
Mathematical Methods in Quantum Mechanics

With Applications to Schrödinger Operators

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Abstract. This manuscript provides a self-contained introduction to mathematical methods in quantum mechanics (spectral theory) with applications to Schrödinger operators. The first part covers mathematical foundations of quantum mechanics from self-adjointness, the spectral theorem, quantum dynamics (including Stone's and the RAGE theorem) to perturbation theory for self-adjoint operators.

The second part starts with a detailed study of the free Schrödinger operator respectively position, momentum and angular momentum operators. Then we develop Weyl-Titchmarsh theory for Sturm-Liouville operators and apply it to spherically symmetric problems, in particular to the hydrogen atom. Next we investigate self-adjointness of atomic Schrödinger operators and their essential spectrum, in particular the HVZ theorem. Finally we have a look at scattering theory and prove asymptotic completeness in the short range case.

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Preface

Overview

The present manuscript was written for my course *Schrödinger Operators* held at the University of Vienna in Winter 1999, Summer 2002, and Summer 2005. It is supposed to give a brief but rather self contained introduction to the mathematical methods of quantum mechanics with a view towards applications to Schrödinger operators. The applications presented are highly selective and many important and interesting items are not touched.

The first part is a stripped down introduction to spectral theory of unbounded operators where I try to introduce only those topics which are needed for the applications later on. This has the advantage that you will not get drowned in results which are never used again before you get to the applications. In particular, I am not trying to provide an encyclopedic reference. Nevertheless I still feel that the first part should give you a solid background covering all important results which are usually taken for granted in more advanced books and research papers.

My approach is built around the spectral theorem as the central object. Hence I try to get to it as quickly as possible. Moreover, I do not take the detour over bounded operators but I go straight for the unbounded case. In addition, existence of spectral measures is established via the Herglotz rather than the Riesz representation theorem since this approach paves the way for an investigation of spectral types via boundary values of the resolvent as the spectral parameter approaches the real line.

The second part starts with the free Schrödinger equation and computes the free resolvent and time evolution. In addition, I discuss position, momentum, and angular momentum operators via algebraic methods. This is usually found in any physics textbook on quantum mechanics, with the only difference that I include some technical details which are usually not found there. Furthermore, I compute the spectrum of the hydrogen atom, again I try to provide some mathematical details not found in physics textbooks. Further topics are nondegeneracy of the ground state, spectra of atoms (the HVZ theorem) and scattering theory.

Prerequisites

I assume some previous experience with Hilbert spaces and bounded linear operators which should be covered in any basic course on functional analysis. However, while this assumption is reasonable for mathematics students, it might not always be for physics students. For this reason there is a preliminary chapter reviewing all necessary results (including proofs). In addition, there is an appendix (again with proofs) providing all necessary results from measure theory.

Readers guide

There is some intentional overlap between Chapter 0, Chapter 1 and Chapter 2. Hence, provided you have the necessary background, you can start reading in Chapter 1 or even Chapter 2. Chapters 2, 3 are key chapters and you should study them in detail (except for Section 2.5 which can be skipped on first reading). Chapter 4 should give you an idea of how the spectral theorem is used. You should have a look at (e.g.) the first section and you can come back to the remaining ones as needed. Chapter 5 contains two key results from quantum dynamics, Stone's theorem and the RAGE theorem. In particular the RAGE theorem shows the connections between long time behavior and spectral types. Finally, Chapter 6 is again of central importance and should be studied in detail.

The chapters in the second part are mostly independent of each others except for the first one, Chapter 7, which is a prerequisite for all others except for Chapter 9.

If you are interested in one dimensional models (Sturm-Liouville equations), Chapter 9 is all you need.

If you are interested in atoms, read Chapter 7, Chapter 10, and Chapter 11. In particular, you can skip the separation of variables (Sections 10.3

and 10.4, which require Chapter 9) method for computing the eigenvalues of the Hydrogen atom if you are happy with the fact that there are countably many which accumulate at the bottom of the continuous spectrum.

If you are interested in scattering theory, read Chapter 7, the first two sections of Chapter 10, and Chapter 12. Chapter 5 is one of the key prerequisites in this case.

Availability

It is available from

<http://www.mat.univie.ac.at/~gerald/ftp/book-schroe/>

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Part 0

Preliminaries

A first look at Banach and Hilbert spaces

I assume that the reader has some basic familiarity with measure theory and functional analysis. For convenience, some facts needed from Banach and L^p spaces are reviewed in this chapter. A crash course in measure theory can be found in the appendix. If you feel comfortable with terms like *Lebesgue L^p spaces*, *Banach space*, or *bounded linear operator*, you can skip this entire chapter. However, you might want to at least browse through it to refresh your memory.

0.1. Warm up: Metric and topological spaces

Before we begin I want to recall some basic facts from metric and topological spaces. I presume that you are familiar with these topics from your calculus course. A good reference is [8].

A **metric space** is a space X together with a function $d : X \times X \rightarrow \mathbb{R}$ such that

- (i) $d(x, y) \geq 0$
- (ii) $d(x, y) = 0$ if and only if $x = y$
- (iii) $d(x, y) = d(y, x)$
- (iv) $d(x, z) \leq d(x, y) + d(y, z)$ (triangle inequality)

If (ii) does not hold, d is called a **semi-metric**.

Example. Euclidean space \mathbb{R}^n together with $d(x, y) = (\sum_{k=1}^n (x_k - y_k)^2)^{1/2}$ is a metric space and so is \mathbb{C}^n together with $d(x, y) = (\sum_{k=1}^n |x_k - y_k|^2)^{1/2}$. \diamond

The set

$$B_r(x) = \{y \in X \mid d(x, y) < r\} \quad (0.1)$$

is called an **open ball** around x with radius $r > 0$. A point x of some set U is called an **interior point** of U if U contains some ball around x . If x is an interior point of U , then U is also called a **neighborhood** of x . A point x is called a **limit point** of U if $B_r(x) \cap (U \setminus \{x\}) \neq \emptyset$ for every ball. Note that a limit point must not lie in U , but U contains points arbitrarily close to x . Moreover, x is not a limit point of U if and only if it is an interior point of the complement of U .

Example. Consider \mathbb{R} with the usual metric and let $U = (-1, 1)$. Then every point $x \in U$ is an interior point of U . The points ± 1 are limit points of U . \diamond

A set consisting only of interior points is called **open**. The family of open sets \mathcal{O} satisfies the following properties

- (i) $\emptyset, X \in \mathcal{O}$
- (ii) $O_1, O_2 \in \mathcal{O}$ implies $O_1 \cap O_2 \in \mathcal{O}$
- (iii) $\{O_\alpha\} \subseteq \mathcal{O}$ implies $\bigcup_\alpha O_\alpha \in \mathcal{O}$

That is, \mathcal{O} is closed under finite intersections and arbitrary unions.

In general, a space X together with a family of sets \mathcal{O} , the open sets, satisfying (i)–(iii) is called a **topological space**. The notions of interior point, limit point, and neighborhood carry over to topological spaces if we replace open ball by open set.

There are usually different choices for the topology. Two usually not very interesting examples are the **trivial topology** $\mathcal{O} = \{\emptyset, X\}$ and the **discrete topology** $\mathcal{O} = \mathfrak{P}(X)$ (the powerset of X). Given two topologies \mathcal{O}_1 and \mathcal{O}_2 on X , \mathcal{O}_1 is called **weaker** (or **coarser**) than \mathcal{O}_2 if and only if $\mathcal{O}_1 \subseteq \mathcal{O}_2$.

Example. Note that different metrics can give rise to the same topology. For example, we can equip \mathbb{R}^n (or \mathbb{C}^n) with the Euclidean distance as before, or we could also use

$$\tilde{d}(x, y) = \sum_{k=1}^n |x_k - y_k| \quad (0.2)$$

Since

$$\frac{1}{\sqrt{n}} \sum_{k=1}^n |x_k| \leq \sqrt{\sum_{k=1}^n |x_k|^2} \leq \sum_{k=1}^n |x_k| \quad (0.3)$$

shows $B_{r/\sqrt{n}}((x, y)) \subseteq \tilde{B}_r((x, y)) \subseteq B_r((x, y))$, where B, \tilde{B} are balls computed using d, \tilde{d} , respectively. Hence the topology is the same for both metrics. \diamond

Example. We can always replace a metric d by the bounded metric

$$\tilde{d}(x, y) = \frac{d(x, y)}{1 + d(x, y)} \quad (0.4)$$

without changing the topology. \diamond

Every subspace Y of a topological space X becomes a topological space of its own if we call $O \subseteq Y$ open if there is some open set $\tilde{O} \subseteq X$ such that $O = \tilde{O} \cap Y$ (**induced topology**).

Example. The set $(0, 1] \subseteq \mathbb{R}$ is not open in the topology of $X = \mathbb{R}$, but it is open in the induced topology when considered as a subset of $Y = [-1, 1]$. \diamond

A family of open sets $\mathcal{B} \subseteq \mathcal{O}$ is called a **base** for the topology if for each x and each neighborhood $U(x)$, there is some set $O \in \mathcal{B}$ with $x \in O \subseteq U$. Since $O = \bigcap_{x \in O} U(x)$ we have

Lemma 0.1. *If $\mathcal{B} \subseteq \mathcal{O}$ is a base for the topology, then every open set can be written as a union of elements from \mathcal{B} .*

If there exists a countable base, then X is called **second countable**.

Example. By construction the open balls $B_{1/n}(x)$ are a base for the topology in a metric space. In the case of \mathbb{R}^n (or \mathbb{C}^n) it even suffices to take balls with rational center and hence \mathbb{R}^n (and \mathbb{C}^n) are second countable. \diamond

A topological space is called **Hausdorff space** if for two different points there are always two disjoint neighborhoods.

Example. Any metric space is a Hausdorff space: Given two different points x and y the balls $B_{d/2}(x)$ and $B_{d/2}(y)$, where $d = d(x, y) > 0$, are disjoint neighborhoods (a semi-metric space will not be Hausdorff). \diamond

The complement of an open set is called a **closed set**. It follows from de Morgan's rules that the family of closed sets \mathcal{C} satisfies

- (i) $\emptyset, X \in \mathcal{C}$
- (ii) $C_1, C_2 \in \mathcal{C}$ implies $C_1 \cup C_2 \in \mathcal{C}$
- (iii) $\{C_\alpha\} \subseteq \mathcal{C}$ implies $\bigcap_\alpha C_\alpha \in \mathcal{C}$

That is, closed sets are closed under finite unions and arbitrary intersections.

The smallest closed set containing a given set U is called the **closure**

$$\bar{U} = \bigcap_{C \in \mathcal{C}, U \subseteq C} C, \quad (0.5)$$

and the largest open set contained in a given set U is called the **interior**

$$U^\circ = \bigcup_{O \in \mathcal{O}, O \subseteq U} O. \quad (0.6)$$

It is straightforward to check that

Lemma 0.2. *Let X be a topological space, then the interior of U is the set of all interior points of U and the closure of U is the set of all limit points of U .*

A sequence $(x_n)_{n=1}^{\infty} \subseteq X$ is said to **converge** to some point $x \in X$ if $d(x, x_n) \rightarrow 0$. We write $\lim_{n \rightarrow \infty} x_n = x$ as usual in this case. Clearly the limit is unique if it exists (this is not true for a semi-metric).

Every convergent sequence is a **Cauchy sequence**, that is, for every $\varepsilon > 0$ there is some $N \in \mathbb{N}$ such that

$$d(x_n, x_m) \leq \varepsilon \quad n, m \geq N. \quad (0.7)$$

If the converse is also true, that is, if every Cauchy sequence has a limit, then X is called **complete**.

Example. Both \mathbb{R}^n and \mathbb{C}^n are complete metric spaces. \diamond

A point x is clearly a limit point of U if and only if there is some sequence $x_n \in U$ converging to x . Hence

Lemma 0.3. *A closed subset of a complete metric space is again a complete metric space.*

Note that convergence can also be equivalently formulated in terms of topological terms: A sequence x_n converges to x if and only if for every neighborhood U of x there is some $N \in \mathbb{N}$ such that $x_n \in U$ for $n \geq N$. In a Hausdorff space the limit is unique.

A metric space is called **separable** if it contains a countable dense set. A set U is called **dense**, if its closure is all of X , that is if $\bar{U} = X$.

Lemma 0.4. *Let X be a separable metric space. Every subset of X is again separable.*

Proof. Let $A = \{x_n\}_{n \in \mathbb{N}}$ be a dense set in X . The only problem is that $A \cap Y$ might contain no elements at all. However, some elements of A must be at least arbitrarily close: Let $J \subseteq \mathbb{N}^2$ be the set of all pairs (n, m) for which $B_{1/m}(x_n) \cap Y \neq \emptyset$ and choose some $y_{n,m} \in B_{1/m}(x_n) \cap Y$ for all $(n, m) \in J$. Then $B = \{y_{n,m}\}_{(n,m) \in J} \subseteq Y$ is countable. To see that B is dense choose $y \in Y$. Then there is some sequence x_{n_k} with $d(x_{n_k}, y) < 1/4$. Hence $(n_k, k) \in J$ and $d(y_{n_k, k}, y) \leq d(y_{n_k, k}, x_{n_k}) + d(x_{n_k}, y) \leq 2/k \rightarrow 0$. \square

A function between metric spaces X and Y is called continuous at a point $x \in X$ if for every $\varepsilon > 0$ we can find a $\delta > 0$ such that

$$d_Y(f(x), f(y)) \leq \varepsilon \quad \text{if} \quad d_X(x, y) < \delta. \quad (0.8)$$

If f is continuous at every point it is called **continuous**.

Lemma 0.5. *Let X be a metric space. The following are equivalent*

- (i) f is continuous at x (i.e., (0.8) holds).
- (ii) $f(x_n) \rightarrow f(x)$ whenever $x_n \rightarrow x$
- (iii) For every neighborhood V of $f(x)$, $f^{-1}(V)$ is a neighborhood of x .

Proof. (i) \Rightarrow (ii) is obvious. (ii) \Rightarrow (iii): If (iii) does not hold there is a neighborhood V of $f(x)$ such that $B_\delta(x) \not\subseteq f^{-1}(V)$ for every δ . Hence we can choose a sequence $x_n \in B_{1/n}(x)$ such that $f(x_n) \notin f^{-1}(V)$. Thus $x_n \rightarrow x$ but $f(x_n) \not\rightarrow f(x)$. (iii) \Rightarrow (i): Choose $V = B_\varepsilon(f(x))$ and observe that by (iii) $B_\delta(x) \subseteq f^{-1}(V)$ for some δ . \square

The last item implies that f is continuous if and only if the inverse image of every open (closed) set is again open (closed).

Note: In a topological space, (iii) is used as definition for continuity. However, in general (ii) and (iii) will no longer be equivalent unless one uses generalized sequences, so called nets, where the index set \mathbb{N} is replaced by arbitrary directed sets.

If X and Y are metric spaces then $X \times Y$ together with

$$d((x_1, y_1), (x_2, y_2)) = d_X(x_1, x_2) + d_Y(y_1, y_2) \quad (0.9)$$

is a metric space. A sequence (x_n, y_n) converges to (x, y) if and only if $x_n \rightarrow x$ and $y_n \rightarrow y$. In particular, the projections onto the first $(x, y) \mapsto x$ respectively onto the second $(x, y) \mapsto y$ coordinate are continuous.

In particular, by

$$|d(x_n, y_n) - d(x, y)| \leq d(x_n, x) + d(y_n, y) \quad (0.10)$$

we see that $d : X \times X \rightarrow \mathbb{R}$ is continuous.

Example. If we consider $\mathbb{R} \times \mathbb{R}$ we do not get the Euclidean distance of \mathbb{R}^2 unless we modify (0.9) as follows:

$$\tilde{d}((x_1, y_1), (x_2, y_2)) = \sqrt{d_X(x_1, x_2)^2 + d_Y(y_1, y_2)^2}. \quad (0.11)$$

As noted in our previous example, the topology (and thus also convergence/continuity) is independent of this choice. \diamond

If X and Y are just topological spaces, the **product topology** is defined by calling $O \subseteq X \times Y$ open if for every point $(x, y) \in O$ there are open neighborhoods U of x and V of y such that $U \times V \subseteq O$. In the case of metric spaces this clearly agrees with the topology defined via the product metric (0.9).

A **cover** of a set $Y \subseteq X$ is a family of sets $\{U_\alpha\}$ such that $Y \subseteq \bigcup_\alpha U_\alpha$. A cover is called open if all U_α are open. A subset of $\{U_\alpha\}$ is called a **subcover**.

A subset $K \subset X$ is called **compact** if every open cover has a finite subcover.

Lemma 0.6. *A topological space is compact if and only if it has the **finite intersection property**: The intersection of a family of closed sets is empty if and only if the intersection of some finite subfamily is empty.*

Proof. By taking complements, to every family of open sets there is a corresponding family of closed sets and vice versa. Moreover, the open sets are a cover if and only if the corresponding closed sets have empty intersection. \square

A subset $K \subset X$ is called **sequentially compact** if every sequence has a convergent subsequence.

Lemma 0.7. *Let X be a topological space.*

- (i) *The continuous image of a compact set is compact.*
- (ii) *Every closed subset of a compact set is compact.*
- (iii) *If X is Hausdorff, any compact set is closed.*
- (iv) *The product of compact sets is compact.*
- (v) *A compact set is also sequentially compact.*

Proof. (i) Just observe that if $\{O_\alpha\}$ is an open cover for $f(Y)$, then $\{f^{-1}(O_\alpha)\}$ is one for Y .

(ii) Let $\{O_\alpha\}$ be an open cover for the closed subset Y . Then $\{O_\alpha\} \cup \{X \setminus Y\}$ is an open cover for X .

(iii) Let $Y \subseteq X$ be compact. We show that $X \setminus Y$ is open. Fix $x \in X \setminus Y$ (if $Y = X$ there is nothing to do). By the definition of Hausdorff, for every $y \in Y$ there are disjoint neighborhoods $V(y)$ of y and $U_y(x)$ of x . By compactness of Y , there are y_1, \dots, y_n such that $V(y_j)$ cover Y . But then $U(x) = \bigcup_{j=1}^n U_{y_j}(x)$ is a neighborhood of x which does not intersect Y .

(iv) Let $\{O_\alpha\}$ be an open cover for $X \times Y$. For every $(x, y) \in X \times Y$ there is some $\alpha(x, y)$ such that $(x, y) \in O_{\alpha(x, y)}$. By definition of the product topology there is some open rectangle $U(x, y) \times V(x, y) \subseteq O_{\alpha(x, y)}$. Hence for fixed x , $\{V(x, y)\}_{y \in Y}$ is an open cover of Y . Hence there are finitely many points $y_k(x)$ such $V(x, y_k(x))$ cover Y . Set $U(x) = \bigcap_k U(x, y_k(x))$. Since finite intersections of open sets are open, $\{U(x)\}_{x \in X}$ is an open cover and there are finitely many points x_j such $U(x_j)$ cover X . By construction, $U(x_j) \times V(x_j, y_k(x_j)) \subseteq O_{\alpha(x_j, y_k(x_j))}$ cover $X \times Y$.

(v) Let x_n be a sequence which has no convergent subsequence. Then $K = \{x_n\}$ has no limit points and is hence compact by (ii). For every n

there is a ball $B_{\varepsilon_n}(x_n)$ which contains only finitely many elements of K . However, finitely many suffice to cover K , a contradiction. \square

In a metric space compact and sequentially compact are equivalent.

Lemma 0.8. *Let X be a metric space. Then a subset is compact if and only if it is sequentially compact.*

Proof. First of all note that every cover of open balls with fixed radius $\varepsilon > 0$ has a finite subcover. Since if this were false we could construct a sequence $x_n \in X \setminus \bigcup_{m=1}^{n-1} B_\varepsilon(x_m)$ such that $d(x_n, x_m) > \varepsilon$ for $m < n$.

In particular, we are done if we can show that for every open cover $\{O_\alpha\}$ there is some $\varepsilon > 0$ such that for every x we have $B_\varepsilon(x) \subseteq O_\alpha$ for some $\alpha = \alpha(x)$. Indeed, choosing $\{x_k\}_{k=1}^n$ such that $B_\varepsilon(x_k)$ is a cover, we have that $O_{\alpha(x_k)}$ is a cover as well.

So it remains to show that there is such an ε . If there were none, for every $\varepsilon > 0$ there must be an x such that $B_\varepsilon(x) \not\subseteq O_\alpha$ for every α . Choose $\varepsilon = \frac{1}{n}$ and pick a corresponding x_n . Since X is sequentially compact, it is no restriction to assume x_n converges (after maybe passing to a subsequence). Let $x = \lim x_n$, then x lies in some O_α and hence $B_\varepsilon(x) \subseteq O_\alpha$. But choosing n so large that $\frac{1}{n} < \frac{\varepsilon}{2}$ and $d(x_n, x) < \frac{\varepsilon}{2}$ we have $B_{1/n}(x_n) \subseteq B_\varepsilon(x) \subseteq O_\alpha$ contradicting our assumption. \square

Please also recall the **Heine-Borel theorem**:

Theorem 0.9 (Heine-Borel). *In \mathbb{R}^n (or \mathbb{C}^n) a set is compact if and only if it is bounded and closed.*

Proof. By Lemma 0.7 (ii) and (iii) it suffices to show that a closed interval in $I \subseteq \mathbb{R}$ is compact. Moreover, by Lemma 0.8 it suffices to show that every sequence in $I = [a, b]$ has a convergent subsequence. Let x_n be our sequence and divide $I = [a, \frac{a+b}{2}] \cup [\frac{a+b}{2}, b]$. Then at least one of these two intervals, call it I_1 , contains infinitely many elements of our sequence. Let $y_1 = x_{n_1}$ be the first one. Subdivide I_1 and pick $y_2 = x_{n_2}$, with $n_2 > n_1$ as before. Proceeding like this we obtain a Cauchy sequence y_n (note that by construction $I_{n+1} \subseteq I_n$ and hence $|y_n - y_m| \leq \frac{b-a}{n}$ for $m \geq n$). \square

A topological space is called **locally compact** if every point has a compact neighborhood.

Example. \mathbb{R}^n is locally compact. \diamond

The **distance** between a point $x \in X$ and a subset $Y \subseteq X$ is

$$\text{dist}(x, Y) = \inf_{y \in Y} d(x, y). \quad (0.12)$$

Note that $x \in \bar{Y}$ if and only if $\text{dist}(x, Y) = 0$.

Lemma 0.10. *Let X be a metric space, then*

$$|\text{dist}(x, Y) - \text{dist}(z, Y)| \leq \text{dist}(x, z). \quad (0.13)$$

In particular, $x \mapsto \text{dist}(x, Y)$ is continuous.

Proof. Taking the infimum in the triangle inequality $d(x, y) \leq d(x, z) + d(z, y)$ shows $\text{dist}(x, Y) \leq d(x, z) + \text{dist}(z, Y)$. Hence $\text{dist}(x, Y) - \text{dist}(z, Y) \leq \text{dist}(x, z)$. Interchanging x and z shows $\text{dist}(z, Y) - \text{dist}(x, Y) \leq \text{dist}(x, z)$. \square

Lemma 0.11 (Urysohn). *Suppose C_1 and C_2 are disjoint closed subsets of a metric space X . Then there is a continuous function $f : X \rightarrow [0, 1]$ such that f is zero on C_1 and one on C_2 .*

If X is locally compact and U is compact, one can choose f with compact support.

Proof. To prove the first claim set $f(x) = \frac{\text{dist}(x, C_2)}{\text{dist}(x, C_1) + \text{dist}(x, C_2)}$. For the second claim, observe that there is an open set O such that \bar{O} is compact and $C_1 \subset O \subset \bar{O} \subset X \setminus C_2$. In fact, for every x , there is a ball $B_\varepsilon(x)$ such that $\overline{B_\varepsilon(x)}$ is compact and $\overline{B_\varepsilon(x)} \subset X \setminus C_2$. Since U is compact, finitely many of them cover C_1 and we can choose the union of those balls to be O . Now replace C_2 by $X \setminus \bar{O}$. \square

Note that Urysohn's lemma implies that a metric space is **normal**, that is, for any two disjoint closed sets C_1 and C_2 , there are disjoint open sets O_1 and O_2 such that $C_j \subseteq O_j$, $j = 1, 2$. In fact, choose f as in Urysohn's lemma and set $O_1 = f^{-1}([0, 1/2))$ respectively $O_2 = f^{-1}((1/2, 1])$.

0.2. The Banach space of continuous functions

Now let us have a first look at Banach spaces by investigating set of continuous functions $C(I)$ on a compact interval $I = [a, b] \subset \mathbb{R}$. Since we want to handle complex models, we will always consider complex valued functions!

One way of declaring a distance, well-known from calculus, is the **maximum norm**:

$$\|f(x) - g(x)\|_\infty = \max_{x \in I} |f(x) - g(x)|. \quad (0.14)$$

It is not hard to see that with this definition $C(I)$ becomes a normed linear space:

A **normed linear space** X is a vector space X over \mathbb{C} (or \mathbb{R}) with a real-valued function (the **norm**) $\|\cdot\|$ such that

- $\|f\| \geq 0$ for all $f \in X$ and $\|f\| = 0$ if and only if $f = 0$,

- $\|\lambda f\| = |\lambda| \|f\|$ for all $\lambda \in \mathbb{C}$ and $f \in X$, and
- $\|f + g\| \leq \|f\| + \|g\|$ for all $f, g \in X$ (**triangle inequality**).

From the triangle inequality we also get the inverse triangle inequality (Problem 0.1)

$$\left| \|f\| - \|g\| \right| \leq \|f - g\|. \quad (0.15)$$

Once we have a norm, we have a **distance** $d(f, g) = \|f - g\|$ and hence we know when a sequence of vectors f_n **converges** to a vector f . We will write $f_n \rightarrow f$ or $\lim_{n \rightarrow \infty} f_n = f$, as usual, in this case. Moreover, a mapping $F : X \rightarrow Y$ between two normed spaces is called **continuous** if $f_n \rightarrow f$ implies $F(f_n) \rightarrow F(f)$. In fact, it is not hard to see that the norm, vector addition, and multiplication by scalars are continuous (Problem 0.2).

In addition to the concept of convergence we have also the concept of a **Cauchy sequence** and hence the concept of completeness: A normed space is called **complete** if every Cauchy sequence has a limit. A complete normed space is called a **Banach space**.

Example. The space $\ell^1(\mathbb{N})$ of all sequences $a = (a_j)_{j=1}^{\infty}$ for which the norm

$$\|a\|_1 = \sum_{j=1}^{\infty} |a_j| \quad (0.16)$$

is finite, is a Banach space.

To show this, we need to verify three things: (i) $\ell^1(\mathbb{N})$ is a Vector space, that is closed under addition and scalar multiplication (ii) $\|\cdot\|_1$ satisfies the three requirements for a norm and (iii) $\ell^1(\mathbb{N})$ is complete.

First of all observe

$$\sum_{j=1}^k |a_j + b_j| \leq \sum_{j=1}^k |a_j| + \sum_{j=1}^k |b_j| \leq \|a\|_1 + \|b\|_1 \quad (0.17)$$

for any finite k . Letting $k \rightarrow \infty$ we conclude that $\ell^1(\mathbb{N})$ is closed under addition and that the triangle inequality holds. That $\ell^1(\mathbb{N})$ is closed under scalar multiplication and the two other properties of a norm are straightforward. It remains to show that $\ell^1(\mathbb{N})$ is complete. Let $a^n = (a_j^n)_{j=1}^{\infty}$ be a Cauchy sequence, that is, for given $\varepsilon > 0$ we can find an N_ε such that $\|a^m - a^n\|_1 \leq \varepsilon$ for $m, n \geq N_\varepsilon$. This implies in particular $|a_j^m - a_j^n| \leq \varepsilon$ for any fixed j . Thus a_j^n is a Cauchy sequence for fixed j and by completeness of \mathbb{C} has a limit: $\lim_{n \rightarrow \infty} a_j^n = a_j$. Now consider

$$\sum_{j=1}^k |a_j^m - a_j^n| \leq \varepsilon \quad (0.18)$$

and take $m \rightarrow \infty$:

$$\sum_{j=1}^k |a_j - a_j^n| \leq \varepsilon. \quad (0.19)$$

Since this holds for any finite k we even have $\|a - a_n\|_1 \leq \varepsilon$. Hence $(a - a_n) \in \ell^1(\mathbb{N})$ and since $a_n \in \ell^1(\mathbb{N})$ we finally conclude $a = a_n + (a - a_n) \in \ell^1(\mathbb{N})$. \diamond

Example. The space $\ell^\infty(\mathbb{N})$ of all bounded sequences $a = (a_j)_{j=1}^\infty$ together with the norm

$$\|a\|_\infty = \sup_{j \in \mathbb{N}} |a_j| \quad (0.20)$$

is a Banach space (Problem 0.3). \diamond

Now what about convergence in this space? A sequence of functions $f_n(x)$ converges to f if and only if

$$\lim_{n \rightarrow \infty} \|f - f_n\| = \lim_{n \rightarrow \infty} \sup_{x \in I} |f_n(x) - f(x)| = 0. \quad (0.21)$$

That is, in the language of real analysis, f_n converges uniformly to f . Now let us look at the case where f_n is only a Cauchy sequence. Then $f_n(x)$ is clearly a Cauchy sequence of real numbers for any fixed $x \in I$. In particular, by completeness of \mathbb{C} , there is a limit $f(x)$ for each x . Thus we get a limiting function $f(x)$. Moreover, letting $m \rightarrow \infty$ in

$$|f_m(x) - f_n(x)| \leq \varepsilon \quad \forall m, n > N_\varepsilon, x \in I \quad (0.22)$$

we see

$$|f(x) - f_n(x)| \leq \varepsilon \quad \forall n > N_\varepsilon, x \in I, \quad (0.23)$$

that is, $f_n(x)$ converges uniformly to $f(x)$. However, up to this point we don't know whether it is in our vector space $C(I)$ or not, that is, whether it is continuous or not. Fortunately, there is a well-known result from real analysis which tells us that the uniform limit of continuous functions is again continuous. Hence $f(x) \in C(I)$ and thus every Cauchy sequence in $C(I)$ converges. Or, in other words

Theorem 0.12. $C(I)$ with the maximum norm is a Banach space.

Next we want to know if there is a basis for $C(I)$. In order to have only countable sums, we would even prefer a countable basis. If such a basis exists, that is, if there is a set $\{u_n\} \subset X$ of linearly independent vectors such that every element $f \in X$ can be written as

$$f = \sum_n c_n u_n, \quad c_n \in \mathbb{C}, \quad (0.24)$$

then the **span** $\text{span}\{u_n\}$ (the set of all finite linear combinations) of $\{u_n\}$ is dense in X . A set whose span is dense is called **total** and if we have a total set, we also have a countable dense set (consider only linear combinations

with rational coefficients – show this). A normed linear space containing a countable dense set is called **separable**.

Example. The Banach space $\ell^1(\mathbb{N})$ is separable. In fact, the set of vectors δ^n , with $\delta_n^n = 1$ and $\delta_m^n = 0$, $n \neq m$ is total: Let $a \in \ell^1(\mathbb{N})$ be given and set $a^n = \sum_{k=1}^n a_k \delta^k$, then

$$\|a - a^n\|_1 = \sum_{j=n+1}^{\infty} |a_j| \rightarrow 0 \quad (0.25)$$

since $a_j^n = a_j$ for $1 \leq j \leq n$ and $a_j^n = 0$ for $j > n$. \diamond

Luckily this is also the case for $C(I)$:

Theorem 0.13 (Weierstraß). *Let I be a compact interval. Then the set of polynomials is dense in $C(I)$.*

Proof. Let $f(x) \in C(I)$ be given. By considering $f(x) - f(a) + (f(b) - f(a))(x - b)$ it is no loss to assume that f vanishes at the boundary points. Moreover, without restriction we only consider $I = [-\frac{1}{2}, \frac{1}{2}]$ (why?).

Now the claim follows from the lemma below using

$$u_n(x) = \frac{1}{I_n} (1 - x^2)^n, \quad (0.26)$$

where

$$\begin{aligned} I_n &= \int_{-1}^1 (1 - x^2)^n dx = \frac{n!}{\frac{1}{2}(\frac{1}{2} + 1) \cdots (\frac{1}{2} + n)} \\ &= \sqrt{\pi} \frac{\Gamma(1 + n)}{\Gamma(\frac{3}{2} + n)} = \sqrt{\frac{\pi}{n}} (1 + O(\frac{1}{n})). \end{aligned} \quad (0.27)$$

(Remark: The integral is known as Beta function and the asymptotics follow from Stirling's formula.) \square

Lemma 0.14 (Smoothing). *Let $u_n(x)$ be a sequence of nonnegative continuous functions on $[-1, 1]$ such that*

$$\int_{|x| \leq 1} u_n(x) dx = 1 \quad \text{and} \quad \int_{\delta \leq |x| \leq 1} u_n(x) dx \rightarrow 0, \quad \delta > 0. \quad (0.28)$$

(In other words, u_n has mass one and concentrates near $x = 0$ as $n \rightarrow \infty$.)

Then for every $f \in C[-\frac{1}{2}, \frac{1}{2}]$ which vanishes at the endpoints, $f(-\frac{1}{2}) = f(\frac{1}{2}) = 0$, we have that

$$f_n(x) = \int_{-1/2}^{1/2} u_n(x - y) f(y) dy \quad (0.29)$$

converges uniformly to $f(x)$.

Proof. Since f is uniformly continuous, for given ε we can find a δ (independent of x) such that $|f(x) - f(y)| \leq \varepsilon$ whenever $|x - y| \leq \delta$. Moreover, we can choose n such that $\int_{\delta \leq |y| \leq 1} u_n(y) dy \leq \varepsilon$. Now abbreviate $M = \max f$ and note

$$|f(x) - \int_{-1/2}^{1/2} u_n(x-y) f(x) dy| = |f(x)| |1 - \int_{-1/2}^{1/2} u_n(x-y) dy| \leq M\varepsilon. \quad (0.30)$$

In fact, either the distance of x to one of the boundary points $\pm \frac{1}{2}$ is smaller than δ and hence $|f(x)| \leq \varepsilon$ or otherwise the difference between one and the integral is smaller than ε .

Using this we have

$$\begin{aligned} |f_n(x) - f(x)| &\leq \int_{-1/2}^{1/2} u_n(x-y) |f(y) - f(x)| dy + M\varepsilon \\ &\leq \int_{|y| \leq 1/2, |x-y| \leq \delta} u_n(x-y) |f(y) - f(x)| dy \\ &\quad + \int_{|y| \leq 1/2, |x-y| \geq \delta} u_n(x-y) |f(y) - f(x)| dy + M\varepsilon \\ &= \varepsilon + 2M\varepsilon + M\varepsilon = (1 + 3M)\varepsilon, \end{aligned} \quad (0.31)$$

which proves the claim. \square

Note that f_n will be as smooth as u_n , hence the title smoothing lemma. The same idea is used to approximate noncontinuous functions by smooth ones (of course the convergence will no longer be uniform in this case).

Corollary 0.15. $C(I)$ is separable.

The same is true for $\ell^1(\mathbb{N})$, but not for $\ell^\infty(\mathbb{N})$ (Problem 0.4)!

Problem 0.1. Show that $\| \|f\| - \|g\| \| \leq \|f - g\|$.

Problem 0.2. Show that the norm, vector addition, and multiplication by scalars are continuous. That is, if $f_n \rightarrow f$, $g_n \rightarrow g$, and $\lambda_n \rightarrow \lambda$ then $\|f_n\| \rightarrow \|f\|$, $f_n + g_n \rightarrow f + g$, and $\lambda_n g_n \rightarrow \lambda g$.

Problem 0.3. Show that $\ell^\infty(\mathbb{N})$ is a Banach space.

Problem 0.4. Show that $\ell^\infty(\mathbb{N})$ is not separable (Hint: Consider sequences which take only the value one and zero. How many are there? What is the distance between two such sequences?).

0.3. The geometry of Hilbert spaces

So it looks like $C(I)$ has all the properties we want. However, there is still one thing missing: How should we define orthogonality in $C(I)$? In

Euclidean space, two vectors are called **orthogonal** if their scalar product vanishes, so we would need a scalar product:

Suppose \mathfrak{H} is a vector space. A map $\langle \cdot, \cdot \rangle : \mathfrak{H} \times \mathfrak{H} \rightarrow \mathbb{C}$ is called skew linear form if it is conjugate linear in the first and linear in the second argument, that is,

$$\begin{aligned}\langle \alpha_1 f_1 + \alpha_2 f_2, g \rangle &= \alpha_1^* \langle f_1, g \rangle + \alpha_2^* \langle f_2, g \rangle \\ \langle f, \alpha_1 g_1 + \alpha_2 g_2 \rangle &= \alpha_1 \langle f, g_1 \rangle + \alpha_2 \langle f, g_2 \rangle\end{aligned}, \quad \alpha_1, \alpha_2 \in \mathbb{C}, \quad (0.32)$$

where ‘*’ denotes complex conjugation. A skew linear form satisfying the requirements

- (i) $\langle f, f \rangle > 0$ for $f \neq 0$ (positive definite)
- (ii) $\langle f, g \rangle = \langle g, f \rangle^*$ (symmetry)

is called **inner product** or **scalar product**. Associated with every scalar product is a norm

$$\|f\| = \sqrt{\langle f, f \rangle}. \quad (0.33)$$

The pair $(\mathfrak{H}, \langle \cdot, \cdot \rangle)$ is called **inner product space**. If \mathfrak{H} is complete it is called a **Hilbert space**.

Example. Clearly \mathbb{C}^n with the usual scalar product

$$\langle a, b \rangle = \sum_{j=1}^n a_j^* b_j \quad (0.34)$$

is a (finite dimensional) Hilbert space. \diamond

Example. A somewhat more interesting example is the Hilbert space $\ell^2(\mathbb{N})$, that is, the set of all sequences

$$\left\{ (a_j)_{j=1}^{\infty} \mid \sum_{j=1}^{\infty} |a_j|^2 < \infty \right\} \quad (0.35)$$

with scalar product

$$\langle a, b \rangle = \sum_{j=1}^{\infty} a_j^* b_j. \quad (0.36)$$

(Show that this is in fact a separable Hilbert space! Problem 0.5) \diamond

Of course I still owe you a proof for the claim that $\sqrt{\langle f, f \rangle}$ is indeed a norm. Only the triangle inequality is nontrivial which will follow from the Cauchy-Schwarz inequality below.

