quad \text{and} \quad \lim_{\lambda \rightarrow \infty} E_\lambda u = u. \quad \blacklozenge$$

The following preliminary result was essentially proved during the proof of the spectral theorem for bounded symmetric operators.

Lemma 3.6.2 *Let $E : \mathbb{R} \rightarrow \mathcal{B}(\mathcal{H})$ satisfy parts (i) and (ii) of Definition 2.1.1. Then for all $\mu \in \mathbb{R}$, there exist projections $E_{\mu-}$ and $E_{\mu+}$ such that, for all $u \in \mathcal{H}$,*

$$\lim_{\lambda \nearrow \mu} E_\lambda u = E_{\mu-} u \quad \text{and} \quad \lim_{\lambda \searrow \mu} E_\lambda u = E_{\mu+} u.$$

Now consider a spectral family $(E_\lambda)_{\lambda \in \mathbb{R}}$. For all $u \in \mathcal{H}$, the function

$$\begin{aligned} F_u : \mathbb{R} &\longrightarrow \mathbb{R}, \\ \lambda &\longmapsto F_u(\lambda) := \langle E_\lambda u, u \rangle = \|E_\lambda u\|^2, \end{aligned}$$

is non-decreasing, left-continuous, and satisfies

$$\lim_{\lambda \rightarrow -\infty} F_u(\lambda) = 0 \quad \text{and} \quad \lim_{\lambda \rightarrow \infty} F_u(\lambda) = \|u\|^2.$$

We can in particular associate to each function F_u the corresponding Lebesgue-Stieltjes measure μ_{F_u} which we denote by $\mu_{\|E_\lambda u\|^2}$ (cf. Section B.1). We observe that $\mu_{\|E_\lambda u\|^2}$ is a finite measure on \mathbb{R} , with

$$\mu_{\|E_\lambda u\|^2}(\mathbb{R}) = F_u(\infty) - F_u(-\infty) = \|u\|^2.$$

We now make the following definition.

Definition 3.6.3 Consider a spectral family $(E_\lambda)_{\lambda \in \mathbb{R}}$. We shall say that a function $f : \mathbb{R} \rightarrow \mathbb{C}$ is **E -measurable** if f is $\mu_{\|E_\lambda u\|^2}$ -measurable for all $u \in \mathcal{H}$. \blacklozenge

The scope of this definition is very large. Indeed, all Lebesgue-measurable functions are E -measurable for any spectral family E , as can be seen from Theorem B.1.1 and Theorem B.2.1.

To define the integral with respect to a spectral family, we start with a step function $t : \mathbb{R} \rightarrow \mathbb{C}$,

$$t = \sum_{k=0}^n c_k \chi_{I_k},$$

where the c_k 's are complex constants and the I_k 's are non-empty pairwise disjoint intervals of one of the following forms:

$$(a_k, b_k), \quad [a_k, b_k), \quad (a_k, b_k], \quad [a_k, b_k].$$

The integral of t with respect to the spectral family $(E_\lambda)_{\lambda \in \mathbb{R}}$ is now defined as

$$\int_{\mathbb{R}} t(\lambda) dE_\lambda = \sum_{k=0}^n c_k E(I_k),$$

where

$$E((a, b)) = E_b - E_{a+}, \quad E([a, b)) = E_b - E_a, \quad E((a, b]) = E_{b+} - E_{a+}, \quad E([a, b]) = E_{b+} - E_a$$

if a, b are finite, while

$$E([a, \infty)) = I - E_a, \quad E((-\infty, b]) = E_{b+}, \text{ etc.}$$

For any step function t we have

$$\begin{aligned} \left\| \int t(\lambda) dE_\lambda u \right\|^2 &= \left\langle \sum_{k=0}^n c_k E(I_k) u, \sum_{j=0}^n \bar{c}_j E(I_j) u \right\rangle = \sum_{k=0}^n \sum_{j=0}^n c_k \bar{c}_j \langle E(I_k) u, E(I_j) u \rangle \\ &= \sum_{k=0}^n |c_k|^2 \langle E(I_k) u, u \rangle = \int |t(\lambda)|^2 d\mu_{\|E_\lambda u\|^2}, \end{aligned}$$

where the integral in the right-hand side is a Lebesgue-Stieltjes integral (cf. Appendix B). Here and henceforth, unless otherwise specified, the integrals are taken over \mathbb{R} .

Consider now an E -measurable function $f : \mathbb{R} \rightarrow \mathbb{C}$. By Theorem B.3.1, for all $u \in \mathcal{H}$ such that $f \in L^2(\mathbb{R}, \mu_{\|E_\lambda u\|^2})$, there is a sequence of step functions $(t_n)_{n=1}^\infty$ converging to f in $L^2(\mathbb{R}, \mu_{\|E_\lambda u\|^2})$. This sequence being Cauchy in $L^2(\mathbb{R}, \mu_{\|E_\lambda u\|^2})$ there holds, as $n, m \rightarrow \infty$,

$$\left\| \int t_n(\lambda) dE_\lambda u - \int t_m(\lambda) dE_\lambda u \right\|^2 = \int |t_n(\lambda) - t_m(\lambda)|^2 d\mu_{\|E_\lambda u\|^2} \longrightarrow 0.$$

Therefore, the sequence $(\int t_n(\lambda) dE_\lambda u)_{n=0}^\infty$ is Cauchy in \mathcal{H} , hence convergent, and we let

$$\int f(\lambda) dE_\lambda u = \lim_{n \rightarrow \infty} \int t_n(\lambda) dE_\lambda u.$$

This definition is independent of the choice of the sequence $(t_n)_{n=1}^\infty$, as can be seen by replacing in the above calculation $t_m(\lambda)$ by another sequence $\tilde{t}_n(\lambda)$ converging to $f(\lambda)$ as $n \rightarrow \infty$.

Letting

$$\mathfrak{D}_{E(f)} = \{u \in \mathcal{H}; f \in L^2(\mathbb{R}, \mu_{\|E_\lambda u\|^2})\},$$

we have thus defined a mapping

$$\begin{aligned} E(f) : \mathfrak{D}_{E(f)} &\longrightarrow \mathcal{H}, \\ u &\longmapsto \int f(\lambda) dE_\lambda u. \end{aligned} \tag{3.6.1}$$

Definition 3.6.4 We denote the linear operator (3.6.1) by $\int f(\lambda) dE_\lambda$ and we call it the **integral of f with respect to $(E_\lambda)_{\lambda \in \mathbb{R}}$** . ♦

The following theorem gives the main properties of the integral.

Theorem 3.6.5 Consider a spectral family $(E_\lambda)_{\lambda \in \mathbb{R}}$ and $f : \mathbb{R} \rightarrow \mathbb{C}$ an E -measurable function.

- (a) The domain $\mathfrak{D}_{E(f)}$ is dense in \mathcal{H} .
- (b) The operator $E(f)$ is normal, i.e. $E(f)E(f)^* = E(f)^*E(f)$.
- (c) $u \in \mathfrak{D}_{E(f)} \iff \|E(f)u\|^2 = \int |f|^2 d\mu_{\|E_\lambda u\|^2} < \infty$.
- (d) If f is bounded, then $\mathfrak{D}_{E(f)} = \mathcal{H}$, $E(f) \in \mathcal{B}(\mathcal{H})$, and $\|E(f)\| \leq \text{ess sup}_{\lambda \in \mathbb{R}} |f(\lambda)|$.
- (e) If $f(\lambda) = 1$ for all $\lambda \in \mathbb{R}$, then $E(f) = I$.
- (f) For all $u \in \mathfrak{D}_{E(f)}$,

$$\langle E(f)u, u \rangle = \int f(\lambda) d\mu_{\|E_\lambda u\|^2}.$$

- (g) For $a, b \in \mathbb{C}$ and any E -measurable function $g : \mathbb{R} \rightarrow \mathbb{C}$,

$$aE(f) + bE(g) \subseteq E(af + bg) \quad \text{and} \quad \mathfrak{D}_{E(f)+E(g)} = \mathfrak{D}_{E(|f|+|g|)}.$$

- (h) For any E -measurable function $g : \mathbb{R} \rightarrow \mathbb{C}$,

$$E(f)E(g) \subseteq E(fg) \quad \text{and} \quad \mathfrak{D}_{E(f)E(g)} = \mathfrak{D}_{E(g)} \cap \mathfrak{D}_{E(fg)};$$

- (i) We have

$$E(\bar{f}) = E(f)^* \quad \text{and} \quad \mathfrak{D}_{E(f)^*} = \mathfrak{D}_{E(f)}.$$

(j) For all $\mu \in \mathbb{R}$,

$$E_\mu E(f) \subseteq E(f) E_\mu,$$

with equality if f is bounded.

Proof. See Problem 3.10. □

We now observe that, given a bounded symmetric operator A on \mathcal{H} , Theorem 2.2.1 yields a unique spectral family $(E_\lambda)_{\lambda \in \mathbb{R}}$ in the sense of Definition 2.1.1 — which is, *a fortiori*, a spectral family in the sense of Definition 3.6.1 — such that $A = \int \lambda dE_\lambda$. (For continuous functions, the equivalence between the present theory of integration and that of Chapter 2 in the case where the spectral family has finite bounds is studied in Problem 3.11.) Hence, for a bounded symmetric operator A and its spectral family $(E_\lambda)_{\lambda \in \mathbb{R}}$, we can now make the following definition.

Let $f : [m, M] \rightarrow \mathbb{C}$ be a function whose extension to \mathbb{R} by $f(\lambda) = 0$ for all $\lambda \in \mathbb{R} \setminus [m, M]$ is E -measurable. The operator $f(A)$ is defined as

$$f(A) = E(f) = \int f(\lambda) dE_\lambda.$$

The functions of A have the following properties.

Theorem 3.6.6 *Consider a bounded symmetric operator A and its spectral family $(E_\lambda)_{\lambda \in \mathbb{R}}$ given by Theorem 2.2.1. Let $f, g : \mathbb{R} \rightarrow \mathbb{C}$ be E -measurable functions such that $f(\lambda) = g(\lambda) = 0$ for all $\lambda \in \mathbb{R} \setminus [m, M]$. Then the following holds.*

(a) *If f is bounded, then $f(A) \in \mathcal{B}(\mathcal{H})$ and*

$$\|f(A)\| \leq \operatorname{ess\,sup}_{\lambda \in [m, M]} |f(\lambda)|.$$

(b) *If f and g are bounded, then*

$$f(A)g(A) = \int_m^{M^+} f(\lambda)g(\lambda) dE_\lambda.$$

(c) $f(A)^* = \bar{f}(A)$.

(d) *Any bounded operator which commutes with A commutes with $f(A)$.*

Proof. Parts (a) to (c) are direct consequences of Theorem 3.6.5, and part (d) will be proved in Problem 3.12. □

3.7 The spectral theorem for selfadjoint operators

Our proof of the spectral theorem follows that of Riesz and Lorch, as presented in [RSN90]. Another proof due to von Neumann, based on the Cayley transform, can also be found in [RSN90]. The main idea in Riesz's proof is to reduce the problem to the case of bounded symmetric operators by a limit procedure. We start with the following result.

Lemma 3.7.1 *Let*

$$\mathcal{H}_1, \mathcal{H}_2, \dots, \mathcal{H}_i, \dots$$

be a sequence of closed, pairwise orthogonal, subspaces of the Hilbert space \mathcal{H} , such that $\oplus_i \mathcal{H}_i = \mathcal{H}$. We denote by u_i the projection of any $u \in \mathcal{H}$ onto \mathcal{H}_i . Consider a sequence

$$A_1, A_2, \dots, A_i, \dots$$

of operators in \mathcal{H} such that the restriction $A_i|_{\mathcal{H}_i}$ is a bounded symmetric operator mapping \mathcal{H}_i into itself, for all $i \geq 1$.

Then there exists a unique selfadjoint operator $A : \mathfrak{D}_A \subseteq \mathcal{H} \rightarrow \mathcal{H}$ which coincides with A_i on \mathcal{H}_i , for all $i \geq 1$. The domain of A is defined by

$$\mathfrak{D}_A = \left\{ u \in \mathcal{H} ; \sum_{i=1}^{\infty} \|A_i u_i\|^2 < \infty \right\} \quad (3.7.1)$$

and, for all $u \in \mathfrak{D}_A$,

$$Au = \sum_{i=1}^{\infty} A_i u_i. \quad (3.7.2)$$

Proof. Let us first observe that the operator defined by (3.7.1)–(3.7.2) is linear. Furthermore, \mathfrak{D}_A is dense in \mathcal{H} since, for all $u \in \mathcal{H}$ and all $\varepsilon > 0$, there exists $N \geq 1$ such that

$$\left\| u - \sum_{i=1}^N u_i \right\| < \varepsilon,$$

and clearly $\sum_{i=1}^N u_i \in \mathfrak{D}_A$. Moreover, A is symmetric since, by linearity and continuity of the inner product, and by the pairwise orthogonality of the \mathcal{H}_i s we have, for all $u, v \in \mathfrak{D}_A$,

$$\langle Au, v \rangle = \sum_{i=1}^{\infty} \langle A_i u_i, v_i \rangle = \sum_{i=1}^{\infty} \langle u_i, A_i v_i \rangle = \langle u, Av \rangle.$$

To prove that A is, in fact, selfadjoint, we need only show that $\mathfrak{D}_A = \mathfrak{D}_{A^*}$. To this end, consider an arbitrary $v \in \mathfrak{D}_{A^*}$. Then, for any $u \in \mathfrak{D}_A$,

$$\langle Au, v \rangle = \langle u, A^*v \rangle,$$

and so

$$\sum_{i=1}^{\infty} \langle A_i u_i, v_i \rangle = \sum_{i=1}^{\infty} \langle u_i, (A^*v)_i \rangle.$$

In particular, for any fixed $j \geq 1$, if $u \in \mathcal{H}_j$ we have $u \in \mathfrak{D}_A$, $u_i = \delta_{i,j}u$, and the above identity becomes

$$\langle A_j u, v_j \rangle = \langle u, (A^*v)_j \rangle.$$

But A_j is bounded and symmetric on \mathcal{H}_j , so we deduce that

$$\langle u, (A^*v)_j \rangle = \langle A_j u, v_j \rangle = \langle u, A_j v_j \rangle \text{ for all } u \in \mathcal{H}_j,$$

that is

$$\langle u, (A^*v)_j - A_j v_j \rangle = 0.$$

Choosing $u = (A^*v)_j - A_j v_j$ thus yields $(A^*v)_j = A_j v_j$ for all $j \geq 1$. Hence, by Pythagoras' theorem,

$$\sum_{i=1}^{\infty} \|A_i v_i\|^2 = \sum_{i=1}^{\infty} \|(A^*v)_i\|^2 = \|A^*v\|^2 < \infty,$$

showing that $v \in \mathfrak{D}_A$. Therefore, $\mathfrak{D}_A = \mathfrak{D}_{A^*}$.

To see that A is unique, consider A' selfadjoint which coincides with A_i on \mathcal{H}_i , for all $i \geq 1$. Since A' is selfadjoint, it is closed, and so well defined at every $u \in \mathcal{H}$ for which the series

$$\sum_{i=1}^{\infty} A' u_i = \lim_{n \rightarrow \infty} \sum_{i=1}^n A' u_i \tag{3.7.3}$$

is convergent. Indeed, given $u \in \mathcal{H}$, we have that $\sum_{i=1}^n u_i \in \mathfrak{D}_{A'}$ for all $n \in \mathbb{N}$ and $\sum_{i=1}^n u_i \rightarrow u$ as $n \rightarrow \infty$. If, moreover, $A' \sum_{i=1}^n u_i = \sum_{i=1}^n A' u_i \rightarrow v$ as $n \rightarrow \infty$, then $(u, v) \in \mathbf{G}_{A'}$ and we deduce that $u \in \mathfrak{D}_{A'}$ and $v = A'u$. Since $A' u_i = A_i u_i$ and all terms in (3.7.3) are pairwise orthogonal, the series is convergent if and only if $\sum_{i=1}^{\infty} \|A_i u_i\|^2 < \infty$. Therefore, $\mathfrak{D}_A \subseteq \mathfrak{D}_{A'}$ and, for all $u \in \mathfrak{D}_A$, $A'u = Au$. That is, $A \subseteq A'$. But A is selfadjoint and hence maximal symmetric, so we must have $A' = A$. The proof is complete. \square

The operator A constructed in Lemma 3.7.1 is unbounded unless all the operators A_i possess a common bound. We have thus found a way to construct unbounded selfadjoint operators from bounded symmetric ones. A remarkable result is that, in fact, any selfadjoint operator can be decomposed in this way.

Lemma 3.7.2 *Consider a selfadjoint operator A acting in \mathcal{H} . There exists a sequence*

$$\mathcal{H}_1, \mathcal{H}_2, \dots, \mathcal{H}_i, \dots$$

of closed, pairwise orthogonal, subspaces of \mathcal{H} , such that $\oplus_i \mathcal{H}_i = \mathcal{H}$ and the restriction $A|_{\mathcal{H}_i}$ is a bounded symmetric operator mapping \mathcal{H}_i into itself, for all $i \geq 1$. Moreover, the restriction to \mathcal{H}_i of any bounded operator T such that $T \circ A$ is a bounded operator mapping \mathcal{H}_i into itself, for all $i \geq 1$.

Proof. Consider the operators of Theorem 3.4.3:

$$\mathbf{B} = (I + A^2)^{-1} \quad \text{and} \quad \mathbf{C} = A\mathbf{B} = A(I + A^2)^{-1}.$$

\mathbf{B} is bounded symmetric and satisfies $0 \leq \mathbf{B} \leq I$. By the spectral theorem for bounded symmetric operators, \mathbf{B} has a unique spectral family $(F_\lambda)_{\lambda \in \mathbb{R}}$ with bounds 0 and 1, such that

$$\mathbf{B} = \int_0^{1+} \lambda dF_\lambda.$$

We now show that F is continuous at $\lambda = 0$, i.e. for all $u \in \mathcal{H}$, $F_{0+}u = \lim_{\lambda \searrow 0} F_\lambda u = F_0 u = 0$. We start by recalling that, by Theorem 2.2.1, the strong limit F_{0+} exists. But for all $\lambda > 0$, there is a sequence $(\mu_n)_{n=1}^\infty \subset \mathbb{R}$ which converges to 0 and such that $0 < \mu_n < \lambda$ for all $n \geq 1$. Since $F_\lambda F_{\mu_n} = F_{\mu_n}$ for all $n \geq 1$, the boundedness of F_λ then implies, for all $u \in \mathcal{H}$,

$$F_\lambda F_{0+}u = \lim_{n \rightarrow \infty} F_\lambda F_{\mu_n}u = \lim_{n \rightarrow \infty} F_{\mu_n}u = F_{0+}u.$$

We now fix $0 < \varepsilon < 1$ for the rest of the proof. For any partition $\Pi = (\lambda_k)_{k=0}^m$ of $[0, 1 + \varepsilon]$, we define

$$S_\Pi = \sum_{k=1}^m \lambda_k (F_{\lambda_k} - F_{\lambda_{k-1}}).$$

Note that, by Theorem 2.2.1, $S_\Pi \rightarrow \mathbf{B}$ as $|\Pi| \rightarrow 0$. Since

$$\begin{aligned} S_\Pi F_{0+} &= \sum_{k=1}^m \lambda_k (F_{\lambda_k} - F_{\lambda_{k-1}}) F_{0+} \\ &= \lambda_1 (F_{0+} - F_0) + \sum_{k=2}^m \lambda_k (F_{0+} - F_{0+}) \\ &= \lambda_1 F_{0+}, \end{aligned}$$

letting $|\Pi| \rightarrow 0$ we get $\mathbf{B}F_{0+} = 0$, hence $F_{0+} = 0$ (as \mathbf{B} is invertible).

We then define the projections

$$P_1 = F_{1+\varepsilon} - F_{\frac{1}{2}}, \quad P_i = F_{\frac{1}{i}} - F_{\frac{1}{i+1}}, \quad i \geq 2,$$

and we let $\mathcal{H}_i = \text{rge } P_i$. We observe that the closed subspaces \mathcal{H}_i are pairwise orthogonal and satisfy $\bigoplus_i \mathcal{H}_i = \mathcal{H}$ since $P_i P_j = 0$ for $i \neq j$ and

$$\sum_{i=1}^{\infty} P_i = F_{1+\varepsilon} - F_{0+} = I.$$

We need to show that the restriction of A to \mathcal{H}_i is a bounded symmetric operator mapping \mathcal{H}_i to itself, for all $i \geq 1$. By Lemma 3.3.2, if $P_i \lrcorner A$, then $P_i A P_i = A P_i$ and so $A|_{\mathcal{H}_i}$ maps \mathcal{H}_i to itself. Moreover, if $A P_i \in \mathcal{B}(\mathcal{H})$, we will have in particular that $\mathcal{H}_i \subset \mathfrak{D}_A$ and so, for all $u, v \in \mathcal{H}_i$,

$$\langle A|_{\mathcal{H}_i} u, v \rangle = \langle A u, v \rangle = \langle u, A v \rangle = \langle u, A|_{\mathcal{H}_i} v \rangle,$$

showing that $A|_{\mathcal{H}_i}$ is a bounded symmetric operator on \mathcal{H}_i .

Thus, we need only show $P_i \lrcorner A$ and $A P_i \in \mathcal{B}(\mathcal{H})$. By Corollary 3.5.7, $B \lrcorner A$ and $C B = B C$. By part (d) of Theorem 3.6.6, C also commutes with all F -measurable functions of B . Consider then the bounded functions $s_i : [0, 1] \rightarrow \mathbb{R}$ defined for all $i \geq 1$ by

$$s_i(\lambda) = \begin{cases} \frac{1}{\lambda} & \text{if } \lambda \in [\frac{1}{i+1}, \frac{1}{i}), \\ 0 & \text{otherwise.} \end{cases}$$

By Theorem 3.6.6,

$$s_i(B) = \int_0^{1+} s_i(\lambda) dF_\lambda \in \mathcal{B}(\mathcal{H})$$

and

$$s_i(B) B = B s_i(B) = \int_0^{1+} \lambda s_i(\lambda) dF_\lambda = \int \chi_{[\frac{1}{i+1}, \frac{1}{i})} dF_\lambda = P_i.$$

It follows that

$$A P_i = A B s_i(B) = C s_i(B),$$

showing that $A P_i \in \mathcal{B}(\mathcal{H})$. On the other hand, since $B \lrcorner A$ and $C \lrcorner s_i(B)$,

$$P_i A = s_i(B) B A \subseteq s_i(B) A B = s_i(B) C = C s_i(B) = A P_i,$$

that is, $P_i \lrcorner A$.

Finally, consider $T \in \mathcal{B}(\mathcal{H})$ such that $T \lrcorner A$. It follows from part (d) of Corollary 3.5.7 that $T B = B T$. By Theorem 3.6.6, T commutes with any function of B , and so with each $P_i = B s_i(B)$. Therefore, we indeed have $P_i T P_i = T P_i$. This concludes the proof of the lemma. \square

Theorem 3.7.3 (Spectral Theorem II) *Let A be a selfadjoint operator. There exists a unique spectral family $(E_\lambda)_{\lambda \in \mathbb{R}}$ such that*

$$A = \int \lambda dE_\lambda.$$

Furthermore, any bounded operator T such that $T \circ A$ commutes with each E_λ .

We call $(E_\lambda)_{\lambda \in \mathbb{R}}$, the **spectral family of A** .

Proof. By Lemma 3.7.2, there exist pairwise orthogonal closed subspaces

$$\mathcal{H}_1, \mathcal{H}_2, \dots, \mathcal{H}_i, \dots$$

such that $\oplus_i \mathcal{H}_i = \mathcal{H}$, and for which the restriction A_i of A to \mathcal{H}_i is a bounded symmetric operator on \mathcal{H}_i , $i = 1, 2, \dots$. By the spectral theorem for bounded symmetric operators, there exists for each $i \geq 1$ a unique spectral family $(E_{\lambda,i})_{\lambda \in \mathbb{R}}$ on \mathcal{H}_i such that

$$A_i = \int_{m_i}^{M_i^+} \lambda dE_{\lambda,i}.$$

Then, for all $\lambda \in \mathbb{R}$, each $E_{\lambda,i}$ is a bounded symmetric operator on \mathcal{H}_i . Therefore, extending $E_{\lambda,i}$ by zero on \mathcal{H}_j , $j \neq i$, it follows by Lemma 3.7.1 that there exists a unique selfadjoint operator E_λ which reduces to $E_{\lambda,i}$ in each subspace \mathcal{H}_i . Moreover, for all $\lambda \in \mathbb{R}$, the domain of E_λ is \mathcal{H} . Indeed, for all $u \in \mathcal{H}$, denoting by u_i the projection of u onto \mathcal{H}_i , it follows from Pythagoras' theorem that

$$\sum_{i=1}^m \|E_{\lambda,i} u_i\|^2 \leq \sum_{i=1}^m \|u_i\|^2 = \left\| \sum_{i=1}^m u_i \right\|^2.$$

Hence, letting $m \rightarrow \infty$, we get

$$\sum_{i=1}^{\infty} \|E_{\lambda,i} u_i\|^2 \leq \|u\|^2,$$

showing that $u \in \mathcal{D}_{E_\lambda}$ and $\|E_\lambda\| \leq 1$. E_λ is thus a bounded symmetric operator, for all $\lambda \in \mathbb{R}$.

Next we prove that $E_\lambda^2 = E_\lambda$, so that E_λ is a projection. For all $i \geq 1$ we have

$$E_\lambda^2 u_i = E_{\lambda,i}^2 u_i = E_{\lambda,i} u_i = E_\lambda u_i.$$

Hence, the selfadjoint operators E_λ^2 and E_λ coincide on \mathcal{H}_i for all $i \geq 1$ and so $E_\lambda^2 = E_\lambda$.

We now show that, for $\lambda < \mu$, $E_\lambda \leq E_\mu$. For any $u = \sum_{i=1}^{\infty} u_i \in \mathcal{H}$, using pairwise orthogonality of \mathcal{H}_i and \mathcal{H}_j ,

$$\langle (E_\lambda - E_\mu)u, u \rangle = \left\langle (E_\lambda - E_\mu) \sum_{i=1}^{\infty} u_i, \sum_{j=1}^{\infty} u_j \right\rangle = \sum_{i=1}^{\infty} \langle (E_{\lambda,i} - E_{\mu,i})u_i, u_i \rangle \leq 0.$$

We now prove that the family $(E_\lambda)_{\lambda \in \mathbb{R}}$ is strongly left-continuous. By Lemma 3.6.2, for all $\mu \in \mathbb{R}$ the left pointwise limit $E_{\mu-}$ is a projection. We need only show that $E_{\mu-}$ and E_μ coincide on each \mathcal{H}_i . But this is clear since, for all $u_i \in \mathcal{H}_i$,

$$E_{\mu-}u_i = \lim_{\lambda \nearrow \mu} E_\lambda u_i = \lim_{\lambda \nearrow \mu} E_{\lambda,i}u_i = E_{\mu,i}u_i = E_\mu u_i.$$

To finish proving that $(E_\lambda)_{\lambda \in \mathbb{R}}$ is a spectral family, it only remains to show that, for all $u \in \mathcal{H}$,

$$\lim_{\lambda \rightarrow -\infty} E_\lambda u = 0 \quad \text{and} \quad \lim_{\lambda \rightarrow \infty} E_\lambda u = u. \quad (3.7.4)$$

Let us first recall that, for all $i \geq 1$, the spectral family $(E_{\lambda,i})_{\lambda \in \mathbb{R}}$ is bounded by the lower and upper bounds m_i and M_i of A_i . Now fix $u \in \mathcal{H}$ and consider $\epsilon > 0$. There exists $N_\epsilon \geq 1$ such that

$$\left\| \sum_{i=N_\epsilon+1}^{\infty} u_i \right\| \leq \epsilon$$

and, since $\|E_\lambda\| \leq 1$,

$$\|E_\lambda u\| \leq \left\| \sum_{i=1}^{N_\epsilon} E_{\lambda,i} u_i \right\| + \left\| E_\lambda \sum_{i=N_\epsilon+1}^{\infty} u_i \right\| \leq \left\| \sum_{i=1}^{N_\epsilon} E_{\lambda,i} u_i \right\| + \epsilon. \quad (3.7.5)$$

Putting $m_\epsilon = \min_{1 \leq i \leq N_\epsilon} m_i$, we have $\sum_{i=1}^{N_\epsilon} E_{\lambda,i} u_i = 0$ for all $\lambda \leq m_\epsilon$. It then follows from (3.7.5) that

$$\|E_\lambda u\| \leq \epsilon \quad \text{for all } \lambda \leq m_\epsilon,$$

showing the first statement of (3.7.4).