A vector $f \in \mathfrak{H}$ is called **normalized** or **unit vector** if $\|f\| = 1$. Two vectors $f, g \in \mathfrak{H}$ are called **orthogonal** or **perpendicular** ($f \perp g$) if $\langle f, g \rangle = 0$ and **parallel** if one is a multiple of the other.

For two orthogonal vectors we have the **Pythagorean theorem**:

$$\|f + g\|^2 = \|f\|^2 + \|g\|^2, \quad f \perp g, \quad (0.37)$$

which is one line of computation.

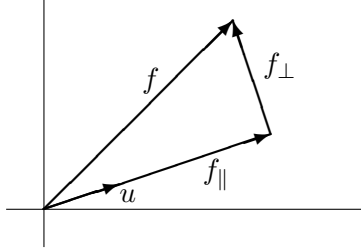
Suppose u is a unit vector, then the projection of f in the direction of u is given by

$$f_{\parallel} = \langle u, f \rangle u \quad (0.38)$$

and f_{\perp} defined via

$$f_{\perp} = f - \langle u, f \rangle u \quad (0.39)$$

is perpendicular to u since $\langle u, f_{\perp} \rangle = \langle u, f - \langle u, f \rangle u \rangle = \langle u, f \rangle - \langle u, f \rangle \langle u, u \rangle = 0$.



Taking any other vector parallel to u it is easy to see

$$\|f - \alpha u\|^2 = \|f_{\perp} + (f_{\parallel} - \alpha u)\|^2 = \|f_{\perp}\|^2 + |\langle u, f \rangle - \alpha|^2 \quad (0.40)$$

and hence $f_{\parallel} = \langle u, f \rangle u$ is the unique vector parallel to u which is closest to f .

As a first consequence we obtain the **Cauchy-Schwarz-Bunjakowski** inequality:

Theorem 0.16 (Cauchy-Schwarz-Bunjakowski). *Let \mathfrak{H}_0 be an inner product space, then for every $f, g \in \mathfrak{H}_0$ we have*

$$|\langle f, g \rangle| \leq \|f\| \|g\| \quad (0.41)$$

with equality if and only if f and g are parallel.

Proof. It suffices to prove the case $\|g\| = 1$. But then the claim follows from $\|f\|^2 = |\langle g, f \rangle|^2 + \|f_{\perp}\|^2$. \square

Note that the Cauchy-Schwarz inequality entails that the scalar product is continuous in both variables, that is, if $f_n \rightarrow f$ and $g_n \rightarrow g$ we have $\langle f_n, g_n \rangle \rightarrow \langle f, g \rangle$.

As another consequence we infer that the map $\|\cdot\|$ is indeed a norm.

$$\|f + g\|^2 = \|f\|^2 + \langle f, g \rangle + \langle g, f \rangle + \|g\|^2 \leq (\|f\| + \|g\|)^2. \quad (0.42)$$

But let us return to $C(I)$. Can we find a scalar product which has the maximum norm as associated norm? Unfortunately the answer is no! The

reason is that the maximum norm does not satisfy the parallelogram law (Problem 0.7).

Theorem 0.17 (Jordan-von Neumann). *A norm is associated with a scalar product if and only if the **parallelogram law***

$$\|f + g\|^2 + \|f - g\|^2 = 2\|f\|^2 + 2\|g\|^2 \quad (0.43)$$

holds.

In this case the scalar product can be recovered from its norm by virtue of the **polarization identity**

$$\langle f, g \rangle = \frac{1}{4} (\|f + g\|^2 - \|f - g\|^2 + i\|f - ig\|^2 - i\|f + ig\|^2). \quad (0.44)$$

Proof. If an inner product space is given, verification of the parallelogram law and the polarization identity is straight forward (Problem 0.6).

To show the converse, we define

$$s(f, g) = \frac{1}{4} (\|f + g\|^2 - \|f - g\|^2 + i\|f - ig\|^2 - i\|f + ig\|^2). \quad (0.45)$$

Then $s(f, f) = \|f\|^2$ and $s(f, g) = s(g, f)^*$ are straightforward to check. Moreover, another straightforward computation using the parallelogram law shows

$$s(f, g) + s(f, h) = 2s(f, \frac{g+h}{2}). \quad (0.46)$$

Now choosing $h = 0$ (and using $s(f, 0) = 0$) shows $s(f, g) = 2s(f, \frac{g}{2})$ and thus $s(f, g) + s(f, h) = s(f, g+h)$. Furthermore, by induction we infer $\frac{m}{2^n} s(f, g) = s(f, \frac{m}{2^n} g)$, that is $\lambda s(f, g) = s(f, \lambda g)$ for every positive rational λ . By continuity (check this!) this holds for all $\lambda > 0$ and $s(f, -g) = -s(f, g)$ respectively $s(f, ig) = i s(f, g)$ finishes the proof. \square

Note that the parallelogram law and the polarization identity even hold for skew linear forms (Problem 0.6).

But how do we define a scalar product on $C(I)$? One possibility is

$$\langle f, g \rangle = \int_a^b f^*(x)g(x)dx. \quad (0.47)$$

The corresponding inner product space is denoted by $\mathcal{L}_{cont}^2(I)$. Note that we have

$$\|f\| \leq \sqrt{|b-a|} \|f\|_\infty \quad (0.48)$$

and hence the maximum norm is stronger than the \mathcal{L}_{cont}^2 norm.

Suppose we have two norms $\|\cdot\|_1$ and $\|\cdot\|_2$ on a space X . Then $\|\cdot\|_2$ is said to be **stronger** than $\|\cdot\|_1$ if there is a constant $m > 0$ such that

$$\|f\|_1 \leq m\|f\|_2. \quad (0.49)$$

It is straightforward to check that

Lemma 0.18. *If $\|\cdot\|_2$ is stronger than $\|\cdot\|_1$, then any $\|\cdot\|_2$ Cauchy sequence is also a $\|\cdot\|_1$ Cauchy sequence.*

Hence if a function $F : X \rightarrow Y$ is continuous in $(X, \|\cdot\|_1)$ it is also continuous in $(X, \|\cdot\|_2)$ and if a set is dense in $(X, \|\cdot\|_2)$ it is also dense in $(X, \|\cdot\|_1)$.

In particular, \mathcal{L}_{cont}^2 is separable. But is it also complete? Unfortunately the answer is no:

Example. Take $I = [0, 2]$ and define

$$f_n(x) = \begin{cases} 0, & 0 \leq x \leq 1 - \frac{1}{n} \\ 1 + n(x - 1), & 1 - \frac{1}{n} \leq x \leq 1 \\ 1, & 1 \leq x \leq 2 \end{cases} \quad (0.50)$$

then $f_n(x)$ is a Cauchy sequence in \mathcal{L}_{cont}^2 , but there is no limit in \mathcal{L}_{cont}^2 ! Clearly the limit should be the step function which is 0 for $0 \leq x < 1$ and 1 for $1 \leq x \leq 2$, but this step function is discontinuous (Problem 0.8)! \diamond

This shows that in infinite dimensional spaces different norms will give rise to different convergent sequences! In fact, the key to solving problems in infinite dimensional spaces is often finding the right norm! This is something which cannot happen in the finite dimensional case.

Theorem 0.19. *If X is a finite dimensional case, then all norms are equivalent. That is, for given two norms $\|\cdot\|_1$ and $\|\cdot\|_2$ there are constants m_1 and m_2 such that*

$$\frac{1}{m_2} \|f\|_1 \leq \|f\|_2 \leq m_1 \|f\|_1. \quad (0.51)$$

Proof. Clearly we can choose a basis u_j , $1 \leq j \leq n$, and assume that $\|\cdot\|_2$ is the usual Euclidean norm, $\|\sum_j \alpha_j u_j\|_2^2 = \sum_j |\alpha_j|^2$. Let $f = \sum_j \alpha_j u_j$, then by the triangle and Cauchy Schwartz inequalities

$$\|f\|_1 \leq \sum_j |\alpha_j| \|u_j\|_1 \leq \sqrt{\sum_j \|u_j\|_1^2} \|f\|_2 \quad (0.52)$$

and we can choose $m_2 = \sqrt{\sum_j \|u_j\|_1^2}$.

In particular, if f_n is convergent with respect to $\|\cdot\|_2$ it is also convergent with respect to $\|\cdot\|_1$. Thus $\|\cdot\|_1$ is continuous with respect to $\|\cdot\|_2$ and attains its minimum $m > 0$ on the unit sphere (which is compact by the Heine-Borel theorem). Now choose $m_1 = 1/m$. \square

Problem 0.5. *Show that $\ell^2(\mathbb{N})$ is a separable Hilbert space.*

Problem 0.6. Let $s(f, g)$ be a skew linear form and $p(f) = s(f, f)$ the associated quadratic form. Prove the parallelogram law

$$p(f + g) + p(f - g) = 2p(f) + 2p(g) \quad (0.53)$$

and the polarization identity

$$s(f, g) = \frac{1}{4} (p(f + g) - p(f - g) + ip(f - ig) - ip(f + ig)). \quad (0.54)$$

Problem 0.7. Show that the maximum norm (on $C[0, 1]$) does not satisfy the parallelogram law.

Problem 0.8. Prove the claims made about f_n , defined in (0.50), in the last example.

0.4. Completeness

Since \mathcal{L}_{cont}^2 is not complete, how can we obtain a Hilbert space out of it? Well the answer is simple: take the **completion**.

If X is a (incomplete) normed space, consider the set of all Cauchy sequences \tilde{X} . Call two Cauchy sequences equivalent if their difference converges to zero and denote by \bar{X} the set of all equivalence classes. It is easy to see that \bar{X} (and \tilde{X}) inherit the vector space structure from X . Moreover,

Lemma 0.20. If x_n is a Cauchy sequence, then $\|x_n\|$ converges.

Consequently the norm of a Cauchy sequence $(x_n)_{n=1}^\infty$ can be defined by $\|(x_n)_{n=1}^\infty\| = \lim_{n \rightarrow \infty} \|x_n\|$ and is independent of the equivalence class (show this!). Thus \bar{X} is a normed space (\tilde{X} is not! why?).

Theorem 0.21. \bar{X} is a Banach space containing X as a dense subspace if we identify $x \in X$ with the equivalence class of all sequences converging to x .

Proof. (Outline) It remains to show that \bar{X} is complete. Let $\xi_n = [(x_{n,j})_{j=1}^\infty]$ be a Cauchy sequence in \bar{X} . Then it is not hard to see that $\xi = [(x_{j,j})_{j=1}^\infty]$ is its limit. \square

Let me remark that the completion \bar{X} is unique. More precisely any other complete space which contains X as a dense subset is isomorphic to \bar{X} . This can for example be seen by showing that the identity map on X has a unique extension to \bar{X} (compare Theorem 0.24 below).

In particular it is no restriction to assume that a normed linear space or an inner product space is complete. However, in the important case of \mathcal{L}_{cont}^2 it is somewhat inconvenient to work with equivalence classes of Cauchy sequences and hence we will give a different characterization using the Lebesgue integral later.

0.5. Bounded operators

A linear map A between two normed spaces X and Y will be called a **(linear) operator**

$$A : \mathfrak{D}(A) \subseteq X \rightarrow Y. \quad (0.55)$$

The linear subspace $\mathfrak{D}(A)$ on which A is defined, is called the **domain** of A and is usually required to be dense. The **kernel**

$$\text{Ker}(A) = \{f \in \mathfrak{D}(A) \mid Af = 0\} \quad (0.56)$$

and **range**

$$\text{Ran}(A) = \{Af \mid f \in \mathfrak{D}(A)\} = A\mathfrak{D}(A) \quad (0.57)$$

are defined as usual. The operator A is called **bounded** if the following operator norm

$$\|A\| = \sup_{\|f\|_X=1} \|Af\|_Y \quad (0.58)$$

is finite.

The set of all bounded linear operators from X to Y is denoted by $\mathfrak{L}(X, Y)$. If $X = Y$ we write $\mathfrak{L}(X, X) = \mathfrak{L}(X)$.

Theorem 0.22. *The space $\mathfrak{L}(X, Y)$ together with the operator norm (0.58) is a normed space. It is a Banach space if Y is.*

Proof. That (0.58) is indeed a norm is straightforward. If Y is complete and A_n is a Cauchy sequence of operators, then $A_n f$ converges to an element g for every f . Define a new operator A via $Af = g$. By continuity of the vector operations, A is linear and by continuity of the norm $\|Af\| = \lim_{n \rightarrow \infty} \|A_n f\| \leq (\lim_{n \rightarrow \infty} \|A_n\|)\|f\|$ it is bounded. Furthermore, given $\varepsilon > 0$ there is some N such that $\|A_n - A_m\| \leq \varepsilon$ for $n, m \geq N$ and thus $\|A_n f - A_m f\| \leq \varepsilon \|f\|$. Taking the limit $m \rightarrow \infty$ we see $\|A_n f - Af\| \leq \varepsilon \|f\|$, that is $A_n \rightarrow A$. \square

By construction, a bounded operator is Lipschitz continuous

$$\|Af\|_Y \leq \|A\| \|f\|_X \quad (0.59)$$

and hence continuous. The converse is also true

Theorem 0.23. *An operator A is bounded if and only if it is continuous.*

Proof. Suppose A is continuous but not bounded. Then there is a sequence of unit vectors u_n such that $\|Au_n\| \geq n$. Then $f_n = \frac{1}{n}u_n$ converges to 0 but $\|Af_n\| \geq 1$ does not converge to 0. \square

Moreover, if A is bounded and densely defined, it is no restriction to assume that it is defined on all of X .

Theorem 0.24. *Let $A \in \mathfrak{L}(X, Y)$ and let Y be a Banach space. If $\mathfrak{D}(A)$ is dense, there is a unique (continuous) extension of A to X , which has the same norm.*

Proof. Since a bounded operator maps Cauchy sequences to Cauchy sequences, this extension can only be given by

$$Af = \lim_{n \rightarrow \infty} Af_n, \quad f_n \in \mathfrak{D}(A), \quad f \in X. \quad (0.60)$$

To show that this definition is independent of the sequence $f_n \rightarrow f$, let $g_n \rightarrow f$ be a second sequence and observe

$$\|Af_n - Ag_n\| = \|A(f_n - g_n)\| \leq \|A\| \|f_n - g_n\| \rightarrow 0. \quad (0.61)$$

From continuity of vector addition and scalar multiplication it follows that our extension is linear. Finally, from continuity of the norm we conclude that the norm does not increase. \square

An operator in $\mathfrak{L}(X, \mathbb{C})$ is called a **bounded linear functional** and the space $X^* = \mathfrak{L}(X, \mathbb{C})$ is called the dual space of X . A sequence f_n is said to **converge weakly** $f_n \rightarrow f$ if $\ell(f_n) \rightarrow \ell(f)$ for every $\ell \in X^*$.

The Banach space of bounded linear operators $\mathfrak{L}(X)$ even has a multiplication given by composition. Clearly this multiplication satisfies

$$(A + B)C = AC + BC, \quad A(B + C) = AB + AC, \quad A, B, C \in \mathfrak{L}(X) \quad (0.62)$$

and

$$(AB)C = A(BC), \quad \alpha(AB) = (\alpha A)B = A(\alpha B), \quad \alpha \in \mathbb{C}. \quad (0.63)$$

Moreover, it is easy to see that we have

$$\|AB\| \leq \|A\| \|B\|. \quad (0.64)$$

However, note that our multiplication is not commutative (unless X is one dimensional). We even have an **identity**, the identity operator \mathbb{I} satisfying $\|\mathbb{I}\| = 1$.

A Banach space together with a multiplication satisfying the above requirements is called a **Banach algebra**. In particular, note that (0.64) ensures that multiplication is continuous.

Problem 0.9. *Show that the integral operator*

$$(Kf)(x) = \int_0^1 K(x, y)f(y)dy, \quad (0.65)$$

where $K(x, y) \in C([0, 1] \times [0, 1])$, defined on $\mathfrak{D}(K) = C[0, 1]$ is a bounded operator both in $X = C[0, 1]$ (max norm) and $X = \mathcal{L}_{cont}^2(0, 1)$.

Problem 0.10. *Show that the differential operator $A = \frac{d}{dx}$ defined on $\mathfrak{D}(A) = C^1[0, 1] \subset C[0, 1]$ is an unbounded operator.*

Problem 0.11. Show that $\|AB\| \leq \|A\|\|B\|$ for every $A, B \in \mathfrak{L}(X)$.

Problem 0.12. Show that the multiplication in a Banach algebra X is continuous: $x_n \rightarrow x$ and $y_n \rightarrow y$ implies $x_n y_n \rightarrow xy$.

0.6. Lebesgue L^p spaces

We fix some measure space (X, Σ, μ) and define the L^p norm by

$$\|f\|_p = \left(\int_X |f|^p d\mu \right)^{1/p}, \quad 1 \leq p \quad (0.66)$$

and denote by $\mathcal{L}^p(X, d\mu)$ the set of all complex valued measurable functions for which $\|f\|_p$ is finite. First of all note that $\mathcal{L}^p(X, d\mu)$ is a linear space, since $|f + g|^p \leq 2^p \max(|f|, |g|)^p \leq 2^p \max(|f|^p, |g|^p) \leq 2^p(|f|^p + |g|^p)$. Of course our hope is that $\mathcal{L}^p(X, d\mu)$ is a Banach space. However, there is a small technical problem (recall that a property is said to hold almost everywhere if the set where it fails to hold is contained in a set of measure zero):

Lemma 0.25. Let f be measurable, then

$$\int_X |f|^p d\mu = 0 \quad (0.67)$$

if and only if $f(x) = 0$ almost everywhere with respect to μ .

Proof. Observe that we have $A = \{x | f(x) \neq 0\} = \bigcap_n A_n$, where $A_n = \{x | |f(x)| > \frac{1}{n}\}$. If $\int |f|^p d\mu = 0$ we must have $\mu(A_n) = 0$ for every n and hence $\mu(A) = \lim_{n \rightarrow \infty} \mu(A_n) = 0$. The converse is obvious. \square

Note that the proof also shows that if f is not 0 almost everywhere, there is an $\varepsilon > 0$ such that $\mu(\{x | |f(x)| \geq \varepsilon\}) > 0$.

Example. Let λ be the Lebesgue measure on \mathbb{R} . Then the characteristic function of the rationals $\chi_{\mathbb{Q}}$ is zero a.e. (with respect to λ). Let Θ be the Dirac measure centered at 0, then $f(x) = 0$ a.e. (with respect to Θ) if and only if $f(0) = 0$. \diamond

Thus $\|f\|_p = 0$ only implies $f(x) = 0$ for almost every x , but not for all! Hence $\|\cdot\|_p$ is not a norm on $\mathcal{L}^p(X, d\mu)$. The way out of this misery is to identify functions which are equal almost everywhere: Let

$$\mathcal{N}(X, d\mu) = \{f | f(x) = 0 \text{ } \mu\text{-almost everywhere}\}. \quad (0.68)$$

Then $\mathcal{N}(X, d\mu)$ is a linear subspace of $\mathcal{L}^p(X, d\mu)$ and we can consider the quotient space

$$L^p(X, d\mu) = \mathcal{L}^p(X, d\mu) / \mathcal{N}(X, d\mu). \quad (0.69)$$

If $d\mu$ is the Lebesgue measure on $X \subseteq \mathbb{R}^n$ we simply write $L^p(X)$. Observe that $\|f\|_p$ is well defined on $L^p(X, d\mu)$.

Even though the elements of $L^p(X, d\mu)$ are strictly speaking equivalence classes of functions, we will still call them functions for notational convenience. However, note that for $f \in L^p(X, d\mu)$ the value $f(x)$ is not well defined (unless there is a continuous representative and different continuous functions are in different equivalence classes, e.g., in the case of Lebesgue measure).

With this modification we are back in business since $L^p(X, d\mu)$ turns out to be a Banach space. We will show this in the following sections.

But before that let us also define $L^\infty(X, d\mu)$. It should be the set of bounded measurable functions $B(X)$ together with the sup norm. The only problem is that if we want to identify functions equal almost everywhere, the supremum is no longer independent of the equivalence class. The solution is the **essential supremum**

$$\|f\|_\infty = \inf\{C \mid \mu(\{x \mid |f(x)| > C\}) = 0\}. \quad (0.70)$$

That is, C is an essential bound if $|f(x)| \leq C$ almost everywhere and the essential supremum is the infimum over all essential bounds.

Example. If λ is the Lebesgue measure, then the essential sup of $\chi_{\mathbb{Q}}$ with respect to λ is 0. If Θ is the Dirac measure centered at 0, then the essential sup of $\chi_{\mathbb{Q}}$ with respect to Θ is 1 (since $\chi_{\mathbb{Q}}(0) = 1$, and $x = 0$ is the only point which counts for Θ). \diamond

As before we set

$$L^\infty(X, d\mu) = B(X)/\mathcal{N}(X, d\mu) \quad (0.71)$$

and observe that $\|f\|_\infty$ is independent of the equivalence class.

If you wonder where the ∞ comes from, have a look at Problem 0.13.

As a preparation for proving that L^p is a Banach space, we will need Hölder's inequality, which plays a central role in the theory of L^p spaces. In particular, it will imply Minkowski's inequality, which is just the triangle inequality for L^p .

Theorem 0.26 (Hölder's inequality). *Let p and q be dual indices, that is,*

$$\frac{1}{p} + \frac{1}{q} = 1 \quad (0.72)$$

with $1 \leq p \leq \infty$. If $f \in L^p(X, d\mu)$ and $g \in L^q(X, d\mu)$ then $fg \in L^1(X, d\mu)$ and

$$\|fg\|_1 \leq \|f\|_p \|g\|_q. \quad (0.73)$$

Proof. The case $p = 1, q = \infty$ (respectively $p = \infty, q = 1$) follows directly from the properties of the integral and hence it remains to consider $1 < p, q < \infty$.

First of all it is no restriction to assume $\|f\|_p = \|g\|_q = 1$. Then, using the elementary inequality (Problem 0.14)

$$a^{1/p}b^{1/q} \leq \frac{1}{p}a + \frac{1}{q}b, \quad a, b \geq 0, \quad (0.74)$$

with $a = |f|^p$ and $b = |g|^q$ and integrating over X gives

$$\int_X |f g| d\mu \leq \frac{1}{p} \int_X |f|^p d\mu + \frac{1}{q} \int_X |g|^q d\mu = 1 \quad (0.75)$$

and finishes the proof. \square

As a consequence we also get

Theorem 0.27 (Minkowski's inequality). *Let $f, g \in L^p(X, d\mu)$, then*

$$\|f + g\|_p \leq \|f\|_p + \|g\|_p. \quad (0.76)$$

Proof. Since the cases $p = 1, \infty$ are straightforward, we only consider $1 < p < \infty$. Using $|f + g|^p \leq |f| |f + g|^{p-1} + |g| |f + g|^{p-1}$ we obtain from Hölder's inequality (note $(p-1)q = p$)

$$\begin{aligned} \|f + g\|_p^p &\leq \|f\|_p \|(f + g)^{p-1}\|_q + \|g\|_p \|(f + g)^{p-1}\|_q \\ &= (\|f\|_p + \|g\|_p) \|(f + g)\|_p^{p-1}. \end{aligned} \quad (0.77)$$

\square

This shows that $L^p(X, d\mu)$ is a normed linear space. Finally it remains to show that $L^p(X, d\mu)$ is complete.

Theorem 0.28. *The space $L^p(X, d\mu)$ is a Banach space.*

Proof. Suppose f_n is a Cauchy sequence. It suffices to show that some subsequence converges (show this). Hence we can drop some terms such that

$$\|f_{n+1} - f_n\|_p \leq \frac{1}{2^n}. \quad (0.78)$$

Now consider $g_n = f_n - f_{n-1}$ (set $f_0 = 0$). Then

$$G(x) = \sum_{k=1}^{\infty} |g_k(x)| \quad (0.79)$$

is in L^p . This follows from

$$\left\| \sum_{k=1}^n |g_k| \right\|_p \leq \sum_{k=1}^n \|g_k(x)\|_p \leq \|f_1\|_p + \frac{1}{2} \quad (0.80)$$

using the monotone convergence theorem. In particular, $G(x) < \infty$ almost everywhere and the sum

$$\sum_{n=1}^{\infty} g_n(x) = \lim_{n \rightarrow \infty} f_n(x) \quad (0.81)$$

is absolutely convergent for those x . Now let $f(x)$ be this limit. Since $|f(x) - f_n(x)|^p$ converges to zero almost everywhere and $|f(x) - f_n(x)|^p \leq 2^p G(x)^p \in L^1$, dominated convergence shows $\|f - f_n\|_p \rightarrow 0$. \square

In particular, in the proof of the last theorem we have seen:

Corollary 0.29. *If $\|f_n - f\|_p \rightarrow 0$ then there is a subsequence which converges pointwise almost everywhere.*

It even turns out that L^p is separable.

Lemma 0.30. *Suppose X is a second countable topological space (i.e., it has a countable basis) and μ is a regular Borel measure. Then $L^p(X, d\mu)$, $1 \leq p < \infty$ is separable.*

Proof. The set of all characteristic functions $\chi_A(x)$ with $A \in \Sigma$ and $\mu(A) < \infty$, is total by construction of the integral. Now our strategy is as follows: Using outer regularity we can restrict A to open sets and using the existence of a countable base, we can restrict A to open sets from this base.

Fix A . By outer regularity, there is a decreasing sequence of open sets O_n such that $\mu(O_n) \rightarrow \mu(A)$. Since $\mu(A) < \infty$ it is no restriction to assume $\mu(O_n) < \infty$, and thus $\mu(O_n \setminus A) = \mu(O_n) - \mu(A) \rightarrow 0$. Now dominated convergence implies $\|\chi_A - \chi_{O_n}\|_p \rightarrow 0$. Thus the set of all characteristic functions $\chi_O(x)$ with O open and $\mu(O) < \infty$, is total. Finally let \mathcal{B} be a countable basis for the topology. Then, every open set O can be written as $O = \bigcup_{j=1}^{\infty} \tilde{O}_j$ with $\tilde{O}_j \in \mathcal{B}$. Moreover, by considering the set of all finite unions of elements from \mathcal{B} it is no restriction to assume $\bigcup_{j=1}^n \tilde{O}_j \in \mathcal{B}$. Hence there is an increasing sequence $\tilde{O}_n \nearrow O$ with $\tilde{O}_n \in \mathcal{B}$. By monotone convergence, $\|\chi_O - \chi_{\tilde{O}_n}\|_p \rightarrow 0$ and hence the set of all characteristic functions $\chi_{\tilde{O}}$ with $\tilde{O} \in \mathcal{B}$ is total. \square

To finish this chapter, let us show that continuous functions are dense in L^p .

Theorem 0.31. *Let X be a locally compact metric space and let μ be a σ -finite regular Borel measure. Then the set $C_c(X)$ of continuous functions with compact support is dense in $L^p(X, d\mu)$, $1 \leq p < \infty$.*

Proof. As in the previous proof the set of all characteristic functions $\chi_K(x)$ with K compact is total (using inner regularity). Hence it suffices to show

that $\chi_K(x)$ can be approximated by continuous functions. By outer regularity there is an open set $O \supset K$ such that $\mu(O \setminus K) \leq \varepsilon$. By Urysohn's lemma (Lemma 0.11) there is a continuous function f_ε which is one on K and 0 outside O . Since

$$\int_X |\chi_K - f_\varepsilon|^p d\mu = \int_{O \setminus K} |f_\varepsilon|^p d\mu \leq \mu(O \setminus K) \leq \varepsilon \quad (0.82)$$

we have $\|f_\varepsilon - \chi_K\| \rightarrow 0$ and we are done. \square

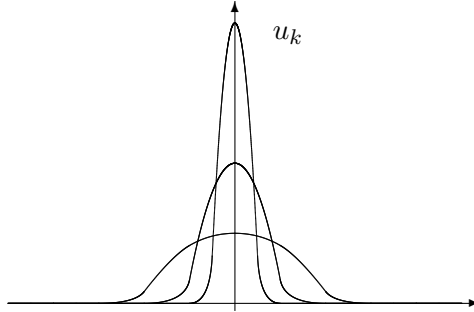
If X is some subset of \mathbb{R}^n we can do even better.

A nonnegative function $u \in C_c^\infty(\mathbb{R}^n)$ is called a **mollifier** if

$$\int_{\mathbb{R}^n} u(x) dx = 1 \quad (0.83)$$

The standard mollifier is $u(x) = \exp(\frac{1}{|x|^2-1})$ for $|x| < 1$ and $u(x) = 0$ else.

If we scale a mollifier according to $u_k(x) = k^n u(kx)$ such that its mass is preserved ($\|u_k\|_1 = 1$) and it concentrates more and more around the origin



we have the following result (Problem 0.17):

Lemma 0.32. *Let u be a mollifier in \mathbb{R}^n and set $u_k(x) = k^n u(kx)$. Then for any (uniformly) continuous function $f : \mathbb{R}^n \rightarrow \mathbb{C}$ we have that*

$$f_k(x) = \int_{\mathbb{R}^n} u_k(x-y) f(y) dy \quad (0.84)$$

is in $C^\infty(\mathbb{R}^n)$ and converges to f (uniformly).

Now we are ready to prove

Theorem 0.33. *If $X \subseteq \mathbb{R}^n$ and μ is a Borel measure, then the set $C_c^\infty(X)$ of all smooth functions with compact support is dense in $L^p(X, d\mu)$, $1 \leq p < \infty$.*

Proof. By our previous result it suffices to show that any continuous function $f(x)$ with compact support can be approximated by smooth ones. By setting $f(x) = 0$ for $x \notin X$, it is no restriction to assume $X = \mathbb{R}^n$. Now choose a mollifier u and observe that f_k has compact support (since f

has). Moreover, since f has compact support it is uniformly continuous and $f_k \rightarrow f$ uniformly. But this implies $f_k \rightarrow f$ in L^p . \square

Problem 0.13. Suppose $\mu(X) < \infty$. Show that

$$\lim_{p \rightarrow \infty} \|f\|_p = \|f\|_\infty \quad (0.85)$$

for any bounded measurable function.

Problem 0.14. Prove (0.74). (Hint: Show that $f(x) = (1-t) + tx - x^t$, $x > 0$, $0 < t < 1$ satisfies $f(a/b) \geq 0 = f(1)$.)

Problem 0.15. Show the following generalization of Hölder's inequality

$$\|fg\|_r \leq \|f\|_p \|g\|_q, \quad (0.86)$$

where $\frac{1}{p} + \frac{1}{q} = \frac{1}{r}$.

Problem 0.16 (Lyapunov inequality). Let $0 < \theta < 1$. Show that if $f \in L^{p_1} \cap L^{p_2}$, then $f \in L^p$ and

$$\|f\|_p \leq \|f\|_{p_1}^\theta \|f\|_{p_2}^{1-\theta}, \quad (0.87)$$

where $\frac{1}{p} = \frac{\theta}{p_1} + \frac{1-\theta}{p_2}$.

Problem 0.17. Prove Lemma 0.32. (Hint: To show that f_k is smooth use Problem A.7 and A.8.)

Problem 0.18. Construct a function $f \in L^p(0,1)$ which has a pole at every rational number in $[0,1]$. (Hint: Start with the function $f_0(x) = |x|^{-\alpha}$ which has a single pole at 0, then $f_j(x) = f_0(x - x_j)$ has a pole at x_j .)

0.7. Appendix: The uniform boundedness principle

Recall that the interior of a set is the largest open subset (that is, the union of all open subsets). A set is called **nowhere dense** if its closure has empty interior. The key to several important theorems about Banach spaces is the observation that a Banach space cannot be the countable union of nowhere dense sets.

Theorem 0.34 (Baire category theorem). Let X be a complete metric space, then X cannot be the countable union of nowhere dense sets.

Proof. Suppose $X = \bigcup_{n=1}^{\infty} X_n$. We can assume that the sets X_n are closed and none of them contains a ball, that is, $X \setminus X_n$ is open and nonempty for every n . We will construct a Cauchy sequence x_n which stays away from all X_n .

Since $X \setminus X_1$ is open and nonempty there is a closed ball $B_{r_1}(x_1) \subseteq X \setminus X_1$. Reducing r_1 a little, we can even assume $\overline{B_{r_1}(x_1)} \subseteq X \setminus X_1$. Moreover, since X_2 cannot contain $B_{r_1}(x_1)$ there is some $x_2 \in B_{r_1}(x_1)$ that is not in X_2 . Since $B_{r_1}(x_1) \cap (X \setminus X_2)$ is open there is a closed ball $\overline{B_{r_2}(x_2)} \subseteq B_{r_1}(x_1) \cap (X \setminus X_2)$. Proceeding by induction we obtain a sequence of balls such that

$$\overline{B_{r_n}(x_n)} \subseteq B_{r_{n-1}}(x_{n-1}) \cap (X \setminus X_n). \quad (0.88)$$

Now observe that in every step we can choose r_n as small as we please, hence without loss of generality $r_n \rightarrow 0$. Since by construction $x_n \in \overline{B_{r_n}(x_n)}$ for $n \geq N$, we conclude that x_n is Cauchy and converges to some point $x \in X$. But $x \in \overline{B_{r_n}(x_n)} \subseteq X \setminus X_n$ for every n , contradicting our assumption that the X_n cover X . \square

(Sets which can be written as countable union of nowhere dense sets are called of first category. All other sets are second category. Hence the name category theorem.)

In other words, if $X_n \subseteq X$ is a sequence of closed subsets which cover X , at least one X_n contains a ball of radius $\varepsilon > 0$.

Now we come to the first important consequence, the **uniform boundedness principle**.

Theorem 0.35 (Banach-Steinhaus). *Let X be a Banach space and Y some normed linear space. Let $\{A_\alpha\} \subseteq \mathfrak{L}(X, Y)$ be a family of bounded operators. Suppose $\|A_\alpha x\| \leq C(x)$ is bounded for fixed $x \in X$, then $\|A_\alpha\| \leq C$ is uniformly bounded.*

Proof. Let

$$X_n = \{x \mid \|A_\alpha x\| \leq n \text{ for all } \alpha\} = \bigcap_{\alpha} \{x \mid \|A_\alpha x\| \leq n\}, \quad (0.89)$$

then $\bigcup_n X_n = X$ by assumption. Moreover, by continuity of A_α and the norm, each X_n is an intersection of closed sets and hence closed. By Baire's theorem at least one contains a ball of positive radius: $B_\varepsilon(x_0) \subset X_n$. Now observe

$$\|A_\alpha y\| \leq \|A_\alpha(y + x_0)\| + \|A_\alpha x_0\| \leq n + \|A_\alpha x_0\| \quad (0.90)$$

for $\|y\| < \varepsilon$. Setting $y = \varepsilon \frac{x}{\|x\|}$ we obtain

$$\|A_\alpha x\| \leq \frac{n + C(x_0)}{\varepsilon} \|x\| \quad (0.91)$$

for any x . \square

Part 1

**Mathematical
Foundations of
Quantum Mechanics**

Hilbert spaces

The phase space in classical mechanics is the Euclidean space \mathbb{R}^{2n} (for the n position and n momentum coordinates). In quantum mechanics the phase space is always a Hilbert space \mathfrak{H} . Hence the geometry of Hilbert spaces stands at the outset of our investigations.

1.1. Hilbert spaces

Suppose \mathfrak{H} is a vector space. A map $\langle \cdot, \cdot \rangle : \mathfrak{H} \times \mathfrak{H} \rightarrow \mathbb{C}$ is called skew linear form if it is conjugate linear in the first and linear in the second argument. A positive definite skew linear form is called **inner product** or **scalar product**. Associated with every scalar product is a norm

$$\|\psi\| = \sqrt{\langle \psi, \psi \rangle}. \quad (1.1)$$

The triangle inequality follows from the **Cauchy-Schwarz-Bunjakowski** inequality:

$$|\langle \psi, \varphi \rangle| \leq \|\psi\| \|\varphi\| \quad (1.2)$$

with equality if and only if ψ and φ are parallel.

If \mathfrak{H} is complete with respect to the above norm, it is called a **Hilbert space**. It is no restriction to assume that \mathfrak{H} is complete since one can easily replace it by its completion.

Example. The space $L^2(M, d\mu)$ is a Hilbert space with scalar product given by

$$\langle f, g \rangle = \int_M f(x)^* g(x) d\mu(x). \quad (1.3)$$

Similarly, the set of all square summable sequences $\ell^2(\mathbb{N})$ is a Hilbert space with scalar product

$$\langle f, g \rangle = \sum_{j \in \mathbb{N}} f_j^* g_j. \quad (1.4)$$

(Note that the second example is a special case of the first one; take $M = \mathbb{R}$ and μ a sum of Dirac measures.) \diamond

A vector $\psi \in \mathfrak{H}$ is called **normalized** or **unit vector** if $\|\psi\| = 1$. Two vectors $\psi, \varphi \in \mathfrak{H}$ are called **orthogonal** or **perpendicular** ($\psi \perp \varphi$) if $\langle \psi, \varphi \rangle = 0$ and **parallel** if one is a multiple of the other. If ψ and φ are orthogonal we have the **Pythagorean theorem**:

$$\|\psi + \varphi\|^2 = \|\psi\|^2 + \|\varphi\|^2, \quad \psi \perp \varphi, \quad (1.5)$$

which is straightforward to check.

Suppose φ is a unit vector, then the projection of ψ in the direction of φ is given by

$$\psi_{\parallel} = \langle \varphi, \psi \rangle \varphi \quad (1.6)$$

and ψ_{\perp} defined via

$$\psi_{\perp} = \psi - \langle \varphi, \psi \rangle \varphi \quad (1.7)$$

is perpendicular to φ .

These results can also be generalized to more than one vector. A set of vectors $\{\varphi_j\}$ is called **orthonormal set** if $\langle \varphi_j, \varphi_k \rangle = 0$ for $j \neq k$ and $\langle \varphi_j, \varphi_j \rangle = 1$.