On the other hand, for all $\epsilon > 0$, there exists $N_\epsilon \geq 1$ such that $\left\| \sum_{i=N_\epsilon+1}^{\infty} u_i \right\| < \frac{1}{2}\epsilon$ and so

$$\begin{aligned} \|E_\lambda u - u\| &\leq \left\| \sum_{i=1}^{N_\epsilon} E_{\lambda,i} u_i - u_i \right\| + \left\| (E_\lambda - I) \sum_{i=N_\epsilon+1}^{\infty} u_i \right\| \\ &\leq \left\| \sum_{i=1}^{N_\epsilon} E_{\lambda,i} u_i - u_i \right\| + 2 \left\| \sum_{i=N_\epsilon+1}^{\infty} u_i \right\| \\ &\leq \left\| \sum_{i=1}^{N_\epsilon} E_{\lambda,i} u_i - u_i \right\| + \epsilon. \end{aligned} \quad (3.7.6)$$

Hence, letting $M_\epsilon = \max_{1 \leq i \leq N_\epsilon} M_i$, we have

$$\sum_{i=1}^{N_\epsilon} E_{\lambda,i} u_i = \sum_{i=1}^{N_\epsilon} u_i \quad \text{for all } \lambda \geq M_\epsilon,$$

and it then follows from (3.7.6) that

$$\|E_\lambda u - u\| < \epsilon \quad \text{for all } \lambda \geq M_\epsilon.$$

This proves the second statement in (3.7.4).

We now show that the spectral family $(E_\lambda)_{\lambda \in \mathbb{R}}$ satisfies

$$A = \int \lambda dE_\lambda.$$

Theorem 3.6.5 ensures that $\int \lambda dE_\lambda$ is a selfadjoint operator since $f(\lambda) = \lambda$ is real-valued. By Lemma 3.7.1 it thus suffices to show that $\int \lambda dE_\lambda$ and A coincide on each \mathcal{H}_i . To see this, consider a sequence of step functions $(t_j)_{j=1}^\infty$ of the form

$$t_j = \sum_{k=1}^{n_j} c_k^j \chi_{I_k^j}, \quad j \geq 1,$$

which converges to $f(\lambda) = \lambda$ in $L^2(\mathbb{R}, \mu_{\|E_\lambda u_i\|^2})$ as $j \rightarrow \infty$. Then

$$\begin{aligned} \int \lambda dE_\lambda u_i &= \lim_{j \rightarrow \infty} \int t_j(\lambda) dE_\lambda u_i = \lim_{j \rightarrow \infty} \sum_{k=1}^{n_j} c_k^j E(I_k^j) u_i \\ &= \lim_{j \rightarrow \infty} \sum_{k=1}^{n_j} c_k^j E_i(I_k^j) u_i = \int \lambda dE_{\lambda,i} u_i \\ &= \int_{m_i}^{M_i^+} \lambda dE_{\lambda,i} u_i = A_i u_i = A u_i, \end{aligned}$$

where we have used the fact that if, for instance, $I = [a, b]$, then

$$E(I)u_i = (E_{b^+} - E_a)u_i = (E_{b^+,i} - E_{a,i})u_i = E_i(I)u_i.$$

Now, consider an operator $T \in \mathcal{B}(\mathcal{H})$ such that $T \subseteq A$. By Lemma 3.7.2, for each $i \geq 1$, the restriction T_i of T to \mathcal{H}_i satisfies $T_i \in \mathcal{B}(\mathcal{H}_i)$. For all $i \geq 1$, since T_i commutes with A_i , it follows by the spectral theorem for bounded symmetric operators that T_i commutes with $E_{\lambda,i}$ for all $\lambda \in \mathbb{R}$. Therefore, for all $\lambda \in \mathbb{R}$ and all $u \in \mathcal{H}$,

$$TE_\lambda u = T \sum_{i=1}^{\infty} E_{\lambda,i} u_i = \sum_{i=1}^{\infty} T_i E_{\lambda,i} u_i = \sum_{i=1}^{\infty} E_{\lambda,i} T_i u_i = E_\lambda T u.$$

Finally, to prove uniqueness of $(E_\lambda)_{\lambda \in \mathbb{R}}$, consider two spectral families $(E_\lambda)_{\lambda \in \mathbb{R}}$, $(F_\lambda)_{\lambda \in \mathbb{R}}$ such that

$$A = \int \lambda dE_\lambda = \int \lambda dF_\lambda.$$

Letting $X_i := \text{rge}(E_i - E_{i-1})$, $i \in \mathbb{Z}$, we have $\mathcal{H} = \oplus_i X_i$. Since $A = F(f)$ (with $f(\lambda) = \lambda$), Theorem 3.6.5 (j) and the previous paragraph imply that F_μ commutes with E_λ for all $\mu, \lambda \in \mathbb{R}$. It then follows from Lemma 3.3.2 that, for all $\lambda \in \mathbb{R}$ and all $i \in \mathbb{Z}$, $\tilde{E}_{\lambda,i} := E_\lambda|_{X_i}$ and $\tilde{F}_{\lambda,i} := F_\lambda|_{X_i}$ are projections mapping X_i into itself. Furthermore, for all $i \in \mathbb{Z}$, $(\tilde{E}_{\lambda,i})_{\lambda \in \mathbb{R}}$ and $(\tilde{F}_{\lambda,i})_{\lambda \in \mathbb{R}}$ are spectral families acting in X_i and such that

$$A|_{X_i} = \int \lambda d\tilde{E}_{\lambda,i} = \int \lambda d\tilde{F}_{\lambda,i}.$$

By uniqueness of the spectral family in Spectral Theorem I, it follows that $\tilde{E}_{\lambda,i} = \tilde{F}_{\lambda,i}$, for all $\lambda \in \mathbb{R}$ and all $i \in \mathbb{Z}$. \square

Definition 3.7.4 Similarly to the case of bounded symmetric operators, thanks to Theorem 3.7.3 we can now define a function of any selfadjoint operator A . Let $(E_\lambda)_{\lambda \in \mathbb{R}}$ be the spectral family of A . For any E -measurable function f , we write

$$f(A) = E(f) = \int f(\lambda) dE_\lambda. \blacklozenge$$

Problems

1. Consider an operator $T : \mathfrak{D}_T \subset \mathcal{H} \rightarrow \mathcal{H}$, and suppose that T is bounded on \mathfrak{D}_T , in the sense that there is a constant $C \geq 0$ such that $\|Tu\| \leq C\|u\|$, $u \in \mathfrak{D}_T$. Show that T can be extended to a bounded linear operator on \mathcal{H} .
2. Let $S : \mathfrak{D}_S \subset \mathcal{H} \rightarrow \mathcal{H}$ be a one-to-one operator. Consider the following additional properties:
 - (i) S is closed.
 - (ii) $\text{rge } S$ is dense.
 - (iii) $\text{rge } S$ is closed.
 - (iv) There is a constant C such that $\|Su\| \geq C\|u\|$ for all $u \in \mathfrak{D}_S$.
 - (a) Prove that (i)–(iii) imply (iv). *Hint:* Apply the Closed Graph Theorem to S^{-1} .

- (b) Prove that (ii)–(iv) imply (i).
 - (c) Prove that (i) and (iv) imply (iii).
3. Prove that, if T^{-1} , T^* and $(T^{-1})^*$ exist, then $(T^*)^{-1}$ also exists, and $(T^{-1})^* = (T^*)^{-1}$.
 4. (a) Show that a densely defined operator T is closable if and only if T^* is densely defined, in which case $\overline{T} = T^{**}$.
(b) Prove that, if a densely defined operator T is closable, then $(\overline{T})^* = T^*$.
 5. We define an operator T on $L^2(\mathbb{R})$ by $(Tu)(x) = \phi(x)u(x)$, where $\phi : \mathbb{R} \rightarrow \mathbb{C}$ is a bounded function. Show that T is bounded and compute its norm. Find T^* . Under what condition is $T = T^*$? If S is defined by $(Su)(x) = \psi(x)u(x)$ with $\psi : \mathbb{R} \rightarrow \mathbb{C}$ bounded, find TS and $(TS)^*$.
 6. For T defined as in the previous problem, suppose now $\lim_{x \rightarrow \infty} |\phi(x)| = \infty$. What is the domain of definition of T ? Show that T is unbounded and find T^* .
 7. Let $\mathcal{H} = L^2(0, 1)$ and consider the differential operator $D_1 : \mathfrak{D}_{D_1} \subset \mathcal{H} \rightarrow \mathcal{H}$ defined by

$$D_1 := i \frac{d}{dx}, \quad \mathfrak{D}_{D_1} := \{u \in AC[0, 1]; u' \in L^2(0, 1) \text{ and } u(0) = u(1) = 0\}.$$

Recall: $AC[0, 1]$ is the space of *absolutely continuous* functions in $[0, 1]$; see [KF80, Sec. 33]. The Lebesgue version of the fundamental theorem of calculus states the following:

- ★ If $f \in AC[0, 1]$ then it is differentiable a.e. in $[0, 1]$, $f' \in L^1(0, 1)$ and $f(x) = f(0) + \int_0^x f'(y) dy$.
- ★ If $g \in L^1(0, 1)$ and $f(x) = \int_0^x g(y) dy$, then $f \in AC[0, 1]$ and $f' = g$ a.e.

- (a) Show that D_1 is unbounded and symmetric.
- (b) Prove that the adjoint D_1^* of D_1 is given by

$$D_1^* = i \frac{d}{dx}, \quad \mathfrak{D}_{D_1^*} = \mathfrak{D} := \{u \in AC[0, 1]; u' \in L^2(0, 1)\}.$$

Hint: To prove that $\mathfrak{D}_{D_1^*} \subset \mathfrak{D}$, consider $v \in \mathfrak{D}_{D_1^*}$ and make clever use of the relation $\langle D_1 u, v \rangle = \langle u, D_1^* v \rangle$, for a well chosen $u \in \mathfrak{D}_{D_1}$ (constructed using v and $D_1^* v$).

- (c) Prove that $D_1^{**} = D_1$.
- (d) Now consider $\mathcal{H} = L^2(\mathbb{R})$ and the operator $D_2 : \mathfrak{D}_{D_2} \subset \mathcal{H} \rightarrow \mathcal{H}$ defined by $D_2 := i \frac{d}{dx}$ and

$$\mathfrak{D}_{D_2} := \{u \in L^2(\mathbb{R}); u' \in L^2(\mathbb{R}) \text{ and } u \in AC[a, b] \text{ for any } -\infty < a < b < \infty\}.$$

Prove that D_2 is selfadjoint.

8. Let again $\mathcal{H} = L^2(0, 1)$ and consider now $D_3 : \mathfrak{D}_{D_3} \subset \mathcal{H} \rightarrow \mathcal{H}$ defined by

$$D_3 := i \frac{d}{dx}, \quad \mathfrak{D}_{D_3} := C_c^1(0, 1).$$

- (a) Show that D_3 is unbounded.
 (b) Prove that the adjoint D_3^* of D_3 exists and is given by

$$D_3^* = i \frac{d}{dx}, \quad \mathfrak{D}_{D_3^*} = \{u \in AC[0, 1]; u' \in L^2(0, 1)\}.$$

- (c) Observe the inclusion relations between $\mathfrak{D}_{D_3}, \mathfrak{D}_{D_3^*}$ and $\mathfrak{D}_{D_1}, \mathfrak{D}_{D_1^*}$.
 (d) Prove that the closure $\overline{D_3}$ of D_3 is given by

$$\overline{D_3} = i \frac{d}{dx}, \quad \mathfrak{D}_{\overline{D_3}} = \{u \in AC[0, 1]; u' \in L^2[0, 1] \text{ and } u(0) = u(1) = 0\}.$$

9. Consider the multiplication operator in $\mathcal{H} = L^2(\mathbb{R})$ defined by

$$(Xu)(x) := xu(x), \quad \mathfrak{D}_X := \{u \in L^2(\mathbb{R}); xu(x) \in L^2(\mathbb{R})\}.$$

Show that X is an unbounded selfadjoint operator. Find its spectrum and its spectral family.

10. Prove Theorem 3.6.5.
 11. Show that, given a spectral family $(E_\lambda)_{\lambda \in \mathbb{R}}$ with finite lower and upper bounds $m < M$, the integral of any continuous function $f : [m, M] \rightarrow \mathbb{C}$ in the sense of Definition 3.6.4 coincides with that of Definition 2.1.3.
 12. Prove part (d) of Theorem 3.6.6.

Chapter 4

Applications to quantum mechanics

In this chapter we will define and study elementary properties of the basic observables of the quantum mechanical particle on the real line: energy, position, momentum. In quantum mechanics, physical observables are represented by selfadjoint operators acting in a Hilbert space \mathcal{H} , the elements of which represent the possible states of the system. The fundamental postulates of quantum mechanics will be formulated in Section 4.2.

As usual in physics, but perhaps even more in quantum mechanics, an important role is played by the symmetries of the system. Indeed, by Noether's theorem, each symmetry group gives rise to a conserved physical quantity. Some of the most important symmetries of quantum mechanical systems can be expressed by the action on the Hilbert space \mathcal{H} of one-parameter unitary groups.