Lemma 1.1. *Suppose $\{\varphi_j\}_{j=0}^n$ is an orthonormal set. Then every $\psi \in \mathfrak{H}$ can be written as*

$$\psi = \psi_{\parallel} + \psi_{\perp}, \quad \psi_{\parallel} = \sum_{j=0}^n \langle \varphi_j, \psi \rangle \varphi_j, \quad (1.8)$$

where ψ_{\parallel} and ψ_{\perp} are orthogonal. Moreover, $\langle \varphi_j, \psi_{\perp} \rangle = 0$ for all $1 \leq j \leq n$. In particular,

$$\|\psi\|^2 = \sum_{j=0}^n |\langle \varphi_j, \psi \rangle|^2 + \|\psi_{\perp}\|^2. \quad (1.9)$$

Moreover, every $\hat{\psi}$ in the span of $\{\varphi_j\}_{j=0}^n$ satisfies

$$\|\psi - \hat{\psi}\| \geq \|\psi_{\perp}\| \quad (1.10)$$

with equality holding if and only if $\hat{\psi} = \psi_{\parallel}$. In other words, ψ_{\parallel} is uniquely characterized as the vector in the span of $\{\varphi_j\}_{j=0}^n$ being closest to ψ .

Proof. A straightforward calculation shows $\langle \varphi_j, \psi - \psi_{\parallel} \rangle = 0$ and hence ψ_{\parallel} and $\psi_{\perp} = \psi - \psi_{\parallel}$ are orthogonal. The formula for the norm follows by applying (1.5) iteratively.

Now, fix a vector

$$\hat{\psi} = \sum_{j=0}^n c_j \varphi_j. \quad (1.11)$$

in the span of $\{\varphi_j\}_{j=0}^n$. Then one computes

$$\begin{aligned} \|\psi - \hat{\psi}\|^2 &= \|\psi_{\parallel} + \psi_{\perp} - \hat{\psi}\|^2 = \|\psi_{\perp}\|^2 + \|\psi_{\parallel} - \hat{\psi}\|^2 \\ &= \|\psi_{\perp}\|^2 + \sum_{j=0}^n |c_j - \langle \varphi_j, \psi \rangle|^2 \end{aligned} \quad (1.12)$$

from which the last claim follows. \square

From (1.9) we obtain **Bessel's inequality**

$$\sum_{j=0}^n |\langle \varphi_j, \psi \rangle|^2 \leq \|\psi\|^2 \quad (1.13)$$

with equality holding if and only if ψ lies in the span of $\{\varphi_j\}_{j=0}^n$.

Recall that a scalar product can be recovered from its norm by virtue of the **polarization identity**

$$\langle \varphi, \psi \rangle = \frac{1}{4} (\|\varphi + \psi\|^2 - \|\varphi - \psi\|^2 + i\|\varphi - i\psi\|^2 - i\|\varphi + i\psi\|^2). \quad (1.14)$$

A bijective operator $U \in \mathcal{L}(\mathfrak{H}_1, \mathfrak{H}_2)$ is called **unitary** if U preserves scalar products:

$$\langle U\varphi, U\psi \rangle_2 = \langle \varphi, \psi \rangle_1, \quad \varphi, \psi \in \mathfrak{H}_1. \quad (1.15)$$

By the polarization identity this is the case if and only if U preserves norms: $\|U\psi\|_2 = \|\psi\|_1$ for all $\psi \in \mathfrak{H}_1$. The two Hilbert space \mathfrak{H}_1 and \mathfrak{H}_2 are called **unitarily equivalent** in this case.

Problem 1.1. *The operator $S : \ell^2(\mathbb{N}) \rightarrow \ell^2(\mathbb{N})$, $(a_1, a_2, a_3, \dots) \mapsto (0, a_1, a_2, \dots)$ clearly satisfies $\|Sa\| = \|a\|$. Is it unitary?*

1.2. Orthonormal bases

Of course, since we cannot assume \mathfrak{H} to be a finite dimensional vector space, we need to generalize Lemma 1.1 to arbitrary orthonormal sets $\{\varphi_j\}_{j \in J}$. We start by assuming that J is countable. Then Bessel's inequality (1.13) shows that

$$\sum_{j \in J} |\langle \varphi_j, \psi \rangle|^2 \quad (1.16)$$

converges absolutely. Moreover, for any finite subset $K \subset J$ we have

$$\left\| \sum_{j \in K} \langle \varphi_j, \psi \rangle \varphi_j \right\|^2 = \sum_{j \in K} |\langle \varphi_j, \psi \rangle|^2 \quad (1.17)$$

by the Pythagorean theorem and thus $\sum_{j \in J} \langle \varphi_j, \psi \rangle \varphi_j$ is Cauchy if and only if $\sum_{j \in J} |\langle \varphi_j, \psi \rangle|^2$ is. Now let J be arbitrary. Again, Bessel's inequality shows that for any given $\varepsilon > 0$ there are at most finitely many j for which $|\langle \varphi_j, \psi \rangle| \geq \varepsilon$. Hence there are at most countably many j for which $|\langle \varphi_j, \psi \rangle| > 0$. Thus it follows that

$$\sum_{j \in J} |\langle \varphi_j, \psi \rangle|^2 \quad (1.18)$$

is well-defined and so is

$$\sum_{j \in J} \langle \varphi_j, \psi \rangle \varphi_j. \quad (1.19)$$

In particular, by continuity of the scalar product we see that Lemma 1.1 holds for arbitrary orthonormal sets without modifications.

Theorem 1.2. *Suppose $\{\varphi_j\}_{j \in J}$ is an orthonormal set. Then every $\psi \in \mathfrak{H}$ can be written as*

$$\psi = \psi_{\parallel} + \psi_{\perp}, \quad \psi_{\parallel} = \sum_{j \in J} \langle \varphi_j, \psi \rangle \varphi_j, \quad (1.20)$$

where ψ_{\parallel} and ψ_{\perp} are orthogonal. Moreover, $\langle \varphi_j, \psi_{\perp} \rangle = 0$ for all $j \in J$. In particular,

$$\|\psi\|^2 = \sum_{j \in J} |\langle \varphi_j, \psi \rangle|^2 + \|\psi_{\perp}\|^2. \quad (1.21)$$

Moreover, every $\hat{\psi}$ in the span of $\{\varphi_j\}_{j \in J}$ satisfies

$$\|\psi - \hat{\psi}\| \geq \|\psi_{\perp}\| \quad (1.22)$$

with equality holding if and only if $\hat{\psi} = \psi_{\parallel}$. In other words, ψ_{\parallel} is uniquely characterized as the vector in the span of $\{\varphi_j\}_{j \in J}$ being closest to ψ .

Note that from Bessel's inequality (which of course still holds) it follows that the map $\psi \rightarrow \psi_{\parallel}$ is continuous.

An orthonormal set which is not a proper subset of any other orthonormal set is called an **orthonormal basis** due to following result:

Theorem 1.3. *For an orthonormal set $\{\varphi_j\}_{j \in J}$ the following conditions are equivalent:*

- (i) $\{\varphi_j\}_{j \in J}$ is a maximal orthonormal set.
- (ii) For every vector $\psi \in \mathfrak{H}$ we have

$$\psi = \sum_{j \in J} \langle \varphi_j, \psi \rangle \varphi_j. \quad (1.23)$$

(iii) For every vector $\psi \in \mathfrak{H}$ we have

$$\|\psi\|^2 = \sum_{j \in J} |\langle \varphi_j, \psi \rangle|^2. \quad (1.24)$$

(iv) $\langle \varphi_j, \psi \rangle = 0$ for all $j \in J$ implies $\psi = 0$.

Proof. We will use the notation from Theorem 1.2.

(i) \Rightarrow (ii): If $\psi_{\perp} \neq 0$ then we can normalize ψ_{\perp} to obtain a unit vector $\tilde{\psi}_{\perp}$ which is orthogonal to all vectors φ_j . But then $\{\varphi_j\}_{j \in J} \cup \{\tilde{\psi}_{\perp}\}$ would be a larger orthonormal set, contradicting maximality of $\{\varphi_j\}_{j \in J}$.

(ii) \Rightarrow (iii): Follows since (ii) implies $\psi_{\perp} = 0$.

(iii) \Rightarrow (iv): If $\langle \psi, \varphi_j \rangle = 0$ for all $j \in J$ we conclude $\|\psi\|^2 = 0$ and hence $\psi = 0$.

(iv) \Rightarrow (i): If $\{\varphi_j\}_{j \in J}$ were not maximal, there would be a unit vector φ such that $\{\varphi_j\}_{j \in J} \cup \{\varphi\}$ is larger orthonormal set. But $\langle \varphi_j, \varphi \rangle = 0$ for all $j \in J$ implies $\varphi = 0$ by (iv), a contradiction. \square

Since $\psi \rightarrow \psi_{\parallel}$ is continuous, it suffices to check conditions (ii) and (iii) on a dense set.

Example. The set of functions

$$\varphi_n(x) = \frac{1}{\sqrt{2\pi}} e^{inx}, \quad n \in \mathbb{Z}, \quad (1.25)$$

forms an orthonormal basis for $\mathfrak{H} = L^2(0, 2\pi)$. The corresponding orthogonal expansion is just the ordinary Fourier series. (Problem 1.17) \diamond

A Hilbert space is **separable** if and only if there is a countable orthonormal basis. In fact, if \mathfrak{H} is separable, then there exists a countable total set $\{\psi_j\}_{j=0}^{\infty}$. After throwing away some vectors we can assume that ψ_{n+1} cannot be expressed as a linear combinations of the vectors ψ_0, \dots, ψ_n . Now we can construct an orthonormal basis as follows: We begin by normalizing ψ_0

$$\varphi_0 = \frac{\psi_0}{\|\psi_0\|}. \quad (1.26)$$

Next we take ψ_1 and remove the component parallel to φ_0 and normalize again

$$\varphi_1 = \frac{\psi_1 - \langle \varphi_0, \psi_1 \rangle \varphi_0}{\|\psi_1 - \langle \varphi_0, \psi_1 \rangle \varphi_0\|}. \quad (1.27)$$

Proceeding like this we define recursively

$$\varphi_n = \frac{\psi_n - \sum_{j=0}^{n-1} \langle \varphi_j, \psi_n \rangle \varphi_j}{\|\psi_n - \sum_{j=0}^{n-1} \langle \varphi_j, \psi_n \rangle \varphi_j\|}. \quad (1.28)$$

This procedure is known as **Gram-Schmidt orthogonalization**. Hence we obtain an orthonormal set $\{\varphi_j\}_{j=0}^{\infty}$ such that $\text{span}\{\varphi_j\}_{j=0}^n = \text{span}\{\psi_j\}_{j=0}^n$

for any finite n and thus also for N . Since $\{\psi_j\}_{j=0}^N$ is total, we infer that $\{\varphi_j\}_{j=0}^N$ is an orthonormal basis.

Example. In $L^2(-1, 1)$ we can orthogonalize the polynomial $f_n(x) = x^n$. The resulting polynomials are up to a normalization equal to the Legendre polynomials

$$P_0(x) = 1, \quad P_1(x) = x, \quad P_2(x) = \frac{3x^2 - 1}{2}, \quad \dots \quad (1.29)$$

(which are normalized such that $P_n(1) = 1$). \diamond

If fact, if there is one countable basis, then it follows that any other basis is countable as well.

Theorem 1.4. *If \mathfrak{H} is separable, then every orthonormal basis is countable.*

Proof. We know that there is at least one countable orthonormal basis $\{\varphi_j\}_{j \in J}$. Now let $\{\phi_k\}_{k \in K}$ be a second basis and consider the set $K_j = \{k \in K \mid \langle \phi_k, \varphi_j \rangle \neq 0\}$. Since these are the expansion coefficients of φ_j with respect to $\{\phi_k\}_{k \in K}$, this set is countable. Hence the set $\tilde{K} = \bigcup_{j \in J} K_j$ is countable as well. But $k \in K \setminus \tilde{K}$ implies $\phi_k = 0$ and hence $\tilde{K} = K$. \square

We will assume all Hilbert spaces to be separable.

In particular, it can be shown that $L^2(M, d\mu)$ is separable. Moreover, it turns out that, up to unitary equivalence, there is only one (separable) infinite dimensional Hilbert space:

Let \mathfrak{H} be an infinite dimensional Hilbert space and let $\{\varphi_j\}_{j \in \mathbb{N}}$ be any orthogonal basis. Then the map $U : \mathfrak{H} \rightarrow \ell^2(\mathbb{N})$, $\psi \mapsto (\langle \varphi_j, \psi \rangle)_{j \in \mathbb{N}}$ is unitary (by Theorem 1.3 (iii)). In particular,

Theorem 1.5. *Any separable infinite dimensional Hilbert space is unitarily equivalent to $\ell^2(\mathbb{N})$.*

Let me remark that if \mathfrak{H} is not separable, there still exists an orthonormal basis. However, the proof requires Zorn's lemma: The collection of all orthonormal sets in \mathfrak{H} can be partially ordered by inclusion. Moreover, any linearly ordered chain has an upper bound (the union of all sets in the chain). Hence Zorn's lemma implies the existence of a maximal element, that is, an orthonormal basis.

1.3. The projection theorem and the Riesz lemma

Let $M \subseteq \mathfrak{H}$ be a subset, then $M^\perp = \{\psi \mid \langle \varphi, \psi \rangle = 0, \forall \varphi \in M\}$ is called the **orthogonal complement** of M . By continuity of the scalar product it follows that M^\perp is a closed linear subspace and by linearity that

$(\overline{\text{span}(M)})^\perp = M^\perp$. For example we have $\mathfrak{H}^\perp = \{0\}$ since any vector in \mathfrak{H}^\perp must be in particular orthogonal to all vectors in some orthonormal basis.

Theorem 1.6 (projection theorem). *Let M be a closed linear subspace of a Hilbert space \mathfrak{H} , then every $\psi \in \mathfrak{H}$ can be uniquely written as $\psi = \psi_\parallel + \psi_\perp$ with $\psi_\parallel \in M$ and $\psi_\perp \in M^\perp$. One writes*

$$M \oplus M^\perp = \mathfrak{H} \quad (1.30)$$

in this situation.

Proof. Since M is closed, it is a Hilbert space and has an orthonormal basis $\{\varphi_j\}_{j \in J}$. Hence the result follows from Theorem 1.2. \square

In other words, to every $\psi \in \mathfrak{H}$ we can assign a unique vector ψ_\parallel which is the vector in M closest to ψ . The rest $\psi - \psi_\parallel$ lies in M^\perp . The operator $P_M\psi = \psi_\parallel$ is called the **orthogonal projection** corresponding to M . Note that we have

$$P_M^2 = P_M \quad \text{and} \quad \langle P_M\psi, \varphi \rangle = \langle \psi, P_M\varphi \rangle \quad (1.31)$$

since $\langle P_M\psi, \varphi \rangle = \langle \psi_\parallel, \varphi_\parallel \rangle = \langle \psi, P_M\varphi \rangle$. Clearly we have $P_{M^\perp}\psi = \psi - P_M\psi = \psi_\perp$.

Moreover, we see that the vectors in a closed subspace M are precisely those which are orthogonal to all vectors in M^\perp , that is, $M^{\perp\perp} = M$. If M is an arbitrary subset we have at least

$$M^{\perp\perp} = \overline{\text{span}(M)}. \quad (1.32)$$

Note that by $\mathfrak{H}^\perp = \{0\}$ we see that $M^\perp = \{0\}$ if and only if M is dense.

Finally we turn to **linear functionals**, that is, to operators $\ell : \mathfrak{H} \rightarrow \mathbb{C}$. By the Cauchy-Schwarz inequality we know that $\ell_\varphi : \psi \mapsto \langle \varphi, \psi \rangle$ is a bounded linear functional (with norm $\|\varphi\|$). It turns out that in a Hilbert space every bounded linear functional can be written in this way.

Theorem 1.7 (Riesz lemma). *Suppose ℓ is a bounded linear functional on a Hilbert space \mathfrak{H} . Then there is a vector $\varphi \in \mathfrak{H}$ such that $\ell(\psi) = \langle \varphi, \psi \rangle$ for all $\psi \in \mathfrak{H}$. In other words, a Hilbert space is equivalent to its own dual space $\mathfrak{H}^* = \mathfrak{H}$.*

Proof. If $\ell \equiv 0$ we can choose $\varphi = 0$. Otherwise $\text{Ker}(\ell) = \{\psi \mid \ell(\psi) = 0\}$ is a proper subspace and we can find a unit vector $\tilde{\varphi} \in \text{Ker}(\ell)^\perp$. For every $\psi \in \mathfrak{H}$ we have $\ell(\psi)\tilde{\varphi} - \ell(\tilde{\varphi})\psi \in \text{Ker}(\ell)$ and hence

$$0 = \langle \tilde{\varphi}, \ell(\psi)\tilde{\varphi} - \ell(\tilde{\varphi})\psi \rangle = \ell(\psi) - \ell(\tilde{\varphi})\langle \tilde{\varphi}, \psi \rangle. \quad (1.33)$$

In other words, we can choose $\varphi = \ell(\tilde{\varphi})^*\tilde{\varphi}$. \square

The following easy consequence is left as an exercise.

Corollary 1.8. *Suppose B is a bounded skew linear form, that is,*

$$|B(\psi, \varphi)| \leq C\|\psi\| \|\varphi\|. \quad (1.34)$$

Then there is a unique bounded operator A such that

$$B(\psi, \varphi) = \langle A\psi, \varphi \rangle. \quad (1.35)$$

Problem 1.2. *Show that an orthogonal projection $P_M \neq 0$ has norm one.*

Problem 1.3. *Suppose P_1 and P_2 are orthogonal projections. Show that $P_1 \leq P_2$ (that is $\langle \psi, P_1\psi \rangle \leq \langle \psi, P_2\psi \rangle$) is equivalent to $\text{Ran}(P_1) \subseteq \text{Ran}(P_2)$.*

Problem 1.4. *Prove Corollary 1.8.*

Problem 1.5. *Let $\{\varphi_j\}$ be some orthonormal basis. Show that a bounded linear operator A is uniquely determined by its matrix elements $A_{jk} = \langle \varphi_j, A\varphi_k \rangle$ with respect to this basis.*

Problem 1.6. *Show that $\mathfrak{L}(\mathfrak{H})$ is not separable \mathfrak{H} is infinite dimensional.*

Problem 1.7. *Show $P : L^2(\mathbb{R}) \rightarrow L^2(\mathbb{R})$, $f(x) \mapsto \frac{1}{2}(f(x) + f(-x))$ is a projection. Compute its range and kernel.*

1.4. Orthogonal sums and tensor products

Given two Hilbert spaces \mathfrak{H}_1 and \mathfrak{H}_2 we define their **orthogonal sum** $\mathfrak{H}_1 \oplus \mathfrak{H}_2$ to be the set of all pairs $(\psi_1, \psi_2) \in \mathfrak{H}_1 \times \mathfrak{H}_2$ together with the scalar product

$$\langle (\varphi_1, \varphi_2), (\psi_1, \psi_2) \rangle = \langle \varphi_1, \psi_1 \rangle_1 + \langle \varphi_2, \psi_2 \rangle_2. \quad (1.36)$$

It is left as an exercise to verify that $\mathfrak{H}_1 \oplus \mathfrak{H}_2$ is again a Hilbert space. Moreover, \mathfrak{H}_1 can be identified with $\{(\psi_1, 0) | \psi_1 \in \mathfrak{H}_1\}$ and we can regard \mathfrak{H}_1 as a subspace of $\mathfrak{H}_1 \oplus \mathfrak{H}_2$. Similarly for \mathfrak{H}_2 . It is also custom to write $\psi_1 + \psi_2$ instead of (ψ_1, ψ_2) .

More generally, let \mathfrak{H}_j $j \in \mathbb{N}$, be a countable collection of Hilbert spaces and define

$$\bigoplus_{j=1}^{\infty} \mathfrak{H}_j = \left\{ \sum_{j=1}^{\infty} \psi_j \mid \psi_j \in \mathfrak{H}_j, \sum_{j=1}^{\infty} \|\psi_j\|_j^2 < \infty \right\}, \quad (1.37)$$

which becomes a Hilbert space with the scalar product

$$\left\langle \sum_{j=1}^{\infty} \varphi_j, \sum_{j=1}^{\infty} \psi_j \right\rangle = \sum_{j=1}^{\infty} \langle \varphi_j, \psi_j \rangle_j. \quad (1.38)$$

Suppose \mathfrak{H} and $\tilde{\mathfrak{H}}$ are two Hilbert spaces. Our goal is to construct their tensor product. The elements should be products $\psi \otimes \tilde{\psi}$ of elements $\psi \in \mathfrak{H}$

and $\tilde{\psi} \in \tilde{\mathfrak{H}}$. Hence we start with the set of all finite linear combinations of elements of $\mathfrak{H} \times \tilde{\mathfrak{H}}$

$$\mathcal{F}(\mathfrak{H}, \tilde{\mathfrak{H}}) = \left\{ \sum_{j=1}^n \alpha_j (\psi_j, \tilde{\psi}_j) \mid (\psi_j, \tilde{\psi}_j) \in \mathfrak{H} \times \tilde{\mathfrak{H}}, \alpha_j \in \mathbb{C} \right\}. \quad (1.39)$$

Since we want $(\psi_1 + \psi_2) \otimes \tilde{\psi} = \psi_1 \otimes \tilde{\psi} + \psi_2 \otimes \tilde{\psi}$, $\psi \otimes (\tilde{\psi}_1 + \tilde{\psi}_2) = \psi \otimes \tilde{\psi}_1 + \psi \otimes \tilde{\psi}_2$, and $(\alpha\psi) \otimes \tilde{\psi} = \psi \otimes (\alpha\tilde{\psi})$ we consider $\mathcal{F}(\mathfrak{H}, \tilde{\mathfrak{H}})/\mathcal{N}(\mathfrak{H}, \tilde{\mathfrak{H}})$, where

$$\mathcal{N}(\mathfrak{H}, \tilde{\mathfrak{H}}) = \text{span} \left\{ \sum_{j,k=1}^n \alpha_j \beta_k (\psi_j, \tilde{\psi}_k) - \left(\sum_{j=1}^n \alpha_j \psi_j, \sum_{k=1}^n \beta_k \tilde{\psi}_k \right) \right\} \quad (1.40)$$

and write $\psi \otimes \tilde{\psi}$ for the equivalence class of $(\psi, \tilde{\psi})$.

Next we define

$$\langle \psi \otimes \tilde{\psi}, \phi \otimes \tilde{\phi} \rangle = \langle \psi, \phi \rangle \langle \tilde{\psi}, \tilde{\phi} \rangle \quad (1.41)$$

which extends to a skew linear form on $\mathcal{F}(\mathfrak{H}, \tilde{\mathfrak{H}})/\mathcal{N}(\mathfrak{H}, \tilde{\mathfrak{H}})$. To show that we obtain a scalar product, we need to ensure positivity. Let $\psi = \sum_i \alpha_i \psi_i \otimes \tilde{\psi}_i \neq 0$ and pick orthonormal bases $\varphi_j, \tilde{\varphi}_k$ for $\text{span}\{\psi_i\}, \text{span}\{\tilde{\psi}_i\}$, respectively. Then

$$\psi = \sum_{j,k} \alpha_{jk} \varphi_j \otimes \tilde{\varphi}_k, \quad \alpha_{jk} = \sum_i \alpha_i \langle \varphi_j, \psi_i \rangle \langle \tilde{\varphi}_k, \tilde{\psi}_i \rangle \quad (1.42)$$

and we compute

$$\langle \psi, \psi \rangle = \sum_{j,k} |\alpha_{jk}|^2 > 0. \quad (1.43)$$

The completion of $\mathcal{F}(\mathfrak{H}, \tilde{\mathfrak{H}})/\mathcal{N}(\mathfrak{H}, \tilde{\mathfrak{H}})$ with respect to the induced norm is called the **tensor product** $\mathfrak{H} \otimes \tilde{\mathfrak{H}}$ of \mathfrak{H} and $\tilde{\mathfrak{H}}$.

Lemma 1.9. *If $\varphi_j, \tilde{\varphi}_k$ are orthonormal bases for $\mathfrak{H}, \tilde{\mathfrak{H}}$, respectively, then $\varphi_j \otimes \tilde{\varphi}_k$ is an orthonormal basis for $\mathfrak{H} \otimes \tilde{\mathfrak{H}}$.*

Proof. That $\varphi_j \otimes \tilde{\varphi}_k$ is an orthonormal set is immediate from (1.41). Moreover, since $\text{span}\{\varphi_j\}, \text{span}\{\tilde{\varphi}_k\}$ is dense in $\mathfrak{H}, \tilde{\mathfrak{H}}$, respectively, it is easy to see that $\varphi_j \otimes \tilde{\varphi}_k$ is dense in $\mathcal{F}(\mathfrak{H}, \tilde{\mathfrak{H}})/\mathcal{N}(\mathfrak{H}, \tilde{\mathfrak{H}})$. But the latter is dense in $\mathfrak{H} \otimes \tilde{\mathfrak{H}}$. \square

Example. We have $\mathfrak{H} \otimes \mathbb{C}^n = \mathfrak{H}^n$. \diamond

Example. Let $(M, d\mu)$ and $(\tilde{M}, d\tilde{\mu})$ be two measure spaces. Then we have $L^2(M, d\mu) \otimes L^2(\tilde{M}, d\tilde{\mu}) = L^2(M \times \tilde{M}, d\mu \times d\tilde{\mu})$.

Clearly we have $L^2(M, d\mu) \otimes L^2(\tilde{M}, d\tilde{\mu}) \subseteq L^2(M \times \tilde{M}, d\mu \times d\tilde{\mu})$. Now take an orthonormal basis $\varphi_j \otimes \tilde{\varphi}_k$ for $L^2(M, d\mu) \otimes L^2(\tilde{M}, d\tilde{\mu})$ as in our previous lemma. Then

$$\int_M \int_{\tilde{M}} (\varphi_j(x) \tilde{\varphi}_k(y))^* f(x, y) d\mu(x) d\tilde{\mu}(y) = 0 \quad (1.44)$$

implies

$$\int_M \varphi_j(x)^* f_k(x) d\mu(x) = 0, \quad f_k(x) = \int_{\tilde{M}} \tilde{\varphi}_k(y)^* f(x, y) d\tilde{\mu}(y) \quad (1.45)$$

and hence $f_k(x) = 0$ μ -a.e. x . But this implies $f(x, y) = 0$ for μ -a.e. x and $\tilde{\mu}$ -a.e. y and thus $f = 0$. Hence $\varphi_j \otimes \tilde{\varphi}_k$ is a basis for $L^2(M \times \tilde{M}, d\mu \times d\tilde{\mu})$ and equality follows. \diamond

It is straightforward to extend the tensor product to any finite number of Hilbert spaces. We even note

$$\left(\bigoplus_{j=1}^{\infty} \mathfrak{H}_j \right) \otimes \mathfrak{H} = \bigoplus_{j=1}^{\infty} (\mathfrak{H}_j \otimes \mathfrak{H}), \quad (1.46)$$

where equality has to be understood in the sense, that both spaces are unitarily equivalent by virtue of the identification

$$\left(\sum_{j=1}^{\infty} \psi_j \right) \otimes \psi = \sum_{j=1}^{\infty} \psi_j \otimes \psi. \quad (1.47)$$

Problem 1.8. We have $\psi \otimes \tilde{\psi} = \phi \otimes \tilde{\phi}$ if and only if there is some $\alpha \in \mathbb{C} \setminus \{0\}$ such that $\psi = \alpha\phi$ and $\tilde{\psi} = \alpha^{-1}\tilde{\phi}$.

Problem 1.9. Show (1.46)

1.5. The C^* algebra of bounded linear operators

We start by introducing a conjugation for operators on a Hilbert space \mathfrak{H} . Let $A \in \mathfrak{L}(\mathfrak{H})$, then the **adjoint operator** is defined via

$$\langle \varphi, A^* \psi \rangle = \langle A \varphi, \psi \rangle \quad (1.48)$$

(compare Corollary 1.8).

Example. If $\mathfrak{H} = \mathbb{C}^n$ and $A = (a_{jk})_{1 \leq j, k \leq n}$, then $A^* = (a_{kj}^*)_{1 \leq j, k \leq n}$. \diamond

Lemma 1.10. Let $A, B \in \mathfrak{L}(\mathfrak{H})$, then

- (i) $(A + B)^* = A^* + B^*$, $(\alpha A)^* = \alpha^* A^*$,
- (ii) $A^{**} = A$,
- (iii) $(AB)^* = B^* A^*$,
- (iv) $\|A\| = \|A^*\|$ and $\|A\|^2 = \|A^* A\| = \|A A^*\|$.

Proof. (i) and (ii) are obvious. (iii) follows from $\langle \varphi, (AB)\psi \rangle = \langle A^* \varphi, B\psi \rangle = \langle B^* A^* \varphi, \psi \rangle$. (iv) follows from

$$\|A^*\| = \sup_{\|\varphi\|=\|\psi\|=1} |\langle \psi, A^* \varphi \rangle| = \sup_{\|\varphi\|=\|\psi\|=1} |\langle A \psi, \varphi \rangle| = \|A\|. \quad (1.49)$$

and

$$\begin{aligned} \|A^*A\| &= \sup_{\|\varphi\|=\|\psi\|=1} |\langle \varphi, A^*A\psi \rangle| = \sup_{\|\varphi\|=\|\psi\|=1} |\langle A\varphi, A\psi \rangle| \\ &= \sup_{\|\varphi\|=1} \|A\varphi\|^2 = \|A\|^2, \end{aligned} \quad (1.50)$$

where we have used $\|\varphi\| = \sup_{\|\psi\|=1} |\langle \psi, \varphi \rangle|$. \square

As a consequence of $\|A^*\| = \|A\|$ observe that taking the adjoint is continuous.

In general, a Banach algebra \mathcal{A} together with an **involution**

$$(a+b)^* = a^* + b^*, \quad (\alpha a)^* = \alpha^* a^*, \quad a^{**} = a, \quad (ab)^* = b^* a^*, \quad (1.51)$$

satisfying

$$\|a\|^2 = \|a^*a\| \quad (1.52)$$

is called a C^* **algebra**. The element a^* is called the adjoint of a . Note that $\|a^*\| = \|a\|$ follows from (1.52) and $\|aa^*\| \leq \|a\|\|a^*\|$.

Any subalgebra which is also closed under involution, is called a $*$ -algebra. An **ideal** is a subspace $\mathcal{I} \subseteq \mathcal{A}$ such that $a \in \mathcal{I}$, $b \in \mathcal{A}$ implies $ab \in \mathcal{I}$ and $ba \in \mathcal{I}$. If it is closed under the adjoint map it is called a $*$ -ideal. Note that if there is an identity e we have $e^* = e$ and hence $(a^{-1})^* = (a^*)^{-1}$ (show this).

Example. The continuous function $C(I)$ together with complex conjugation form a commutative C^* algebra. \diamond

An element $a \in \mathcal{A}$ is called **normal** if $aa^* = a^*a$, **self-adjoint** if $a = a^*$, **unitary** if $aa^* = a^*a = \mathbb{I}$, (orthogonal) **projection** if $a = a^* = a^2$, and **positive** if $a = bb^*$ for some $b \in \mathcal{A}$. Clearly both self-adjoint and unitary elements are normal.

Problem 1.10. Let $A \in \mathfrak{L}(\mathfrak{H})$. Show that A is normal if and only if

$$\|A\psi\| = \|A^*\psi\|, \quad \forall \psi \in \mathfrak{H}. \quad (1.53)$$

(Hint: Problem 0.6)

Problem 1.11. Show that $U : \mathfrak{H} \rightarrow \mathfrak{H}$ is unitary if and only if $U^{-1} = U^*$.

Problem 1.12. Compute the adjoint of $S : \ell^2(\mathbb{N}) \rightarrow \ell^2(\mathbb{N})$, $(a_1, a_2, a_3, \dots) \mapsto (0, a_1, a_2, \dots)$.

1.6. Weak and strong convergence

Sometimes a weaker notion of convergence is useful: We say that ψ_n **converges weakly** to ψ and write

$$\text{w-lim}_{n \rightarrow \infty} \psi_n = \psi \quad \text{or} \quad \psi_n \rightharpoonup \psi. \quad (1.54)$$

if $\langle \varphi, \psi_n \rangle \rightarrow \langle \varphi, \psi \rangle$ for every $\varphi \in \mathfrak{H}$ (show that a weak limit is unique).

Example. Let φ_n be an (infinite) orthonormal set. Then $\langle \psi, \varphi_n \rangle \rightarrow 0$ for every ψ since these are just the expansion coefficients of ψ . (φ_n does not converge to 0, since $\|\varphi_n\| = 1$.) \diamond

Clearly $\psi_n \rightarrow \psi$ implies $\psi_n \rightharpoonup \psi$ and hence this notion of convergence is indeed weaker. Moreover, the weak limit is unique, since $\langle \varphi, \psi_n \rangle \rightarrow \langle \varphi, \psi \rangle$ and $\langle \varphi, \psi_n \rangle \rightarrow \langle \varphi, \tilde{\psi} \rangle$ implies $\langle \varphi, (\psi - \tilde{\psi}) \rangle = 0$. A sequence ψ_n is called **weak Cauchy sequence** if $\langle \varphi, \psi_n \rangle$ is Cauchy for every $\varphi \in \mathfrak{H}$.

Lemma 1.11. *Let \mathfrak{H} be a Hilbert space.*

- (i) $\psi_n \rightharpoonup \psi$ implies $\|\psi\| \leq \liminf \|\psi_n\|$.
- (ii) Every weak Cauchy sequence ψ_n is bounded: $\|\psi_n\| \leq C$.
- (iii) Every weak Cauchy sequence converges weakly.
- (iv) For a weakly convergent sequence $\psi_n \rightharpoonup \psi$ we have: $\psi_n \rightarrow \psi$ if and only if $\limsup \|\psi_n\| \leq \|\psi\|$.

Proof. (i) Observe

$$\|\psi\|^2 = \langle \psi, \psi \rangle = \liminf \langle \psi, \psi_n \rangle \leq \|\psi\| \liminf \|\psi_n\|. \quad (1.55)$$

(ii) For every φ we have that $|\langle \varphi, \psi_n \rangle| \leq C(\varphi)$ is bounded. Hence by the uniform boundedness principle we have $\|\psi_n\| = \|\langle \psi_n, \cdot \rangle\| \leq C$.

(iii) Let φ_m be an orthonormal basis and define $c_m = \lim_{n \rightarrow \infty} \langle \varphi_m, \psi_n \rangle$. Then $\psi = \sum_m c_m \varphi_m$ is the desired limit.

(iv) By (i) we have $\lim \|\psi_n\| = \|\psi\|$ and hence

$$\|\psi - \psi_n\|^2 = \|\psi\|^2 - 2\operatorname{Re}(\langle \psi, \psi_n \rangle) + \|\psi_n\|^2 \rightarrow 0. \quad (1.56)$$

The converse is straightforward. \square

Clearly an orthonormal basis does not have a norm convergent subsequence. Hence the unit ball in an infinite dimensional Hilbert space is never compact. However, we can at least extract weakly convergent subsequences:

Lemma 1.12. *Let \mathfrak{H} be a Hilbert space. Every bounded sequence ψ_n has weakly convergent subsequence.*

Proof. Let φ_k be an ONB, then by the usual diagonal sequence argument we can find a subsequence ψ_{n_m} such that $\langle \varphi_k, \psi_{n_m} \rangle$ converges for all k . Since ψ_n is bounded, $\langle \varphi, \psi_{n_m} \rangle$ converges for every $\varphi \in \mathfrak{H}$ and hence ψ_{n_m} is a weak Cauchy sequence. \square

Finally, let me remark that similar concepts can be introduced for operators. This is of particular importance for the case of unbounded operators, where convergence in the operator norm makes no sense at all.

A sequence of operators A_n is said to **converge strongly** to A ,

$$\text{s-lim}_{n \rightarrow \infty} A_n = A \quad :\Leftrightarrow \quad A_n \psi \rightarrow A \psi \quad \forall x \in \mathfrak{D}(A) \subseteq \mathfrak{D}(A_n). \quad (1.57)$$

It is said to **converge weakly** to A ,

$$\text{w-lim}_{n \rightarrow \infty} A_n = A \quad :\Leftrightarrow \quad A_n \psi \rightharpoonup A \psi \quad \forall \psi \in \mathfrak{D}(A) \subseteq \mathfrak{D}(A_n). \quad (1.58)$$

Clearly norm convergence implies strong convergence and strong convergence implies weak convergence.

Example. Consider the operator $S_n \in \mathfrak{L}(\ell^2(\mathbb{N}))$ which shifts a sequence n places to the left

$$S_n(x_1, x_2, \dots) = (x_{n+1}, x_{n+2}, \dots). \quad (1.59)$$

and the operator $S_n^* \in \mathfrak{L}(\ell^2(\mathbb{N}))$ which shifts a sequence n places to the right and fills up the first n places with zeros

$$S_n^*(x_1, x_2, \dots) = (\underbrace{0, \dots, 0}_{n \text{ places}}, x_1, x_2, \dots). \quad (1.60)$$

Then S_n converges to zero strongly but not in norm and S_n^* converges weakly to zero but not strongly. \diamond

Note that this example also shows that taking adjoints is not continuous with respect to strong convergence! If $A_n \xrightarrow{s} A$ we only have

$$\langle \varphi, A_n^* \psi \rangle = \langle A_n \varphi, \psi \rangle \rightarrow \langle A \varphi, \psi \rangle = \langle \varphi, A^* \psi \rangle \quad (1.61)$$

and hence $A_n^* \rightharpoonup A^*$ in general. However, if A_n and A are normal we have

$$\|(A_n - A)^* \psi\| = \|(A_n - A) \psi\| \quad (1.62)$$

and hence $A_n^* \xrightarrow{s} A^*$ in this case. Thus at least for normal operators taking adjoints is continuous with respect to strong convergence.