4.1 Representation of one-parameter unitary groups

An operator $U : \mathcal{H} \rightarrow \mathcal{H}$ is called **unitary** if it is surjective and, for all $u, v \in \mathcal{H}$,

$$\langle Uu, Uv \rangle = \langle u, v \rangle.$$

It then follows easily that $\|U\| = 1$, and that U is invertible with $U^{-1} = U^*$ (Problem 4.1).

Definition 4.1.1 We call **one-parameter unitary group** a mapping $U : \mathbb{R} \rightarrow \mathcal{B}(\mathcal{H})$ such that $U(t) \equiv U_t$ is unitary for all $t \in \mathbb{R}$, with

$$U_0 = I \quad \text{and} \quad U_t U_s = U_{t+s} \quad \text{for all } t, s \in \mathbb{R}.$$

A one-parameter unitary group is said to be **strongly continuous** if, for all $u \in \mathcal{H}$, the mapping $t \mapsto U_t u$ is continuous on \mathbb{R} . ♦

It follows directly from the definition that a one-parameter unitary group $(U_t)_{t \in \mathbb{R}}$ satisfies

$$U_{-t} = (U_t)^* = (U_t)^{-1}.$$

We also observe that if $(U_t)_{t \in \mathbb{R}}$ is **weakly continuous**, in the sense that, for all $u, v \in \mathcal{H}$, $t \mapsto \langle U_t u, v \rangle$ is continuous on \mathbb{R} , then $(U_t)_{t \in \mathbb{R}}$ is in fact strongly continuous (Problem 4.2). We now define the central object of the theory of one-parameter unitary groups.

Definition 4.1.2 Let $(U_t)_{t \in \mathbb{R}}$ be a strongly continuous one-parameter unitary group. The **infinitesimal generator** of $(U_t)_{t \in \mathbb{R}}$ is the operator G defined on the domain

$$\mathfrak{D}_G = \left\{ u \in \mathcal{H}; \lim_{t \rightarrow 0} \frac{1}{t} (U_t - I)u \text{ exists} \right\}$$

by

$$Gu = \lim_{t \rightarrow 0} \frac{1}{t} (U_t - I)u. \quad \blacklozenge$$

The following result is a first step towards the characterization of strongly continuous (one-parameter) unitary groups.

Theorem 4.1.3 Let A be a selfadjoint operator acting in \mathcal{H} and $(E_\lambda)_{\lambda \in \mathbb{R}}$ be its spectral family. Then

$$U_t = e^{itA} = \int e^{it\lambda} dE_\lambda, \quad t \in \mathbb{R}, \quad (4.1.1)$$

defines a strongly continuous unitary group with infinitesimal generator iA . Furthermore, if $u \in \mathfrak{D}_A$ then $U_t u \in \mathfrak{D}_A$ for all $t \in \mathbb{R}$.

Proof. Since the function $f(\lambda) = e^{it\lambda}$ is bounded on \mathbb{R} for all $t \in \mathbb{R}$, it follows by Theorem 3.6.5 that, for all $t \in \mathbb{R}$, $U_t \in \mathcal{B}(\mathcal{H})$ and

$$U_t^* = \int \overline{e^{it\lambda}} dE_\lambda = \int e^{-it\lambda} dE_\lambda = U_{-t}.$$

Hence, by Theorem 3.6.5,

$$U_t^* U_t = U_{-t} U_t = \int e^{-it\lambda} e^{it\lambda} dE_\lambda = \int 1 dE_\lambda = I.$$

Thus, every U_t is unitary. Moreover, using again Theorem 3.6.5,

$$U_t U_s = \int e^{it\lambda} e^{is\lambda} dE_\lambda = \int e^{i(t+s)\lambda} dE_\lambda = U_{t+s} \quad \text{for all } t, s \in \mathbb{R}.$$

Therefore, $(U_t)_{t \in \mathbb{R}}$ is a one-parameter unitary group. We now show that it is strongly continuous. Since for all $x, y \in \mathbb{R}$ we have

$$|e^{ix} - e^{iy}| = 2 \left| \sin \frac{x-y}{2} \right|,$$

it follows by Theorem 3.6.5 that, for any given $u \in \mathcal{H}$ and all $s, t \in \mathbb{R}$,

$$\|U_t u - U_s u\|^2 = \left\| \int (e^{it\lambda} - e^{is\lambda}) dE_\lambda u \right\|^2 = \int |e^{it\lambda} - e^{is\lambda}|^2 d\mu_{\|E_\lambda u\|^2} = 4 \int \left| \sin \frac{(t-s)\lambda}{2} \right|^2 d\mu_{\|E_\lambda u\|^2}.$$

But since

$$\left| \sin \frac{(t-s)\lambda}{2} \right|^2 \leq 1 \quad \text{and} \quad \lim_{s \rightarrow t} \left| \sin \frac{(t-s)\lambda}{2} \right|^2 = 0,$$

it follows by dominated convergence (Theorem B.2.5) that

$$\lim_{s \rightarrow t} \|U_t u - U_s u\| = 0,$$

showing that $(U_t)_{t \in \mathbb{R}}$ is indeed strongly continuous.

Let us now show that the infinitesimal generator G of $(U_t)_{t \in \mathbb{R}}$ is equal to iA . We first observe that, for all $u \in \mathfrak{D}_A$ and all $t \neq 0$,

$$\left\| \left[\frac{1}{t}(U_t - I) - iA \right] u \right\|^2 = \int \left| \frac{1}{t}(e^{it\lambda} - 1) - i\lambda \right|^2 d\mu_{\|E_\lambda u\|^2}.$$

But since

$$\lim_{t \rightarrow 0} \frac{1}{t}(e^{it\lambda} - 1) = i\lambda,$$

it follows that

$$\lim_{t \rightarrow 0} \left\| \frac{1}{t}(e^{it\lambda} - 1) - i\lambda \right\|^2 = 0. \quad (4.1.2)$$

On the other hand, by the mean-value theorem, $\left| \frac{1}{t}(e^{it\lambda} - 1) \right| \leq |\lambda|$, and so

$$\left| \frac{1}{t}(e^{it\lambda} - 1) - i\lambda \right|^2 \leq (|\lambda| + |\lambda|)^2 = 4\lambda^2. \quad (4.1.3)$$

Moreover, the function $4\lambda^2$ is $\mu_{\|E_\lambda u\|^2}$ -integrable for any $u \in \mathfrak{D}_A$ since, by Theorem 3.6.5 (c),

$$\int \lambda^2 d\mu_{\|E_\lambda u\|^2} = \|Au\|^2 < \infty.$$

It therefore follows from (4.1.2), (4.1.3) and the dominated convergence theorem that, for all $u \in \mathfrak{D}_A$,

$$\lim_{t \rightarrow 0} \left\| \left[\frac{1}{t}(U_t - I) - iA \right] u \right\|^2 = \lim_{t \rightarrow 0} \int \left| \frac{1}{t}(e^{it\lambda} - 1) - i\lambda \right|^2 d\mu_{\|E_\lambda u\|^2} = 0,$$

and so

$$Gu = \lim_{t \rightarrow 0} \frac{1}{t} (U_t - I)u = iAu \quad \text{for all } u \in \mathfrak{D}_A,$$

showing that $G \supseteq iA$. To see that $G = iA$, it remains to show that $\mathfrak{D}_G \subseteq \mathfrak{D}_A$. To this end, consider $u \in \mathfrak{D}_G$, i.e. $u \in \mathcal{H}$ such that the limit

$$\lim_{t \rightarrow 0} \frac{1}{t} (U_t - I)u \quad \text{exists.}$$

In this case we have

$$\|Gu\|^2 = \lim_{t \rightarrow 0} \left\| \frac{1}{t} (U_t - I)u \right\|^2 = \lim_{t \rightarrow 0} \left\| \int \frac{1}{t} (e^{it\lambda} - 1) dE_\lambda u \right\|^2 = \lim_{t \rightarrow 0} \int \left| \frac{1}{t} (e^{it\lambda} - 1) \right|^2 d\mu_{\|E_\lambda u\|^2}.$$

Now, since

$$\lim_{t \rightarrow 0} \left| \frac{1}{t} (e^{it\lambda} - 1) \right|^2 = \lambda^2,$$

it follows by Fatou's lemma (Theorem B.2.4) that

$$\int \lambda^2 d\mu_{\|E_\lambda u\|^2} \leq \liminf_{t \rightarrow 0} \int \left| \frac{1}{t} (e^{it\lambda} - 1) \right|^2 d\mu_{\|E_\lambda u\|^2} = \|Gu\|^2.$$

By Theorem 3.6.5 (c), this shows that $u \in \mathfrak{D}_A$.

We finally show that, if $u \in \mathfrak{D}_A$ then $U_t u \in \mathfrak{D}_A$ for all $t \in \mathbb{R}$. First, by Theorem 3.6.5 (h), $E_\lambda U_t = U_t E_\lambda$ for all $t \in \mathbb{R}$ and all $\lambda \in \mathbb{R}$. Hence, since every U_t is unitary, we have for all $\lambda \in \mathbb{R}$ and all $t \in \mathbb{R}$ that

$$\|E_\lambda U_t u\|^2 = \langle E_\lambda U_t u, E_\lambda U_t u \rangle = \langle U_t E_\lambda u, U_t E_\lambda u \rangle = \|E_\lambda u\|^2.$$

It follows that

$$\int \lambda^2 d\mu_{\|E_\lambda(U_t u)\|^2} = \int \lambda^2 d\mu_{\|E_\lambda u\|^2} < \infty,$$

and so $U_t u \in \mathfrak{D}_A$, which concludes the proof of the theorem. \square

The next theorem, due to Marshall H. Stone, shows that, in fact, any strongly continuous one-parameter unitary group is of the form (4.1.1), for a uniquely defined selfadjoint A .

Theorem 4.1.4 (Stone's Theorem) *Let $(U_t)_{t \in \mathbb{R}}$ be a strongly continuous one-parameter unitary group. There exists a unique selfadjoint operator A such that*

$$U_t = e^{itA} \quad \text{for all } t \in \mathbb{R}.$$

Furthermore, $U_t \downarrow A$ for all $t \in \mathbb{R}$.

Proof. See Problem 4.3. \square

4.2 A glimpse of quantum mechanics

A self-contained exposition of the theory of quantum mechanics would largely exceed the scope of these notes. We refer the interested reader to the classic works [Dir58, Mes99, VN55]. Let us just mention that quantum mechanics typically describes microscopic systems, in the order of atomic length scales and below. At this level, the description of physical systems cannot rely any more on the macroscopic concepts we experience in our everyday lives. In fact, atoms and subatomic particles turn out to have very peculiar properties when we try to express them in terms of our macroscopic perception of the world. For instance, a most striking feature is that it is not possible in general to assign a precise position in space to a quantum mechanical particle, nor a precise speed (or rather momentum = mass · speed). The Heisenberg uncertainty principle, which is one of the cornerstones of quantum mechanics, indeed states that the respective standard deviations Δq and Δp of the position q and the momentum p of a particle satisfy

$$\Delta q \Delta p \geq \hbar/2 \quad (4.2.1)$$

where $\hbar = h/2\pi$ is the reduced Planck constant, with the Planck constant $h \simeq 6.626 \cdot 10^{-34} \text{ J} \cdot \text{s}$. And this is not a matter of ‘not being able to’ measure things more precisely, but rather a fundamental obstruction of Nature. In fact, as we shall see below, this restriction is due to the status of physical observables in quantum theory. The constant h is named after Max Planck, who was the first to propose a physical model in which electromagnetic radiation could only be emitted as integer multiples — called *quanta* — of the fundamental unit h (1900). In fact, Planck introduced this assumption as a trick to resolve an apparent paradox in the description of the black-body radiation, and did not himself believe in this ‘quantized’ emission process in real physical terms. The corpuscular nature of light was later fully assumed by Einstein in his work on the photoelectric effect (1905) which owed him the Nobel prize in physics in 1921.¹

We shall soon see that the conceptual framework of quantum mechanics is in sharp contrast with that of classical mechanics. In classical mechanics, the observables of a point-like particle are (smooth) functions $f(\mathbf{q}, \mathbf{p})$, where $(\mathbf{q}, \mathbf{p}) \in \mathbb{R}^3 \times \mathbb{R}^3$ are the position and the momentum of the particle. For example, the Hamiltonian (energy)

$$H(\mathbf{q}, \mathbf{p}) = \frac{\mathbf{p} \cdot \mathbf{p}}{2m} + V(\mathbf{q})$$

describes a particle in a potential field $V : \mathbb{R}^3 \rightarrow \mathbb{R}$. It emerged from various attempts to obtain a satisfactory theory of atoms at the beginning of the last century (most notably from the works of Max Planck, Albert Einstein, Niels Bohr, Werner Heisenberg, Erwin Schrödinger, Max Born, Pascual Jordan, Wolfgang Pauli and Paul Dirac) that this classical description of the world dramatically fails

¹Ironically, Einstein later became one of the fiercest opponents of quantum physics.

to account for microscopic phenomena, such as the very stability of atoms², and their emitting of light only at certain universal discrete frequencies (Balmer series). To cut a long story short, on the one hand Heisenberg realized that atomic observables were best represented by (infinite) matrices, a theory now referred to as *matrix mechanics* (1925). A stunning consequence of this new paradigm is that the product of quantum observables is non-commutative. We shall see that this results in particular in the famous *uncertainty principle* mentioned above. On the other hand, Schrödinger derived a theory describing the evolution of a quantum particle through a ‘wave function’,³ therefore known as *wave mechanics* (1926). It should be noted that Schrödinger’s theory is a dynamical one, where the central equation — known as the *Schrödinger equation* — governs the time evolution of the wave function. On the other hand, Heisenberg’s matrix mechanics only describes the stationary states of the system. Apart from this difference, the complete equivalence of the two theories was proved mathematically by Dirac shortly thereafter⁴ and is presented in his famous book *The Principles of Quantum Mechanics* (1930) [Dir58].