Lemma 1.13. *Suppose A_n is a sequence of bounded operators.*

- (i) $\text{s-lim}_{n \rightarrow \infty} A_n = A$ implies $\|A\| \leq \liminf \|A_n\|$.
- (ii) Every strong Cauchy sequence A_n is bounded: $\|A_n\| \leq C$.
- (iii) If $A_n y \rightarrow A y$ for y in a dense set and $\|A_n\| \leq C$, then $\text{s-lim}_{n \rightarrow \infty} A_n = A$.

The same result holds if strong convergence is replaced by weak convergence.

Proof. (i) and (ii) follow as in Lemma 1.11 (i).

(ii) Just use

$$\begin{aligned} \|A_n \psi - A \psi\| &\leq \|A_n \psi - A_n \varphi\| + \|A_n \varphi - A \varphi\| + \|A \varphi - A \psi\| \\ &\leq 2C \|\psi - \varphi\| + \|A_n \varphi - A \varphi\| \end{aligned} \quad (1.63)$$

and choose φ in the dense subspace such that $\|\psi - \varphi\| \leq \frac{\varepsilon}{4C}$ and n large such that $\|A_n\varphi - A\varphi\| \leq \frac{\varepsilon}{2}$.

The case of weak convergence is left as an exercise. \square

Problem 1.13. Suppose $\psi_n \rightarrow \psi$ and $\varphi_n \rightarrow \varphi$. Then $\langle \psi_n, \varphi_n \rangle \rightarrow \langle \psi, \varphi \rangle$.

Problem 1.14. Let $\{\varphi_j\}$ be some orthonormal basis. Show that $\psi_n \rightarrow \varphi$ if and only if ψ_n is bounded and $\langle \varphi_j, \psi_n \rangle \rightarrow \langle \varphi_j, \psi \rangle$ for every j . Show that this is wrong without the boundedness assumption.

Problem 1.15. Let $\{\varphi_j\}_{j=1}^{\infty}$ be some orthonormal basis and define

$$\|\psi\|_w = \sum_{j=1}^{\infty} \frac{1}{2^j} |\langle \varphi_j, \psi \rangle|. \quad (1.64)$$

Show that $\|\cdot\|_w$ is a norm. Show that $\psi_n \rightarrow \varphi$ if and only if $\|\psi_n - \psi\|_w \rightarrow 0$.

Problem 1.16. A subspace $M \subseteq \mathfrak{H}$ is closed if and only if every weak Cauchy sequence in M has a limit in M . (Hint: $\overline{M} = M^{\perp\perp}$.)

1.7. Appendix: The Stone–Weierstraß theorem

In case of a self-adjoint operator, the spectral theorem will show that the closed $*$ -algebra generated by this operator is isomorphic to the C^* algebra of continuous functions $C(K)$ over some compact set. Hence it is important to be able to identify dense sets:

Theorem 1.14 (Stone–Weierstraß, real version). Suppose K is a compact set and let $C(K, \mathbb{R})$ be the Banach algebra of continuous functions (with the sup norm).

If $F \subset C(K, \mathbb{R})$ contains the identity 1 and separates points (i.e., for every $x_1 \neq x_2$ there is some function $f \in F$ such that $f(x_1) \neq f(x_2)$), then the algebra generated by F is dense.

Proof. Denote by A the algebra generated by F . Note that if $f \in \overline{A}$, we have $|f| \in \overline{A}$: By the Weierstraß approximation theorem (Theorem 0.13) there is a polynomial $p_n(t)$ such that $||t| - p_n(t)| < \frac{1}{n}$ and hence $p_n(f) \rightarrow |f|$.

In particular, if $f, g \in \overline{A}$, we also have

$$\max\{f, g\} = \frac{(f+g) + |f-g|}{2}, \quad \min\{f, g\} = \frac{(f+g) - |f-g|}{2} \quad (1.65)$$

in \overline{A} .

Now fix $f \in C(K, \mathbb{R})$. We need to find some $f_\varepsilon \in \overline{A}$ with $\|f - f_\varepsilon\|_\infty < \varepsilon$.

First of all, since A separates points, observe that for given $y, z \in K$ there is a function $f_{y,z} \in A$ such that $f_{y,z}(y) = f(y)$ and $f_{y,z}(z) = f(z)$

(show this). Next, for every $y \in K$ there is a neighborhood $U(y)$ such that

$$f_{y,z}(x) > f(x) - \varepsilon, \quad x \in U(y) \quad (1.66)$$

and since K is compact, finitely many, say $U(y_1), \dots, U(y_j)$, cover K . Then

$$f_z = \max\{f_{y_1,z}, \dots, f_{y_j,z}\} \in \overline{A} \quad (1.67)$$

and satisfies $f_z > f - \varepsilon$ by construction. Since $f_z(z) = f(z)$ for every $z \in K$ there is a neighborhood $V(z)$ such that

$$f_z(x) < f(x) + \varepsilon, \quad x \in V(z) \quad (1.68)$$

and a corresponding finite cover $V(z_1), \dots, V(z_k)$. Now

$$f_\varepsilon = \min\{f_{z_1}, \dots, f_{z_k}\} \in \overline{A} \quad (1.69)$$

satisfies $f_\varepsilon < f + \varepsilon$. Since $f - \varepsilon < f_{z_l} < f_\varepsilon$, we have found a required function. \square

Theorem 1.15 (Stone–Weierstraß). *Suppose K is a compact set and let $C(K)$ be the C^* algebra of continuous functions (with the sup norm).*

If $F \subset C(K)$ contains the identity 1 and separates points, then the $$ -algebra generated by F is dense.*

Proof. Just observe that $\tilde{F} = \{\operatorname{Re}(f), \operatorname{Im}(f) \mid f \in F\}$ satisfies the assumption of the real version. Hence any real-valued continuous functions can be approximated by elements from \tilde{F} , in particular this holds for the real and imaginary part for any given complex-valued function. \square

Note that the additional requirement of being closed under complex conjugation is crucial: The functions holomorphic on the unit ball and continuous on the boundary separate points, but they are not dense (since the uniform limit of holomorphic functions is again holomorphic).

Corollary 1.16. *Suppose K is a compact set and let $C(K)$ be the C^* algebra of continuous functions (with the sup norm).*

If $F \subset C(K)$ separates points, then the closure of the $$ -algebra generated by F is either $C(K)$ or $\{f \in C(K) \mid f(t_0) = 0\}$ for some $t_0 \in K$.*

Proof. There are two possibilities, either all $f \in F$ vanish at one point $t_0 \in K$ (there can be at most one such point since F separates points) or there is no such point. If there is no such point we can proceed as in the proof of the Stone–Weierstraß theorem to show that the identity can be approximated by elements in \overline{A} (note that to show $|f| \in \overline{A}$ if $f \in \overline{A}$ we do not need the identity, since p_n can be chosen to contain no constant term). If there is such a t_0 , the identity is clearly missing from \overline{A} . However, adding the identity to \overline{A} we get $\overline{A} + \mathbb{C} = C(K)$ and it is easy to see that $\overline{A} = \{f \in C(K) \mid f(t_0) = 0\}$. \square

Problem 1.17. Show that the set of functions $\varphi_n(x) = \frac{1}{\sqrt{2\pi}}e^{inx}$, $n \in \mathbb{Z}$, form an orthonormal basis for $\mathfrak{H} = L^2(0, 2\pi)$.

Problem 1.18. Show that the $*$ -algebra generated by $f_z(t) = \frac{1}{t-z}$, $z \in \mathbb{C}$, is dense in the C^* algebra $C_\infty(\mathbb{R})$ of continuous functions vanishing at infinity. (Hint: Add ∞ to \mathbb{R} to make it compact.)

Self-adjointness and spectrum

2.1. Some quantum mechanics

In quantum mechanics, a single particle living in \mathbb{R}^3 is described by a complex-valued function (the **wave function**)

$$\psi(x, t), \quad (x, t) \in \mathbb{R}^3 \times \mathbb{R}, \quad (2.1)$$

where x corresponds to a point in space and t corresponds to time. The quantity $\rho_t(x) = |\psi(x, t)|^2$ is interpreted as the **probability density** of the particle at the time t . In particular, ψ must be normalized according to

$$\int_{\mathbb{R}^3} |\psi(x, t)|^2 d^3x = 1, \quad t \in \mathbb{R}. \quad (2.2)$$

The location x of the particle is a quantity which can be observed (i.e., measured) and is hence called **observable**. Due to our probabilistic interpretation it is also a random variable whose **expectation** is given by

$$\mathbb{E}_\psi(x) = \int_{\mathbb{R}^3} x |\psi(x, t)|^2 d^3x. \quad (2.3)$$

In a real life setting, it will not be possible to measure x directly and one will only be able to measure certain functions of x . For example, it is possible to check whether the particle is inside a certain area Ω of space (e.g., inside a detector). The corresponding observable is the characteristic function $\chi_\Omega(x)$ of this set. In particular, the number

$$\mathbb{E}_\psi(\chi_\Omega) = \int_{\mathbb{R}^3} \chi_\Omega(x) |\psi(x, t)|^2 d^3x = \int_{\Omega} |\psi(x, t)|^2 d^3x \quad (2.4)$$

corresponds to the probability of finding the particle inside $\Omega \subseteq \mathbb{R}^3$. An important point to observe is that, in contradistinction to classical mechanics, the particle is no longer localized at a certain point. In particular, the **mean-square deviation** (or **variance**) $\Delta_\psi(x)^2 = \mathbb{E}_\psi(x^2) - \mathbb{E}_\psi(x)^2$ is always nonzero.

In general, the **configuration space** (or **phase space**) of a quantum system is a (complex) Hilbert space \mathfrak{H} and the possible states of this system are represented by the elements ψ having norm one, $\|\psi\| = 1$.

An observable a corresponds to a linear operator A in this Hilbert space and its expectation, if the system is in the state ψ , is given by the real number

$$\mathbb{E}_\psi(A) = \langle \psi, A\psi \rangle = \langle A\psi, \psi \rangle, \quad (2.5)$$

where $\langle \cdot, \cdot \rangle$ denotes the scalar product of \mathfrak{H} . Similarly, the mean-square deviation is given by

$$\Delta_\psi(A)^2 = \mathbb{E}_\psi(A^2) - \mathbb{E}_\psi(A)^2 = \|(A - \mathbb{E}_\psi(A))\psi\|^2. \quad (2.6)$$

Note that $\Delta_\psi(A)$ vanishes if and only if ψ is an eigenstate corresponding to the eigenvalue $\mathbb{E}_\psi(A)$, that is, $A\psi = \mathbb{E}_\psi(A)\psi$.

From a physical point of view, (2.5) should make sense for any $\psi \in \mathfrak{H}$. However, this is not in the cards as our simple example of one particle already shows. In fact, the reader is invited to find a square integrable function $\psi(x)$ for which $x\psi(x)$ is no longer square integrable. The deeper reason behind this nuisance is that $\mathbb{E}_\psi(x)$ can attain arbitrary large values if the particle is not confined to a finite domain, which renders the corresponding operator unbounded. But unbounded operators cannot be defined on the entire Hilbert space in a natural way by the closed graph theorem (Theorem 2.7 below).

Hence, A will only be defined on a subset $\mathfrak{D}(A) \subseteq \mathfrak{H}$ called the **domain** of A . Since we want A to at least be defined for *most* states, we require $\mathfrak{D}(A)$ to be dense.

However, it should be noted that there is no general prescription how to find the operator corresponding to a given observable.

Now let us turn to the time evolution of such a quantum mechanical system. Given an initial state $\psi(0)$ of the system, there should be a unique $\psi(t)$ representing the state of the system at time $t \in \mathbb{R}$. We will write

$$\psi(t) = U(t)\psi(0). \quad (2.7)$$

Moreover, it follows from physical experiments, that **superposition of states** holds, that is, $U(t)(\alpha_1\psi_1(0) + \alpha_2\psi_2(0)) = \alpha_1\psi_1(t) + \alpha_2\psi_2(t)$ ($|\alpha_1|^2 + |\alpha_2|^2 = 1$). In other words, $U(t)$ should be a linear operator. Moreover,

since $\psi(t)$ is a state (i.e., $\|\psi(t)\| = 1$), we have

$$\|U(t)\psi\| = \|\psi\|. \quad (2.8)$$

Such operators are called **unitary**. Next, since we have assumed uniqueness of solutions to the initial value problem, we must have

$$U(0) = \mathbb{I}, \quad U(t+s) = U(t)U(s). \quad (2.9)$$

A family of unitary operators $U(t)$ having this property is called a **one-parameter unitary group**. In addition, it is natural to assume that this group is **strongly continuous**

$$\lim_{t \rightarrow t_0} U(t)\psi = U(t_0)\psi, \quad \psi \in \mathfrak{H}. \quad (2.10)$$

Each such group has an **infinitesimal generator** defined by

$$H\psi = \lim_{t \rightarrow 0} \frac{i}{t}(U(t)\psi - \psi), \quad \mathfrak{D}(H) = \{\psi \in \mathfrak{H} \mid \lim_{t \rightarrow 0} \frac{1}{t}(U(t)\psi - \psi) \text{ exists}\}. \quad (2.11)$$

This operator is called the **Hamiltonian** and corresponds to the energy of the system. If $\psi(0) \in \mathfrak{D}(H)$, then $\psi(t)$ is a solution of the **Schrödinger equation** (in suitable units)

$$i \frac{d}{dt} \psi(t) = H\psi(t). \quad (2.12)$$

This equation will be the main subject of our course.

In summary, we have the following **axioms of quantum mechanics**.

Axiom 1. The configuration space of a quantum system is a complex separable Hilbert space \mathfrak{H} and the possible states of this system are represented by the elements of \mathfrak{H} which have norm one.

Axiom 2. Each observable a corresponds to a linear operator A defined maximally on a dense subset $\mathfrak{D}(A)$. Moreover, the operator corresponding to a polynomial $P_n(a) = \sum_{j=0}^n \alpha_j a^j$, $\alpha_j \in \mathbb{R}$, is $P_n(A) = \sum_{j=0}^n \alpha_j A^j$, $\mathfrak{D}(P_n(A)) = \mathfrak{D}(A^n) = \{\psi \in \mathfrak{D}(A) \mid A\psi \in \mathfrak{D}(A^{n-1})\}$ ($A^0 = \mathbb{I}$).

Axiom 3. The expectation value for a measurement of a , when the system is in the state $\psi \in \mathfrak{D}(A)$, is given by (2.5), which must be real for all $\psi \in \mathfrak{D}(A)$.

Axiom 4. The time evolution is given by a strongly continuous one-parameter unitary group $U(t)$. The generator of this group corresponds to the energy of the system.

In the following sections we will try to draw some mathematical consequences from these assumptions:

First we will see that Axiom 2 and 3 imply that observables correspond to self-adjoint operators. Hence these operators play a central role in quantum mechanics and we will derive some of their basic properties. Another crucial role is played by the set of all possible expectation values for the measurement of a , which is connected with the spectrum $\sigma(A)$ of the corresponding operator A .

The problem of defining functions of an observable will lead us to the spectral theorem (in the next chapter), which generalizes the diagonalization of symmetric matrices.

Axiom 4 will be the topic of Chapter 5.

2.2. Self-adjoint operators

Let \mathfrak{H} be a (complex separable) Hilbert space. A **linear operator** is a linear mapping

$$A : \mathfrak{D}(A) \rightarrow \mathfrak{H}, \quad (2.13)$$

where $\mathfrak{D}(A)$ is a linear subspace of \mathfrak{H} , called the **domain** of A . It is called **bounded** if the operator norm

$$\|A\| = \sup_{\|\psi\|=1} \|A\psi\| = \sup_{\|\varphi\|=\|\psi\|=1} |\langle \psi, A\varphi \rangle| \quad (2.14)$$

is finite. The second equality follows since equality in $|\langle \psi, A\varphi \rangle| \leq \|\psi\| \|A\varphi\|$ is attained when $A\varphi = z\psi$ for some $z \in \mathbb{C}$. If A is bounded it is no restriction to assume $\mathfrak{D}(A) = \mathfrak{H}$ and we will always do so. The Banach space of all bounded linear operators is denoted by $\mathfrak{L}(\mathfrak{H})$.

The expression $\langle \psi, A\psi \rangle$ encountered in the previous section is called the **quadratic form**

$$q_A(\psi) = \langle \psi, A\psi \rangle, \quad \psi \in \mathfrak{D}(A), \quad (2.15)$$

associated to A . An operator can be reconstructed from its quadratic form via the **polarization identity**

$$\langle \varphi, A\psi \rangle = \frac{1}{4} (q_A(\varphi + \psi) - q_A(\varphi - \psi) + iq_A(\varphi - i\psi) - iq_A(\varphi + i\psi)). \quad (2.16)$$

A densely defined linear operator A is called **symmetric** (or **Hermitian**) if

$$\langle \varphi, A\psi \rangle = \langle A\varphi, \psi \rangle, \quad \psi, \varphi \in \mathfrak{D}(A). \quad (2.17)$$

The justification for this definition is provided by the following

Lemma 2.1. *A densely defined operator A is symmetric if and only if the corresponding quadratic form is real-valued.*

Proof. Clearly (2.17) implies that $\text{Im}(q_A(\psi)) = 0$. Conversely, taking the imaginary part of the identity

$$q_A(\psi + i\varphi) = q_A(\psi) + q_A(\varphi) + i(\langle \psi, A\varphi \rangle - \langle \varphi, A\psi \rangle) \quad (2.18)$$

shows $\text{Re}\langle A\varphi, \psi \rangle = \text{Re}\langle \varphi, A\psi \rangle$. Replacing φ by $i\varphi$ in this last equation shows $\text{Im}\langle A\varphi, \psi \rangle = \text{Im}\langle \varphi, A\psi \rangle$ and finishes the proof. \square

In other words, a densely defined operator A is symmetric if and only if

$$\langle \psi, A\psi \rangle = \langle A\psi, \psi \rangle, \quad \psi \in \mathfrak{D}(A). \quad (2.19)$$

This already narrows the class of admissible operators to the class of symmetric operators by Axiom 3. Next, let us tackle the issue of the correct domain.

By Axiom 2, A should be defined maximally, that is, if \tilde{A} is another symmetric operator such that $A \subseteq \tilde{A}$, then $A = \tilde{A}$. Here we write $A \subseteq \tilde{A}$ if $\mathfrak{D}(A) \subseteq \mathfrak{D}(\tilde{A})$ and $A\psi = \tilde{A}\psi$ for all $\psi \in \mathfrak{D}(A)$. In addition, we write $A = \tilde{A}$ if both $\tilde{A} \subseteq A$ and $A \subseteq \tilde{A}$ hold.

The **adjoint operator** A^* of a densely defined linear operator A is defined by

$$\begin{aligned} \mathfrak{D}(A^*) &= \{\psi \in \mathfrak{H} \mid \exists \tilde{\psi} \in \mathfrak{H} : \langle \psi, A\varphi \rangle = \langle \tilde{\psi}, \varphi \rangle, \forall \varphi \in \mathfrak{D}(A)\} \\ A^*\psi &= \tilde{\psi} \end{aligned} \quad (2.20)$$

The requirement that $\mathfrak{D}(A)$ is dense implies that A^* is well-defined. However, note that $\mathfrak{D}(A^*)$ might not be dense in general. In fact, it might contain no vectors other than 0.

Clearly we have $(\alpha A)^* = \alpha^* A^*$ for $\alpha \in \mathbb{C}$ and $(A + B)^* \supseteq A^* + B^*$ provided $\mathfrak{D}(A + B) = \mathfrak{D}(A) \cap \mathfrak{D}(B)$ is dense. However, equality will not hold in general unless one operator is bounded (Problem 2.1).

For later use, note that (Problem 2.2)

$$\text{Ker}(A^*) = \text{Ran}(A)^\perp. \quad (2.21)$$

For symmetric operators we clearly have $A \subseteq A^*$. If in addition, $A = A^*$ holds, then A is called **self-adjoint**. Our goal is to show that observables correspond to self-adjoint operators. This is for example true in the case of the position operator x , which is a special case of a multiplication operator.

Example. (Multiplication operator) Consider the multiplication operator

$$(Af)(x) = A(x)f(x), \quad \mathfrak{D}(A) = \{f \in L^2(\mathbb{R}^n, d\mu) \mid Af \in L^2(\mathbb{R}^n, d\mu)\}, \quad (2.22)$$

given by multiplication with the measurable function $A : \mathbb{R}^n \rightarrow \mathbb{C}$. First of all note that $\mathfrak{D}(A)$ is dense. In fact, consider $\Omega_n = \{x \in \mathbb{R}^n \mid |A(x)| \leq n\} \nearrow \mathbb{R}^n$. Then, for every $f \in L^2(\mathbb{R}^n, d\mu)$ the function $f_n = \chi_{\Omega_n} f \in \mathfrak{D}(A)$ converges to f as $n \rightarrow \infty$ by dominated convergence.

Next, let us compute the adjoint of A . Performing a formal computation we have for $h, f \in \mathfrak{D}(A)$ that

$$\langle h, Af \rangle = \int h(x)^* A(x) f(x) d\mu(x) = \int (A(x)^* h(x))^* f(x) d\mu(x) = \langle \tilde{A}h, f \rangle, \quad (2.23)$$

where \tilde{A} is multiplication by $A(x)^*$,

$$(\tilde{A}f)(x) = A(x)^* f(x), \quad \mathfrak{D}(\tilde{A}) = \{f \in L^2(\mathbb{R}^n, d\mu) \mid \tilde{A}f \in L^2(\mathbb{R}^n, d\mu)\}. \quad (2.24)$$

Note $\mathfrak{D}(\tilde{A}) = \mathfrak{D}(A)$. At first sight this seems to show that the adjoint of A is \tilde{A} . But for our calculation we had to assume $h \in \mathfrak{D}(A)$ and there might be some functions in $\mathfrak{D}(A^*)$ which do not satisfy this requirement! In particular, our calculation only shows $\tilde{A} \subseteq A^*$. To show that equality holds, we need to work a little harder:

If $h \in \mathfrak{D}(A^*)$ there is some $g \in L^2(\mathbb{R}^n, d\mu)$ such that

$$\int h(x)^* A(x) f(x) d\mu(x) = \int g(x)^* f(x) d\mu(x), \quad f \in \mathfrak{D}(A), \quad (2.25)$$

and thus

$$\int (h(x)A(x)^* - g(x))^* f(x) d\mu(x) = 0, \quad f \in \mathfrak{D}(A). \quad (2.26)$$

In particular,

$$\int \chi_{\Omega_n}(x)(h(x)A(x)^* - g(x))^* f(x) d\mu(x) = 0, \quad f \in L^2(\mathbb{R}^n, d\mu), \quad (2.27)$$

which shows that $\chi_{\Omega_n}(h(x)A(x)^* - g(x))^* \in L^2(\mathbb{R}^n, d\mu)$ vanishes. Since n is arbitrary, we even have $h(x)A(x)^* = g(x) \in L^2(\mathbb{R}^n, d\mu)$ and thus A^* is multiplication by $A(x)^*$ and $\mathfrak{D}(A^*) = \mathfrak{D}(A)$.

In particular, A is self-adjoint if A is real-valued. In the general case we have at least $\|Af\| = \|A^*f\|$ for all $f \in \mathfrak{D}(A) = \mathfrak{D}(A^*)$. Such operators are called normal. \diamond

Now note that

$$A \subseteq B \Rightarrow B^* \subseteq A^*, \quad (2.28)$$

that is, increasing the domain of A implies decreasing the domain of A^* . Thus there is no point in trying to extend the domain of a self-adjoint operator further. In fact, if A is self-adjoint and B is a symmetric extension, we infer $A \subseteq B \subseteq B^* \subseteq A^* = A$ implying $A = B$.

Corollary 2.2. *Self-adjoint operators are maximal, that is, they do not have any symmetric extensions.*

Furthermore, if A^* is densely defined (which is the case if A is symmetric) we can consider A^{**} . From the definition (2.20) it is clear that $A \subseteq A^{**}$ and

thus A^{**} is an extension of A . This extension is closely related to extending a linear subspace M via $M^{\perp\perp} = \overline{M}$ (as we will see a bit later) and thus is called the **closure** $\overline{A} = A^{**}$ of A .

If A is symmetric we have $A \subseteq A^*$ and hence $\overline{A} = A^{**} \subseteq A^*$, that is, \overline{A} lies between A and A^* . Moreover, $\langle \psi, A^* \varphi \rangle = \langle \overline{A} \psi, \varphi \rangle$ for all $\psi \in \mathfrak{D}(\overline{A})$, $\varphi \in \mathfrak{D}(A^*)$ implies that \overline{A} is symmetric since $A^* \varphi = \overline{A} \varphi$ for $\varphi \in \mathfrak{D}(\overline{A})$.

Example. (Differential operator) Take $\mathfrak{H} = L^2(0, 2\pi)$.

(i). Consider the operator

$$A_0 f = -i \frac{d}{dx} f, \quad \mathfrak{D}(A_0) = \{f \in C^1[0, 2\pi] \mid f(0) = f(2\pi) = 0\}. \quad (2.29)$$

That A_0 is symmetric can be shown by a simple integration by parts (do this). Note that the *boundary conditions* $f(0) = f(2\pi) = 0$ are chosen such that the boundary terms occurring from integration by parts vanish. However, this will also follow once we have computed A_0^* . If $g \in \mathfrak{D}(A_0^*)$ we must have

$$\int_0^{2\pi} g(x)^* (-i f'(x)) dx = \int_0^{2\pi} \tilde{g}(x)^* f(x) dx \quad (2.30)$$

for some $\tilde{g} \in L^2(0, 2\pi)$. Integration by parts shows

$$\int_0^{2\pi} f'(x) \left(g(x) - i \int_0^x \tilde{g}(t) dt \right)^* dx = 0 \quad (2.31)$$

and hence $g(x) - i \int_0^x \tilde{g}(t) dt \in \{f' \mid f \in \mathfrak{D}(A_0)\}^\perp$. But $\{f' \mid f \in \mathfrak{D}(A_0)\} = \{h \in C(0, 2\pi) \mid \int_0^{2\pi} h(t) dt = 0\}$ implying $g(x) = g(0) + i \int_0^x \tilde{g}(t) dt$ since $\overline{\{f' \mid f \in \mathfrak{D}(A_0)\}} = \{h \in \mathfrak{H} \mid \langle 1, h \rangle = 0\} = \{1\}^\perp$ and $\{1\}^{\perp\perp} = \text{span}\{1\}$. Thus $g \in AC[0, 2\pi]$, where

$$AC[a, b] = \{f \in C[a, b] \mid f(x) = f(a) + \int_a^x g(t) dt, g \in L^1(a, b)\} \quad (2.32)$$

denotes the set of all absolutely continuous functions (see Section 2.6). In summary, $g \in \mathfrak{D}(A_0^*)$ implies $g \in AC[0, 2\pi]$ and $A_0^* g = \tilde{g} = -ig'$. Conversely, for every $g \in H^1(0, 2\pi) = \{f \in AC[0, 2\pi] \mid f' \in L^2(0, 2\pi)\}$ (2.30) holds with $\tilde{g} = -ig'$ and we conclude

$$A_0^* f = -i \frac{d}{dx} f, \quad \mathfrak{D}(A_0^*) = H^1(0, 2\pi). \quad (2.33)$$

In particular, A is symmetric but not self-adjoint. Since $A^{**} \subseteq A^*$ we compute

$$0 = \langle g, \overline{A_0} f \rangle - \langle A_0^* g, f \rangle = i(f(0)g(0)^* - f(2\pi)g(2\pi)^*) \quad (2.34)$$

and since the boundary values of $g \in \mathfrak{D}(A_0^*)$ can be prescribed arbitrary, we must have $f(0) = f(2\pi) = 0$. Thus

$$\overline{A_0}f = -i\frac{d}{dx}f, \quad \mathfrak{D}(\overline{A_0}) = \{f \in \mathfrak{D}(A_0^*) \mid f(0) = f(2\pi) = 0\}. \quad (2.35)$$

(ii). Now let us take

$$Af = -i\frac{d}{dx}f, \quad \mathfrak{D}(A) = \{f \in C^1[0, 2\pi] \mid f(0) = f(2\pi)\}. \quad (2.36)$$

which is clearly an extension of A_0 . Thus $A^* \subseteq A_0^*$ and we compute

$$0 = \langle g, Af \rangle - \langle A^*g, f \rangle = if(0)(g(0)^* - g(2\pi)^*). \quad (2.37)$$

Since this must hold for all $f \in \mathfrak{D}(A)$ we conclude $g(0) = g(2\pi)$ and

$$A^*f = -i\frac{d}{dx}f, \quad \mathfrak{D}(A^*) = \{f \in H^1(0, 2\pi) \mid f(0) = f(2\pi)\}. \quad (2.38)$$

Similarly, as before, $\overline{A} = A^*$ and thus \overline{A} is self-adjoint. \diamond

One might suspect that there is no big difference between the two symmetric operators A_0 and A from the previous example, since they coincide on a dense set of vectors. However, the converse is true: For example, the first operator A_0 has no eigenvectors at all (i.e., solutions of the equation $A_0\psi = z\psi$, $z \in \mathbb{C}$) whereas the second one has an orthonormal basis of eigenvectors!

Example. Compute the eigenvectors of A_0 and A from the previous example.

(i). By definition an eigenvector is a (nonzero) solution of $A_0u = zu$, $z \in \mathbb{C}$, that is, a solution of the ordinary differential equation

$$u'(x) = zu(x) \quad (2.39)$$

satisfying the boundary conditions $u(0) = u(2\pi) = 0$ (since we must have $u \in \mathfrak{D}(A_0)$). The general solution of the differential equation is $u(x) = u(0)e^{izx}$ and the boundary conditions imply $u(x) = 0$. Hence there are no eigenvectors.

(ii). Now we look for solutions of $Au = zu$, that is the same differential equation as before, but now subject to the boundary condition $u(0) = u(2\pi)$. Again the general solution is $u(x) = u(0)e^{izx}$ and the boundary condition requires $u(0) = u(0)e^{2\pi iz}$. Thus there are two possibilities. Either $u(0) = 0$ (which is of no use for us) or $z \in \mathbb{Z}$. In particular, we see that all eigenvectors are given by

$$u_n(x) = \frac{1}{\sqrt{2\pi}}e^{inx}, \quad n \in \mathbb{Z}, \quad (2.40)$$

which are well-known to form an orthonormal basis. \diamond

We will see a bit later that this is a consequence of self-adjointness of \overline{A} . Hence it will be important to know whether a given operator is self-adjoint or not. Our example shows that symmetry is easy to check (in case of differential operators it usually boils down to integration by parts), but computing the adjoint of an operator is a nontrivial job even in simple situations. However, we will learn soon that self-adjointness is a much stronger property than symmetry justifying the additional effort needed to prove it.

On the other hand, if a given symmetric operator A turns out not to be self-adjoint, this raises the question of self-adjoint extensions. Two cases need to be distinguished. If \overline{A} is self-adjoint, then there is only one self-adjoint extension (if B is another one, we have $\overline{A} \subseteq B$ and hence $\overline{A} = B$ by Corollary 2.2). In this case A is called **essentially self-adjoint** and $\mathfrak{D}(A)$ is called a **core** for \overline{A} . Otherwise there might be more than one self-adjoint extension or none at all. This situation is more delicate and will be investigated in Section 2.5.

Since we have seen that computing A^* is not always easy, a criterion for self-adjointness not involving A^* will be useful.

Lemma 2.3. *Let A be symmetric such that $\text{Ran}(A + z) = \text{Ran}(A + z^*) = \mathfrak{H}$ for one $z \in \mathbb{C}$. Then A is self-adjoint.*

Proof. Let $\psi \in \mathfrak{D}(A^*)$ and $A^*\psi = \tilde{\psi}$. Since $\text{Ran}(A + z^*) = \mathfrak{H}$, there is a $\vartheta \in \mathfrak{D}(A)$ such that $(A + z^*)\vartheta = \tilde{\psi} + z^*\psi$. Now we compute

$$\langle \psi, (A + z)\varphi \rangle = \langle \tilde{\psi} + z^*\psi, \varphi \rangle = \langle (A + z^*)\vartheta, \varphi \rangle = \langle \vartheta, (A + z)\varphi \rangle, \quad \varphi \in \mathfrak{D}(A), \quad (2.41)$$

and hence $\psi = \vartheta \in \mathfrak{D}(A)$ since $\text{Ran}(A + z) = \mathfrak{H}$. \square

To proceed further, we will need more information on the closure of an operator. We will use a different approach which avoids the use of the adjoint operator. We will establish equivalence with our original definition in Lemma 2.4.

The simplest way of extending an operator A is to take the closure of its **graph** $\Gamma(A) = \{(\psi, A\psi) \mid \psi \in \mathfrak{D}(A)\} \subset \mathfrak{H}^2$. That is, if $(\psi_n, A\psi_n) \rightarrow (\psi, \tilde{\psi})$ we might try to define $A\psi = \tilde{\psi}$. For $A\psi$ to be well-defined, we need that $(\psi_n, A\psi_n) \rightarrow (0, \tilde{\psi})$ implies $\tilde{\psi} = 0$. In this case A is called **closable** and the unique operator \overline{A} which satisfies $\Gamma(\overline{A}) = \overline{\Gamma(A)}$ is called the **closure** of A . Clearly, A is called **closed** if $\overline{A} = A$, which is the case if and only if the graph of A is closed. Equivalently, A is closed if and only if $\Gamma(A)$ equipped with the **graph norm** $\|\psi\|_{\Gamma(A)}^2 = \|\psi\|^2 + \|A\psi\|^2$ is a Hilbert space (i.e., closed). A bounded operator is closed if and only if its domain is closed (show this!).

Example. Let us compute the closure of the operator A_0 from the previous example without the use of the adjoint operator. Let $f \in \mathfrak{D}(\overline{A_0})$ and let $f_n \in \mathfrak{D}(A_0)$ be a sequence such that $f_n \rightarrow f$, $A_0 f_n \rightarrow -ig$. Then $f'_n \rightarrow g$ and hence $f(x) = \int_0^x g(t)dt$. Thus $f \in AC[0, 2\pi]$ and $f(0) = 0$. Moreover $f(2\pi) = \lim_{n \rightarrow \infty} \int_0^{2\pi} f'_n(t)dt = 0$. Conversely, any such f can be approximated by functions in $\mathfrak{D}(A_0)$ (show this). \diamond

Next, let us collect a few important results.

Lemma 2.4. *Suppose A is a densely defined operator.*

- (i) A^* is closed.
- (ii) A is closable if and only if $\mathfrak{D}(A^*)$ is dense and $\overline{A} = A^{**}$ respectively $(\overline{A})^* = A^*$ in this case.
- (iii) If A is injective and the $\text{Ran}(A)$ is dense, then $(A^*)^{-1} = (A^{-1})^*$. If A is closable and \overline{A} is injective, then $\overline{A}^{-1} = \overline{A^{-1}}$.

Proof. Let us consider the following two unitary operators from \mathfrak{H}^2 to itself

$$U(\varphi, \psi) = (\psi, -\varphi), \quad V(\varphi, \psi) = (\psi, \varphi). \quad (2.42)$$

(i). From

$$\begin{aligned} \Gamma(A^*) &= \{(\varphi, \tilde{\varphi}) \in \mathfrak{H}^2 \mid \langle \varphi, A\psi \rangle = \langle \tilde{\varphi}, \psi \rangle \forall \varphi \in \mathfrak{D}(A^*)\} \\ &= \{(\varphi, \tilde{\varphi}) \in \mathfrak{H}^2 \mid \langle (-\tilde{\varphi}, \varphi), (\psi, \tilde{\psi}) \rangle_{\Gamma(A)} = 0 \forall (\psi, \tilde{\psi}) \in \Gamma(A)\} \\ &= U(\Gamma(A)^\perp) = (U\Gamma(A))^\perp \end{aligned} \quad (2.43)$$

we conclude that A^* is closed.

(ii). From

$$\begin{aligned} \overline{\Gamma(A)} &= \Gamma(A)^{\perp\perp} = (U\Gamma(A^*))^\perp \\ &= \{(\psi, \tilde{\psi}) \mid \langle \psi, A^*\varphi \rangle - \langle \tilde{\psi}, \varphi \rangle = 0, \forall \varphi \in \mathfrak{D}(A^*)\} \end{aligned} \quad (2.44)$$

we see that $(0, \tilde{\psi}) \in \overline{\Gamma(A)}$ if and only if $\tilde{\psi} \in \mathfrak{D}(A^*)^\perp$. Hence A is closable if and only if $\mathfrak{D}(A^*)$ is dense. In this case, equation (2.43) also shows $\overline{A}^* = A^*$. Moreover, replacing A by A^* in (2.43) and comparing with the last formula shows $A^{**} = \overline{A}$.

(iii). Next note that (provided A is injective)

$$\Gamma(A^{-1}) = V\Gamma(A). \quad (2.45)$$

Hence if $\text{Ran}(A)$ is dense, then $\text{Ker}(A^*) = \text{Ran}(A)^\perp = \{0\}$ and

$$\Gamma((A^*)^{-1}) = V\Gamma(A^*) = VU\Gamma(A)^\perp = UV\Gamma(A)^\perp = U(V\Gamma(A))^\perp \quad (2.46)$$

shows that $(A^*)^{-1} = (A^{-1})^*$. Similarly, if A is closable and \bar{A} is injective, then $\bar{A}^{-1} = \overline{A^{-1}}$ by

$$\Gamma(\bar{A}^{-1}) = V\Gamma(\bar{A}) = \overline{V\Gamma(A)} = \Gamma(\overline{A^{-1}}). \quad (2.47)$$

□

If $A \in \mathfrak{L}(\mathfrak{H})$ we clearly have $\mathfrak{D}(A^*) = \mathfrak{H}$ and by Corollary 1.8 $A \in \mathfrak{L}(\mathfrak{H})$. In particular, since $\bar{A} = A^{**}$ we obtain

Theorem 2.5. *We have $\bar{A} \in \mathfrak{L}(\mathfrak{H})$ if and only if $A^* \in \mathfrak{L}(\mathfrak{H})$.*

Now we can also generalize Lemma 2.3 to the case of essential self-adjoint operators.

Lemma 2.6. *A symmetric operator A is essentially self-adjoint if and only if one of the following conditions holds for one $z \in \mathbb{C} \setminus \mathbb{R}$.*

- $\overline{\text{Ran}(A+z)} = \overline{\text{Ran}(A+z^*)} = \mathfrak{H}$.
- $\text{Ker}(A^*+z) = \text{Ker}(A^*+z^*) = \{0\}$.

If A is non-negative, that is $\langle \psi, A\psi \rangle \geq 0$ for all $\psi \in \mathfrak{D}(A)$, we can also admit $z \in (-\infty, 0)$.

Proof. As noted earlier $\text{Ker}(A^*) = \text{Ran}(A)^\perp$, and hence the two conditions are equivalent. By taking the closure of A it is no restriction to assume that A is closed. Let $z = x + iy$. From

$$\|(A-z)\psi\|^2 = \|(A-x)\psi - iy\psi\|^2 = \|(A-x)\psi\|^2 + y^2\|\psi\|^2 \geq y^2\|\psi\|^2, \quad (2.48)$$

we infer that $\text{Ker}(A-z) = \{0\}$ and hence $(A-z)^{-1}$ exists. Moreover, setting $\psi = (A-z)^{-1}\varphi$ ($y \neq 0$) shows $\|(A-z)^{-1}\| \leq |y|^{-1}$. Hence $(A-z)^{-1}$ is bounded and closed. Since it is densely defined by assumption, its domain $\text{Ran}(A+z)$ must be equal to \mathfrak{H} . Replacing z by z^* and applying Lemma 2.3 finishes the general case. The argument for the non-negative case with $z < 0$ is similar using $\varepsilon\|\psi\|^2 \leq |\langle \psi, (A+\varepsilon)\psi \rangle|^2 \leq \|\psi\|\|(A+\varepsilon)\psi\|$ which shows $(A+\varepsilon)^{-1} \leq \varepsilon^{-1}$, $\varepsilon > 0$. □

In addition, we can also prove the closed graph theorem which shows that an unbounded operator cannot be defined on the entire Hilbert space.

Theorem 2.7 (closed graph). *Let \mathfrak{H}_1 and \mathfrak{H}_2 be two Hilbert spaces and A an operator defined on all of \mathfrak{H}_1 . Then A is bounded if and only if $\Gamma(A)$ is closed.*

Proof. If A is bounded then it is easy to see that $\Gamma(A)$ is closed. So let us assume that $\Gamma(A)$ is closed. Then A^* is well defined and for all unit vectors

$\varphi \in \mathfrak{D}(A^*)$ we have that the linear functional $\ell_\varphi(\psi) = \langle A^*\varphi, \psi \rangle$ is pointwise bounded

$$\|\ell_\varphi(\psi)\| = |\langle \varphi, A\psi \rangle| \leq \|A\psi\|. \quad (2.49)$$

Hence by the uniform boundedness principle there is a constant C such that $\|\ell_\varphi\| = \|A^*\varphi\| \leq C$. That is, A^* is bounded and so is $A = A^{**}$. \square

Finally we want to draw some further consequences of Axiom 2 and show that observables correspond to self-adjoint operators. Since self-adjoint operators are already maximal, the difficult part remaining is to show that an observable has at least one self-adjoint extension. There is a good way of doing this for non-negative operators and hence we will consider this case first.

An operator is called **non-negative** (resp. **positive**) if $\langle \psi, A\psi \rangle \geq 0$ (resp. > 0 for $\psi \neq 0$) for all $\psi \in \mathfrak{D}(A)$. If A is positive, the map $(\varphi, \psi) \mapsto \langle \varphi, A\psi \rangle$ is a scalar product. However, there might be sequences which are Cauchy with respect to this scalar product but not with respect to our original one. To avoid this, we introduce the scalar product

$$\langle \varphi, \psi \rangle_A = \langle \varphi, (A + 1)\psi \rangle, \quad A \geq 0, \quad (2.50)$$

defined on $\mathfrak{D}(A)$, which satisfies $\|\psi\| \leq \|\psi\|_A$. Let \mathfrak{H}_A be the completion of $\mathfrak{D}(A)$ with respect to the above scalar product. We claim that \mathfrak{H}_A can be regarded as a subspace of \mathfrak{H} , that is, $\mathfrak{D}(A) \subseteq \mathfrak{H}_A \subseteq \mathfrak{H}$.

If (ψ_n) is a Cauchy sequence in $\mathfrak{D}(A)$, then it is also Cauchy in \mathfrak{H} (since $\|\psi\| \leq \|\psi\|_A$ by assumption) and hence we can identify it with the limit of (ψ_n) regarded as a sequence in \mathfrak{H} . For this identification to be unique, we need to show that if $(\psi_n) \subset \mathfrak{D}(A)$ is a Cauchy sequence in \mathfrak{H}_A such that $\|\psi_n\| \rightarrow 0$, then $\|\psi_n\|_A \rightarrow 0$. This follows from

$$\begin{aligned} \|\psi_n\|_A^2 &= \langle \psi_n, \psi_n - \psi_m \rangle_A + \langle \psi_n, \psi_m \rangle_A \\ &\leq \|\psi_n\|_A \|\psi_n - \psi_m\|_A + \|\psi_n\| \|(A + 1)\psi_m\| \end{aligned} \quad (2.51)$$

since the right hand side can be made arbitrarily small choosing m, n large.

Clearly the quadratic form q_A can be extended to every $\psi \in \mathfrak{H}_A$ by setting

$$q_A(\psi) = \langle \psi, \psi \rangle_A - \|\psi\|^2, \quad \psi \in \mathfrak{Q}(A) = \mathfrak{H}_A. \quad (2.52)$$

The set $\mathfrak{Q}(A)$ is also called the **form domain** of A .

Example. (Multiplication operator) Let A be multiplication by $A(x) \geq 0$ in $L^2(\mathbb{R}^n, d\mu)$. Then

$$\mathfrak{Q}(A) = \mathfrak{D}(A^{1/2}) = \{f \in L^2(\mathbb{R}^n, d\mu) \mid A^{1/2}f \in L^2(\mathbb{R}^n, d\mu)\} \quad (2.53)$$

and

$$q_A(x) = \int_{\mathbb{R}^n} A(x)|f(x)|^2 d\mu(x) \quad (2.54)$$

(show this). \diamond

Now we come to our extension result. Note that $A + 1$ is injective and the best we can hope for is that for a non-negative extension \tilde{A} , $\tilde{A} + 1$ is a bijection from $\mathfrak{D}(\tilde{A})$ onto \mathfrak{H} .

Lemma 2.8. *Suppose A is a non-negative operator, then there is a non-negative extension \tilde{A} such that $\text{Ran}(\tilde{A} + 1) = \mathfrak{H}$.*

Proof. Let us define an operator \tilde{A} by

$$\begin{aligned} \mathfrak{D}(\tilde{A}) &= \{\psi \in \mathfrak{H}_A \mid \exists \tilde{\psi} \in \mathfrak{H} : \langle \varphi, \psi \rangle_A = \langle \varphi, \tilde{\psi} \rangle, \forall \varphi \in \mathfrak{H}_A\} \\ \tilde{A}\psi &= \tilde{\psi} - \psi \end{aligned} \quad (2.55)$$

Since \mathfrak{H}_A is dense, $\tilde{\psi}$ is well-defined. Moreover, it is straightforward to see that \tilde{A} is a non-negative extension of A .

It is also not hard to see that $\text{Ran}(\tilde{A} + 1) = \mathfrak{H}$. Indeed, for any $\tilde{\psi} \in \mathfrak{H}$, $\varphi \mapsto \langle \tilde{\psi}, \varphi \rangle$ is bounded linear functional on \mathfrak{H}_A . Hence there is an element $\psi \in \mathfrak{H}_A$ such that $\langle \tilde{\psi}, \varphi \rangle = \langle \psi, \varphi \rangle_A$ for all $\varphi \in \mathfrak{H}_A$. By the definition of \tilde{A} , $(\tilde{A} + 1)\psi = \tilde{\psi}$ and hence $\tilde{A} + 1$ is onto. \square

Now it is time for another

Example. Let us take $\mathfrak{H} = L^2(0, \pi)$ and consider the operator

$$Af = -\frac{d^2}{dx^2}f, \quad \mathfrak{D}(A) = \{f \in C^2[0, \pi] \mid f(0) = f(\pi) = 0\}, \quad (2.56)$$

which corresponds to the one-dimensional model of a particle confined to a box.

(i). First of all, using integration by parts twice, it is straightforward to check that A is symmetric

$$\int_0^\pi g(x)^*(-f'')(x)dx = \int_0^\pi g'(x)^*f'(x)dx = \int_0^\pi (-g'')(x)^*f(x)dx. \quad (2.57)$$

Note that the *boundary conditions* $f(0) = f(\pi) = 0$ are chosen such that the boundary terms occurring from integration by parts vanish. Moreover, the same calculation also shows that A is positive

$$\int_0^\pi f(x)^*(-f'')(x)dx = \int_0^\pi |f'(x)|^2dx > 0, \quad f \neq 0. \quad (2.58)$$

(ii). Next let us show $\mathfrak{H}_A = \{f \in H^1(0, \pi) \mid f(0) = f(\pi) = 0\}$. In fact, since

$$\langle g, f \rangle_A = \int_0^\pi (g'(x)^*f'(x) + g(x)^*f(x)) dx, \quad (2.59)$$

we see that f_n is Cauchy in \mathfrak{H}_A if and only if both f_n and f'_n are Cauchy in $L^2(0, \pi)$. Thus $f_n \rightarrow f$ and $f'_n \rightarrow g$ in $L^2(0, \pi)$ and $f_n(x) = \int_0^x f'_n(t)dt$

implies $f(x) = \int_0^x g(t)dt$. Thus $f \in AC[0, \pi]$. Moreover, $f(0) = 0$ is obvious and from $0 = f_n(\pi) = \int_0^\pi f'_n(t)dt$ we have $f(\pi) = \lim_{n \rightarrow \infty} \int_0^\pi f'_n(t)dt = 0$. So we have $\mathfrak{H}_A \subseteq \{f \in H^1(0, \pi) \mid f(0) = f(\pi) = 0\}$. To see the converse approximate f' by smooth functions g_n . Using $g_n - \int_0^\pi g_n(t)dt$ instead of g_n it is no restriction to assume $\int_0^\pi g_n(t)dt = 0$. Now define $f_n(x) = \int_0^x g_n(t)dt$ and note $f_n \in \mathfrak{D}(A) \rightarrow f$.

(iii). Finally, let us compute the extension \tilde{A} . We have $f \in \mathfrak{D}(\tilde{A})$ if for all $g \in \mathfrak{H}_A$ there is an \tilde{f} such that $\langle g, f \rangle_A = \langle g, \tilde{f} \rangle$. That is,

$$\int_0^\pi g'(x)^* f'(x) dx = \int_0^\pi g(x)^* (\tilde{f}(x) - f(x)) dx. \quad (2.60)$$

Integration by parts on the right hand side shows

$$\int_0^\pi g'(x)^* f'(x) dx = - \int_0^\pi g'(x)^* \int_0^x (\tilde{f}(t) - f(t)) dt dx \quad (2.61)$$

or equivalently

$$\int_0^\pi g'(x)^* \left(f'(x) + \int_0^x (\tilde{f}(t) - f(t)) dt \right) dx = 0. \quad (2.62)$$

Now observe $\{g' \in \mathfrak{H} \mid g \in \mathfrak{H}_A\} = \{h \in \mathfrak{H} \mid \int_0^\pi h(t)dt = 0\} = \{1\}^\perp$ and thus $f'(x) + \int_0^x (\tilde{f}(t) - f(t))dt \in \{1\}^{\perp\perp} = \text{span}\{1\}$. So we see $f \in H^2(0, \pi) = \{f \in AC[0, \pi] \mid f' \in H^1(0, \pi)\}$ and $\tilde{A}f = -f''$. The converse is easy and hence

$$\tilde{A}f = -\frac{d^2}{dx^2}f, \quad \mathfrak{D}(\tilde{A}) = \{f \in H^2[0, \pi] \mid f(0) = f(\pi) = 0\}. \quad (2.63)$$

◇

Now let us apply this result to operators A corresponding to observables. Since A will, in general, not satisfy the assumptions of our lemma, we will consider $1 + A^2$, $\mathfrak{D}(1 + A^2) = \mathfrak{D}(A^2)$, instead, which has a symmetric extension whose range is \mathfrak{H} . By our requirement for observables, $1 + A^2$ is maximally defined and hence is equal to this extension. In other words, $\text{Ran}(1 + A^2) = \mathfrak{H}$. Moreover, for any $\varphi \in \mathfrak{H}$ there is a $\psi \in \mathfrak{D}(A^2)$ such that

$$(A - i)(A + i)\psi = (A + i)(A - i)\psi = \varphi \quad (2.64)$$

and since $(A \pm i)\psi \in \mathfrak{D}(A)$, we infer $\text{Ran}(A \pm i) = \mathfrak{H}$. As an immediate consequence we obtain

Corollary 2.9. *Observables correspond to self-adjoint operators.*

But there is another important consequence of the results which is worth while mentioning.

Theorem 2.10 (Friedrichs extension). *Let A be a semi-bounded symmetric operator, that is,*

$$q_A(\psi) = \langle \psi, A\psi \rangle \geq \gamma \|\psi\|^2, \quad \gamma \in \mathbb{R}. \quad (2.65)$$

Then there is a self-adjoint extension \tilde{A} which is also bounded from below by γ and which satisfies $\mathfrak{D}(\tilde{A}) \subseteq \mathfrak{H}_{A-\gamma}$.

Proof. Replacing A by $A - \gamma$ we can reduce it to the case considered in Lemma 2.8. The rest is straightforward. \square

Problem 2.1. *Show $(\alpha A)^* = \alpha^* A^*$ and $(A+B)^* \supseteq A^* + B^*$ (where $\mathfrak{D}(A^* + B^*) = \mathfrak{D}(A^*) \cap \mathfrak{D}(B^*)$) with equality if one operator is bounded. Give an example where equality does not hold.*

Problem 2.2. *Show (2.21).*

Problem 2.3. *Show that if A is normal, so is $A + z$ for any $z \in \mathbb{C}$.*

Problem 2.4. *Show that normal operators are closed.*

Problem 2.5. *Show that the kernel of a closed operator is closed.*

Problem 2.6. *Show that if A is bounded and B closed, then BA is closed.*

Problem 2.7. *Let $A = -\frac{d^2}{dx^2}$, $\mathfrak{D}(A) = \{f \in H^2(0, \pi) \mid f(0) = f(\pi) = 0\}$ and let $\psi(x) = \frac{1}{2\sqrt{\pi}}x(\pi - x)$. Find the error in the following argument: Since A is symmetric we have $1 = \langle A\psi, A\psi \rangle = \langle \psi, A^2\psi \rangle = 0$.*

Problem 2.8. *Suppose A is a closed operator. Show that A^*A (with $\mathfrak{D}(A^*A) = \{\psi \in \mathfrak{D}(A) \mid A\psi \in \mathfrak{D}(A^*)\}$) is self-adjoint. (Hint: $A^*A \geq 0$.)*

Problem 2.9. *Show that A is normal if and only if $AA^* = A^*A$.*

2.3. Resolvents and spectra

Let A be a (densely defined) closed operator. The **resolvent set** of A is defined by

$$\rho(A) = \{z \in \mathbb{C} \mid (A - z)^{-1} \in \mathfrak{L}(\mathfrak{H})\}. \quad (2.66)$$

More precisely, $z \in \rho(A)$ if and only if $(A - z) : \mathfrak{D}(A) \rightarrow \mathfrak{H}$ is bijective and its inverse is bounded. By the closed graph theorem (Theorem 2.7), it suffices to check that $A - z$ is bijective. The complement of the resolvent set is called the **spectrum**

$$\sigma(A) = \mathbb{C} \setminus \rho(A) \quad (2.67)$$

of A . In particular, $z \in \sigma(A)$ if $A - z$ has a nontrivial kernel. A vector $\psi \in \text{Ker}(A - z)$ is called an **eigenvector** and z is called **eigenvalue** in this case.

The function

$$\begin{aligned} R_A : \rho(A) &\rightarrow \mathfrak{L}(\mathfrak{H}) \\ z &\mapsto (A - z)^{-1} \end{aligned} \quad (2.68)$$

is called **resolvent** of A . Note the convenient formula

$$R_A(z)^* = ((A - z)^{-1})^* = ((A - z)^*)^{-1} = (A^* - z^*)^{-1} = R_{A^*}(z^*). \quad (2.69)$$

In particular,

$$\rho(A^*) = \rho(A)^*. \quad (2.70)$$

Example. (Multiplication operator) Consider again the multiplication operator

$$(Af)(x) = A(x)f(x), \quad \mathfrak{D}(A) = \{f \in L^2(\mathbb{R}^n, d\mu) \mid Af \in L^2(\mathbb{R}^n, d\mu)\}, \quad (2.71)$$

given by multiplication with the measurable function $A : \mathbb{R}^n \rightarrow \mathbb{C}$. Clearly $(A - z)^{-1}$ is given by the multiplication operator

$$\begin{aligned} (A - z)^{-1}f(x) &= \frac{1}{A(x) - z}f(x), \\ \mathfrak{D}((A - z)^{-1}) &= \{f \in L^2(\mathbb{R}^n, d\mu) \mid \frac{1}{A - z}f \in L^2(\mathbb{R}^n, d\mu)\} \end{aligned} \quad (2.72)$$

whenever this operator is bounded. But $\|(A - z)^{-1}\| = \|\frac{1}{A - z}\|_\infty \leq \frac{1}{\varepsilon}$ is equivalent to $\mu(\{x \mid |A(x) - z| \geq \varepsilon\}) = 0$ and hence

$$\rho(A) = \{z \in \mathbb{C} \mid \exists \varepsilon > 0 : \mu(\{x \mid |A(x) - z| \leq \varepsilon\}) = 0\}. \quad (2.73)$$

Moreover, z is an eigenvalue of A if $\mu(A^{-1}(\{z\})) > 0$ and $\chi_{A^{-1}(\{z\})}$ is a corresponding eigenfunction in this case. \diamond

Example. (Differential operator) Consider again the differential operator

$$Af = -i\frac{d}{dx}f, \quad \mathfrak{D}(A) = \{f \in AC[0, 2\pi] \mid f' \in L^2, f(0) = f(2\pi)\} \quad (2.74)$$

in $L^2(0, 2\pi)$. We already know that the eigenvalues of A are the integers and that the corresponding normalized eigenfunctions

$$u_n(x) = \frac{1}{\sqrt{2\pi}}e^{inx} \quad (2.75)$$

form an orthonormal basis.

To compute the resolvent we must find the solution of the corresponding inhomogeneous equation $-if'(x) - zf(x) = g(x)$. By the variation of constants formula the solution is given by (this can also be easily verified directly)

$$f(x) = f(0)e^{izx} + i \int_0^x e^{iz(x-t)}g(t)dt. \quad (2.76)$$

Since f must lie in the domain of A , we must have $f(0) = f(2\pi)$ which gives

$$f(0) = \frac{i}{e^{-2\pi iz} - 1} \int_0^{2\pi} e^{-izt} g(t) dt, \quad z \in \mathbb{C} \setminus \mathbb{Z}. \quad (2.77)$$

(Since $z \in \mathbb{Z}$ are the eigenvalues, the inverse cannot exist in this case.) Hence

$$(A - z)^{-1}g(x) = \int_0^{2\pi} G(z, x, t)g(t)dt, \quad (2.78)$$

where

$$G(z, x, t) = e^{iz(x-t)} \begin{cases} \frac{-i}{1 - e^{-2\pi iz}}, & t > x \\ \frac{i}{1 - e^{2\pi iz}}, & t < x \end{cases}, \quad z \in \mathbb{C} \setminus \mathbb{Z}. \quad (2.79)$$

In particular $\sigma(A) = \mathbb{Z}$. \diamond

If $z, z' \in \rho(A)$, we have the **first resolvent formula**

$$R_A(z) - R_A(z') = (z - z')R_A(z)R_A(z') = (z - z')R_A(z')R_A(z). \quad (2.80)$$

In fact,

$$\begin{aligned} (A - z)^{-1} - (z - z')(A - z)^{-1}(A - z')^{-1} = \\ (A - z)^{-1}(1 - (z - A + A - z')(A - z')^{-1}) = (A - z')^{-1}, \end{aligned} \quad (2.81)$$

which proves the first equality. The second follows after interchanging z and z' . Now fix $z' = z_0$ and use (2.80) recursively to obtain

$$R_A(z) = \sum_{j=0}^n (z - z_0)^j R_A(z_0)^{j+1} + (z - z_0)^{n+1} R_A(z_0)^{n+1} R_A(z). \quad (2.82)$$

The sequence of bounded operators

$$R_n = \sum_{j=0}^n (z - z_0)^j R_A(z_0)^{j+1} \quad (2.83)$$

converges to a bounded operator if $|z - z_0| < \|R_A(z_0)\|^{-1}$ and clearly we expect $z \in \rho(A)$ and $R_n \rightarrow R_A(z)$ in this case. Let $R_\infty = \lim_{n \rightarrow \infty} R_n$ and set $\varphi_n = R_n \psi$, $\varphi = R_\infty \psi$ for some $\psi \in \mathfrak{H}$. Then a quick calculation shows

$$AR_n \psi = \psi + (z - z_0)\varphi_{n-1} + z_0\varphi_n. \quad (2.84)$$

Hence $(\varphi_n, A\varphi_n) \rightarrow (\varphi, \psi + z\varphi)$ shows $\varphi \in \mathfrak{D}(A)$ (since A is closed) and $(A - z)R_\infty \psi = \psi$. Similarly, for $\psi \in \mathfrak{D}(A)$,

$$R_n A \psi = \psi + (z - z_0)\varphi_{n-1} + z_0\varphi_n \quad (2.85)$$

and hence $R_\infty(A - z)\psi = \psi$ after taking the limit. Thus $R_\infty = R_A(z)$ as anticipated.

If A is bounded, a similar argument verifies the **Neumann series** for the resolvent

$$\begin{aligned} R_A(z) &= -\sum_{j=0}^{n-1} \frac{A^j}{z^{j+1}} + \frac{1}{z^n} A^n R_A(z) \\ &= -\sum_{j=0}^{\infty} \frac{A^j}{z^{j+1}}, \quad |z| > \|A\|. \end{aligned} \quad (2.86)$$

In summary we have proved the following

Theorem 2.11. *The resolvent set $\rho(A)$ is open and $R_A : \rho(A) \rightarrow \mathfrak{L}(\mathfrak{H})$ is holomorphic, that is, it has an absolutely convergent power series expansion around every point $z_0 \in \rho(A)$. In addition,*

$$\|R_A(z)\| \geq \text{dist}(z, \sigma(A))^{-1} \quad (2.87)$$

and if A is bounded we have $\{z \in \mathbb{C} \mid |z| > \|A\|\} \subseteq \rho(A)$.

As a consequence we obtain the useful

Lemma 2.12. *We have $z \in \sigma(A)$ if there is a sequence $\psi_n \in \mathfrak{D}(A)$ such that $\|\psi_n\| = 1$ and $\|(A - z)\psi_n\| \rightarrow 0$. If z is a boundary point of $\rho(A)$, then the converse is also true. Such a sequence is called **Weyl sequence**.*

Proof. Let ψ_n be a Weyl sequence. Then $z \in \rho(A)$ is impossible by $1 = \|\psi_n\| = \|R_A(z)(A - z)\psi_n\| \leq \|R_A(z)\| \|(A - z)\psi_n\| \rightarrow 0$. Conversely, by (2.87) there is a sequence $z_n \rightarrow z$ and corresponding vectors $\varphi_n \in \mathfrak{H}$ such that $\|R_A(z)\varphi_n\| \|\varphi_n\|^{-1} \rightarrow \infty$. Let $\psi_n = R_A(z_n)\varphi_n$ and rescale φ_n such that $\|\psi_n\| = 1$. Then $\|\varphi_n\| \rightarrow 0$ and hence

$$\|(A - z)\psi_n\| = \|\varphi_n + (z_n - z)\psi_n\| \leq \|\varphi_n\| + |z - z_n| \rightarrow 0 \quad (2.88)$$

shows that ψ_n is a Weyl sequence. \square

Let us also note the following spectral mapping result.

Lemma 2.13. *Suppose A is injective, then*

$$\sigma(A^{-1}) \setminus \{0\} = (\sigma(A) \setminus \{0\})^{-1}. \quad (2.89)$$

In addition, we have $A\psi = z\psi$ if and only if $A^{-1}\psi = z^{-1}\psi$.

Proof. Suppose $z \in \rho(A) \setminus \{0\}$. Then we claim

$$R_{A^{-1}}(z^{-1}) = -zAR_A(z) = -z - R_A(z). \quad (2.90)$$

In fact, the right hand side is a bounded operator from $\mathfrak{H} \rightarrow \text{Ran}(A) = \mathfrak{D}(A^{-1})$ and

$$(A^{-1} - z^{-1})(-zAR_A(z))\varphi = (-z + A)R_A(z)\varphi = \varphi, \quad \varphi \in \mathfrak{H}. \quad (2.91)$$

Conversely, if $\psi \in \mathfrak{D}(A^{-1}) = \text{Ran}(A)$ we have $\psi = A\varphi$ and hence

$$(-zAR_A(z))(A^{-1} - z^{-1})\psi = AR_A(z)((A - z)\varphi) = A\varphi = \psi. \quad (2.92)$$

Thus $z^{-1} \in \rho(A^{-1})$. The rest follows after interchanging the roles of A and A^{-1} . \square

Next, let us characterize the spectra of self-adjoint operators.

Theorem 2.14. *Let A be symmetric. Then A is self-adjoint if and only if $\sigma(A) \subseteq \mathbb{R}$ and $A \geq 0$ if and only if $\sigma(A) \subseteq [0, \infty)$. Moreover, $\|R_A(z)\| \leq |\text{Im}(z)|^{-1}$ and, if $A \geq 0$, $\|R_A(\lambda)\| \leq |\lambda|^{-1}$, $\lambda < 0$.*

Proof. If $\sigma(A) \subseteq \mathbb{R}$, then $\text{Ran}(A + z) = \mathfrak{H}$, $z \in \mathbb{C} \setminus \mathbb{R}$, and hence A is self-adjoint by Lemma 2.6. Conversely, if A is self-adjoint (resp. $A \geq 0$), then $R_A(z)$ exists for $z \in \mathbb{C} \setminus \mathbb{R}$ (resp. $z \in \mathbb{C} \setminus (-\infty, 0]$) and satisfies the given estimates as has been shown in the proof of Lemma 2.6. \square

In particular, we obtain

Theorem 2.15. *Let A be self-adjoint, then*

$$\inf \sigma(A) = \inf_{\psi \in \mathfrak{D}(A), \|\psi\|=1} \langle \psi, A\psi \rangle. \quad (2.93)$$

For the eigenvalues and corresponding eigenfunctions we have:

Lemma 2.16. *Let A be symmetric. Then all eigenvalues are real and eigenvectors corresponding to different eigenvalues are orthogonal.*

Proof. If $A\psi_j = \lambda_j\psi_j$, $j = 1, 2$, we have

$$\lambda_1 \|\psi_1\|^2 = \langle \psi_1, \lambda_1 \psi_1 \rangle = \langle \psi_1, A\psi_1 \rangle = \langle \psi_1, A\psi_1 \rangle = \langle \lambda_1 \psi_1, \psi_1 \rangle = \lambda_1^* \|\psi_1\|^2 \quad (2.94)$$

and

$$(\lambda_1 - \lambda_2) \langle \psi_1, \psi_2 \rangle = \langle A\psi_1, \psi_2 \rangle - \langle A\psi_1, \psi_2 \rangle = 0, \quad (2.95)$$

finishing the proof. \square

The result does not imply that two linearly independent eigenfunctions to the same eigenvalue are orthogonal. However, it is no restriction to assume that they are since we can use Gram-Schmidt to find an orthonormal basis for $\text{Ker}(A - \lambda)$. If \mathfrak{H} is finite dimensional, we can always find an orthonormal basis of eigenvectors. In the infinite dimensional case this is no longer true in general. However, if there is an orthonormal basis of eigenvectors, then A is essentially self-adjoint.

Theorem 2.17. *Suppose A is a symmetric operator which has an orthonormal basis of eigenfunctions $\{\varphi_j\}$, then A is essentially self-adjoint. In particular, it is essentially self-adjoint on $\text{span}\{\varphi_j\}$.*

Proof. Consider the set of all finite linear combinations $\psi = \sum_{j=0}^n c_j \varphi_j$ which is dense in \mathfrak{H} . Then $\phi = \sum_{j=0}^n \frac{c_j}{\lambda_j \pm i} \varphi_j \in \mathfrak{D}(A)$ and $(A \pm i)\phi = \psi$ shows that $\text{Ran}(A \pm i)$ is dense. \square

In addition, we note the following asymptotic expansion for the resolvent.

Lemma 2.18. *Suppose A is self-adjoint. For every $\psi \in \mathfrak{H}$ we have*

$$\lim_{\text{Im}(z) \rightarrow \infty} \|AR_A(z)\psi\| = 0. \quad (2.96)$$

In particular, if $\psi \in \mathfrak{D}(A^n)$, then

$$R_A(z)\psi = -\sum_{j=0}^n \frac{A^j \psi}{z^{j+1}} + o\left(\frac{1}{z^{n+1}}\right), \quad \text{as } \text{Im}(z) \rightarrow \infty. \quad (2.97)$$

Proof. It suffices to prove the first claim since the second then follows as in (2.86).

Write $\psi = \tilde{\psi} + \varphi$, where $\tilde{\psi} \in \mathfrak{D}(A)$ and $\|\varphi\| \leq \varepsilon$. Then

$$\begin{aligned} \|AR_A(z)\psi\| &\leq \|R_A(z)A\tilde{\psi}\| + \|AR_A(z)\varphi\| \\ &\leq \frac{\|A\tilde{\psi}\|}{\text{Im}(z)} + \|\varphi\|, \end{aligned} \quad (2.98)$$

by (2.48), finishing the proof. \square

Similarly, we can characterize the spectra of unitary operators. Recall that a bijection U is called unitary if $\langle U\psi, U\psi \rangle = \langle \psi, U^*U\psi \rangle = \langle \psi, \psi \rangle$. Thus U is unitary if and only if

$$U^* = U^{-1}. \quad (2.99)$$

Theorem 2.19. *Let U be unitary, then $\sigma(U) \subseteq \{z \in \mathbb{C} \mid |z| = 1\}$. All eigenvalues have modulus one and eigenvectors corresponding to different eigenvalues are orthogonal.*

Proof. Since $\|U\| \leq 1$ we have $\sigma(U) \subseteq \{z \in \mathbb{C} \mid |z| \leq 1\}$. Moreover, U^{-1} is also unitary and hence $\sigma(U) \subseteq \{z \in \mathbb{C} \mid |z| \geq 1\}$ by Lemma 2.13. If $U\psi_j = z_j\psi_j$, $j = 1, 2$ we have

$$(z_1 - z_2)\langle \psi_1, \psi_2 \rangle = \langle U^*\psi_1, \psi_2 \rangle - \langle \psi_1, U\psi_2 \rangle = 0 \quad (2.100)$$

since $U\psi = z\psi$ implies $U^*\psi = U^{-1}\psi = z^{-1}\psi = z^*\psi$. \square

Problem 2.10. *What is the spectrum of an orthogonal projection?*

Problem 2.11. *Compute the resolvent of $Af = f'$, $\mathfrak{D}(A) = \{f \in H^1[0, 1] \mid f(0) = 0\}$ and show that unbounded operators can have empty spectrum.*

Problem 2.12. *Compute the eigenvalues and eigenvectors of $A = -\frac{d^2}{dx^2}$, $\mathfrak{D}(A) = \{f \in H^2(0, \pi) \mid f(0) = f(\pi) = 0\}$. Compute the resolvent of A .*

Problem 2.13. Find a Weyl sequence for the self-adjoint operator $A = -\frac{d^2}{dx^2}$, $\mathfrak{D}(A) = H^2(\mathbb{R})$ for $z \in (0, \infty)$. What is $\sigma(A)$? (Hint: Cut off the solutions of $-u''(x) = zu(x)$ outside a finite ball.)

Problem 2.14. Suppose A is bounded. Show that the spectrum of AA^* and A^*A coincide away from 0 by showing

$$R_{AA^*}(z) = \frac{1}{z} (AR_{A^*A}(z)A^* - 1), \quad R_{A^*A}(z) = \frac{1}{z} (A^*R_{AA^*}(z)A - 1). \quad (2.101)$$

2.4. Orthogonal sums of operators

Let \mathfrak{H}_j , $j = 1, 2$, be two given Hilbert spaces and let $A_j : \mathfrak{D}(A_j) \rightarrow \mathfrak{H}_j$ be two given operators. Setting $\mathfrak{H} = \mathfrak{H}_1 \oplus \mathfrak{H}_2$ we can define an operator

$$A = A_1 \oplus A_2, \quad \mathfrak{D}(A) = \mathfrak{D}(A_1) \oplus \mathfrak{D}(A_2) \quad (2.102)$$

by setting $A(\psi_1 + \psi_2) = A_1\psi_1 + A_2\psi_2$ for $\psi_j \in \mathfrak{D}(A_j)$. Clearly A is closed, (essentially) self-adjoint, etc., if and only if both A_1 and A_2 are. The same considerations apply to countable orthogonal sums

$$A = \bigoplus_j A_j, \quad \mathfrak{D}(A) = \bigoplus_j \mathfrak{D}(A_j) \quad (2.103)$$

and we have

Theorem 2.20. Suppose A_j are self-adjoint operators on \mathfrak{H}_j , then $A = \bigoplus_j A_j$ is self-adjoint and

$$R_A(z) = \bigoplus_j R_{A_j}(z), \quad z \in \rho(A) = \mathbb{C} \setminus \sigma(A) \quad (2.104)$$

where

$$\sigma(A) = \overline{\bigcup_j \sigma(A_j)} \quad (2.105)$$

(the closure can be omitted if there are only finitely many terms).

Proof. By $\text{Ran}(A \pm i) = (A \pm i)\mathfrak{D}(A) = \bigoplus_j (A_j \pm i)\mathfrak{D}(A_j) = \bigoplus_j \mathfrak{H}_j = \mathfrak{H}$ we see that A is self-adjoint. Moreover, if $z \in \sigma(A_j)$ there is a corresponding Weyl sequence $\psi_n \in \mathfrak{D}(A_j) \subseteq \mathfrak{D}(A)$ and hence $z \in \sigma(A)$. Conversely, if $z \notin \overline{\bigcup_j \sigma(A_j)}$ set $\varepsilon = d(z, \bigcup_j \sigma(A_j)) > 0$, then $\|R_{A_j}(z)\| \leq \varepsilon^{-1}$ and hence $\|\bigoplus_j R_{A_j}(z)\| \leq \varepsilon^{-1}$ shows that $z \in \rho(A)$. \square

Conversely, given an operator A it might be useful to write A as orthogonal sum and investigate each part separately.

Let $\mathfrak{H}_1 \subseteq \mathfrak{H}$ be a closed subspace and let P_1 be the corresponding projector. We say that \mathfrak{H}_1 **reduces** the operator A if $P_1A \subseteq AP_1$. Note that this

implies $P_1\mathfrak{D}(A) \subseteq \mathfrak{D}(A)$. Moreover, if we set $\mathfrak{H}_2 = \mathfrak{H}_1^\perp$, we have $\mathfrak{H} = \mathfrak{H}_1 \oplus \mathfrak{H}_2$ and $P_2 = \mathbb{I} - P_1$ reduces A as well.

Lemma 2.21. *Suppose $\mathfrak{H}_1 \subseteq \mathfrak{H}$ reduces A , then $A = A_1 \oplus A_2$, where*

$$A_j\psi = A\psi, \quad \mathfrak{D}(A_j) = P_j\mathfrak{D}(A) \subseteq \mathfrak{D}(A). \quad (2.106)$$

If A is closable, then \mathfrak{H}_1 also reduces \overline{A} and

$$\overline{A} = \overline{A_1} \oplus \overline{A_2}. \quad (2.107)$$

Proof. As already noted, $P_1\mathfrak{D}(A) \subseteq \mathfrak{D}(A)$ and hence $P_2\mathfrak{D}(A) = (\mathbb{I} - P_1)\mathfrak{D}(A) \subseteq \mathfrak{D}(A)$. Thus we see $\mathfrak{D}(A) = \mathfrak{D}(A_1) \oplus \mathfrak{D}(A_2)$. Moreover, if $\psi \in \mathfrak{D}(A_j)$ we have $A\psi = AP_j\psi = P_jA\psi \in \mathfrak{H}_j$ and thus $A_j : \mathfrak{D}(A_j) \rightarrow \mathfrak{H}_j$ which proves the first claim.

Now let us turn to the second claim. Clearly $\overline{A} \subseteq \overline{A_1} \oplus \overline{A_2}$. Conversely, suppose $\psi \in \mathfrak{D}(\overline{A})$, then there is a sequence $\psi_n \in \mathfrak{D}(A)$ such that $\psi_n \rightarrow \psi$ and $A\psi_n \rightarrow A\psi$. Then $P_j\psi_n \rightarrow P_j\psi$ and $AP_j\psi_n = P_jA\psi_n \rightarrow PA\psi$. In particular, $P_j\psi \in \mathfrak{D}(\overline{A})$ and $AP_j\psi = PA\psi$. \square

If A is self-adjoint, then \mathfrak{H}_1 reduces A if $P_1\mathfrak{D}(A) \subseteq \mathfrak{D}(A)$ and $AP_1\psi \in \mathfrak{H}_1$ for every $\psi \in \mathfrak{D}(A)$. In fact, if $\psi \in \mathfrak{D}(A)$ we can write $\psi = \psi_1 \oplus \psi_2$, $\psi_j = P_j\psi \in \mathfrak{D}(A)$. Since $AP_1\psi = A\psi_1$ and $P_1A\psi = P_1A\psi_1 + P_1A\psi_2 = A\psi_1 + P_1A\psi_2$ we need to show $P_1A\psi_2 = 0$. But this follows since

$$\langle \varphi, P_1A\psi_2 \rangle = \langle AP_1\varphi, \psi_2 \rangle = 0 \quad (2.108)$$

for every $\varphi \in \mathfrak{D}(A)$.