Thus, following three decades of intense creative work from a bunch of brilliant theoretical physicists, a new coherent theory was finally born. And it very soon turned out that a natural mathematical framework to describe the theory was that of (unbounded) operators acting in a Hilbert space. A complete set of axioms for the new physics was formulated by von Neumann in *Mathematical Foundations of Quantum Mechanics* (1932) [VN55], while parts of the mathematical theory was developed independently by Marshall H. Stone in his great book *Linear Transformations in Hilbert Space* (1932) [Sto32]. We shall now state the basic postulates of quantum mechanics in this Hilbert space formalism.

The basic postulates of quantum mechanics

The following postulates pertain to *quantum systems*, that is, systems which are best described by the laws of quantum mechanics, which rely crucially on the notion of *measurement device*. Indeed, since we don’t have any macroscopic intuition of quantum systems, the only thing the theory describes/predicts is the results of measurements performed on the system under given experimental conditions. The so-called ‘Copenhagen interpretation’ of quantum mechanics — largely personified by Bohr — pushed this new paradigm so far as to claim that it is irrelevant to attempt any interpretation of the theory in terms of elements of *physical reality* (a notion that was the object of

²According to Newtonian mechanics and Maxwell’s theory of electromagnetics, the electron radiating electromagnetic energy while orbiting about the nucleus would very quickly collapse to it.

³The idea of representing a particle as an oscillatory phenomenon was motivated by earlier considerations from Einstein and de Broglie, pointing that both light and matter can behave either like waves or like particles depending on the experimental setting, the now famous ‘wave/particle duality’.

⁴This is at least the official version, see the Handout for an interesting discussion on the history and equivalence of the two theories.

intense debates, notably between Einstein and Bohr), outside the scope of measurement devices. For instance, there exists no such thing as the position of an electron, so long as the electron is not detected experimentally by an external *observer* (another notion prone to vast philosophical debate)!

Postulate I At any given time, a (pure)⁵ state of the system is represented by a vector $\psi \neq 0$ of a complex separable Hilbert space \mathcal{H} . Furthermore, for all $c \in \mathbb{C} \setminus \{0\}$, the vector $c\psi$ represents the same state as ψ . Thus, the states of the system are in one-to-one correspondence with the rays

$$\{c\psi; c \in \mathbb{C}\} \subseteq \mathcal{H}, \quad \psi \in \mathcal{H} \setminus \{0\},$$

or, equivalently, with the orthogonal projections P_ψ onto these one-dimensional subspaces.

Postulate II An **observable** of the system is a selfadjoint operator A acting in \mathcal{H} .

Postulate III The result of a **measurement** of A can only be a real number $\lambda \in \sigma(A)$.

Postulate IV If the system is in state ψ , then the **probability** of finding a value in the (Borel) set $\Lambda \subset \mathbb{R}$ when measuring A is given by

$$\text{Prob}_\psi\{\text{meas. of } A \in \Lambda\} = \frac{\mu_{\|E_\lambda\psi\|^2}(\Lambda)}{\|\psi\|^2}, \quad (4.2.2)$$

where $(E_\lambda)_{\lambda \in \mathbb{R}}$ is the spectral family of A .

Postulate V The time evolution of the system is unitary. Denoting by $\psi_t \in \mathcal{H}$ the state of the system at time $t \in \mathbb{R}$, this means that $\|\psi_t\| = \|\psi_{t_0}\|$ for any $t \in \mathbb{R}$ and any initial time $t_0 \in \mathbb{R}$.

Postulate VI If the system is in state ψ , then immediately after a measurement of A yielding an **eigenvalue** $\lambda \in \sigma_p(A)$ the system is in state $P_\lambda\psi$, where P_λ is the projector onto the eigenspace corresponding to λ .

Remark 4.2.1 By Postulate IV, the **mean value** of A , calculated over a large number of systems all prepared in state ψ , is given by

$$\langle A \rangle_\psi = \frac{\langle A\psi, \psi \rangle}{\|\psi\|^2} = \frac{\int_{\mathbb{R}} \lambda d\mu_{\|E_\lambda\psi\|^2}}{\|\psi\|^2}. \quad (4.2.3)$$

⁵There is also a notion of mixed state, which will not be addressed in these notes.

Remark 4.2.2 If the vector ψ is **normalized** so that $\|\psi\| = 1$, formulas (4.2.2) and (4.2.3) take the simple forms

$$\text{Prob}_\psi\{\text{meas. of } A \in \Lambda\} = \mu_{\|E_\Lambda\psi\|^2}(\Lambda) \quad (4.2.4)$$

and

$$\langle A \rangle_\psi = \int \lambda \, d\mu_{\|E_\lambda\psi\|^2}. \quad (4.2.5)$$

Note that, in this case, $\mu_{\|E_\lambda\psi\|^2}$ is a probability measure on \mathbb{R} , as

$$1 = \|\psi\|^2 = \int d\mu_{\|E_\lambda\psi\|^2}.$$

Then, in particular, for any $\lambda \in \mathbb{R}$,

$$\begin{aligned} \text{Prob}_\psi\{\text{meas. of } A = \lambda\} &= \mu_{\|E_\lambda\psi\|^2}(\{\lambda\}) \\ &= \langle (E_{\lambda+} - E_\lambda)\psi, \psi \rangle \\ &= \begin{cases} 0 & \text{if } \lambda \notin \sigma_p(A), \\ \langle P_\lambda\psi, \psi \rangle & \text{if } \lambda \in \sigma_p(A), \end{cases} \end{aligned}$$

where P_λ is the projector onto the eigenspace corresponding to λ . In the special case when $\lambda \in \sigma_p(A)$ and the corresponding eigenspace is one-dimensional and spanned by a normalized ϕ_λ , one recovers the classical textbook formula

$$\begin{aligned} \text{Prob}_\psi\{\text{meas. of } A = \lambda\} &= \langle \langle \psi, \phi_\lambda \rangle \phi_\lambda, \psi \rangle \\ &= \langle \psi, \phi_\lambda \rangle \langle \phi_\lambda, \psi \rangle \\ &= |\langle \phi_\lambda, \psi \rangle|^2. \end{aligned}$$

Finally, Postulate V ensures that, if $\|\psi_0\| = 1$ then $\|\psi_t\| = 1$ and $\mu_{\|E_\lambda\psi_t\|^2}$ remains a probability measure for all times $t \in \mathbb{R}$.

Time evolution: Stone's theorem and the existence of dynamics

We say that a quantum system with state space \mathcal{H} is **invariant under time translations** if its evolution in time is governed by a strongly continuous one-parameter unitary group $(U_t)_{t \in \mathbb{R}}$ on \mathcal{H} . That is, if the system at time $t = 0$ is in the initial state ψ_0 , then its state at time t is

$$\psi_t = U_t \psi_0.$$

Hence, the evolution is unitary and Postulate V is indeed satisfied.⁶

To see that the system is indeed insensitive to time translations, observe that the evolution from state ψ_{t_0} to state ψ_{t_1} is given by

$$\psi_{t_1} = U_{t_1}\psi_0 = U_{t_1}U_{t_0}^{-1}U_{t_0}\psi_0 = U_{t_1}U_{-t_0}\psi_{t_0} = U_{t_1-t_0}\psi_{t_0},$$

and so depends only on the elapsed time $t_1 - t_0$, and not on the initial time t_0 . Thus, if one translates the origin of time, this translation disappears in the difference, so the evolution is identical in the new time frame.

Now, Stone's theorem ensures that there exists an infinitesimal generator G of the group $(U_t)_{t \in \mathbb{R}}$, such that iG is selfadjoint. We recall that the domain of G is given by

$$\mathfrak{D}_G = \left\{ \psi \in H ; \lim_{t \rightarrow 0} \frac{1}{t}(U_t - I)\psi \text{ exists} \right\},$$

and that

$$G\psi = \lim_{t \rightarrow 0} \frac{1}{t}(U_t - I)\psi \quad \text{for all } \psi \in \mathfrak{D}_G.$$

We define the selfadjoint **Hamiltonian** H by

$$H = i\hbar G.$$

This operator represents the **energy** of the system.

By Theorem 4.1.3, if $\psi \in \mathfrak{D}_G = \mathfrak{D}_H$ then $U_t\psi \in \mathfrak{D}_H$ for all $t \in \mathbb{R}$. Therefore, given any initial state $\psi_0 \in \mathfrak{D}_H$, we have for all $t \in \mathbb{R}$

$$\partial_t \psi_t = \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon}(\psi_{t+\varepsilon} - \psi_t) = \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon}(U_\varepsilon - I)\psi_t = G\psi_t = -\frac{i}{\hbar}H\psi_t.$$

That is,

$$i\hbar \partial_t \psi_t = H\psi_t.$$

This is the **Schrödinger equation** corresponding to the Hamiltonian H . Thus, by Stone's theorem, to determine the dynamics of the system, it is equivalent to know the unitary group $(U_t)_{t \in \mathbb{R}}$ or the Hamiltonian H .

We now verify that, **if the system is invariant under time translations then the energy is a constant of the motion**, i.e. that the mean value of H does not change under the time evolution

⁶The more difficult case when the system is not invariant under time translations is described by two-parameter unitary groups and will not be discussed here.

of the system.⁷ Indeed, by Stone's theorem, $U_t H \psi = H U_t \psi$ for all $\psi \in \mathfrak{D}_H$. Hence, if $\psi_0 \in \mathfrak{D}_H$ is normalized, we have for all $t \in \mathbb{R}$

$$\langle H \rangle_{\psi_t} = \langle \psi_t, H \psi_t \rangle = \langle U_t \psi_0, H U_t \psi_0 \rangle = \langle U_t \psi_0, U_t H \psi_0 \rangle = \langle \psi_0, H \psi_0 \rangle = \langle H \rangle_{\psi_0}.$$

In view of Remark 4.2.2, the only exact values of the energy of a system that can be measured in a laboratory are the eigenvalues of the Hamiltonian H . The corresponding eigenvectors are called **bound states**. This is the surprising discovery physicists from the early 20th century made by studying spectral rays of light emission by atoms, and observing only discrete sets of frequencies (characteristic of each atom). It is thus of utmost importance in the framework of quantum mechanics to understand the spectral structure of Hamiltonians describing atomic systems. A thorough analysis of this issue can be found in [RS]. (In Volume I a proof of Stone's theorem can be found, as well as interesting historical remarks about the mathematical formalization of quantum mechanics.) Basic examples of Hamiltonians will be given at the end of the next section.

4.3 The quantum particle on \mathbb{R}

The quantum particle on the real line \mathbb{R} is the system characterized by the following properties.

- (A) To any (Borel) set $\Delta \subseteq \mathbb{R}$ one can associate a measurement device, i.e. an observable P_Δ called **particle detector**, taking the value 0 or 1 depending on whether the particle is in Δ or not, respectively.
- (B) The set of all operators P_Δ , for $\Delta \subseteq \mathbb{R}$, forms a family of pairwise commuting selfadjoint operators.
- (C) To every $a \in \mathbb{R}$ one can associate a translation of the detectors

$$\tau_a P_\Delta = P_{\Delta - a}, \quad \text{where } \Delta - a = \{x \in \mathbb{R}; x + a \in \Delta\}.$$

Equivalently (see below), the translation can be interpreted as acting on the system rather than on the detectors:

$$U_a \psi = \psi_a, \quad \psi \in \mathcal{H}.$$

- (D) The only observables commuting with all the P_Δ are functions of them.

A natural choice of separable Hilbert space satisfying these properties is $L^2(\mathbb{R})$. Then the state of the system at any time is given by a so-called **wave function** $0 \neq \psi \in L^2(\mathbb{R})$, and the detector P_Δ is defined as

$$(P_\Delta \psi)(x) = \chi_\Delta(x) \psi(x), \quad \psi \in \mathcal{H}, \quad \text{a.e. } x \in \mathbb{R}.$$

⁷This conservation principle is an instance, in the quantum setting, of Noether's theorem.

Interpretation of the wave function ψ , observable position

For any $\Delta \subseteq \mathbb{R}$, the probability of finding the particle in a normalized state ψ in Δ is the mean value of the observable P_Δ . By Remark 4.2.1, it is given by

$$\langle P_\Delta \rangle_\psi = \langle P_\Delta \psi, \psi \rangle = \int_\Delta |\psi(x)|^2 dx.$$

Therefore, the function $|\psi(x)|^2$ is interpreted as the density of probability of observing the particle in state ψ .

The observable position is then naturally represented by the multiplication operator

$$(X\psi)(x) = x\psi(x)$$

on the domain

$$\mathfrak{D}_X = \{\psi \in L^2(\mathbb{R}); x\psi(x) \in L^2(\mathbb{R})\}.$$

Indeed, in view of the above probabilistic interpretation of $|\psi(x)|^2$, the mean value of the position of the particle in state ψ is then the expectation value of the probability measure $|\psi(x)|^2 dx$,

$$\int_{\mathbb{R}} x |\psi(x)|^2 dx = \langle X\psi, \psi \rangle.$$

Physically, it represents the ‘averaged position’ of the particle, when the measurement of position is performed on a large number of copies of the system in the same state ψ . The selfadjoint operator X is therefore called **position operator**.

Observable momentum

In a similar way to how we associated the Hamiltonian operator to the group of time translations, we shall now apply Stone’s theorem to obtain the momentum operator as the infinitesimal generator of space translations on the line.