Problem 2.15. *Show $(A_1 \oplus A_2)^* = A_1^* \oplus A_2^*$.*

2.5. Self-adjoint extensions

It is safe to skip this entire section on first reading.

In many physical applications a symmetric operator is given. If this operator turns out to be essentially self-adjoint, there is a unique self-adjoint extension and everything is fine. However, if it is not, it is important to find out if there are self-adjoint extensions at all (for physical problems there better are) and to classify them.

In Section 2.2 we have seen that A is essentially self-adjoint if $\text{Ker}(A^* - z) = \text{Ker}(A^* - z^*) = \{0\}$ for one $z \in \mathbb{C} \setminus \mathbb{R}$. Hence self-adjointness is related to the dimension of these spaces and one calls the numbers

$$d_\pm(A) = \dim K_\pm, \quad K_\pm = \text{Ran}(A \pm i)^\perp = \text{Ker}(A^* \mp i), \quad (2.109)$$

defect indices of A (we have chosen $z = i$ for simplicity, any other $z \in \mathbb{C} \setminus \mathbb{R}$ would be as good). If $d_-(A) = d_+(A) = 0$ there is one self-adjoint extension of A , namely \overline{A} . But what happens in the general case? Is there more than

one extension, or maybe none at all? These questions can be answered by virtue of the **Cayley transform**

$$V = (A - i)(A + i)^{-1} : \text{Ran}(A + i) \rightarrow \text{Ran}(A - i). \quad (2.110)$$

Theorem 2.22. *The Cayley transform is a bijection from the set of all symmetric operators A to the set of all isometric operators V (i.e., $\|V\varphi\| = \|\varphi\|$ for all $\varphi \in \mathfrak{D}(V)$) for which $\text{Ran}(1 + V)$ is dense.*

Proof. Since A is symmetric we have $\|(A \pm i)\psi\|^2 = \|A\psi\|^2 + \|\psi\|^2$ for all $\psi \in \mathfrak{D}(A)$ by a straightforward computation. And thus for every $\varphi = (A + i)\psi \in \mathfrak{D}(V) = \text{Ran}(A + i)$ we have

$$\|V\varphi\| = \|(A - i)\psi\| = \|(A + i)\psi\| = \|\varphi\|. \quad (2.111)$$

Next observe

$$1 \pm V = ((A - i) \pm (A + i))(A + i)^{-1} = \begin{cases} 2A(A + i)^{-1} \\ 2i(A + i)^{-1} \end{cases}, \quad (2.112)$$

which shows $\mathfrak{D}(A) = \text{Ran}(1 - V)$ and

$$A = i(1 + V)(1 - V)^{-1}. \quad (2.113)$$

Conversely, let V be given and use the last equation to define A .

Since V is isometric we have $\langle (1 \pm V)\varphi, (1 \mp V)\varphi \rangle = \pm 2i\text{Im}\langle V\varphi, \varphi \rangle$ for all $\varphi \in \mathfrak{D}(V)$ by a straightforward computation. And thus for every $\psi = (1 - V)\varphi \in \mathfrak{D}(A) = \text{Ran}(1 - V)$ we have

$$\langle A\psi, \psi \rangle = -i\langle (1 + V)\varphi, (1 - V)\varphi \rangle = i\langle (1 - V)\varphi, (1 + V)\varphi \rangle = \langle \psi, A\psi \rangle, \quad (2.114)$$

that is, A is symmetric. Finally observe

$$A \pm i = ((1 + V) \pm (1 - V))(1 - V)^{-1} = \begin{cases} 2i(1 - V)^{-1} \\ 2iV(1 - V)^{-1} \end{cases}, \quad (2.115)$$

which shows that A is the Cayley transform of V and finishes the proof. \square

Thus A is self-adjoint if and only if its Cayley transform V is unitary. Moreover, finding a self-adjoint extension of A is equivalent to finding a unitary extensions of V and this in turn is equivalent to (taking the closure and) finding a unitary operator from $\mathfrak{D}(V)^\perp$ to $\text{Ran}(V)^\perp$. This is possible if and only if both spaces have the same dimension, that is, if and only if $d_+(A) = d_-(A)$.

Theorem 2.23. *A symmetric operator has self-adjoint extensions if and only if its defect indices are equal.*

In this case let A_1 be a self-adjoint extension, V_1 its Cayley transform. Then

$$\mathfrak{D}(A_1) = \mathfrak{D}(A) + (1 - V_1)K_+ = \{\psi + \varphi_+ - V_1\varphi_+ \mid \psi \in \mathfrak{D}(A), \varphi_+ \in K_+\} \quad (2.116)$$

and

$$A_1(\psi + \varphi_+ - V_1\varphi_+) = A\psi + i\varphi_+ + iV_1\varphi_+. \quad (2.117)$$

Moreover,

$$(A_1 \pm i)^{-1} = (A \pm i)^{-1} \oplus \frac{\mp i}{2} \sum_j \langle \varphi_j^\pm, \cdot \rangle (\varphi_j^\pm - \varphi_j^\mp), \quad (2.118)$$

where $\{\varphi_j^+\}$ is an orthonormal basis for K_+ and $\varphi_j^- = V_1\varphi_j^+$.

Corollary 2.24. *Suppose A is a closed symmetric operator with equal defect indices $d = d_+(A) = d_-(A)$. Then $\dim \text{Ker}(A^* - z^*) = d$ for all $z \in \mathbb{C} \setminus \mathbb{R}$.*

Proof. First of all we note that instead of $z = i$ we could use $V(z) = (A + z^*)(A + z)^{-1}$ for any $z \in \mathbb{C} \setminus \mathbb{R}$. Let $d_\pm(z) = \dim K_\pm(z)$, $K_+(z) = \text{Ran}(A + z)^\perp$ respectively $K_-(z) = \text{Ran}(A + z^*)^\perp$. The same arguments as before show that there is a one to one correspondence between the self-adjoint extensions of A and the unitary operators on $\mathbb{C}^{d(z)}$. Hence $d(z_1) = d(z_2) = d_\pm(A)$. \square

Example. Recall the operator $A = -i\frac{d}{dx}$, $\mathfrak{D}(A) = \{f \in H^1(0, 2\pi) | f(0) = f(2\pi) = 0\}$ with adjoint $A^* = -i\frac{d}{dx}$, $\mathfrak{D}(A^*) = H^1(0, 2\pi)$.

Clearly

$$K_\pm = \text{span}\{e^{\mp x}\} \quad (2.119)$$

is one dimensional and hence all unitary maps are of the form

$$V_\theta e^{2\pi-x} = e^{i\theta} e^x, \quad \theta \in [0, 2\pi). \quad (2.120)$$

The functions in the domain of the corresponding operator A_θ are given by

$$f_\theta(x) = f(x) + \alpha(e^{2\pi-x} - e^{i\theta}e^x), \quad f \in \mathfrak{D}(A), \alpha \in \mathbb{C}. \quad (2.121)$$

In particular, f_θ satisfies

$$f_\theta(2\pi) = e^{i\tilde{\theta}} f_\theta(0), \quad e^{i\tilde{\theta}} = \frac{1 - e^{i\theta}e^{2\pi}}{e^{2\pi} - e^{i\theta}} \quad (2.122)$$

and thus we have

$$\mathfrak{D}(A_\theta) = \{f \in H^1(0, 2\pi) | f(2\pi) = e^{i\tilde{\theta}} f(0)\}. \quad (2.123)$$

\diamond

Concerning closures we note that a bounded operator is closed if and only if its domain is closed and any operator is closed if and only if its inverse is closed. Hence we have

Lemma 2.25. *The following items are equivalent.*

- A is closed.
- $\mathfrak{D}(V) = \text{Ran}(A + i)$ is closed.

- $\text{Ran}(V) = \text{Ran}(A - i)$ is closed.
- V is closed.

Next, we give a useful criterion for the existence of self-adjoint extensions. A skew linear map $C : \mathfrak{H} \rightarrow \mathfrak{H}$ is called a **conjugation** if it satisfies $C^2 = \mathbb{I}$ and $\langle C\psi, C\varphi \rangle = \langle \psi, \varphi \rangle$. The prototypical example is of course complex conjugation $C\psi = \psi^*$. An operator A is called **C -real** if

$$C\mathfrak{D}(A) \subseteq \mathfrak{D}(A), \quad \text{and} \quad AC\psi = CA\psi, \quad \psi \in \mathfrak{D}(A). \quad (2.124)$$

Note that in this case $C\mathfrak{D}(A) = \mathfrak{D}(A)$, since $\mathfrak{D}(A) = C^2\mathfrak{D}(A) \subseteq C\mathfrak{D}(A)$.

Theorem 2.26. *Suppose the symmetric operator A is C -real, then its defect indices are equal.*

Proof. Let $\{\varphi_j\}$ be an orthonormal set in $\text{Ran}(A + i)^\perp$. Then $\{K\varphi_j\}$ is an orthonormal set in $\text{Ran}(A - i)^\perp$. Hence $\{\varphi_j\}$ is an orthonormal basis for $\text{Ran}(A + i)^\perp$ if and only if $\{K\varphi_j\}$ is an orthonormal basis for $\text{Ran}(A - i)^\perp$. Hence the two spaces have the same dimension. \square

Finally, we note the following useful formula for the difference of resolvents of self-adjoint extensions.

Lemma 2.27. *If A_j , $j = 1, 2$ are self-adjoint extensions and if $\{\varphi_j(z)\}$ is an orthonormal basis for $\text{Ker}(A^* - z^*)$, then*

$$(A_1 - z)^{-1} - (A_2 - z)^{-1} = \sum_{j,k} (\alpha_{jk}^1(z) - \alpha_{jk}^2(z)) \langle \varphi_k(z), \cdot \rangle \varphi_k(z^*), \quad (2.125)$$

where

$$\alpha_{jk}^l(z) = \langle \varphi_j(z^*), (A_l - z)^{-1} \varphi_k(z) \rangle. \quad (2.126)$$

Proof. First observe that $((A_1 - z)^{-1} - (A_2 - z)^{-1})\varphi$ is zero for every $\varphi \in \text{Ran}(A - z)$. Hence it suffices to consider it for vectors $\varphi = \sum_j \langle \varphi_j(z), \varphi \rangle \varphi_j(z) \in \text{Ran}(A - z)^\perp$. Hence we have

$$(A_1 - z)^{-1} - (A_2 - z)^{-1} = \sum_j \langle \varphi_j(z), \cdot \rangle \psi_j(z), \quad (2.127)$$

where

$$\psi_j(z) = ((A_1 - z)^{-1} - (A_2 - z)^{-1})\varphi_j(z). \quad (2.128)$$

Now computation the adjoint once using $((A_j - z)^{-1})^* = (A_j - z^*)^{-1}$ and once using $(\sum_j \langle \psi_j, \cdot \rangle \varphi_j)^* = \sum_j \langle \varphi_j, \cdot \rangle \psi_j$ we obtain

$$\sum_j \langle \varphi_j(z^*), \cdot \rangle \psi_j(z^*) = \sum_j \langle \psi_j(z), \cdot \rangle \varphi_j(z). \quad (2.129)$$

Evaluating at $\varphi_k(z)$ implies

$$\psi_k(z) = \sum_j \langle \psi_j(z^*), \varphi_k(z) \rangle \varphi_j(z^*) \quad (2.130)$$

and finishes the proof. \square

Problem 2.16. Compute the defect indices of $A_0 = i\frac{d}{dx}$, $\mathfrak{D}(A_0) = C_c^\infty((0, \infty))$. Can you give a self-adjoint extension of A_0 .

2.6. Appendix: Absolutely continuous functions

Let $(a, b) \subseteq \mathbb{R}$ be some interval. We denote by

$$AC(a, b) = \{f \in C(a, b) \mid f(x) = f(c) + \int_c^x g(t)dt, c \in (a, b), g \in L_{loc}^1(a, b)\} \quad (2.131)$$

the set of all **absolutely continuous functions**. That is, f is absolutely continuous if and only if it can be written as the integral of some locally integrable function. Note that $AC(a, b)$ is a vector space.

By Corollary A.33 $f(x) = f(c) + \int_c^x g(t)dt$ is differentiable a.e. (with respect to Lebesgue measure) and $f'(x) = g(x)$. In particular, g is determined uniquely a.e..

If $[a, b]$ is a compact interval we set

$$AC[a, b] = \{f \in AC(a, b) \mid g \in L^1(a, b)\} \subseteq C[a, b]. \quad (2.132)$$

If $f, g \in AC[a, b]$ we have the formula of partial integration

$$\int_a^b f(x)g'(x) = f(b)g(b) - f(a)g(a) - \int_a^b f'(x)g(x)dx. \quad (2.133)$$

We set

$$H^m(a, b) = \{f \in L^2(a, b) \mid f^{(j)} \in AC(a, b), f^{(j+1)} \in L^2(a, b), 0 \leq j \leq m-1\}. \quad (2.134)$$

Then we have

Lemma 2.28. Suppose $f \in H^m(a, b)$, $m \geq 1$. Then f is bounded and $\lim_{x \downarrow a} f^{(j)}(x)$ respectively $\lim_{x \uparrow b} f^{(j)}(x)$ exist for $0 \leq j \leq m-1$. Moreover, the limit is zero if the endpoint is infinite.

Proof. If the endpoint is finite, then $f^{(j+1)}$ is integrable near this endpoint and hence the claim follows. If the endpoint is infinite, note that

$$|f^{(j)}(x)|^2 = |f^{(j)}(c)|^2 + 2 \int_c^x \operatorname{Re}(f^{(j)}(t)^* f^{(j+1)}(t))dt \quad (2.135)$$

shows that the limit exists (dominated convergence). Since $f^{(j)}$ is square integrable the limit must be zero. \square

Let me remark, that it suffices to check that the function plus the highest derivative is in L^2 , the lower derivatives are then automatically in L^2 . That is,

$$H^m(a, b) = \{f \in L^2(a, b) \mid f^{(j)} \in AC(a, b), 0 \leq j \leq m - 1, f^{(r)} \in L^2(a, b)\}. \quad (2.136)$$

For a finite endpoint this is straightforward. For an infinite endpoint this can also be shown directly, but it is much easier to use the Fourier transform (compare Section 7.1).

Problem 2.17. Show (2.133). (Hint: Fubini)

Problem 2.18. Show that $H^1(a, b)$ together with the norm

$$\|f\|_{2,1}^2 = \int_a^b |f(t)|^2 dt + \int_a^b |f'(t)|^2 dt \quad (2.137)$$

is a Hilbert space.

Problem 2.19. What is the closure of $C_0^\infty(a, b)$ in $H^1(a, b)$? (Hint: Start with the case where (a, b) is finite.)

The spectral theorem

The time evolution of a quantum mechanical system is governed by the Schrödinger equation

$$i\frac{d}{dt}\psi(t) = H\psi(t). \quad (3.1)$$

If $\mathfrak{H} = \mathbb{C}^n$, and H is hence a matrix, this system of ordinary differential equations is solved by the matrix exponential

$$\psi(t) = \exp(-itH)\psi(0). \quad (3.2)$$

This matrix exponential can be defined by a convergent power series

$$\exp(-itH) = \sum_{n=0}^{\infty} \frac{(-it)^n}{n!} H^n. \quad (3.3)$$

For this approach the boundedness of H is crucial, which might not be the case for a quantum system. However, the best way to compute the matrix exponential, and to understand the underlying dynamics, is to diagonalize H . But how do we diagonalize a self-adjoint operator? The answer is known as the spectral theorem.

3.1. The spectral theorem

In this section we want to address the problem of defining functions of a self-adjoint operator A in a natural way, that is, such that

$$(f+g)(A) = f(A)+g(A), \quad (fg)(A) = f(A)g(A), \quad (f^*)(A) = f(A)^*. \quad (3.4)$$

As long as f and g are polynomials, no problems arise. If we want to extend this definition to a larger class of functions, we will need to perform some limiting procedure. Hence we could consider convergent power series or equip the space of polynomials with the sup norm. In both cases this only

works if the operator A is bounded. To overcome this limitation, we will use characteristic functions $\chi_\Omega(A)$ instead of powers A^j . Since $\chi_\Omega(\lambda)^2 = \chi_\Omega(\lambda)$, the corresponding operators should be orthogonal projections. Moreover, we should also have $\chi_{\mathbb{R}}(A) = \mathbb{I}$ and $\chi_\Omega(A) = \sum_{j=1}^n \chi_{\Omega_j}(A)$ for any finite union $\Omega = \bigcup_{j=1}^n \Omega_j$ of disjoint sets. The only remaining problem is of course the definition of $\chi_\Omega(A)$. However, we will defer this problem and begin by developing a functional calculus for a family of characteristic functions $\chi_\Omega(A)$.

Denote the Borel sigma algebra of \mathbb{R} by \mathfrak{B} . A **projection-valued measure** is a map

$$P : \mathfrak{B} \rightarrow \mathfrak{L}(\mathfrak{H}), \quad \Omega \mapsto P(\Omega), \quad (3.5)$$

from the Borel sets to the set of orthogonal projections, that is, $P(\Omega)^* = P(\Omega)$ and $P(\Omega)^2 = P(\Omega)$, such that the following two conditions hold:

- (i) $P(\mathbb{R}) = \mathbb{I}$.
- (ii) If $\Omega = \bigcup_n \Omega_n$ with $\Omega_n \cap \Omega_m = \emptyset$ for $n \neq m$, then $\sum_n P(\Omega_n)\psi = P(\Omega)\psi$ for every $\psi \in \mathfrak{H}$ (strong σ -additivity).

Note that we require strong convergence, $\sum_n P(\Omega_n)\psi = P(\Omega)\psi$, rather than norm convergence, $\sum_n P(\Omega_n) = P(\Omega)$. In fact, norm convergence does not even hold in the simplest case where $\mathfrak{H} = L^2(I)$ and $P(\Omega) = \chi_\Omega$ (multiplication operator), since for a multiplication operator the norm is just the sup norm of the function. Furthermore, it even suffices to require weak convergence, since $w\text{-lim } P_n = P$ for some orthogonal projections implies $s\text{-lim } P_n = P$ by $\langle \psi, P_n \psi \rangle = \langle \psi, P_n^2 \psi \rangle = \langle P_n \psi, P_n \psi \rangle = \|P_n \psi\|^2$ together with Lemma 1.11 (iv).

Example. Let $\mathfrak{H} = \mathbb{C}^n$ and $A \in \text{GL}(n)$ be some symmetric matrix. Let $\lambda_1, \dots, \lambda_m$ be its (distinct) eigenvalues and let P_j be the projections onto the corresponding eigenspaces. Then

$$P_A(\Omega) = \sum_{\{j|\lambda_j \in \Omega\}} P_j \quad (3.6)$$

is a projection valued measure. \diamond

Example. Let $\mathfrak{H} = L^2(\mathbb{R})$ and let f be a real-valued measurable function. Then

$$P(\Omega) = \chi_{f^{-1}(\Omega)} \quad (3.7)$$

is a projection valued measure (Problem 3.2). \diamond

It is straightforward to verify that any projection-valued measure satisfies

$$P(\emptyset) = 0, \quad P(\mathbb{R} \setminus \Omega) = \mathbb{I} - P(\Omega), \quad (3.8)$$

and

$$P(\Omega_1 \cup \Omega_2) + P(\Omega_1 \cap \Omega_2) = P(\Omega_1) + P(\Omega_2). \quad (3.9)$$

Moreover, we also have

$$P(\Omega_1)P(\Omega_2) = P(\Omega_1 \cap \Omega_2). \quad (3.10)$$

Indeed, suppose $\Omega_1 \cap \Omega_2 = \emptyset$ first. Then, taking the square of (3.9) we infer

$$P(\Omega_1)P(\Omega_2) + P(\Omega_2)P(\Omega_1) = 0. \quad (3.11)$$

Multiplying this equation from the right by $P(\Omega_2)$ shows that $P(\Omega_1)P(\Omega_2) = -P(\Omega_2)P(\Omega_1)P(\Omega_2)$ is self-adjoint and thus $P(\Omega_1)P(\Omega_2) = P(\Omega_2)P(\Omega_1) = 0$. For the general case $\Omega_1 \cap \Omega_2 \neq \emptyset$ we now have

$$\begin{aligned} P(\Omega_1)P(\Omega_2) &= (P(\Omega_1 - \Omega_2) + P(\Omega_1 \cap \Omega_2))(P(\Omega_2 - \Omega_1) + P(\Omega_1 \cap \Omega_2)) \\ &= P(\Omega_1 \cap \Omega_2) \end{aligned} \quad (3.12)$$

as stated.

To every projection-valued measure there corresponds a **resolution of the identity**

$$P(\lambda) = P((-\infty, \lambda]) \quad (3.13)$$

which has the properties (Problem 3.3):

- (i) $P(\lambda)$ is an orthogonal projection.
- (ii) $P(\lambda_1) \leq P(\lambda_2)$ (that is $\langle \psi, P(\lambda_1)\psi \rangle \leq \langle \psi, P(\lambda_2)\psi \rangle$) or equivalently $\text{Ran}(P(\lambda_1)) \subseteq \text{Ran}(P(\lambda_2))$ for $\lambda_1 \leq \lambda_2$.
- (iii) $\text{s-lim}_{\lambda_n \downarrow \lambda} P(\lambda_n) = P(\lambda)$ (strong right continuity).
- (iv) $\text{s-lim}_{\lambda \rightarrow -\infty} P(\lambda) = 0$ and $\text{s-lim}_{\lambda \rightarrow +\infty} P(\lambda) = \mathbb{I}$.

As before, strong right continuity is equivalent to weak right continuity.

Picking $\psi \in \mathfrak{H}$, we obtain a finite Borel measure $\mu_\psi(\Omega) = \langle \psi, P(\Omega)\psi \rangle = \|P(\Omega)\psi\|^2$ with $\mu_\psi(\mathbb{R}) = \|\psi\|^2 < \infty$. The corresponding distribution function is given by $\mu(\lambda) = \langle \psi, P(\lambda)\psi \rangle$ and since for every distribution function there is a unique Borel measure (Theorem A.2), for every resolution of the identity there is a unique projection valued measure.

Using the polarization identity (2.16) we also have the following complex Borel measures

$$\mu_{\varphi, \psi}(\Omega) = \langle \varphi, P(\Omega)\psi \rangle = \frac{1}{4}(\mu_{\varphi+\psi}(\Omega) - \mu_{\varphi-\psi}(\Omega) + i\mu_{\varphi-i\psi}(\Omega) - i\mu_{\varphi+i\psi}(\Omega)). \quad (3.14)$$

Note also that, by Cauchy-Schwarz, $|\mu_{\varphi, \psi}(\Omega)| \leq \|\varphi\| \|\psi\|$.

Now let us turn to integration with respect to our projection-valued measure. For any simple function $f = \sum_{j=1}^n \alpha_j \chi_{\Omega_j}$ (where $\Omega_j = f^{-1}(\alpha_j)$)

we set

$$P(f) \equiv \int_{\mathbb{R}} f(\lambda) dP(\lambda) = \sum_{j=1}^n \alpha_j P(\Omega_j). \quad (3.15)$$

In particular, $P(\chi_{\Omega}) = P(\Omega)$. Then $\langle \varphi, P(f)\psi \rangle = \sum_j \alpha_j \mu_{\varphi, \psi}(\Omega_j)$ shows

$$\langle \varphi, P(f)\psi \rangle = \int_{\mathbb{R}} f(\lambda) d\mu_{\varphi, \psi}(\lambda) \quad (3.16)$$

and, by linearity of the integral, the operator P is a linear map from the set of simple functions into the set of bounded linear operators on \mathfrak{H} . Moreover, $\|P(f)\psi\|^2 = \sum_j |\alpha_j|^2 \mu_{\psi}(\Omega_j)$ (the sets Ω_j are disjoint) shows

$$\|P(f)\psi\|^2 = \int_{\mathbb{R}} |f(\lambda)|^2 d\mu_{\psi}(\lambda). \quad (3.17)$$

Equipping the set of simple functions with the sup norm this implies

$$\|P(f)\psi\| \leq \|f\|_{\infty} \|\psi\| \quad (3.18)$$

that P has norm one. Since the simple functions are dense in the Banach space of bounded Borel functions $B(\mathbb{R})$, there is a unique extension of P to a bounded linear operator $P : B(\mathbb{R}) \rightarrow \mathfrak{L}(\mathfrak{H})$ (whose norm is one) from the bounded Borel functions on \mathbb{R} (with sup norm) to the set of bounded linear operators on \mathfrak{H} . In particular, (3.16) and (3.17) remain true.

There is some additional structure behind this extension. Recall that the set $\mathfrak{L}(\mathfrak{H})$ of all bounded linear mappings on \mathfrak{H} forms a C^* algebra. A C^* algebra homomorphism ϕ is a linear map between two C^* algebras which respects both the multiplication and the adjoint, that is, $\phi(ab) = \phi(a)\phi(b)$ and $\phi(a^*) = \phi(a)^*$.

Theorem 3.1. *Let $P(\Omega)$ be a projection-valued measure on \mathfrak{H} . Then the operator*

$$\begin{aligned} P : B(\mathbb{R}) &\rightarrow \mathfrak{L}(\mathfrak{H}) \\ f &\mapsto \int_{\mathbb{R}} f(\lambda) dP(\lambda) \end{aligned} \quad (3.19)$$

is a C^* algebra homomorphism with norm one.

In addition, if $f_n(x) \rightarrow f(x)$ pointwise and if the sequence $\sup_{\lambda \in \mathbb{R}} |f_n(\lambda)|$ is bounded, then $P(f_n) \rightarrow P(f)$ strongly.

Proof. The properties $P(1) = \mathbb{I}$, $P(f^*) = P(f)^*$, and $P(fg) = P(f)P(g)$ are straightforward for simple functions f . For general f they follow from continuity. Hence P is a C^* algebra homomorphism.

The last claim follows from the dominated convergence theorem and (3.17). \square

As a consequence, observe

$$\langle P(g)\varphi, P(f)\psi \rangle = \int_{\mathbb{R}} g^*(\lambda) f(\lambda) d\mu_{\varphi, \psi}(\lambda) \quad (3.20)$$

and thus

$$d\mu_{P(g)\varphi, P(f)\psi} = g^* f d\mu_{\varphi, \psi}. \quad (3.21)$$

Example. Let $\mathfrak{H} = \mathbb{C}^n$ and $A \in \text{GL}(n)$ respectively P_A as in the previous example. Then

$$P_A(f) = \sum_{j=1}^m f(\lambda_j) P_j. \quad (3.22)$$

In particular, $P_A(f) = A$ for $f(\lambda) = \lambda$. \diamond

Next we want to define this operator for unbounded Borel functions. Since we expect the resulting operator to be unbounded, we need a suitable domain first. Motivated by (3.17) we set

$$\mathfrak{D}_f = \left\{ \psi \in \mathfrak{H} \mid \int_{\mathbb{R}} |f(\lambda)|^2 d\mu_{\psi}(\lambda) < \infty \right\}. \quad (3.23)$$

This is clearly a linear subspace of \mathfrak{H} since $\mu_{\alpha\psi}(\Omega) = |\alpha|^2 \mu_{\psi}(\Omega)$ and since $\mu_{\varphi+\psi}(\Omega) \leq 2(\mu_{\varphi}(\Omega) + \mu_{\psi}(\Omega))$ (by the triangle inequality).

For every $\psi \in \mathfrak{D}_f$, the bounded Borel function

$$f_n = \chi_{\Omega_n} f, \quad \Omega_n = \{ \lambda \mid |f(\lambda)| \leq n \}, \quad (3.24)$$

converges to f in the sense of $L^2(\mathbb{R}, d\mu_{\psi})$. Moreover, because of (3.17), $P(f_n)\psi$ converges to some vector $\tilde{\psi}$. We define $P(f)\psi = \tilde{\psi}$. By construction, $P(f)$ is a linear operator such that (3.16) and (3.17) hold.

In addition, \mathfrak{D}_f is dense. Indeed, let Ω_n be defined as in (3.24) and abbreviate $\psi_n = P(\Omega_n)\psi$. Now observe that $d\mu_{\psi_n} = \chi_{\Omega_n} d\mu_{\psi}$ and hence $\psi_n \in \mathfrak{D}_f$. Moreover, $\psi_n \rightarrow \psi$ by (3.17) since $\chi_{\Omega_n} \rightarrow 1$ in $L^2(\mathbb{R}, d\mu_{\psi})$.

The operator $P(f)$ has some additional properties. One calls an unbounded operator A **normal** if $\mathfrak{D}(A) = \mathfrak{D}(A^*)$ and $\|A\psi\| = \|A^*\psi\|$ for all $\psi \in \mathfrak{D}(A)$.

Theorem 3.2. *For any Borel function f , the operator*

$$P(f) = \int_{\mathbb{R}} f(\lambda) dP(\lambda), \quad \mathfrak{D}(P(f)) = \mathfrak{D}_f, \quad (3.25)$$

is normal and satisfies

$$P(f)^* = P(f^*). \quad (3.26)$$

Proof. Let f be given and define f_n, Ω_n as above. Since (3.26) holds for f_n by our previous theorem, we get

$$\langle \varphi, P(f)\psi \rangle = \langle P(f^*)\varphi, \psi \rangle \quad (3.27)$$

for any $\varphi, \psi \in \mathfrak{D}_f = \mathfrak{D}(f^*)$ by continuity. Thus it remains to show that $\mathfrak{D}(P(f)^*) \subseteq \mathfrak{D}_f$. If $\psi \in \mathfrak{D}(P(f)^*)$ we have $\langle \psi, P(f)\varphi \rangle = \langle \tilde{\psi}, \varphi \rangle$ for all $\varphi \in \mathfrak{D}_f$ by definition. Now observe that $P(f_n^*)\psi = P(\Omega_n)\tilde{\psi}$ since we have

$$\langle P(f_n^*)\psi, \varphi \rangle = \langle \psi, P(f_n)\varphi \rangle = \langle \psi, P(f)P(\Omega_n)\varphi \rangle = \langle P(\Omega_n)\tilde{\psi}, \varphi \rangle \quad (3.28)$$

for any $\varphi \in \mathfrak{H}$. To see the second equality use $P(f_n)\varphi = P(f_n\chi_n)\varphi = P(f_m)P(\Omega_n)\varphi$ for $m \geq n$ and let $m \rightarrow \infty$. This proves existence of the limit

$$\lim_{n \rightarrow \infty} \int_{\mathbb{R}} |f_n|^2 d\mu_\psi(\lambda) = \lim_{n \rightarrow \infty} \|P(f_n^*)\psi\|^2 = \lim_{n \rightarrow \infty} \|P(\Omega_n)\tilde{\psi}\|^2 = \|\tilde{\psi}\|^2, \quad (3.29)$$

which implies $f \in L^2(\mathbb{R}, d\mu_\psi)$, that is, $\psi \in \mathfrak{D}_f$. That $P(f)$ is normal follows from $\|P(f)\psi\|^2 = \|P(f^*)\psi\|^2 = \int_{\mathbb{R}} |f(\lambda)|^2 d\mu_\psi$. \square

These considerations seem to indicate some kind of correspondence between the operators $P(f)$ in \mathfrak{H} and f in $L^2(\mathbb{R}, d\mu_\psi)$. Recall that $U : \mathfrak{H} \rightarrow \tilde{\mathfrak{H}}$ is called unitary if it is a bijection which preserves scalar products $\langle U\varphi, U\psi \rangle = \langle \varphi, \psi \rangle$. The operators A in \mathfrak{H} and \tilde{A} in $\tilde{\mathfrak{H}}$ are said to be **unitarily equivalent** if

$$UA = \tilde{A}U, \quad U\mathfrak{D}(A) = \mathfrak{D}(\tilde{A}). \quad (3.30)$$

Clearly, A is self-adjoint if and only if \tilde{A} is and $\sigma(A) = \sigma(\tilde{A})$.

Now let us return to our original problem and consider the subspace

$$\mathfrak{H}_\psi = \{P(f)\psi \mid f \in L^2(\mathbb{R}, d\mu_\psi)\} \subseteq \mathfrak{H}. \quad (3.31)$$

Observe that this subspace is closed: If $\psi_n = P(f_n)\psi$ converges in \mathfrak{H} , then f_n converges to some f in L^2 (since $\|\psi_n - \psi_m\|^2 = \int |f_n - f_m|^2 d\mu_\psi$) and hence $\psi_n \rightarrow P(f)\psi$.

The vector ψ is called **cyclic** if $\mathfrak{H}_\psi = \mathfrak{H}$. By (3.17), the relation

$$U_\psi(P(f)\psi) = f \quad (3.32)$$

defines a unique unitary operator $U_\psi : \mathfrak{H}_\psi \rightarrow L^2(\mathbb{R}, d\mu_\psi)$ such that

$$U_\psi P(f) = fU_\psi, \quad (3.33)$$

where f is identified with its corresponding multiplication operator. Moreover, if f is unbounded we have $U_\psi(\mathfrak{D}_f \cap \mathfrak{H}_\psi) = \mathfrak{D}(f) = \{g \in L^2(\mathbb{R}, d\mu_\psi) \mid fg \in L^2(\mathbb{R}, d\mu_\psi)\}$ (since $\varphi = P(f)\psi$ implies $d\mu_\varphi = |f|^2 d\mu_\psi$) and the above equation still holds.

If ψ is cyclic, our picture is complete. Otherwise we need to extend this approach. A set $\{\psi_j\}_{j \in J}$ (J some index set) is called a set of spectral vectors if $\|\psi_j\| = 1$ and $\mathfrak{H}_{\psi_i} \perp \mathfrak{H}_{\psi_j}$ for all $i \neq j$. A set of spectral vectors is called a **spectral basis** if $\bigoplus_j \mathfrak{H}_{\psi_j} = \mathfrak{H}$. Luckily a spectral basis always exist:

Lemma 3.3. *For every projection valued measure P , there is an (at most countable) spectral basis $\{\psi_n\}$ such that*

$$\mathfrak{H} = \bigoplus_n \mathfrak{H}_{\psi_n} \quad (3.34)$$

and a corresponding unitary operator

$$U = \bigoplus_n U_{\psi_n} : \mathfrak{H} \rightarrow \bigoplus_n L^2(\mathbb{R}, d\mu_{\psi_n}) \quad (3.35)$$

such that for any Borel function f ,

$$UP(f) = fU, \quad U\mathfrak{D}_f = \mathfrak{D}(f). \quad (3.36)$$

Proof. It suffices to show that a spectral basis exists. This can be easily done using a Gram-Schmidt type construction. First of all observe that if $\{\psi_j\}_{j \in J}$ is a spectral set and $\psi \perp \mathfrak{H}_{\psi_j}$ for all j we have $\mathfrak{H}_\psi \perp \mathfrak{H}_{\psi_j}$ for all j . Indeed, $\psi \perp \mathfrak{H}_{\psi_j}$ implies $P(g)\psi \perp \mathfrak{H}_{\psi_j}$ for every bounded function g since $\langle P(g)\psi, P(f)\psi_j \rangle = \langle \psi, P(g^*f)\psi_j \rangle = 0$. But $P(g)\psi$ with g bounded is dense in \mathfrak{H}_ψ implying $\mathfrak{H}_\psi \perp \mathfrak{H}_{\psi_j}$.

Now start with some total set $\{\tilde{\psi}_j\}$. Normalize $\tilde{\psi}_1$ and choose this to be ψ_1 . Move to the first $\tilde{\psi}_j$ which is not in \mathfrak{H}_{ψ_1} , take the orthogonal complement with respect to \mathfrak{H}_{ψ_1} and normalize it. Choose the result to be ψ_2 . Proceeding like this we get a set of spectral vectors $\{\psi_j\}$ such that $\text{span}\{\tilde{\psi}_j\} \subseteq \bigoplus_j \mathfrak{H}_{\psi_j}$. Hence $\mathfrak{H} = \overline{\text{span}\{\tilde{\psi}_j\}} \subseteq \bigoplus_j \mathfrak{H}_{\psi_j}$. \square

It is important to observe that the cardinality of a spectral basis is *not* well-defined (in contradistinction to the cardinality of an ordinary basis of the Hilbert space). However, it can be at most equal to the cardinality of an ordinary basis. In particular, since \mathfrak{H} is separable, it is at most countable. The minimal cardinality of a spectral basis is called **spectral multiplicity** of P . If the spectral multiplicity is one, the spectrum is called **simple**.

Example. Let $\mathfrak{H} = \mathbb{C}^2$ and $A = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$. Then $\psi_1 = (1, 0)$ and $\psi_2 = (0, 1)$ are a spectral basis. However, $\psi = (1, 1)$ is cyclic and hence the spectrum of A is simple. If $A = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ there is no cyclic vector (why) and hence the spectral multiplicity is two. \diamond

Using this canonical form of projection valued measures it is straightforward to prove

Lemma 3.4. *Let f, g be Borel functions and $\alpha, \beta \in \mathbb{C}$. Then we have*

$$\alpha P(f) + \beta P(g) \subseteq P(\alpha f + \beta g), \quad \mathfrak{D}(\alpha P(f) + \beta P(g)) = \mathfrak{D}_{|f|+|g|} \quad (3.37)$$

and

$$P(f)P(g) \subseteq P(fg), \quad \mathfrak{D}(P(f)P(g)) = \mathfrak{D}_g \cap \mathfrak{D}_{fg}. \quad (3.38)$$

Now observe, that to every projection valued measure P we can assign a self-adjoint operator $A = \int_{\mathbb{R}} \lambda dP(\lambda)$. The question is whether we can invert this map. To do this, we consider the resolvent $R_A(z) = \int_{\mathbb{R}} (\lambda - z)^{-1} dP(\lambda)$. By (3.16) the corresponding quadratic form is given by

$$F_\psi(z) = \langle \psi, R_A(z)\psi \rangle = \int_{\mathbb{R}} \frac{1}{\lambda - z} d\mu_\psi(\lambda), \quad (3.39)$$

which is known as the **Borel transform** of the measure μ_ψ . It can be shown (see Section 3.4) that $F_\psi(z)$ is a holomorphic map from the upper half plane to itself. Such functions are called **Herglotz functions**. Moreover, the measure μ_ψ can be reconstructed from $F_\psi(z)$ by **Stieltjes inversion formula**

$$\mu_\psi(\lambda) = \lim_{\delta \downarrow 0} \lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \int_{-\infty}^{\lambda+\delta} \text{Im}(F_\psi(t + i\varepsilon)) dt. \quad (3.40)$$

Conversely, if $F_\psi(z)$ is a Herglotz function satisfying $|F(z)| \leq \frac{M}{\text{Im}(z)}$, then it is the Borel transform of a unique measure μ_ψ (given by Stieltjes inversion formula).

So let A be a given self-adjoint operator and consider the expectation of the resolvent of A ,

$$F_\psi(z) = \langle \psi, R_A(z)\psi \rangle. \quad (3.41)$$

This function is holomorphic for $z \in \rho(A)$ and satisfies

$$F_\psi(z^*) = F_\psi(z)^* \quad \text{and} \quad |F_\psi(z)| \leq \frac{\|\psi\|^2}{\text{Im}(z)} \quad (3.42)$$

(see Theorem 2.14). Moreover, the first resolvent formula (2.80) shows

$$\text{Im}(F_\psi(z)) = \text{Im}(z) \|R_A(z)\psi\|^2 \quad (3.43)$$

that it maps the upper half plane to itself, that is, it is a Herglotz function. So by our above remarks, there is a corresponding measure $\mu_\psi(\lambda)$ given by Stieltjes inversion formula. It is called **spectral measure** corresponding to ψ .

More generally, by polarization, for each $\varphi, \psi \in \mathfrak{H}$ we can find a corresponding complex measure $\mu_{\varphi, \psi}$ such that

$$\langle \varphi, R_A(z)\psi \rangle = \int_{\mathbb{R}} \frac{1}{\lambda - z} d\mu_{\varphi, \psi}(\lambda). \quad (3.44)$$

The measure $\mu_{\varphi, \psi}$ is conjugate linear in φ and linear in ψ . Moreover, a comparison with our previous considerations begs us to define a family of

operators $P_A(\Omega)$ via

$$\langle \varphi, P_A(\Omega)\psi \rangle = \int_{\mathbb{R}} \chi_{\Omega}(\lambda) d\mu_{\varphi, \psi}(\lambda). \quad (3.45)$$

This is indeed possible by Corollary 1.8 since $|\langle \varphi, P_A(\Omega)\psi \rangle| = |\mu_{\varphi, \psi}(\Omega)| \leq \|\varphi\| \|\psi\|$. The operators $P_A(\Omega)$ are non negative ($0 \leq \langle \psi, P_A(\Omega)\psi \rangle \leq 1$) and hence self-adjoint.

Lemma 3.5. *The family of operators $P_A(\Omega)$ forms a projection valued measure.*

Proof. We first show $P_A(\Omega_1)P_A(\Omega_2) = P_A(\Omega_1 \cap \Omega_2)$ in two steps. First observe (using the first resolvent formula (2.80))

$$\begin{aligned} \int_{\mathbb{R}} \frac{1}{\lambda - \tilde{z}} d\mu_{R_A(z^*)\varphi, \psi}(\lambda) &= \langle R_A(z^*)\varphi, R_A(\tilde{z})\psi \rangle = \langle \varphi, R_A(z)R_A(\tilde{z})\psi \rangle \\ &= \frac{1}{z - \tilde{z}} (\langle \varphi, R_A(z)\psi \rangle - \langle \varphi, R_A(\tilde{z})\psi \rangle) \\ &= \frac{1}{z - \tilde{z}} \int_{\mathbb{R}} \left(\frac{1}{\lambda - z} - \frac{1}{\lambda - \tilde{z}} \right) d\mu_{\varphi, \psi}(\lambda) = \int_{\mathbb{R}} \frac{1}{\lambda - \tilde{z}} \frac{d\mu_{\varphi, \psi}(\lambda)}{\lambda - z} \end{aligned} \quad (3.46)$$

implying $d\mu_{R_A(z^*)\varphi, \psi}(\lambda) = (\lambda - z)^{-1} d\mu_{\varphi, \psi}(\lambda)$ since a Herglotz function is uniquely determined by its measure. Secondly we compute

$$\begin{aligned} \int_{\mathbb{R}} \frac{1}{\lambda - z} d\mu_{\varphi, P_A(\Omega)\psi}(\lambda) &= \langle \varphi, R_A(z)P_A(\Omega)\psi \rangle = \langle R_A(z^*)\varphi, P_A(\Omega)\psi \rangle \\ &= \int_{\mathbb{R}} \chi_{\Omega}(\lambda) d\mu_{R_A(z^*)\varphi, \psi}(\lambda) = \int_{\mathbb{R}} \frac{1}{\lambda - z} \chi_{\Omega}(\lambda) d\mu_{\varphi, \psi}(\lambda) \end{aligned}$$

implying $d\mu_{\varphi, P_A(\Omega)\psi}(\lambda) = \chi_{\Omega}(\lambda) d\mu_{\varphi, \psi}(\lambda)$. Equivalently we have

$$\langle \varphi, P_A(\Omega_1)P_A(\Omega_2)\psi \rangle = \langle \varphi, P_A(\Omega_1 \cap \Omega_2)\psi \rangle \quad (3.47)$$

since $\chi_{\Omega_1}\chi_{\Omega_2} = \chi_{\Omega_1 \cap \Omega_2}$. In particular, choosing $\Omega_1 = \Omega_2$, we see that $P_A(\Omega_1)$ is a projector.

The relation $P_A(\mathbb{R}) = \mathbb{I}$ follows from (3.93) below and Lemma 2.18 which imply $\mu_{\psi}(\mathbb{R}) = \|\psi\|^2$.

Now let $\Omega = \bigcup_{n=1}^{\infty} \Omega_n$ with $\Omega_n \cap \Omega_m = \emptyset$ for $n \neq m$. Then

$$\sum_{j=1}^n \langle \psi, P_A(\Omega_j)\psi \rangle = \sum_{j=1}^n \mu_{\psi}(\Omega_j) \rightarrow \langle \psi, P_A(\Omega)\psi \rangle = \mu_{\psi}(\Omega) \quad (3.48)$$

by σ -additivity of μ_{ψ} . Hence P_A is weakly σ -additive which implies strong σ -additivity, as pointed out earlier. \square

Now we can prove the **spectral theorem** for self-adjoint operators.

Theorem 3.6 (Spectral theorem). *To every self-adjoint operator A there corresponds a unique projection valued measure P_A such that*

$$A = \int_{\mathbb{R}} \lambda dP_A(\lambda). \quad (3.49)$$

Proof. Existence has already been established. Moreover, Lemma 3.4 shows that $P_A((\lambda - z)^{-1}) = R_A(z)$, $z \in \mathbb{C} \setminus \mathbb{R}$. Since the measures $\mu_{\varphi, \psi}$ are uniquely determined by the resolvent and the projection valued measure is uniquely determined by the measures $\mu_{\varphi, \psi}$ we are done. \square

The quadratic form of A is given by

$$q_A(\psi) = \int_{\mathbb{R}} \lambda d\mu_{\psi}(\lambda) \quad (3.50)$$

and can be defined for every ψ in the **form domain** self-adjoint operator

$$\mathfrak{D}(A) = \{\psi \in \mathfrak{H} \mid \int_{\mathbb{R}} |\lambda| d\mu_{\psi}(\lambda) < \infty\} \quad (3.51)$$

(which is larger than the domain $\mathfrak{D}(A) = \{\psi \in \mathfrak{H} \mid \int_{\mathbb{R}} \lambda^2 d\mu_{\psi}(\lambda) < \infty\}$). This extends our previous definition for non-negative operators.

Note, that if A and \tilde{A} are unitarily equivalent as in (3.30), then $UR_A(z) = R_{\tilde{A}}(z)U$ and hence

$$d\mu_{\psi} = d\tilde{\mu}_{U\psi}. \quad (3.52)$$

In particular, we have $UP_A(f) = P_{\tilde{A}}(f)U$, $U\mathfrak{D}(P_A(f)) = \mathfrak{D}(P_{\tilde{A}}(f))$.

Finally, let us give a characterization of the spectrum of A in terms of the associated projectors.

Theorem 3.7. *The spectrum of A is given by*

$$\sigma(A) = \{\lambda \in \mathbb{R} \mid P_A((\lambda - \varepsilon, \lambda + \varepsilon)) \neq 0 \text{ for all } \varepsilon > 0\}. \quad (3.53)$$

Proof. Let $\Omega_n = (\lambda_0 - \frac{1}{n}, \lambda_0 + \frac{1}{n})$. Suppose $P_A(\Omega_n) \neq 0$. Then we can find a $\psi_n \in P_A(\Omega_n)\mathfrak{H}$ with $\|\psi_n\| = 1$. Since

$$\begin{aligned} \|(A - \lambda_0)\psi_n\|^2 &= \|(A - \lambda_0)P_A(\Omega_n)\psi_n\|^2 \\ &= \int_{\mathbb{R}} (\lambda - \lambda_0)^2 \chi_{\Omega_n}(\lambda) d\mu_{\psi_n}(\lambda) \leq \frac{1}{n^2} \end{aligned} \quad (3.54)$$

we conclude $\lambda_0 \in \sigma(A)$ by Lemma 2.12.

Conversely, if $P_A((\lambda_0 - \varepsilon, \lambda_0 + \varepsilon)) = 0$, set $f_{\varepsilon}(\lambda) = \chi_{\mathbb{R} \setminus (\lambda_0 - \varepsilon, \lambda_0 + \varepsilon)}(\lambda)(\lambda - \lambda_0)^{-1}$. Then

$$(A - \lambda_0)P_A(f_{\varepsilon}) = P_A((\lambda - \lambda_0)f_{\varepsilon}(\lambda)) = P_A(\mathbb{R} \setminus (\lambda_0 - \varepsilon, \lambda_0 + \varepsilon)) = \mathbb{I}. \quad (3.55)$$

Similarly $P_A(f_{\varepsilon})(A - \lambda_0) = \mathbb{I}|_{\mathfrak{D}(A)}$ and hence $\lambda_0 \in \rho(A)$. \square

Thus $P_A((\lambda_1, \lambda_2)) = 0$ if and only if $(\lambda_1, \lambda_2) \subseteq \rho(A)$ and we have

$$P_A(\sigma(A)) = \mathbb{I} \quad \text{and} \quad P_A(\mathbb{R} \cap \rho(A)) = 0 \quad (3.56)$$

and consequently

$$P_A(f) = P_A(\sigma(A))P_A(f) = P_A(\chi_{\sigma(A)}f). \quad (3.57)$$

In other words, $P_A(f)$ is not affected by the values of f on $\mathbb{R} \setminus \sigma(A)$!

It is clearly more intuitive to write $P_A(f) = f(A)$ and we will do so from now on. This notation is justified by the elementary observation

$$P_A\left(\sum_{j=0}^n \alpha_j \lambda^j\right) = \sum_{j=0}^n \alpha_j A^j. \quad (3.58)$$

Moreover, this also shows that if A is bounded and $f(A)$ can be defined via a convergent power series, then this agrees with our present definition by Theorem 3.1.

Problem 3.1. Show that a self-adjoint operator P is a projection if and only if $\sigma(P) \subseteq \{0, 1\}$.

Problem 3.2. Show that (3.7) is a projection valued measure. What is the corresponding operator?

Problem 3.3. Show that $P(\lambda)$ satisfies the properties (i)–(iv).

Problem 3.4 (Polar decomposition). Let A be a bounded operator and set $|A| = \sqrt{A^*A}$. Show that

$$\||A|\psi\| = \|A\psi\|.$$

Conclude that $\text{Ker}(A) = \text{Ker}(|A|) = \text{Ran}(|A|)^\perp$ and that

$$U = \begin{cases} \varphi = |A|\psi \mapsto A\psi & \text{if } \varphi \in \text{Ran}(|A|) \\ \varphi \mapsto 0 & \text{if } \varphi \in \text{Ker}(|A|) \end{cases}$$

extends to a well-defined **partial isometry**, that is, $U : \text{Ker}(U)^\perp \rightarrow \mathfrak{H}$ is norm preserving.

In particular, we have the **polar decomposition**

$$A = U|A|.$$

Problem 3.5. Compute $|A| = \sqrt{A^*A}$ of $A = \langle \varphi, \cdot \rangle \psi$.

3.2. More on Borel measures

Section 3.1 showed that in order to understand self-adjoint operators, one needs to understand multiplication operators on $L^2(\mathbb{R}, d\mu)$, where $d\mu$ is a finite Borel measure. This is the purpose of the present section.

The set of all **growth points**, that is,

$$\sigma(\mu) = \{\lambda \in \mathbb{R} \mid \mu((\lambda - \varepsilon, \lambda + \varepsilon)) > 0 \text{ for all } \varepsilon > 0\}, \quad (3.59)$$

is called the spectrum of μ . Invoking Moreau's together with Fubini's theorem shows that the Borel transform

$$F(z) = \int_{\mathbb{R}} \frac{1}{\lambda - z} d\mu(\lambda) \quad (3.60)$$

is holomorphic for $z \in \mathbb{C} \setminus \sigma(\mu)$. The converse following from Stieltjes inversion formula. Associated with this measure is the operator

$$Af(\lambda) = \lambda f(\lambda), \quad \mathfrak{D}(A) = \{f \in L^2(\mathbb{R}, d\mu) \mid \lambda f(\lambda) \in L^2(\mathbb{R}, d\mu)\}. \quad (3.61)$$

By Theorem 3.7 the spectrum of A is precisely the spectrum of μ , that is,

$$\sigma(A) = \sigma(\mu). \quad (3.62)$$

Note that $1 \in L^2(\mathbb{R}, d\mu)$ is a cyclic vector for A and that

$$d\mu_{g,f}(\lambda) = g(\lambda)^* f(\lambda) d\mu(\lambda). \quad (3.63)$$

Now what can we say about the function $f(A)$ (which is precisely the multiplication operator by f) of A ? We are only interested in the case where f is real-valued. Introduce the measure

$$(f_*\mu)(\Omega) = \mu(f^{-1}(\Omega)), \quad (3.64)$$

then

$$\int_{\mathbb{R}} g(\lambda) d(f_*\mu)(\lambda) = \int_{\mathbb{R}} g(f(\lambda)) d\mu(\lambda). \quad (3.65)$$

In fact, it suffices to check this formula for simple functions g which follows since $\chi_{\Omega} \circ f = \chi_{f^{-1}(\Omega)}$. In particular, we have

$$P_{f(A)}(\Omega) = \chi_{f^{-1}(\Omega)}. \quad (3.66)$$

It is tempting to conjecture that $f(A)$ is unitarily equivalent to multiplication by λ in $L^2(\mathbb{R}, d(f_*\mu))$ via the map

$$L^2(\mathbb{R}, d(f_*\mu)) \rightarrow L^2(\mathbb{R}, d\mu), \quad g \mapsto g \circ f. \quad (3.67)$$

However, this map is only unitary if its range is $L^2(\mathbb{R}, d\mu)$, that is, if f is injective.

Lemma 3.8. *Suppose f is injective, then*

$$U : L^2(\mathbb{R}, d\mu) \rightarrow L^2(\mathbb{R}, d(f_*\mu)), \quad g \mapsto g \circ f^{-1} \quad (3.68)$$

is a unitary map such that $Uf(\lambda) = \lambda$.

Example. Let $f(\lambda) = \lambda^2$, then $(g \circ f)(\lambda) = g(\lambda^2)$ and the range of the above map is given by the symmetric functions. Note that we can still get a unitary map $L^2(\mathbb{R}, d(f_*\mu)) \oplus L^2(\mathbb{R}, \chi d(f_*\mu)) \rightarrow L^2(\mathbb{R}, d\mu)$, $(g_1, g_2) \mapsto g_1(\lambda^2) + g_2(\lambda^2)(\chi(\lambda) - \chi(-\lambda))$, where $\chi = \chi_{(0, \infty)}$. \diamond

Lemma 3.9. *Let f be real-valued. The spectrum of $f(A)$ is given by*

$$\sigma(f(A)) = \sigma(f_*\mu). \quad (3.69)$$

In particular,

$$\sigma(f(A)) \subseteq \overline{f(\sigma(A))}, \quad (3.70)$$

where equality holds if f is continuous and the closure can be dropped if, in addition, $\sigma(A)$ is bounded (i.e., compact).

Proof. If $\lambda_0 \in \sigma(f_*\mu)$, then the sequence $g_n = \mu(\Omega_n)^{-1/2} \chi_{\Omega_n}$, $\Omega_n = f^{-1}((\lambda_0 - \frac{1}{n}, \lambda_0 + \frac{1}{n}))$, satisfies $\|g_n\| = 1$, $\|(f(A) - \lambda_0)g_n\| < n^{-1}$ and hence $\lambda_0 \in \sigma(f(A))$. Conversely, if $\lambda_0 \notin \sigma(f_*\mu)$, then $\mu(\Omega_n) = 0$ for some n and hence we can change f on Ω_n such that $f(\mathbb{R}) \cap (\lambda_0 - \frac{1}{n}, \lambda_0 + \frac{1}{n}) = \emptyset$ without changing the corresponding operator. Thus $(f(A) - \lambda_0)^{-1} = (f(\lambda) - \lambda_0)^{-1}$ exists and is bounded, implying $\lambda_0 \notin \sigma(f(A))$.

If f is continuous, $f^{-1}(f(\lambda) - \varepsilon, f(\lambda) + \varepsilon)$ contains an open interval around λ and hence $f(\lambda) \in \sigma(f(A))$ if $\lambda \in \sigma(A)$. If, in addition, $\sigma(A)$ is compact, then $f(\sigma(A))$ is compact and hence closed. \square

If two operators with simple spectrum are unitarily equivalent can be read off from the corresponding measures:

Lemma 3.10. *Let A_1, A_2 be self-adjoint operators with simple spectrum and corresponding spectral measures μ_1 and μ_2 of cyclic vectors. Then A_1 and A_2 are unitarily equivalent if and only if μ_1 and μ_2 are mutually absolutely continuous.*

Proof. Without restriction we can assume that A_j is multiplication by λ in $L^2(\mathbb{R}, d\mu_j)$. Let $U : L^2(\mathbb{R}, d\mu_1) \rightarrow L^2(\mathbb{R}, d\mu_2)$ be a unitary map such that $UA_1 = A_2U$. Then we also have $Uf(A_1) = f(A_2)U$ for any bounded Borel Function and hence

$$Uf(\lambda) = Uf(\lambda) \cdot 1 = f(\lambda)U(1)(\lambda) \quad (3.71)$$

and thus U is multiplication by $u(\lambda) = U(1)(\lambda)$. Moreover, since U is unitary we have

$$\mu_1(\Omega) = \int_{\mathbb{R}} |\chi_{\Omega}|^2 d\mu_1 = \int_{\mathbb{R}} |u \chi_{\Omega}|^2 d\mu_2 = \int_{\Omega} |u|^2 d\mu_2, \quad (3.72)$$

that is, $d\mu_1 = |u|^2 d\mu_2$. Reversing the role of A_1 and A_2 we obtain $d\mu_2 = |v|^2 d\mu_1$, where $v = U^{-1}1$.

The converse is left as an exercise (Problem 3.10.) \square

Next we recall the unique decomposition of μ with respect to Lebesgue measure,

$$d\mu = d\mu_{ac} + d\mu_s, \quad (3.73)$$

where μ_{ac} is **absolutely continuous** with respect to Lebesgue measure (i.e., we have $\mu_{ac}(B) = 0$ for all B with Lebesgue measure zero) and μ_s is **singular** with respect to Lebesgue measure (i.e., μ_s is supported, $\mu_s(\mathbb{R} \setminus B) = 0$, on a set B with Lebesgue measure zero). The singular part μ_s can be further decomposed into a **(singularly) continuous** and a **pure point** part,

$$d\mu_s = d\mu_{sc} + d\mu_{pp}, \quad (3.74)$$

where μ_{sc} is continuous on \mathbb{R} and μ_{pp} is a step function. Since the measures $d\mu_{ac}$, $d\mu_{sc}$, and $d\mu_{pp}$ are mutually singular, they have mutually disjoint supports M_{ac} , M_{sc} , and M_{pp} . Note that these sets are *not* unique. We will choose them such that M_{pp} is the set of all jumps of $\mu(\lambda)$ and such that M_{sc} has Lebesgue measure zero.

To the sets M_{ac} , M_{sc} , and M_{pp} correspond projectors $P^{ac} = \chi_{M_{ac}}(A)$, $P^{sc} = \chi_{M_{sc}}(A)$, and $P^{pp} = \chi_{M_{pp}}(A)$ satisfying $P^{ac} + P^{sc} + P^{pp} = \mathbb{I}$. In other words, we have a corresponding direct sum decomposition of both our Hilbert space

$$L^2(\mathbb{R}, d\mu) = L^2(\mathbb{R}, d\mu_{ac}) \oplus L^2(\mathbb{R}, d\mu_{sc}) \oplus L^2(\mathbb{R}, d\mu_{pp}) \quad (3.75)$$

and our operator A

$$A = (AP^{ac}) \oplus (AP^{sc}) \oplus (AP^{pp}). \quad (3.76)$$

The corresponding spectra, $\sigma_{ac}(A) = \sigma(\mu_{ac})$, $\sigma_{sc}(A) = \sigma(\mu_{sc})$, and $\sigma_{pp}(A) = \sigma(\mu_{pp})$ are called the absolutely continuous, singularly continuous, and pure point spectrum of A , respectively.

It is important to observe that $\sigma_{pp}(A)$ is in general not equal to the set of eigenvalues

$$\sigma_p(A) = \{\lambda \in \mathbb{R} \mid \lambda \text{ is an eigenvalue of } A\} \quad (3.77)$$

since we only have $\sigma_{pp}(A) = \overline{\sigma_p(A)}$.

Example. let $\mathfrak{H} = \ell^2(\mathbb{N})$ and let A be given by $A\delta_n = \frac{1}{n}\delta_n$, where δ_n is the sequence which is 1 at the n 'th place and zero else (that is, A is a diagonal matrix with diagonal elements $\frac{1}{n}$). Then $\sigma_p(A) = \{\frac{1}{n} \mid n \in \mathbb{N}\}$ but $\sigma(A) = \sigma_{pp}(A) = \sigma_p(A) \cup \{0\}$. To see this, just observe that δ_n is the eigenvector corresponding to the eigenvalue $\frac{1}{n}$ and for $z \notin \sigma(A)$ we have $R_A(z)\delta_n = \frac{n}{1-nz}\delta_n$. At $z = 0$ this formula still gives the inverse of A , but it is unbounded and hence $0 \in \sigma(A)$ but $0 \notin \sigma_p(A)$. Since a continuous measure cannot live on a single point and hence also not on a countable set, we have $\sigma_{ac}(A) = \sigma_{sc}(A) = \emptyset$. \diamond

Example. An example with purely absolutely continuous spectrum is given by taking μ to be Lebesgue measure. An example with purely singularly continuous spectrum is given by taking μ to be the Cantor measure. \diamond

Problem 3.6. Construct a multiplication operator on $L^2(\mathbb{R})$ which has dense point spectrum.

Problem 3.7. Let λ be Lebesgue measure on \mathbb{R} . Show that if $f \in AC(\mathbb{R})$ with $f' > 0$, then

$$d(f_*\lambda) = \frac{1}{f'(\lambda)} d\lambda. \quad (3.78)$$

Problem 3.8. Let $d\mu(\lambda) = \chi_{[0,1]}(\lambda)d\lambda$ and $f(\lambda) = \chi_{(-\infty,t]}$, $t \in \mathbb{R}$. Compute $f_*\mu$.

Problem 3.9. Let A be the multiplication operator by the Cantor function in $L^2(0,1)$. Compute the spectrum of A . Determine the spectral types.

Problem 3.10. Show the missing direction in the proof of Lemma 3.10.

3.3. Spectral types

Our next aim is to transfer the results of the previous section to arbitrary self-adjoint operators A using Lemma 3.3. To do this we will need a spectral measure which contains the information from all measures in a spectral basis. This will be the case if there is a vector ψ such that for every $\varphi \in \mathfrak{H}$ its spectral measure μ_φ is absolutely continuous with respect to μ_ψ . Such a vector will be called a **maximal spectral vector** of A and μ_ψ will be called a **maximal spectral measure** of A .

Lemma 3.11. For every self-adjoint operator A there is a maximal spectral vector.

Proof. Let $\{\psi_j\}_{j \in J}$ be a spectral basis and choose nonzero numbers ε_j with $\sum_{j \in J} |\varepsilon_j|^2 = 1$. Then I claim that

$$\psi = \sum_{j \in J} \varepsilon_j \psi_j \quad (3.79)$$

is a maximal spectral vector. Let φ be given, then we can write it as $\varphi = \sum_j f_j(A)\psi_j$ and hence $d\mu_\varphi = \sum_j |f_j|^2 d\mu_{\psi_j}$. But $\mu_\psi(\Omega) = \sum_j |\varepsilon_j|^2 \mu_{\psi_j}(\Omega) = 0$ implies $\mu_{\psi_j}(\Omega) = 0$ for every $j \in J$ and thus $\mu_\varphi(\Omega) = 0$. \square

A set $\{\psi_j\}$ of spectral vectors is called **ordered** if ψ_k is a maximal spectral vector for A restricted to $(\bigoplus_{j=1}^{k-1} \mathfrak{H}_{\psi_j})^\perp$. As in the unordered case one can show

Theorem 3.12. *For every self-adjoint operator there is an ordered spectral basis.*

Observe that if $\{\psi_j\}$ is an ordered spectral basis, then $\mu_{\psi_{j+1}}$ is absolutely continuous with respect to μ_{ψ_j} .

If μ is a maximal spectral measure we have $\sigma(A) = \sigma(\mu)$ and the following generalization of Lemma 3.9 holds.

Theorem 3.13 (Spectral mapping). *Let μ be a maximal spectral measure and let f be real-valued. Then the spectrum of $f(A)$ is given by*

$$\sigma(f(A)) = \{\lambda \in \mathbb{R} \mid \mu(f^{-1}(\lambda - \varepsilon, \lambda + \varepsilon)) > 0 \text{ for all } \varepsilon > 0\}. \quad (3.80)$$

In particular,

$$\sigma(f(A)) \subseteq \overline{f(\sigma(A))}, \quad (3.81)$$

where equality holds if f is continuous and the closure can be dropped if, in addition, $\sigma(A)$ is bounded.

Next, we want to introduce the splitting (3.75) for arbitrary self-adjoint operators A . It is tempting to pick a spectral basis and treat each summand in the direct sum separately. However, since it is not clear that this approach is independent of the spectral basis chosen, we use the more sophisticated definition

$$\begin{aligned} \mathfrak{H}_{ac} &= \{\psi \in \mathfrak{H} \mid \mu_\psi \text{ is absolutely continuous}\}, \\ \mathfrak{H}_{sc} &= \{\psi \in \mathfrak{H} \mid \mu_\psi \text{ is singularly continuous}\}, \\ \mathfrak{H}_{pp} &= \{\psi \in \mathfrak{H} \mid \mu_\psi \text{ is pure point}\}. \end{aligned} \quad (3.82)$$

Lemma 3.14. *We have*

$$\mathfrak{H} = \mathfrak{H}_{ac} \oplus \mathfrak{H}_{sc} \oplus \mathfrak{H}_{pp}. \quad (3.83)$$

There are Borel sets M_{xx} such that the projector onto \mathfrak{H}_{xx} is given by $P^{xx} = \chi_{M_{xx}}(A)$, $xx \in \{ac, sc, pp\}$. In particular, the subspaces \mathfrak{H}_{xx} reduce A . For the sets M_{xx} one can choose the corresponding supports of some maximal spectral measure μ .

Proof. We will use the unitary operator U of Lemma 3.3. Pick $\varphi \in \mathfrak{H}$ and write $\varphi = \sum_n \varphi_n$ with $\varphi_n \in \mathfrak{H}_{\psi_n}$. Let $f_n = U\varphi_n$, then, by construction of the unitary operator U , $\varphi_n = f_n(A)\psi_n$ and hence $d\mu_{\varphi_n} = |f_n|^2 d\mu_{\psi_n}$. Moreover, since the subspaces \mathfrak{H}_{ψ_n} are orthogonal, we have

$$d\mu_\varphi = \sum_n |f_n|^2 d\mu_{\psi_n} \quad (3.84)$$

and hence

$$d\mu_{\varphi,xx} = \sum_n |f_n|^2 d\mu_{\psi_n,xx}, \quad xx \in \{ac, sc, pp\}. \quad (3.85)$$

This shows

$$U\mathfrak{H}_{xx} = \bigoplus_n L^2(\mathbb{R}, d\mu_{\psi_n, xx}), \quad xx \in \{ac, sc, pp\} \quad (3.86)$$

and reduces our problem to the considerations of the previous section. \square

The **absolutely continuous, singularly continuous, and pure point spectrum** of A are defined as

$$\sigma_{ac}(A) = \sigma(A|_{\mathfrak{H}_{ac}}), \quad \sigma_{sc}(A) = \sigma(A|_{\mathfrak{H}_{sc}}), \quad \text{and} \quad \sigma_{pp}(A) = \sigma(A|_{\mathfrak{H}_{pp}}), \quad (3.87)$$

respectively. If μ is a maximal spectral measure we have $\sigma_{ac}(A) = \sigma(\mu_{ac})$, $\sigma_{sc}(A) = \sigma(\mu_{sc})$, and $\sigma_{pp}(A) = \sigma(\mu_{pp})$.

If A and \tilde{A} are unitarily equivalent via U , then so are $A|_{\mathfrak{H}_{xx}}$ and $\tilde{A}|_{\mathfrak{H}_{xx}}$ by (3.52). In particular, $\sigma_{xx}(A) = \sigma_{xx}(\tilde{A})$.

Problem 3.11. Compute $\sigma(A)$, $\sigma_{ac}(A)$, $\sigma_{sc}(A)$, and $\sigma_{pp}(A)$ for the multiplication operator $A = \frac{1}{1+x^2}$ in $L^2(\mathbb{R})$. What is its spectral multiplicity?

3.4. Appendix: The Herglotz theorem

A holomorphic function $F : \mathbb{C}_+ \rightarrow \mathbb{C}_+$, $\mathbb{C}_\pm = \{z \in \mathbb{C} \mid \pm \text{Im}(z) > 0\}$, is called a Herglotz function. We can define F on \mathbb{C}_- using $F(z^*) = F(z)^*$.

Suppose μ is a finite Borel measure. Then its Borel transform is defined via

$$F(z) = \int_{\mathbb{R}} \frac{d\mu(\lambda)}{\lambda - z}. \quad (3.88)$$

Theorem 3.15. The Borel transform of a finite Borel measure is a Herglotz function satisfying

$$|F(z)| \leq \frac{\mu(\mathbb{R})}{\text{Im}(z)}, \quad z \in \mathbb{C}_+. \quad (3.89)$$

Moreover, the measure μ can be reconstructed via Stieltjes inversion formula

$$\frac{1}{2}(\mu((\lambda_1, \lambda_2)) + \mu([\lambda_1, \lambda_2])) = \lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \int_{\lambda_1}^{\lambda_2} \text{Im}(F(\lambda + i\varepsilon)) d\lambda. \quad (3.90)$$

Proof. By Morea's and Fubini's theorem, F is holomorphic on \mathbb{C}_+ and the remaining properties follow from $0 < \text{Im}((\lambda - z)^{-1})$ and $|\lambda - z|^{-1} \leq \text{Im}(z)^{-1}$. Stieltjes inversion formula follows from Fubini's theorem and the dominated convergence theorem since

$$\frac{1}{2\pi i} \int_{\lambda_1}^{\lambda_2} \left(\frac{1}{x - \lambda - i\varepsilon} - \frac{1}{x - \lambda + i\varepsilon} \right) d\lambda \rightarrow \frac{1}{2} (\chi_{[\lambda_1, \lambda_2]}(x) + \chi_{(\lambda_1, \lambda_2)}(x)) \quad (3.91)$$

pointwise. \square

Observe

$$\operatorname{Im}(F(z)) = \operatorname{Im}(z) \int_{\mathbb{R}} \frac{d\mu(\lambda)}{|\lambda - z|^2} \quad (3.92)$$

and

$$\lim_{\lambda \rightarrow \infty} \lambda \operatorname{Im}(F(i\lambda)) = \mu(\mathbb{R}). \quad (3.93)$$

The converse of the previous theorem is also true

Theorem 3.16. *Suppose F is a Herglotz function satisfying*

$$|F(z)| \leq \frac{M}{\operatorname{Im}(z)}, \quad z \in \mathbb{C}_+. \quad (3.94)$$

Then there is a unique Borel measure μ , satisfying $\mu(\mathbb{R}) \leq M$, such that F is the Borel transform of μ .

Proof. We abbreviate $F(z) = v(z) + iw(z)$ and $z = x + iy$. Next we choose a contour

$$\Gamma = \{x + i\varepsilon + \lambda | \lambda \in [-R, R]\} \cup \{x + i\varepsilon + Re^{i\varphi} | \varphi \in [0, \pi]\}. \quad (3.95)$$

and note that z lies inside Γ and $z^* + 2i\varepsilon$ lies outside Γ if $0 < \varepsilon < y < R$. Hence we have by Cauchy's formula

$$F(z) = \frac{1}{2\pi i} \int_{\Gamma} \left(\frac{1}{\zeta - z} - \frac{1}{\zeta - z^* - 2i\varepsilon} \right) F(\zeta) d\zeta. \quad (3.96)$$

Inserting the explicit form of Γ we see

$$\begin{aligned} F(z) &= \frac{1}{\pi} \int_{-R}^R \frac{y - \varepsilon}{\lambda^2 + (y - \varepsilon)^2} F(x + i\varepsilon + \lambda) d\lambda \\ &\quad + \frac{i}{\pi} \int_0^\pi \frac{y - \varepsilon}{R^2 e^{2i\varphi} + (y - \varepsilon)^2} F(x + i\varepsilon + Re^{i\varphi}) Re^{i\varphi} d\varphi. \end{aligned} \quad (3.97)$$

The integral over the semi circle vanishes as $R \rightarrow \infty$ and hence we obtain

$$F(z) = \frac{1}{\pi} \int_{\mathbb{R}} \frac{y - \varepsilon}{(\lambda - x)^2 + (y - \varepsilon)^2} F(\lambda + i\varepsilon) d\lambda \quad (3.98)$$

and taking imaginary parts

$$w(z) = \int_{\mathbb{R}} \phi_\varepsilon(\lambda) w_\varepsilon(\lambda) d\lambda, \quad (3.99)$$

where $\phi_\varepsilon(\lambda) = (y - \varepsilon) / ((\lambda - x)^2 + (y - \varepsilon)^2)$ and $w_\varepsilon(\lambda) = w(\lambda + i\varepsilon) / \pi$. Letting $y \rightarrow \infty$ we infer from our bound

$$\int_{\mathbb{R}} w_\varepsilon(\lambda) d\lambda \leq M. \quad (3.100)$$

In particular, since $|\phi_\varepsilon(\lambda) - \phi_0(\lambda)| \leq \text{const } \varepsilon$ we have

$$w(z) = \lim_{\varepsilon \downarrow 0} \int_{\mathbb{R}} \phi_0(\lambda) d\mu_\varepsilon(\lambda), \quad (3.101)$$

where $\mu_\varepsilon(\lambda) = \int_{-\infty}^{\lambda} w_\varepsilon(x) dx$. It remains to establish that the monotone functions μ_ε converge properly. Since $0 \leq \mu_\varepsilon(\lambda) \leq M$, there is a convergent subsequence for fixed λ . Moreover, by the standard diagonal trick, there is even a subsequence ε_n such that $\mu_{\varepsilon_n}(\lambda)$ converges for each rational λ . For irrational λ we set $\mu(\lambda_0) = \inf_{\lambda \geq \lambda_0} \{\mu(\lambda) | \lambda \text{ rational}\}$. Then $\mu(\lambda)$ is monotone, $0 \leq \mu(\lambda_1) \leq \mu(\lambda_2) \leq M$, $\lambda_1 \leq \lambda_2$, and we claim

$$w(z) = \int_{\mathbb{R}} \phi_0(\lambda) d\mu(\lambda). \quad (3.102)$$

Fix $\delta > 0$ and let $\lambda_1 < \lambda_2 < \dots < \lambda_{m+1}$ be rational numbers such that

$$|\lambda_{j+1} - \lambda_j| \leq \delta \quad \text{and} \quad \lambda_1 \leq x - \frac{y^3}{\delta}, \quad \lambda_{m+1} \geq x + \frac{y^3}{\delta}. \quad (3.103)$$

Then (since $|\phi_0'(\lambda)| \leq y^{-2}$)

$$|\phi_0(\lambda) - \phi_0(\lambda_j)| \leq \frac{\delta}{y^2}, \quad \lambda_j \leq \lambda \leq \lambda_{j+1}, \quad (3.104)$$

and

$$|\phi_0(\lambda)| \leq \frac{\delta}{y^2}, \quad \lambda \leq \lambda_1 \text{ or } \lambda_{m+1} \leq \lambda. \quad (3.105)$$

Now observe

$$\begin{aligned} & \left| \int_{\mathbb{R}} \phi_0(\lambda) d\mu(\lambda) - \int_{\mathbb{R}} \phi_0(\lambda) d\mu_{\varepsilon_n}(\lambda) \right| \leq \\ & \left| \int_{\mathbb{R}} \phi_0(\lambda) d\mu(\lambda) - \sum_{j=1}^m \phi_0(\lambda_j) (\mu(\lambda_{j+1}) - \mu(\lambda_j)) \right| \\ & + \left| \sum_{j=1}^m \phi_0(\lambda_j) (\mu(\lambda_{j+1}) - \mu(\lambda_j) - \mu_{\varepsilon_n}(\lambda_{j+1}) + \mu_{\varepsilon_n}(\lambda_j)) \right| \\ & + \left| \int_{\mathbb{R}} \phi_0(\lambda) d\mu_{\varepsilon_n}(\lambda) - \sum_{j=1}^m \phi_0(\lambda_j) (\mu_{\varepsilon_n}(\lambda_{j+1}) - \mu_{\varepsilon_n}(\lambda_j)) \right| \quad (3.106) \end{aligned}$$

The first and third term can be bounded by $2M\delta/y^2$. Moreover, since $\phi_0(y) \leq 1/y$ we can find an $N \in \mathbb{N}$ such that

$$|\mu(\lambda_j) - \mu_{\varepsilon_n}(\lambda_j)| \leq \frac{y}{2m} \delta, \quad n \geq N, \quad (3.107)$$

and hence the second term is bounded by δ . In summary, the difference in (3.106) can be made arbitrarily small.