To each translation $a \in \mathbb{R}$, we associate a transformation acting on the states of the system as mentioned in assumption (C) above. This transformation is explicitly given by

$$(U_a \psi)(x) = \psi_a(x) = \psi(x - a), \quad x \in \mathbb{R}. \quad (4.3.1)$$

It is not difficult to check (see Problem 4.5) that $(U_a)_{a \in \mathbb{R}}$ defines a strongly continuous one-parameter unitary group on $L^2(\mathbb{R})$. By Stone’s theorem, there exists a selfadjoint operator A such that

$$U_a = e^{iaA}, \quad \text{for all } a \in \mathbb{R}.$$

Moreover,

$$iA\psi = \left. \frac{d}{da} \right|_{a=0} U_a \psi = \lim_{a \rightarrow 0} \frac{1}{a} (U_a - I)\psi, \quad \psi \in \mathfrak{D}_A.$$

Hence, for $\psi \in \mathfrak{D}_A$,

$$\begin{aligned} (A\psi)(x) &= \frac{1}{i} \lim_{a \rightarrow 0} \frac{\psi(x-a) - \psi(x)}{a} \\ &= -\frac{1}{i} \lim_{a \rightarrow 0} \frac{\psi(x-a) - \psi(x)}{-a} \\ &= -\frac{1}{i} \frac{d}{dx} \psi(x), \end{aligned}$$

and \mathfrak{D}_A is precisely the subspace of all ψ such that $\psi'(x)$ exists and belongs to $L^2(\mathbb{R})$.

For reasons of physical dimensions, the **momentum operator** P is thus defined by

$$\mathfrak{D}_P = \mathfrak{D}_A = \{u \in L^2(\mathbb{R}); u \in AC[a, b] \text{ for any } -\infty < a < b < \infty \text{ and } u' \in L^2(\mathbb{R})\}$$

and

$$(P\psi)(x) = \frac{\hbar}{i} \frac{d}{dx} \psi(x), \quad x \in \mathbb{R}.$$

Hence,

$$U_a = e^{-\frac{i}{\hbar} a P}, \quad \text{for all } a \in \mathbb{R}.$$

Commutation relation and uncertainty principle

For the particle in a normalized state ψ , given an observable represented by a selfadjoint operator A , we define the **variance** of A by

$$\text{var}_\psi(A) = \left\langle [A - \langle A \rangle_\psi I]^2 \right\rangle_\psi = \int_{\mathbb{R}} [A - \langle A \rangle_\psi I]^2 \psi(x) \overline{\psi(x)} dx$$

(where $\langle \cdot \rangle_\psi$ is the mean value defined in Remark 4.2.1) and its **standard deviation** by

$$\Delta_\psi(A) = \sqrt{\text{var}_\psi(A)}.$$

The following theorem is of fundamental importance in the algebraic structure of quantum mechanics. It will be proved in Problem 4.8.

Theorem 4.3.1 *Let A and B be selfadjoint operators acting in the Hilbert space $L^2(\mathbb{R})$. Then the commutator $C = AB - BA$ satisfies*

$$|\langle C \rangle_\psi| \leq 2\Delta_\psi(A)\Delta_\psi(B),$$

for all $\psi \in \mathfrak{D}_C$.

We will see in Problem 4.7 that the position and momentum operators satisfy the **Heisenberg commutation relation**

$$XP - PX = i\hbar I, \quad (4.3.2)$$

where I is the identity operator on the domain $\mathfrak{D}(XP - PX) = \mathfrak{D}(XP) \cap \mathfrak{D}(PX)$. We then have the following immediate corollary of Theorem 4.3.1.

Corollary 4.3.2 (Heisenberg's Uncertainty Principle) *The position and momentum operators of the quantum particle on the real line satisfy*

$$\Delta_\psi(X)\Delta_\psi(P) \geq \frac{\hbar}{2}.$$

Particle in a potential

The quantum Hamiltonian for the particle in a potential field $V : \mathbb{R} \rightarrow \mathbb{R}$ is constructed by replacing the classical momentum p by $\frac{\hbar}{i} \frac{d}{dx}$ in the total mechanical energy $E = \frac{p^2}{2m} + V(x)$, where m is the mass of the particle. This yields

$$(H\psi)(x) = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V(x)\psi(x), \quad \psi \in \mathfrak{D}_H. \quad (4.3.3)$$

The Schrödinger equation then becomes

$$i\hbar \partial_t \psi_t(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_t(x) + V(x)\psi_t(x).$$

To solve it, one can seek a solution in the form of a **standing wave** $\psi_t(x) = e^{-\frac{i}{\hbar}Et} \varphi(x)$, which yields the **stationary Schrödinger equation** for φ :

$$E\varphi = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \varphi(x) + V(x)\varphi(x),$$

where $E \in \mathbb{R}$ is therefore an eigenvalue of the Hamiltonian H , and φ a corresponding eigenvector.⁸

⁸Note that the same Ansatz yields the stationary Schrödinger equation $E\varphi = H\varphi$ for any time-independent Hamiltonian H .

The spectral theory of **Schrödinger operators** of the form (4.3.3) is very well known. In the typical case of a continuous attractive potential $V < 0$, with $\lim_{|x| \rightarrow \infty} V(x) = 0$, the spectrum of H consists of a finite number of negative isolated eigenvalues of multiplicity one, and the continuous spectrum $\sigma_c(H) = [0, \infty)$. But many other scenarios can occur, as discussed e.g. in [RS]. For instance, in three dimensions, the Hamiltonian of the electron in the hydrogen atom is

$$H\psi = -\frac{\hbar^2}{2m}\Delta\psi + V(|\mathbf{x}|)\psi, \quad \text{where } V(|\mathbf{x}|) = -\frac{e^2}{4\pi\epsilon_0|\mathbf{x}|}, \quad \mathbf{x} \in \mathbb{R}^3.$$

Here e is the electric charge of the electron, ϵ_0 is the vacuum electric permittivity, and $|\mathbf{x}|$ is the distance of the electron to the (fixed) nucleus. In this case there are infinitely many negative eigenvalues ($\propto -1/n^2$, $n = 1, 2, \dots$) corresponding to the bound states of the electron.

In the present one-dimensional case, even though it does not belong to $L^2(\mathbb{R})$, it is instructive to study a solution in the form of a **plane wave** $\varphi(x) = e^{ikx}$ for $k \in \mathbb{R}$. Then our standing wave becomes

$$\psi_t(x) = e^{i(kx - \omega t)}, \quad \text{where } \omega = E/\hbar.$$

Some simple properties of plane wave solutions will be studied in Problem 4.9, in the case where V is a ‘potential barrier’, notably displaying the famous *tunnel effect*.

Problems

1. We say that $U : \mathcal{H} \rightarrow \mathcal{H}$ is unitary if $\langle Uu, Uv \rangle = \langle u, v \rangle$ for all $u, v \in \mathcal{H}$. Show that a unitary operator $U : \mathcal{H} \rightarrow \mathcal{H}$ satisfies: (a) $\|U\| = 1$; (b) U is invertible with $U^{-1} = U^*$ unitary. Then show that, in fact, $U \in \mathcal{B}(\mathcal{H})$ is unitary if and only if $UU^* = U^*U = I$.
2. Show that a weakly continuous one-parameter unitary group is strongly continuous.
3. Prove Theorem 4.1.4.

Strategy: Let $A := -iG$ where G is the infinitesimal generator of $(U_t)_{t \in \mathbb{R}}$, and consider the set \mathfrak{D} of all finite linear combinations of elements of the form

$$u_\phi = \int_{\mathbb{R}} \phi(t) U_t u \, dt,$$

for $u \in \mathcal{H}$ and $\phi \in C_0^\infty(\mathbb{R})$ (see Appendix C for the meaning of this integral). The theorem is then proved in three steps.

- (i) Using the results of Section C.2, show that \mathfrak{D} is dense in \mathcal{H} , and contained in \mathfrak{D}_A .

- (ii) Show that A is symmetric and, in fact, essentially selfadjoint (use Theorem 3.5.6 for this).
- (iii) By differentiating $\|(U_t - e^{it\bar{A}})u\|^2$ with respect to t , show that $U_t = e^{it\bar{A}}$. Conclude.
- 4. Using (??) and the spectral family of the position operator X obtained in Problem 3.9, recover the statement that the probability of finding the particle in a normalized state ψ in the interval $\Delta = [a, b]$ is given by $\int_a^b |\psi(x)|^2 dx$.
- 5. Show that the group of translations acting on $L^2(\mathbb{R})$ as defined in (4.3.1) is a strongly continuous one-parameter unitary group.
- 6. Prove that the domain \mathfrak{D}_P of the momentum operator P given by Stone's theorem coincides with the domain \mathfrak{D}_{D_2} in Problem 3.7 (d), i.e. that $P = -\hbar D_2$.
- 7. Prove (4.3.2).
- 8. Prove Theorem 4.3.1.
Hint: First show that $C = ST - TS$ where $S = A - \langle A \rangle_\psi$ and $T = B - \langle B \rangle_\psi$.
- 9. Consider the stationary Schrödinger equation with a **potential barrier** defined in three regions of \mathbb{R} by: (A) $V(x) = 0$ for $x < 0$, (B) $V(x) = V_0 > 0$ for $0 \leq x \leq a$, (C) $V(x) = 0$ for $x > a$. Seek solutions in the three regions with the same given energy $E > 0$, $E \neq V_0$, in the following forms:

$$\begin{aligned}\varphi_A(x) &= A_r e^{ik_A x} + A_l e^{-ik_A x}, \\ \varphi_B(x) &= B_r e^{ik_B x} + B_l e^{-ik_B x}, \\ \varphi_C(x) &= C_r e^{ik_C x} + C_l e^{-ik_C x},\end{aligned}$$

with k_A, k_B, k_C to be determined as functions of E . The indices 'r' and 'l' stand for the direction of the velocity vector of each wave component, respectively 'right' and 'left'.

Now the global solution is obtained by 'gluing' together the solutions $\varphi_A, \varphi_B, \varphi_C$. Find the relations between the coefficients so that the global solution is continuous everywhere, as well as its derivative.

Tunnel effect: We define the **transmission coefficient** t and the **reflection coefficient** r as follows. Consider the solution for which $A_r = 1$ (particle coming from the left), $A_l = r$ (reflection), $C_l = 0$ (no particle coming from the right), and $C_r = t$ (transmission). The number $|t|^2$ is the probability for the particle to be transmitted through the barrier and $|r|^2$ the probability of it being reflected by the barrier. Find the explicit expressions of t and r , in terms of k_A, k_B, k_C and a . Verify that $|t|^2 + |r|^2 = 1$ (conservation of the particle).

Now discuss the two cases $E < V_0$ and $E > V_0$. Decide if the particle is always transmitted or always reflected in each case. How do the results contrast with the situation of a classical particle with the same energy?

Appendix A

The Riemann-Stieltjes integral

In this appendix we will extend the Riemann integral to measures generated by functions of ‘bounded variation’.

A.1 Functions of bounded variation

Let $[a, b] \subset \mathbb{R}$ be a non-empty compact interval. A **partition** Π of $[a, b]$ is a finite sequence of numbers $(\lambda_k)_{k=0}^n$ such that

$$a = \lambda_0 < \lambda_1 < \cdots < \lambda_n = b.$$

The size of Π is the positive number

$$|\Pi| := \max_{k=1, \dots, n} \lambda_k - \lambda_{k-1}.$$

We denote $\mathfrak{P}[a, b]$ the set of all partitions of $[a, b]$.

A function $\phi : [a, b] \rightarrow \mathbb{R}$ is said to have **bounded variation** if there exists a constant $C \geq 0$ such that

$$\sum_{k=1}^n |\phi(\lambda_k) - \phi(\lambda_{k-1})| \leq C,$$

for any partition $\Pi = (\lambda_k)_{k=0}^n \in \mathfrak{P}[a, b]$. If ϕ has bounded variation in $[a, b]$ we define for all $x, y \in [a, b]$ such that $x < y$ the **total variation** of ϕ in $[x, y]$ as the positive number

$$V_x^y(\phi) := \sup_{\Pi \in \mathfrak{P}[x, y]} \sum_{k=1}^n |\phi(\lambda_k) - \phi(\lambda_{k-1})|.$$

The functions of bounded variation in $[a, b]$ form a vector space, denoted $BV[a, b]$.

The following theorems are proved in [KF80], pp. 329 and 330.

Theorem A.1.1 *Let $\phi \in BV[a, b]$. If $a < c < d \leq b$ then*

$$V_a^d(\phi) = V_a^c(\phi) + V_c^d(\phi).$$

Theorem A.1.2 *Let $\phi \in BV[a, b]$. If ϕ is left-continuous at a point $x_0 \in [a, b]$, then the function $x \mapsto V_a^x(\phi)$ is also left-continuous at x_0 .*

A.2 Definition of the integral

Let us now consider a continuous function $f : [a, b] \rightarrow \mathbb{R}$ and a function of bounded variation $\phi \in BV[a, b]$. For any partition $\Pi = (\lambda_k)_{k=0}^n$ and any real numbers

$$\mu_k \in [\lambda_k, \lambda_{k-1}], \quad k = 1, \dots, n,$$

we let

$$S_\Pi = \sum_{k=1}^n f(\mu_k)(\phi(\lambda_k) - \phi(\lambda_{k-1})).$$

Theorem A.2.1 *Let $f : [a, b] \rightarrow \mathbb{R}$ continuous and $\phi \in BV[a, b]$. There exists a unique number $I \in \mathbb{R}$ satisfying: for all $\varepsilon > 0$ there exists $\delta > 0$ such that if Π is a partition of $[a, b]$ satisfying $|\Pi| < \delta$, then*

$$|S_\Pi - I| < \varepsilon.$$

Furthermore, the number I is independent of the choice of points μ_k .

Proof. Let $\varepsilon > 0$. Since f continuous in a compact set, it is uniformly continuous. So there exists δ_ε such that for all $x, y \in [a, b]$ $|x - y| < \delta_\varepsilon \implies$

$$|f(x) - f(y)| \leq \frac{\varepsilon}{2V_a^b(\phi)},$$

where $V_a^b(\phi)$ is the total variation of ϕ in $[a, b]$.

Let us now show that for any two partitions $\Pi, \Pi' \in \mathfrak{P}[a, b]$ we have

$$|\Pi|, |\Pi'| < \delta_\varepsilon \implies |S_\Pi - S_{\Pi'}| \leq \varepsilon, \tag{A.2.1}$$

independently of the choice of points μ_k used to compute the partial sums S_Π et $S_{\Pi'}$. We denote by $(\lambda_k)_{k=0}^n$ the partition Π and we consider the partition $\bar{\Pi} = \Pi \cup \Pi'$, which we index as follows:

$$\bar{\lambda}_0 = \lambda_0 < \bar{\lambda}_1 < \dots < \bar{\lambda}_{k_1} = \lambda_1 < \bar{\lambda}_{k_1+1} < \dots < \bar{\lambda}_{k_2} = \lambda_2 < \dots < \bar{\lambda}_{k_n} = \lambda_n.$$

Fixing arbitrarily $\mu_i \in [\lambda_i, \lambda_{i-1}]$, $k = 1, \dots, n$, and $\bar{\mu}_j \in [\bar{\lambda}_j, \bar{\lambda}_{j-1}]$, $j = 1, \dots, k_n$, we have

$$S_{\Pi} = \sum_{i=1}^n \sum_{j=k_{i-1}+1}^{k_i} f(\bar{\mu}_j) [\phi(\bar{\lambda}_j) - \phi(\bar{\lambda}_{j-1})].$$

Furthermore, since for all $i = 1, \dots, n$

$$\sum_{j=k_{i-1}+1}^{k_i} \phi(\bar{\lambda}_j) - \phi(\bar{\lambda}_{j-1}) = \phi(\bar{\lambda}_{k_i}) - \phi(\bar{\lambda}_{k_{i-1}}) = \phi(\lambda_i) - \phi(\lambda_{i-1}),$$

we can write S_{Π} as

$$S_{\Pi} = \sum_{i=1}^n \sum_{j=k_{i-1}+1}^{k_i} f(\mu_i) [\phi(\bar{\lambda}_j) - \phi(\bar{\lambda}_{j-1})].$$

Since $|\Pi| < \delta_\varepsilon$, we now have that, for all $i = 1, \dots, n$ and all $j = k_{i-1} + 1, \dots, k_i$,

$$|\bar{\mu}_j - \mu_i| < \lambda_i - \lambda_{i-1} < \delta_\varepsilon \implies |f(\bar{\mu}_j) - f(\mu_i)| < \frac{\varepsilon}{2V_a^b(\phi)}.$$

Therefore,

$$\begin{aligned} |S_{\Pi} - S_{\bar{\Pi}}| &\leq \sum_{i=1}^n \sum_{j=k_{i-1}+1}^{k_i} |f(\bar{\mu}_j) - f(\mu_i)| |\phi(\bar{\lambda}_j) - \phi(\bar{\lambda}_{j-1})| \\ &\leq \frac{\varepsilon}{2V_a^b(\phi)} \sum_{j=1}^{k_n} |\phi(\bar{\lambda}_j) - \phi(\bar{\lambda}_{j-1})| \leq \frac{\varepsilon}{2}. \end{aligned}$$

Similarly, we also have $|S_{\Pi'} - S_{\bar{\Pi}}| \leq \varepsilon/2$. Thus, as expected,

$$|S_{\Pi} - S_{\Pi'}| \leq |S_{\Pi} - S_{\bar{\Pi}}| + |S_{\bar{\Pi}} - S_{\Pi'}| \leq \varepsilon.$$

Let us now consider a sequence of partitions $(\Pi_n)_{n=1}^\infty$ satisfying $\lim_{n \rightarrow \infty} |\Pi_n| = 0$. There exists $M \geq 1$ such that $|\Pi_n| < \delta_\varepsilon$ for all $n \geq M$. It then follows from (A.2.1) that $|S_{\Pi_n} - S_{\Pi_m}| < \varepsilon$, for all $n, m \geq M$. Hence $(S_{\Pi_n})_{n=1}^\infty$ is a Cauchy sequence in \mathbb{R} . So there exists $I \in \mathbb{R}$ and $N \geq 1$ such that $|S_{\Pi_N} - I| < \varepsilon/2$. Finally, by (A.2.1), any partition Π smaller than $\delta_{\varepsilon/2}$ satisfies

$$|S_{\Pi} - I| \leq |S_{\Pi} - S_{\Pi_N}| + |S_{\Pi_N} - I| \leq \varepsilon.$$

This concludes the proof of the theorem. \square

The limit I in Theorem A.2.1 is called the **Riemann-Stieltjes integral** of f with respect to ϕ . We denote it as

$$\int_a^b f(x) d\phi(x) \quad \text{ore merely as} \quad \int_a^b f d\phi.$$

A.3 Some properties of the Riemann-Stieltjes integral

The following elementary properties are direct consequences of the definition and of Theorem A.2.1.

Properties A.3.1 Consider two continuous functions $f, g : [a, b] \rightarrow \mathbb{R}$, two functions of bounded variation $\phi, \psi \in BV[a, b]$, $c \in (a, b)$ and $\alpha \in \mathbb{R}$. Then there holds:

- (a) $\int_a^b f \, d\phi = \int_a^c f \, d\phi + \int_c^b f \, d\phi$;
- (b) $\int_a^b \alpha f \, d\phi = \alpha \int_a^b f \, d\phi$;
- (c) $\int_a^b (f + g) \, d\phi = \int_a^b f \, d\phi + \int_a^b g \, d\phi$;
- (d) $\int_a^b f \, d\phi + \int_a^b f \, d\psi = \int_a^b f \, d(\phi + \psi)$. ♦

We next state the integral form of the mean-value theorem for Riemann-Stieltjes integrals.

Theorem A.3.2 Consider $\phi \in BV[a, b]$ and $f : [a, b] \rightarrow \mathbb{R}$ continuous. Then

$$\left| \int_a^b f \, d\phi \right| \leq \sup_{x \in [a, b]} |f(x)| V_a^b(\phi).$$

Proof. Let $\Pi = (\lambda_k)_{k=0}^n$ be a partition of $[a, b]$. Then

$$\left| \sum_{k=1}^n f(\lambda_k) [\phi(\lambda_k) - \phi(\lambda_{k-1})] \right| \leq \sup_{x \in [a, b]} |f(x)| \sum_{k=1}^n |\phi(\lambda_k) - \phi(\lambda_{k-1})| \leq \sup_{x \in [a, b]} |f(x)| V_a^b(\phi).$$

The result follows by considering a sequence of partitions, the size of which converges to zero. \square

Here is now the analogue of the uniform convergence theorem for Riemann integrals.

Theorem A.3.3 Let $\phi \in BV[a, b]$ and consider a sequence $(f_n)_{n=1}^\infty$ of real continuous functions defined on $[a, b]$, converging uniformly to a function f . Then there holds

$$\lim_{n \rightarrow \infty} \int_a^b f_n \, d\phi = \int_a^b f \, d\phi.$$

Proof. Let us first observe that, since f is continuous, its Riemann-Stieltjes integral w.r.t. ϕ exists. Now consider $\varepsilon > 0$ arbitrary. Since $(f_n)_{n=1}^\infty$ converges uniformly to f , there exists $N \geq 1$ such that, for all $n \geq N$,

$$\sup_{x \in [a, b]} |f_n(x) - f(x)| \leq \frac{\varepsilon}{V_a^b(\phi)}.$$

Then take a sequence of partitions $(\Pi_m)_{m=1}^\infty$ of $[a, b]$ such that $\lim_{m \rightarrow \infty} |\Pi_m| = 0$. Denoting by $(\lambda_k^m)_{k=1}^{l_m}$ partition Π_m we have, for all $n \geq N$ and all $m \geq 1$,

$$\begin{aligned} \left| \sum_{k=1}^{l_m} f_n(\lambda_k^m) [\phi(\lambda_k^m) - \phi(\lambda_{k-1}^m)] - \sum_{k=1}^{l_m} f(\lambda_k^m) [\phi(\lambda_k^m) - \phi(\lambda_{k-1}^m)] \right| \\ \leq \sum_{k=1}^{l_m} |f_n(\lambda_k^m) - f(\lambda_k^m)| |\phi(\lambda_k^m) - \phi(\lambda_{k-1}^m)| \\ \leq \sup_{x \in [a, b]} |f_n(x) - f(x)| V_a^b(\phi) \leq \varepsilon. \end{aligned}$$

For any fixed $n \geq N$, we let $m \rightarrow \infty$ and we get, thanks to Theorem A.2.1,

$$\left| \int_a^b f_n d\phi - \int_a^b f d\phi \right| \leq \varepsilon.$$

□

The following theorem is used in Chapter 2.

Theorem A.3.4 *Let $\phi \in BV[a, b]$ and suppose that ϕ is left-continuous in $[a, b]$. If, for any continuous function $f : [a, b] \rightarrow \mathbb{R}$, there holds*

$$\int_a^b f d\phi = 0,$$

then $\phi(x) = \phi(a)$ for all $x \in [a, b]$.

Proof. Fix $x_0 \in (a, b)$ and choose $N \in \mathbb{N}$ so that $x_0 - 1/N > a$. For any $n \geq N$, we define a continuous function $f_n : [a, b] \rightarrow \mathbb{R}$ by

$$f_n(x) = \begin{cases} 1 & \text{if } x \in [a, x_0 - \frac{1}{n}], \\ -nx + nt & \text{if } x \in [x_0 - \frac{1}{n}, x_0], \\ 0 & \text{if } x \in [x_0, b]. \end{cases}$$

Then, for all $n \geq N$,

$$\begin{aligned} 0 &= \int_a^b f_n d\phi = \int_a^{x_0 - \frac{1}{n}} 1 d\phi + \int_{x_0 - \frac{1}{n}}^{x_0} (-nx + nx_0) d\phi(x) + \int_{x_0}^b 0 d\phi \\ &= \phi(x_0 - \frac{1}{n}) - \phi(a) + \int_{x_0 - \frac{1}{n}}^{x_0} (-nx + nx_0) d\phi(x). \end{aligned} \tag{A.3.1}$$

However by Theorem A.3.2 we have, for all $n \geq N$,

$$0 \leq \left| \int_{x_0 - \frac{1}{n}}^{x_0} (-nx + nx_0) d\phi(x) \right| \leq V_{x_0 - \frac{1}{n}}^{x_0}(\phi).$$

Furthermore, by Theorem A.1.1 we can express the total variation of ϕ in $[x_0 - \frac{1}{n}, x_0]$ as

$$V_{x_0 - \frac{1}{n}}^{x_0}(\phi) = V_a^{x_0}(\phi) - V_a^{x_0 - \frac{1}{n}}(\phi).$$

Since ϕ is left-continuous, Theorem A.1.2 yields

$$\lim_{n \rightarrow \infty} V_{x_0 - \frac{1}{n}}^{x_0}(\phi) = V_a^{x_0}(\phi) - \lim_{n \rightarrow \infty} V_a^{x_0 - \frac{1}{n}}(\phi) = 0.$$

Thus,

$$\lim_{n \rightarrow \infty} \int_{x_0 - \frac{1}{n}}^{x_0} (-nx + nx_0) d\phi(x) = 0.$$

Hence, letting $n \rightarrow \infty$ in (A.3.1), the left continuity of ϕ implies that

$$0 = \lim_{n \rightarrow \infty} \phi(x_0 - \frac{1}{n}) - \phi(a) = \phi(x_0) - \phi(a).$$

Since $x_0 \in (a, b)$ is arbitrary, we have proved that $\phi(x) = \phi(a)$ for all $x \in [a, b)$, and it follows that

$$\phi(b) = \lim_{x \nearrow b} \phi(x) = \phi(a),$$

which finishes the proof. □

Appendix B

The Lebesgue-Stieltjes integral

B.1 Lebesgue-Stieltjes measures

A measure can be associated with any non-decreasing left-continuous function $F : \mathbb{R} \rightarrow \mathbb{R}$ in the following way. Write $F(\lambda^+) = \lim_{\mu \searrow \lambda} F(\mu)$ for all $\lambda \in \mathbb{R}$. The following theorem guarantees the existence of a measure μ_F defined on the Borel sets \mathcal{B} of \mathbb{R} such that

$$\begin{aligned}\mu_F[a, b) &= F(b) - F(a) \\ \mu_F(a, b] &= F(b^+) - F(a^+) \\ \mu_F(a, b) &= F(b) - F(a^+)\end{aligned}$$

for any $a, b \in \mathbb{R}$ with $a < b$, and

$$\mu_F[a, b] = F(b^+) - F(a),$$

for $a, b \in \mathbb{R}$ with $a \leq b$. The total mass of μ_F is given by

$$\mu_F(\mathbb{R}) = F(\infty) - F(-\infty)$$

and can be finite or infinite.

Theorem B.1.1 *Consider an non-decreasing left-continuous function $F : \mathbb{R} \rightarrow \mathbb{R}$. There exists a unique measure μ_F defined on \mathcal{B} such that $\mu_F[a, b) = F(b) - F(a)$ for any $a, b \in \mathbb{R}$ with $a < b$.*

Proof. See [SS05, p. 282]. □

We call **Lebesgue-Stieltjes measure** associated to F the measure μ_F . This measure can be extended to a complete measure on the σ -algebra $\Sigma_F \supset \mathcal{B}$ of all μ_F -measurable sets.

Remark B.1.2 Any measure μ on \mathcal{B} which is finite on bounded intervals is, in fact, a Lebesgue-Stieltjes measure. Indeed $\mu = \mu_F$, where

$$F(x) := \begin{cases} -\mu[-x, 0) & \text{if } x < 0, \\ 0 & \text{if } x = 0, \\ \mu[0, x) & \text{if } x > 0, \end{cases}$$

is non-decreasing and left-continuous. See [SS05, p. 282] for details.

In the remainder of this section, F will always denote a non-decreasing left-continuous function.

B.2 The Lebesgue-Stieltjes integral

The Lebesgue-Stieltjes integral with respect to F is merely defined as the Lebesgue integral associated with the measure μ_F . We shall briefly recall here one possible construction in the context of interest to these notes. We essentially follow [KF80], where more details can be found.

The first step is to define the integral of **simple functions**, i.e. functions of the form

$$s = \sum_{k=1}^{\infty} c_k \chi_{A_k}, \tag{B.2.1}$$

where χ_A denotes the characteristic function of A , the sets A_k are μ_F -measurable and pairwise disjoint, and the numbers $c_k \in \mathbb{R}$, $k \geq 1$, are distincts. Then s is called Lebesgue-Stieltjes integrable with respect to F if the series

$$\sum_{k=1}^{\infty} c_k \mu_F(A_k)$$

is absolutely convergent. In this case the Lebesgue-Stieltjes integral of s with respect to F is defined as

$$\int s \, d\mu_F = \sum_{k=1}^{\infty} c_k \mu_F(A_k).$$

Hence, the definition of the integral for simple functions is quite straightforward. To extend it to general measurable functions, one then benefits from the following theorem. Recall that a function $f : \mathbb{R} \rightarrow \mathbb{R}$ is called **measurable** if

$$f^{-1}(A) \text{ is measurable for any measurable set } A.$$

Theorem B.2.1 *A function f is μ_F -measurable if and only if there exists a sequence $(s_n)_{n=1}^{\infty}$ of simple functions converging uniformly to f .*

Definition B.2.2 A μ_F -measurable function f is called **Lebesgue-Stieltjes integrable with respect to F** , or simply **μ_F -integrable**, if there is a sequence $(s_n)_{n=1}^\infty$ of μ_F -integrable simple functions which converges uniformly to f . In this case we call **Lebesgue-Stieltjes integral with respect to F** of the function f the limit

$$\int f \, d\mu_F = \lim_{n \rightarrow \infty} \int_A s_n \, d\mu_F.$$

One shows in particular that the above limit exists, is finite, and does not depend on the choice of the sequence of simple functions $(s_n)_{n=1}^\infty$, see [KF80, p. 296] for more details.

For a complex function $f : \mathbb{R} \rightarrow \mathbb{C}$, writing $f = g + ih$ with $g = \Re f$ and $h = \Im f$, we say that f is Lebesgue-Stieltjes integrable with respect to F if both g and h are. In this case, the integral of f is simply defined as

$$\int f \, d\mu_F = \int g \, d\mu_F + i \int h \, d\mu_F.$$

The following theorem ensures that the Riemann-Stieltjes integral and the Lebesgue-Stieltjes integral coincide for continuous functions.

Theorem B.2.3 *Let $f : [a, b] \rightarrow \mathbb{R}$ be a continuous function and $F : \mathbb{R} \rightarrow \mathbb{R}$ be non-decreasing and left-continuous. Then*

$$\int_a^b f \, dF = \int_{[a,b)} f \, d\mu_F.$$

Proof. Consider a sequence $(\Pi_n)_{n=1}^\infty$ of partitions of $[a, b]$ given as

$$\Pi_n : \quad a = \lambda_0^n < \lambda_1^n < \cdots < \lambda_{m_n-1}^n < \lambda_{m_n}^n = b,$$

and such that $\lim_{n \rightarrow \infty} |\Pi_n| = 0$. For all $n \geq 1$ we define a simple function $\psi_n : [a, b) \rightarrow \mathbb{R}$ by

$$\psi_n(x) = f(\lambda_k^n) \quad \text{if } x \in [\lambda_k^n, \lambda_{k+1}^n), \quad \text{for } k = 0, \dots, m_n - 1.$$

Each ψ_n is μ_F -integrable over $[a, b)$ and it follows from the uniform continuity of f that the sequence $(\psi_n)_{n=1}^\infty$ converges uniformly to f . Furthermore,

$$S_{\Pi_n} = \int_{[a,b)} \psi_n \, d\mu_F$$

and so, letting $n \rightarrow \infty$, Theorem A.2.1 implies that

$$\int_a^b f \, dF = \int_{[a,b)} f \, d\mu_F.$$

□

We now state, without proofs, some important convergence results. We say that a sequence of functions $(f_n)_{n=1}^\infty$ **converges μ_F -almost everywhere** to a function f , and we simply write $f_n \rightarrow f$ a.e. if the context is clear, provided there exists a μ_F -measurable set N such that $\mu_F(N) = 0$ and

$$\lim_{n \rightarrow \infty} f_n(x) = f(x) \quad \text{for all } x \in \mathbb{R} \setminus N.$$

Similarly, any pointwise property holding everywhere except on a set N such that $\mu_F(N) = 0$ will be said to hold **μ_F -almost everywhere**, or merely almost everywhere if the context is clear.

Theorem B.2.4 (Fatou's Lemma) *Let $(f_n)_{n=1}^\infty$ be a sequence of μ_F -measurable functions such that $f_n \geq 0$ a.e. for all $n \geq 1$. If $f_n \rightarrow f$ a.e. then*

$$\int f \, d\mu_F \leq \liminf_{n \rightarrow \infty} \int f_n \, d\mu_F.$$

The proof of this result can be found on p. 61 of [SS05].

Theorem B.2.5 (Dominated Convergence) *Let $(f_n)_{n=1}^\infty$ be a sequence of μ_F -measurable functions such that $f_n \rightarrow f$ a.e. If there exists a μ_F -integrable function g such that $|f_n| \leq g$ for all $n \geq 1$, then*

$$\lim_{n \rightarrow \infty} \int |f_n - f| \, d\mu_F = 0$$

and so

$$\lim_{n \rightarrow \infty} \int f_n \, d\mu_F = \int f \, d\mu_F.$$

The proof of this result can be found on p. 67 of [SS05]. An equivalent formulation is given on p. 303 of [KF80].

B.3 The Hilbert space $L^2(\mathbb{R}, \mu_F)$

The space $L^2(\mathbb{R}, \mu_F)$ is defined similarly to the case where μ_F is the Lebesgue measure on \mathbb{R} . It consists of equivalence classes of functions μ_F -measurable $f : \mathbb{R} \rightarrow \mathbb{C}$ such that $|f|^2$ is μ_F -integrable over \mathbb{R} , the equivalence relation being given by

$$f \sim_{\mu_F} g \iff f = g \text{ } \mu_F\text{-a.e.}$$

Endowed with the inner product

$$\langle f, g \rangle_{L^2(\mathbb{R}, \mu_F)} = \int f \bar{g} \, d\mu_F, \quad f, g \in L^2(\mathbb{R}, \mu_F),$$

it is a Hilbert space.

The definition of the integral with respect to a spectral family in Chapter 3 is based on the following result. A proof can be found in [Wei80, p. 25]. It can also be deduced from the proof of the separability of $L^2(\mathbb{R})$ in [SS05, p. 160].

We call **step function** a function $t : \mathbb{R} \rightarrow \mathbb{C}$ that can be written as

$$t = \sum_{k=0}^n c_k \chi_{I_k}$$

for a finite number of non-empty pairwise disjoint intervals $I_k \subseteq \mathbb{R}$ of the form

$$(a_k, b_k), \quad [a_k, b_k), \quad (a_k, b_k] \quad \text{or} \quad [a_k, b_k],$$

and corresponding constants $c_k \in \mathbb{C}$.

Theorem B.3.1 *Step functions are dense in $L^2(\mathbb{R}, \mu_F)$.*

Appendix C

The Banach space-valued Riemann integral

Throughout this appendix we consider a Banach space \mathcal{X} and a continuous function $F : [a, b] \rightarrow \mathcal{X}$ where $a, b \in \mathbb{R}$ with $a < b$.

C.1 Definition and existence

The function F being continuous, it is uniformly continuous over the compact interval $[a, b]$. That is, for all $\varepsilon > 0$, there exists $\delta > 0$ such that, for all $t, s \in [a, b]$,

$$|t - s| < \delta \implies \|F(t) - F(s)\| < \varepsilon.$$

On the other hand, $F : [a, b] \rightarrow \mathcal{X}$ is bounded, that is,

$$\sup_{t \in [a, b]} \|F(t)\| < \infty.$$

In fact, this supremum is achieved at some point in $[a, b]$.

In perfect analogy with the real-valued Riemann integral, for any partition Π of $[a, b]$,

$$\Pi : \quad a = \lambda_0 < \lambda_1 < \cdots < \lambda_{m-1} < \lambda_m = b,$$

and any sequence of points

$$\mu_k \in [\lambda_{k-1}, \lambda_k], \quad k = 1, \dots, m,$$

we consider the sum

$$S_\Pi = \sum_{k=1}^m (\lambda_k - \lambda_{k-1}) F(\mu_k).$$

Theorem C.1.1 *Let $F : [a, b] \rightarrow \mathcal{X}$ be continuous. There exists a unique $Y \in \mathcal{X}$ such that, for all $\varepsilon > 0$, there exists $\delta > 0$ such that, for any partition Π of $[a, b]$ satisfying $|\Pi| < \delta$, we have*

$$\|S_\Pi - Y\| < \varepsilon.$$

The element $Y \in \mathcal{X}$ given by Theorem C.1.1 is called the **Riemann integral** of F over $[a, b]$, and we write

$$Y = \int_a^b F(t) \, dt.$$

The proof of this result is virtually identical to those of Theorem A.2.1 and Lemma 2.1.2. We therefore leave as an easy revision exercise the obvious changes of notation required.

The integral defined by Theorem C.1.1 is of course linear. That is, if $F, G : [a, b] \rightarrow \mathcal{X}$ are continuous and $\alpha, \beta \in \mathbb{R}$, then

$$\int_a^b (\alpha F(t) + \beta G(t)) \, dt = \alpha \int_a^b F(t) \, dt + \beta \int_a^b G(t) \, dt.$$

Furthermore, it is easily seen that

$$\left\| \int_a^b F(t) \, dt \right\| \leq \int_a^b \|F(t)\| \, dt.$$

C.2 Some useful results

Lemma C.2.1 *Let $T \in \mathcal{B}(\mathcal{X})$ and $F : [a, b] \rightarrow \mathcal{X}$ continuous. The composition $T \circ F$ is continuous and we have*

$$T \int_a^b F(t) \, dt = \int_a^b TF(t) \, dt.$$

Proof. The continuity of the composition follows from

$$\|TF(t) - TF(s)\| = \|T(F(t) - F(s))\| \leq \|T\| \|F(t) - F(s)\|.$$

Consider now a sequence $(\Pi_n)_{n=1}^\infty$ of partitions of $[a, b]$, given as

$$\Pi_n : \quad a = \lambda_0^n < \lambda_1^n < \cdots < \lambda_{m_n-1}^n < \lambda_{m_n}^n = b,$$

and such that $\lim_{n \rightarrow \infty} |\Pi_n| = 0$. We then have

$$TS_{\Pi_n} = T \sum_{k=1}^{m_n} (\lambda_k^n - \lambda_{k-1}^n) F(\lambda_k^n) = \sum_{k=1}^{m_n} (\lambda_k^n - \lambda_{k-1}^n) TF(\lambda_k^n),$$

and so by continuity of T and Theorem C.1.1, the result follows by letting $n \rightarrow \infty$. □

Theorem C.2.2 *Let $\phi : [a, b] \rightarrow \mathbb{R}$ and $F : [a, b] \rightarrow \mathcal{X}$ be continuous functions. The product ϕF defined by $\phi F(t) = \phi(t)F(t)$ is continuous and we have*

$$\left\| \int \phi(t)F(t) dt \right\| \leq \int |\phi(t)| dt \sup_{s \in [a, b]} \|F(s)\|.$$

Proof. The continuity of ϕF follows from

$$\begin{aligned} \|\phi(t)F(t) - \phi(s)F(s)\| &\leq \|\phi(t)F(t) - \phi(s)F(t)\| + \|\phi(s)F(t) - \phi(s)F(s)\| \\ &\leq |\phi(t) - \phi(s)| \|F(t)\| + |\phi(s)| \|F(t) - F(s)\|. \end{aligned}$$

Consider now a sequence $(\Pi_n)_{n=1}^\infty$ of partitions of $[a, b]$, given as

$$\Pi_n : a = \lambda_0^n < \lambda_1^n < \cdots < \lambda_{m_n-1}^n < \lambda_{m_n}^n = b,$$

and such that $\lim_{n \rightarrow \infty} |\Pi_n| = 0$. We then have

$$\begin{aligned} \|S_{\Pi_n}\| &= \left\| \sum_{k=1}^{m_n} (\lambda_k^n - \lambda_{k-1}^n) \phi(\lambda_k^n) F(\lambda_k^n) \right\| \leq \sum_{k=1}^{m_n} (\lambda_k^n - \lambda_{k-1}^n) |\phi(\lambda_k^n)| \|F(\lambda_k^n)\| \\ &\leq \sum_{k=1}^{m_n} (\lambda_k^n - \lambda_{k-1}^n) |\phi(\lambda_k^n)| \sup_{s \in [a, b]} \|F(s)\|, \end{aligned}$$

and so letting $n \rightarrow \infty$ the result follows by continuity of the norm, by Theorem C.1.1, and the fact that

$$\lim_{n \rightarrow \infty} \sum_{k=1}^{m_n} (\lambda_k^n - \lambda_{k-1}^n) |\phi(\lambda_k^n)| = \int_a^b |\phi(t)| dt.$$

□

Finally, we have the following uniform convergence theorem.

Theorem C.2.3 *Consider a sequence $(F_n)_{n=1}^\infty$ of continuous functions $F_n : [a, b] \rightarrow \mathcal{X}$ and a continuous function $F : [a, b] \rightarrow \mathcal{X}$. Suppose $(F_n)_{n=1}^\infty$ converges uniformly to F . That is, for all $\varepsilon > 0$ there exists $N \geq 1$ such that*

$$n \geq N \implies \sup_{s \in [a, b]} \|F_n(s) - F(s)\| < \varepsilon.$$

Then we have

$$\lim_{n \rightarrow \infty} \int_a^b F_n(t) dt = \int_a^b F(t) dt.$$

Proof. Applying Theorem C.2.2 to $\phi(s) \equiv 1$, we have, for all $n \geq 1$,

$$\left\| \int_a^b F_n(t) \, dt - \int_a^b F(t) \, dt \right\| \leq (b-a) \sup_{t \in [a,b]} \|F_n(t) - F(t)\|.$$

The result then follows from the uniform convergence of $(F_n)_{n=1}^\infty$ to F . □

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