Now $F(z)$ and $\int_{\mathbb{R}} (\lambda - z)^{-1} d\mu(\lambda)$ have the same imaginary part and thus they only differ by a real constant. By our bound this constant must be zero. \square

The Radon-Nikodym derivative of μ can be obtained from the boundary values of F .

Theorem 3.17. *Let μ be a finite Borel measure and F its Borel transform, then*

$$(\underline{D}\mu)(\lambda) \leq \liminf_{\varepsilon \downarrow 0} \frac{1}{\pi} F(\lambda + i\varepsilon) \leq \limsup_{\varepsilon \downarrow 0} \frac{1}{\pi} F(\lambda + i\varepsilon) \leq (\overline{D}\mu)(\lambda). \quad (3.108)$$

Proof. We need to estimate

$$\operatorname{Im}(F(\lambda + i\varepsilon)) = \int_{\mathbb{R}} K_{\varepsilon}(t) d\mu(t), \quad K_{\varepsilon}(t) = \frac{\varepsilon}{t^2 + \varepsilon^2}. \quad (3.109)$$

We first split the integral into two parts

$$\operatorname{Im}(F(\lambda + i\varepsilon)) = \int_{I_{\delta}} K_{\varepsilon}(t - \lambda) d\mu(t) + \int_{\mathbb{R} \setminus I_{\delta}} K_{\varepsilon}(t - \lambda) \mu(t), \quad I_{\delta} = (\lambda - \delta, \lambda + \delta). \quad (3.110)$$

Clearly the second part can be estimated by

$$\int_{\mathbb{R} \setminus I_{\delta}} K_{\varepsilon}(t - \lambda) \mu(t) \leq K_{\varepsilon}(\delta) \mu(\mathbb{R}). \quad (3.111)$$

To estimate the first part we integrate

$$K'_{\varepsilon}(s) ds d\mu(t) \quad (3.112)$$

over the triangle $\{(s, t) | \lambda - s < t < \lambda + s, 0 < s < \delta\} = \{(s, t) | \lambda - \delta < t < \lambda + \delta, t - \lambda < s < \delta\}$ and obtain

$$\int_0^{\delta} \mu(I_s) K'_{\varepsilon}(s) ds = \int_{I_{\delta}} (K(\delta) - K_{\varepsilon}(t - \lambda)) d\mu(t). \quad (3.113)$$

Now suppose there are constants c and C such that $c \leq \frac{\mu(I_s)}{2s} \leq C$, $0 \leq s \leq \delta$, then

$$2c \arctan\left(\frac{\delta}{\varepsilon}\right) \leq \int_{I_{\delta}} K_{\varepsilon}(t - \lambda) d\mu(t) \leq 2C \arctan\left(\frac{\delta}{\varepsilon}\right) \quad (3.114)$$

since

$$\delta K_{\varepsilon}(\delta) + \int_0^{\delta} -s K'_{\varepsilon}(s) ds = \arctan\left(\frac{\delta}{\varepsilon}\right). \quad (3.115)$$

Thus the claim follows combining both estimates. \square

As a consequence of Theorem A.34 and Theorem A.35 we obtain

Theorem 3.18. *Let μ be a finite Borel measure and F its Borel transform, then the limit*

$$\operatorname{Im}(F(\lambda)) = \lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \operatorname{Im}(F(\lambda + i\varepsilon)) \quad (3.116)$$

exists a.e. with respect to both μ and Lebesgue measure (finite or infinite) and

$$(D\mu)(\lambda) = \frac{1}{\pi} \operatorname{Im}(F(\lambda)) \quad (3.117)$$

whenever $(D\mu)(\lambda)$ exists.

Moreover, the set $\{\lambda | F(\lambda) = \infty\}$ is a support for the singularly and $\{\lambda | F(\lambda) < \infty\}$ is a support for the absolutely continuous part.

In particular,

Corollary 3.19. *The measure μ is purely absolutely continuous on I if $\limsup_{\varepsilon \downarrow 0} \operatorname{Im}(F(\lambda + i\varepsilon)) < \infty$ for all $\lambda \in I$.*

Applications of the spectral theorem

This chapter can be mostly skipped on first reading. You might want to have a look at the first section and then come back to the remaining ones later.

Now let us show how the spectral theorem can be used. We will give a few typical applications:

Firstly we will derive an operator valued version of Stieltjes' inversion formula. To do this, we need to show how to integrate a family of functions of A with respect to a parameter. Moreover, we will show that these integrals can be evaluated by computing the corresponding integrals of the complex valued functions.

Secondly we will consider commuting operators and show how certain facts, which are known to hold for the resolvent of an operator A , can be established for a larger class of functions.

Then we will show how the eigenvalues below the essential spectrum and dimension of $\text{Ran}P_A(\Omega)$ can be estimated using the quadratic form.

Finally, we will investigate tensor products of operators.

4.1. Integral formulas

We begin with the first task by having a closer look at the projector $P_A(\Omega)$. They project onto subspaces corresponding to expectation values in the set Ω . In particular, the number

$$\langle \psi, \chi_\Omega(A)\psi \rangle \tag{4.1}$$

is the probability for a measurement of a to lie in Ω . In addition, we have

$$\langle \psi, A\psi \rangle = \int_{\Omega} \lambda d\mu_{\psi}(\lambda) \in \text{hull}(\Omega), \quad \psi \in P_A(\Omega)\mathfrak{H}, \quad \|\psi\| = 1, \quad (4.2)$$

where $\text{hull}(\Omega)$ is the convex hull of Ω .

The space $\text{Ran}\chi_{\{\lambda_0\}}(A)$ is called the **eigenspace** corresponding to λ_0 since we have

$$\langle \varphi, A\psi \rangle = \int_{\mathbb{R}} \lambda \chi_{\{\lambda_0\}}(\lambda) d\mu_{\varphi, \psi}(\lambda) = \lambda_0 \int_{\mathbb{R}} d\mu_{\varphi, \psi}(\lambda) = \lambda_0 \langle \varphi, \psi \rangle \quad (4.3)$$

and hence $A\psi = \lambda_0\psi$ for all $\psi \in \text{Ran}\chi_{\{\lambda_0\}}(A)$. The dimension of the eigenspace is called the **multiplicity** of the eigenvalue.

Moreover, since

$$\lim_{\varepsilon \downarrow 0} \frac{-i\varepsilon}{\lambda - \lambda_0 - i\varepsilon} = \chi_{\{\lambda_0\}}(\lambda) \quad (4.4)$$

we infer from Theorem 3.1 that

$$\lim_{\varepsilon \downarrow 0} -i\varepsilon R_A(\lambda_0 + i\varepsilon)\psi = \chi_{\{\lambda_0\}}(A)\psi. \quad (4.5)$$

Similarly, we can obtain an operator valued version of Stieltjes' inversion formula. But first we need to recall a few facts from integration in Banach spaces.

We will consider the case of mappings $f : I \rightarrow X$ where $I = [t_0, t_1] \subset \mathbb{R}$ is a compact interval and X is a Banach space. As before, a function $f : I \rightarrow X$ is called simple if the image of f is finite, $f(I) = \{x_i\}_{i=1}^n$, and if each inverse image $f^{-1}(x_i)$, $1 \leq i \leq n$, is a Borel set. The set of simple functions $S(I, X)$ forms a linear space and can be equipped with the sup norm

$$\|f\|_{\infty} = \sup_{t \in I} \|f(t)\|. \quad (4.6)$$

The corresponding Banach space obtained after completion is called the set of regulated functions $R(I, X)$.

Observe that $C(I, X) \subset R(I, X)$. In fact, consider the simple function $f_n = \sum_{i=0}^{n-1} f(s_i)\chi_{[s_i, s_{i+1})}$, where $s_i = t_0 + i\frac{t_1-t_0}{n}$. Since $f \in C(I, X)$ is uniformly continuous, we infer that f_n converges uniformly to f .

For $f \in S(I, X)$ we can define a linear map $\int : S(I, X) \rightarrow X$ by

$$\int_I f(t)dt = \sum_{i=1}^n x_i |f^{-1}(x_i)|, \quad (4.7)$$

where $|\Omega|$ denotes the Lebesgue measure of Ω . This map satisfies

$$\left\| \int_I f(t)dt \right\| \leq \|f\|_{\infty}(t_1 - t_0) \quad (4.8)$$

and hence it can be extended uniquely to a linear map $\int : R(I, X) \rightarrow X$ with the same norm $(t_1 - t_0)$ by Theorem 0.24. We even have

$$\left\| \int_I f(t) dt \right\| \leq \int_I \|f(t)\| dt, \quad (4.9)$$

which clearly holds for $f \in S(I, X)$ and thus for all $f \in R(I, X)$ by continuity. In addition, if $\ell \in X^*$ is a continuous linear functional, then

$$\ell\left(\int_I f(t) dt\right) = \int_I \ell(f(t)) dt, \quad f \in R(I, X). \quad (4.10)$$

In particular, if $A(t) \in R(I, \mathfrak{L}(\mathfrak{H}))$, then

$$\left(\int_I A(t) dt\right) \psi = \int_I (A(t)\psi) dt. \quad (4.11)$$

If $I = \mathbb{R}$, we say that $f : I \rightarrow X$ is integrable if $f \in R([-r, r], X)$ for all $r > 0$ and if $\|f(t)\|$ is integrable. In this case we can set

$$\int_{\mathbb{R}} f(t) dt = \lim_{r \rightarrow \infty} \int_{[-r, r]} f(t) dt \quad (4.12)$$

and (4.9) and (4.10) still hold.

We will use the standard notation $\int_{t_2}^{t_3} f(s) ds = \int_I \chi_{(t_2, t_3)}(s) f(s) ds$ and $\int_{t_3}^{t_2} f(s) ds = -\int_{t_2}^{t_3} f(s) ds$.

We write $f \in C^1(I, X)$ if

$$\frac{d}{dt} f(t) = \lim_{\varepsilon \rightarrow 0} \frac{f(t + \varepsilon) - f(t)}{\varepsilon} \quad (4.13)$$

exists for all $t \in I$. In particular, if $f \in C(I, X)$, then $F(t) = \int_{t_0}^t f(s) ds \in C^1(I, X)$ and $dF/dt = f$ as can be seen from

$$\|F(t + \varepsilon) - F(t) - f(t)\varepsilon\| = \left\| \int_t^{t+\varepsilon} (f(s) - f(t)) ds \right\| \leq |\varepsilon| \sup_{s \in [t, t+\varepsilon]} \|f(s) - f(t)\|. \quad (4.14)$$

The important facts for us are the following two results.

Lemma 4.1. *Suppose $f : I \times \mathbb{R} \rightarrow \mathbb{C}$ is a bounded Borel function such that $f(\cdot, \lambda)$ and set $F(\lambda) = \int_I f(t, \lambda) dt$. Let A be self-adjoint. Then $f(t, A) \in R(I, \mathfrak{L}(\mathfrak{H}))$ and*

$$F(A) = \int_I f(t, A) dt \quad \text{respectively} \quad F(A)\psi = \int_I f(t, A)\psi dt. \quad (4.15)$$

Proof. That $f(t, A) \in R(I, \mathfrak{L}(\mathfrak{H}))$ follows from the spectral theorem, since it is no restriction to assume that A is multiplication by λ in some L^2 space.

We compute

$$\begin{aligned}
\langle \varphi, \left(\int_I f(t, A) dt \right) \psi \rangle &= \int_I \langle \varphi, f(t, A) \psi \rangle dt \\
&= \int_I \int_{\mathbb{R}} f(t, \lambda) d\mu_{\varphi, \psi}(\lambda) dt \\
&= \int_{\mathbb{R}} \int_I f(t, \lambda) dt d\mu_{\varphi, \psi}(\lambda) \\
&= \int_{\mathbb{R}} F(\lambda) d\mu_{\varphi, \psi}(\lambda) = \langle \varphi, F(A) \psi \rangle \quad (4.16)
\end{aligned}$$

by Fubini's theorem and hence the first claim follows. \square

Lemma 4.2. *Suppose $f : \mathbb{R} \rightarrow \mathfrak{L}(\mathfrak{H})$ is integrable and $A \in \mathfrak{L}(\mathfrak{H})$. Then*

$$A \int_{\mathbb{R}} f(t) dt = \int_{\mathbb{R}} A f(t) dt \quad \text{respectively} \quad \int_{\mathbb{R}} f(t) dt A = \int_{\mathbb{R}} f(t) A dt. \quad (4.17)$$

Proof. It suffices to prove the case where f is simple and of compact support. But for such functions the claim is straightforward. \square

Now we can prove Stone's formula.

Theorem 4.3 (Stone's formula). *Let A be self-adjoint, then*

$$\frac{1}{2\pi i} \int_{\lambda_1}^{\lambda_2} (R_A(\lambda + i\varepsilon) - R_A(\lambda - i\varepsilon)) d\lambda \rightarrow \frac{1}{2} (P_A([\lambda_1, \lambda_2]) + P_A((\lambda_1, \lambda_2))) \quad (4.18)$$

strongly.

Proof. The result follows combining Lemma 4.1 with Theorem 3.1 and (3.91). \square

Problem 4.1. *Let Γ be a differentiable Jordan curve in $\rho(A)$. Show*

$$\chi_{\Omega}(A) = \int_{\Gamma} R_A(z) dz, \quad (4.19)$$

where Ω is the intersection of the interior of Γ with \mathbb{R} .

4.2. Commuting operators

Now we come to commuting operators. As a preparation we can now prove

Lemma 4.4. *Let $K \subseteq \mathbb{R}$ be closed. And let $C_{\infty}(K)$ be the set of all continuous functions on K which vanish at ∞ (if K is unbounded) with the sup norm. The $*$ -algebra generated by the function*

$$\lambda \mapsto \frac{1}{\lambda - z} \quad (4.20)$$

for one $z \in \mathbb{C} \setminus K$ is dense in $C_{\infty}(K)$.

Proof. If K is compact, the claim follows directly from the complex Stone–Weierstraß theorem since $(\lambda_1 - z)^{-1} = (\lambda_2 - z)^{-1}$ implies $\lambda_1 = \lambda_2$. Otherwise, replace K by $\tilde{K} = K \cup \{\infty\}$, which is compact, and set $(\infty - z)^{-1} = 0$. Then we can again apply the complex Stone–Weierstraß theorem to conclude that our $*$ -subalgebra is equal to $\{f \in C(\tilde{K}) \mid f(\infty) = 0\}$ which is equivalent to $C_\infty(K)$. \square

We say that two bounded operators A, B **commute** if

$$[A, B] = AB - BA = 0. \quad (4.21)$$

If A or B is unbounded, we soon run into trouble with this definition since the above expression might not even make sense for any nonzero vector (e.g., take $B = \langle \varphi, \cdot \rangle \psi$ with $\psi \notin \mathfrak{D}(A)$). To avoid this nuisance we will replace A by a bounded function of A . A good candidate is the resolvent. Hence if A is self-adjoint and B is bounded we will say that A and B commute if

$$[R_A(z), B] = [R_A(z^*), B] = 0 \quad (4.22)$$

for one $z \in \rho(A)$.

Lemma 4.5. *Suppose A is self-adjoint and commutes with the bounded operator B . Then*

$$[f(A), B] = 0 \quad (4.23)$$

for any bounded Borel function f . If f is unbounded, the claim holds for any $\psi \in \mathfrak{D}(f(A))$.

Proof. Equation (4.22) tell us that (4.23) holds for any f in the $*$ -subalgebra generated by $R_A(z)$. Since this subalgebra is dense in $C_\infty(\sigma(A))$, the claim follows for all such $f \in C_\infty(\sigma(A))$. Next fix $\psi \in \mathfrak{H}$ and let f be bounded. Choose a sequence $f_n \in C_\infty(\sigma(A))$ converging to f in $L^2(\mathbb{R}, d\mu_\psi)$. Then

$$Bf(A)\psi = \lim_{n \rightarrow \infty} Bf_n(A)\psi = \lim_{n \rightarrow \infty} f_n(A)B\psi = f(A)B\psi. \quad (4.24)$$

If f is unbounded, let $\psi \in \mathfrak{D}(f(A))$ and choose f_n as in (3.24). Then

$$f(A)B\psi = \lim_{n \rightarrow \infty} f_n(A)B\psi = \lim_{n \rightarrow \infty} Bf_n(A)\psi \quad (4.25)$$

shows $f \in L^2(\mathbb{R}, d\mu_{B\psi})$ (i.e., $B\psi \in \mathfrak{D}(f(A))$) and $f(A)B\psi = BF(A)\psi$. \square

Corollary 4.6. *If A is self-adjoint and bounded, then (4.22) holds if and only if (4.21) holds.*

Proof. Since $\sigma(A)$ is compact, we have $\lambda \in C_\infty(\sigma(A))$ and hence (4.21) follows from (4.23) by our lemma. Conversely, since B commutes with any polynomial of A , the claim follows from the Neumann series. \square

As another consequence we obtain

Theorem 4.7. *Suppose A is self-adjoint and has simple spectrum. A bounded operator B commutes with A if and only if $B = f(A)$ for some bounded Borel function.*

Proof. Let ψ be a cyclic vector for A . By our unitary equivalence it is no restriction to assume $\mathfrak{H} = L^2(\mathbb{R}, d\mu_\psi)$. Then

$$Bg(\lambda) = Bg(\lambda) \cdot 1 = g(\lambda)(B1)(\lambda) \quad (4.26)$$

since B commutes with the multiplication operator $g(\lambda)$. Hence B is multiplication by $f(\lambda) = (B1)(\lambda)$. \square

The assumption that the spectrum of A is simple is crucial as the example $A = \mathbb{I}$ shows. Note also that the functions $\exp(-itA)$ can also be used instead of resolvents.

Lemma 4.8. *Suppose A is self-adjoint and B is bounded. Then B commutes with A if and only if*

$$[e^{-iAt}, B] = 0 \quad (4.27)$$

for all $t \in \mathbb{R}$.

Proof. It suffices to show $[\hat{f}(A), B] = 0$ for $f \in \mathcal{S}(\mathbb{R})$, since these functions are dense in $C_\infty(\mathbb{R})$ by the complex Stone–Weierstraß theorem. Here \hat{f} denotes the Fourier transform of f , see Section 7.1. But for such f we have

$$[\hat{f}(A), B] = \frac{1}{\sqrt{2\pi}} \left[\int_{\mathbb{R}} f(t)e^{-iAt} dt, B \right] = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} f(t)[e^{-iAt}, B] dt = 0 \quad (4.28)$$

by Lemma 4.2. \square

The extension to the case where B is self-adjoint and unbounded is straightforward. We say that A and B commute in this case if

$$[R_A(z_1), R_B(z_2)] = [R_A(z_1^*), R_B(z_2)] = 0 \quad (4.29)$$

for one $z_1 \in \rho(A)$ and one $z_2 \in \rho(B)$ (the claim for z_2^* follows by taking adjoints). From our above analysis it follows that this is equivalent to

$$[e^{-iAt}, e^{-iBs}] = 0, \quad t, s \in \mathbb{R}, \quad (4.30)$$

respectively

$$[f(A), g(B)] = 0 \quad (4.31)$$

for arbitrary bounded Borel functions f and g .

4.3. The min-max theorem

In many applications a self-adjoint operator has a number of eigenvalues below the bottom of the essential spectrum. The essential spectrum is obtained from the spectrum by removing all discrete eigenvalues with finite multiplicity (we will have a closer look at it in Section 6.2). In general there is no way of computing the lowest eigenvalues and their corresponding eigenfunctions explicitly. However, one often has some idea how the eigenfunctions might approximately look like.

So suppose we have a normalized function ψ_1 which is an approximation for the eigenfunction φ_1 of the lowest eigenvalue E_1 . Then by Theorem 2.15 we know that

$$\langle \psi_1, A\psi_1 \rangle \geq \langle \varphi_1, A\varphi_1 \rangle = E_1. \quad (4.32)$$

If we add some free parameters to ψ_1 , one can optimize them and obtain quite good upper bounds for the first eigenvalue.

But is there also something one can say about the next eigenvalues? Suppose we know the first eigenfunction φ_1 , then we can restrict A to the orthogonal complement of φ_1 and proceed as before: E_2 will be the infimum over all expectations restricted to this subspace. If we restrict to the orthogonal complement of an approximating eigenfunction ψ_1 , there will still be a component in the direction of φ_1 left and hence the infimum of the expectations will be lower than E_2 . Thus the optimal choice $\psi_1 = \varphi_1$ will give the maximal value E_2 .

More precisely, let $\{\varphi_j\}_{j=1}^N$ be an orthonormal basis for the space spanned by the eigenfunctions corresponding to eigenvalues below the essential spectrum. Assume they satisfy $(A - E_j)\varphi_j = 0$, where $E_j \leq E_{j+1}$ are the eigenvalues (counted according to their multiplicity). If the number of eigenvalues N is finite we set $E_j = \inf \sigma_{\text{ess}}(A)$ for $j > N$ and choose φ_j orthonormal such that $\|(A - E_j)\varphi_j\| \leq \varepsilon$.

Define

$$U(\psi_1, \dots, \psi_n) = \{\psi \in \mathfrak{D}(A) \mid \|\psi\| = 1, \psi \in \text{span}\{\psi_1, \dots, \psi_n\}^\perp\}. \quad (4.33)$$

(i) We have

$$\inf_{\psi \in U(\psi_1, \dots, \psi_{n-1})} \langle \psi, A\psi \rangle \leq E_n + O(\varepsilon). \quad (4.34)$$

In fact, set $\psi = \sum_{j=1}^n \alpha_j \varphi_j$ and choose α_j such that $\psi \in U(\psi_1, \dots, \psi_{n-1})$, then

$$\langle \psi, A\psi \rangle = \sum_{j=1}^n |\alpha_j|^2 E_j + O(\varepsilon) \leq E_n + O(\varepsilon) \quad (4.35)$$

and the claim follows.

(ii) We have

$$\inf_{\psi \in U(\varphi_1, \dots, \varphi_{n-1})} \langle \psi, A\psi \rangle \geq E_n - O(\varepsilon). \quad (4.36)$$

In fact, set $\psi = \varphi_n$.

Since ε can be chosen arbitrarily small we have proven

Theorem 4.9 (Min-Max). *Let A be self-adjoint and let $E_1 \leq E_2 \leq E_3 \cdots$ be the eigenvalues of A below the essential spectrum respectively the infimum of the essential spectrum once there are no more eigenvalues left. Then*

$$E_n = \sup_{\psi_1, \dots, \psi_{n-1}} \inf_{\psi \in U(\psi_1, \dots, \psi_{n-1})} \langle \psi, A\psi \rangle. \quad (4.37)$$

Clearly the same result holds if $\mathfrak{D}(A)$ is replaced by the quadratic form domain $\mathfrak{Q}(A)$ in the definition of U . In addition, as long as E_n is an eigenvalue, the sup and inf are in fact max and min, explaining the name.

Corollary 4.10. *Suppose A and B are self-adjoint operators with $A \geq B$ (i.e. $A - B \geq 0$), then $E_n(A) \geq E_n(B)$.*

Problem 4.2. *Suppose A, A_n are bounded and $A_n \rightarrow A$. Then $E_k(A_n) \rightarrow E_k(A)$. (Hint $\|A - A_n\| \leq \varepsilon$ is equivalent to $A - \varepsilon \leq A \leq A + \varepsilon$.)*

4.4. Estimating eigenspaces

Next, we show that the dimension of the range of $P_A(\Omega)$ can be estimated if we have some functions which lie approximately in this space.

Theorem 4.11. *Suppose A is a self-adjoint operator and ψ_j , $1 \leq j \leq k$, are linearly independent elements of a \mathfrak{H} .*

(i). *Let $\lambda \in \mathbb{R}$, $\psi_j \in \mathfrak{Q}(A)$. If*

$$\langle \psi, A\psi \rangle < \lambda \|\psi\|^2 \quad (4.38)$$

for any nonzero linear combination $\psi = \sum_{j=1}^k c_j \psi_j$, then

$$\dim \text{Ran } P_A((-\infty, \lambda)) \geq k. \quad (4.39)$$

Similarly, $\langle \psi, A\psi \rangle > \lambda \|\psi\|^2$ implies $\dim \text{Ran } P_A((\lambda, \infty)) \geq k$.

(ii). *Let $\lambda_1 < \lambda_2$, $\psi_j \in \mathfrak{D}(A)$. If*

$$\|(A - \frac{\lambda_2 + \lambda_1}{2})\psi\| < \frac{\lambda_2 - \lambda_1}{2} \|\psi\| \quad (4.40)$$

for any nonzero linear combination $\psi = \sum_{j=1}^k c_j \psi_j$, then

$$\dim \text{Ran } P_A((\lambda_1, \lambda_2)) \geq k. \quad (4.41)$$

Proof. (i). Let $M = \text{span}\{\psi_j\} \subseteq \mathfrak{H}$. We claim $\dim P_A((-\infty, \lambda))M = \dim M = k$. For this it suffices to show $\text{Ker}P_A((-\infty, \lambda))|_M = \{0\}$. Suppose $P_A((-\infty, \lambda))\psi = 0$, $\psi \neq 0$. Then we see that for any nonzero linear combination ψ

$$\begin{aligned} \langle \psi, A\psi \rangle &= \int_{\mathbb{R}} \eta d\mu_\psi(\eta) = \int_{[\lambda, \infty)} \eta d\mu_\psi(\eta) \\ &\geq \lambda \int_{[\lambda, \infty)} d\mu_\psi(\eta) = \lambda \|\psi\|^2. \end{aligned} \quad (4.42)$$

This contradicts our assumption (4.38).

(ii). Using the same notation as before we need to show $\text{Ker}P_A((\lambda_1, \lambda_2))|_M = \{0\}$. If $P_A((\lambda_1, \lambda_2))\psi = 0$, $\psi \neq 0$, then,

$$\begin{aligned} \|(A - \frac{\lambda_2 + \lambda_1}{2})\psi\|^2 &= \int_{\mathbb{R}} (x - \frac{\lambda_2 + \lambda_1}{2})^2 d\mu_\psi(x) = \int_{\Omega} x^2 d\mu_\psi(x + \frac{\lambda_2 + \lambda_1}{2}) \\ &\geq \frac{(\lambda_2 - \lambda_1)^2}{4} \int_{\Omega} d\mu_\psi(x + \frac{\lambda_2 + \lambda_1}{2}) = \frac{(\lambda_2 - \lambda_1)^2}{4} \|\psi\|^2, \end{aligned} \quad (4.43)$$

where $\Omega = (-\infty, -(\lambda_2 - \lambda_1)/2] \cup [(\lambda_2 - \lambda_1)/2, \infty)$. But this is a contradiction as before. \square

4.5. Tensor products of operators

Suppose A_j , $1 \leq j \leq n$, are self-adjoint operators on \mathfrak{H}_j . For every monomial $\lambda_1^{n_1} \cdots \lambda_n^{n_n}$ we can define

$$(A_1^{n_1} \otimes \cdots \otimes A_n^{n_n})\psi_1 \otimes \cdots \otimes \psi_n = (A_1^{n_1}\psi_1) \otimes \cdots \otimes (A_n^{n_n}\psi_n), \quad \psi_j \in \mathfrak{D}(A_j^{n_j}). \quad (4.44)$$

Hence for every polynomial $P(\lambda_1, \dots, \lambda_n)$ of degree N we can define

$$P(A_1, \dots, A_n)\psi_1 \otimes \cdots \otimes \psi_n, \quad \psi_j \in \mathfrak{D}(A_j^N), \quad (4.45)$$

and extend this definition to obtain a linear operator on the set

$$\mathfrak{D} = \text{span}\{\psi_1 \otimes \cdots \otimes \psi_n \mid \psi_j \in \mathfrak{D}(A_j^N)\}. \quad (4.46)$$

Moreover, if P is real-valued, then the operator $P(A_1, \dots, A_n)$ on \mathfrak{D} is symmetric and we can consider its closure, which will again be denoted by $P(A_1, \dots, A_n)$.

Theorem 4.12. *Suppose A_j , $1 \leq j \leq n$, are self-adjoint operators on \mathfrak{H}_j and let $P(\lambda_1, \dots, \lambda_n)$ be a real-valued polynomial and define $P(A_1, \dots, A_n)$ as above.*

Then $P(A_1, \dots, A_n)$ is self-adjoint and its spectrum is the closure of the range of P on the product of the spectra of the A_j , that is,

$$\sigma(P(A_1, \dots, A_n)) = \overline{P(\sigma(A_1), \dots, \sigma(A_n))}. \quad (4.47)$$

Proof. By the spectral theorem it is no restriction to assume that A_j is multiplication by λ_j on $L^2(\mathbb{R}, d\mu_j)$ and $P(A_1, \dots, A_n)$ is hence multiplication by $P(\lambda_1, \dots, \lambda_n)$ on $L^2(\mathbb{R}^n, d\mu_1 \times \dots \times d\mu_n)$. Since \mathfrak{D} contains the set of all functions $\psi_1(\lambda_1) \cdots \psi_n(\lambda_n)$ for which $\psi_j \in L^2_c(\mathbb{R}, d\mu_j)$ it follows that the domain of the closure of P contains $L^2_c(\mathbb{R}^n, d\mu_1 \times \dots \times d\mu_n)$. Hence P is the maximally defined multiplication operator by $P(\lambda_1, \dots, \lambda_n)$, which is self-adjoint.

Now let $\lambda = P(\lambda_1, \dots, \lambda_n)$ with $\lambda_j \in \sigma(A_j)$. Then there exists Weyl sequences $\psi_{j,k} \in \mathfrak{D}(A_j^N)$ with $(A_j - \lambda_j)\psi_{j,k} \rightarrow 0$ as $k \rightarrow \infty$. Then, $(P - \lambda)\psi_k \rightarrow 0$, where $\psi_k = \psi_{1,k} \otimes \dots \otimes \psi_{n,k}$ and hence $\lambda \in \sigma(P)$. Conversely, if $\lambda \notin \overline{P(\sigma(A_1), \dots, \sigma(A_n))}$, then $|P(\lambda_1, \dots, \lambda_n) - \lambda| \geq \varepsilon$ for a.e. λ_j with respect to μ_j and hence $(P - \lambda)^{-1}$ exists and is bounded, that is $\lambda \in \rho(P)$. \square

The two main cases of interest are $A_1 \otimes A_2$, in which case

$$\sigma(A_1 \otimes A_2) = \overline{\sigma(A_1)\sigma(A_2)} = \overline{\{\lambda_1\lambda_2 \mid \lambda_j \in \sigma(A_j)\}}, \quad (4.48)$$

and $A_1 \otimes \mathbb{I} + \mathbb{I} \otimes A_2$, in which case

$$\sigma(A_1 \otimes \mathbb{I} + \mathbb{I} \otimes A_2) = \overline{\sigma(A_1) + \sigma(A_2)} = \overline{\{\lambda_1 + \lambda_2 \mid \lambda_j \in \sigma(A_j)\}}. \quad (4.49)$$

Quantum dynamics

As in the finite dimensional case, the solution of the Schrödinger equation

$$i\frac{d}{dt}\psi(t) = H\psi(t) \quad (5.1)$$

is given by

$$\psi(t) = \exp(-itH)\psi(0). \quad (5.2)$$

A detailed investigation of this formula will be our first task. Moreover, in the finite dimensional case the dynamics is understood once the eigenvalues are known and the same is true in our case once we know the spectrum. Note that, like any Hamiltonian system from classical mechanics, our system is not hyperbolic (i.e., the spectrum is not away from the real axis) and hence simple results like, all solutions tend to the equilibrium position cannot be expected.

5.1. The time evolution and Stone's theorem

In this section we want to have a look at the initial value problem associated with the Schrödinger equation (2.12) in the Hilbert space \mathfrak{H} . If \mathfrak{H} is one-dimensional (and hence A is a real number), the solution is given by

$$\psi(t) = e^{-itA}\psi(0). \quad (5.3)$$

Our hope is that this formula also applies in the general case and that we can reconstruct a one-parameter unitary group $U(t)$ from its generator A (compare (2.11)) via $U(t) = \exp(-itA)$. We first investigate the family of operators $\exp(-itA)$.

Theorem 5.1. *Let A be self-adjoint and let $U(t) = \exp(-itA)$.*

(i). *$U(t)$ is a strongly continuous one-parameter unitary group.*

(ii). The limit $\lim_{t \rightarrow 0} \frac{1}{t}(U(t)\psi - \psi)$ exists if and only if $\psi \in \mathfrak{D}(A)$ in which case $\lim_{t \rightarrow 0} \frac{1}{t}(U(t)\psi - \psi) = -iA\psi$.

(iii). $U(t)\mathfrak{D}(A) = \mathfrak{D}(A)$ and $AU(t) = U(t)A$.

Proof. The group property (i) follows directly from Theorem 3.1 and the corresponding statements for the function $\exp(-it\lambda)$. To prove strong continuity observe that

$$\begin{aligned} \lim_{t \rightarrow t_0} \|e^{-itA}\psi - e^{-it_0A}\psi\|^2 &= \lim_{t \rightarrow t_0} \int_{\mathbb{R}} |e^{-it\lambda} - e^{-it_0\lambda}|^2 d\mu_\psi(\lambda) \\ &= \int_{\mathbb{R}} \lim_{t \rightarrow t_0} |e^{-it\lambda} - e^{-it_0\lambda}|^2 d\mu_\psi(\lambda) = 0 \end{aligned} \quad (5.4)$$

by the dominated convergence theorem.

Similarly, if $\psi \in \mathfrak{D}(A)$ we obtain

$$\lim_{t \rightarrow 0} \left\| \frac{1}{t}(e^{-itA}\psi - \psi) + iA\psi \right\|^2 = \lim_{t \rightarrow 0} \int_{\mathbb{R}} \left| \frac{1}{t}(e^{-it\lambda} - 1) + i\lambda \right|^2 d\mu_\psi(\lambda) = 0 \quad (5.5)$$

since $|e^{it\lambda} - 1| \leq |t\lambda|$. Now let \tilde{A} be the generator defined as in (2.11). Then \tilde{A} is a symmetric extension of A since we have

$$\langle \varphi, \tilde{A}\psi \rangle = \lim_{t \rightarrow 0} \langle \varphi, \frac{i}{t}(U(t) - 1)\psi \rangle = \lim_{t \rightarrow 0} \langle \frac{i}{-t}(U(-t) - 1)\varphi, \psi \rangle = \langle \tilde{A}\varphi, \psi \rangle \quad (5.6)$$

and hence $\tilde{A} = A$ by Corollary 2.2. This settles (ii).

To see (iii) replace $\psi \rightarrow U(s)\psi$ in (ii). \square

For our original problem this implies that formula (5.3) is indeed the solution to the initial value problem of the Schrödinger equation. Moreover,

$$\langle U(t)\psi, AU(t)\psi \rangle = \langle U(t)\psi, U(t)A\psi \rangle = \langle \psi, A\psi \rangle \quad (5.7)$$

shows that the expectations of A are time independent. This corresponds to conservation of energy.

On the other hand, the generator of the time evolution of a quantum mechanical system should always be a self-adjoint operator since it corresponds to an observable (energy). Moreover, there should be a one to one correspondence between the unitary group and its generator. This is ensured by Stone's theorem.

Theorem 5.2 (Stone). *Let $U(t)$ be a weakly continuous one-parameter unitary group. Then its generator A is self-adjoint and $U(t) = \exp(-itA)$.*

Proof. First of all observe that weak continuity together with Lemma 1.11 (iv) shows that $U(t)$ is in fact strongly continuous.

Next we show that A is densely defined. Pick $\psi \in \mathfrak{H}$ and set

$$\psi_\tau = \int_0^\tau U(t)\psi dt \quad (5.8)$$

(the integral is defined as in Section 4.1) implying $\lim_{\tau \rightarrow 0} \tau^{-1}\psi_\tau = \psi$. Moreover,

$$\begin{aligned} \frac{1}{t}(U(t)\psi_\tau - \psi_\tau) &= \frac{1}{t} \int_t^{t+\tau} U(s)\psi ds - \frac{1}{t} \int_0^\tau U(s)\psi ds \\ &= \frac{1}{t} \int_\tau^{\tau+t} U(s)\psi ds - \frac{1}{t} \int_0^t U(s)\psi ds \\ &= \frac{1}{t} U(\tau) \int_0^t U(s)\psi ds - \frac{1}{t} \int_0^t U(s)\psi ds \rightarrow U(\tau)\psi - \psi \end{aligned} \quad (5.9)$$

as $t \rightarrow 0$ shows $\psi_\tau \in \mathfrak{D}(A)$. As in the proof of the previous theorem, we can show that A is symmetric and that $U(t)\mathfrak{D}(A) = \mathfrak{D}(A)$.

Next, let us prove that A is essentially self-adjoint. By Lemma 2.6 it suffices to prove $\text{Ker}(A^* - z^*) = \{0\}$ for $z \in \mathbb{C} \setminus \mathbb{R}$. Suppose $A^*\varphi = z^*\varphi$, then for each $\psi \in \mathfrak{D}(A)$ we have

$$\begin{aligned} \frac{d}{dt} \langle \varphi, U(t)\psi \rangle &= \langle \varphi, -iAU(t)\psi \rangle = -i \langle A^*\varphi, U(t)\psi \rangle \\ &= -iz \langle \varphi, U(t)\psi \rangle \end{aligned} \quad (5.10)$$

and hence $\langle \varphi, U(t)\psi \rangle = \exp(-izt) \langle \varphi, \psi \rangle$. Since the left hand side is bounded for all $t \in \mathbb{R}$ and the exponential on the right hand side is not, we must have $\langle \varphi, \psi \rangle = 0$ implying $\varphi = 0$ since $\mathfrak{D}(A)$ is dense.

So A is essentially self-adjoint and we can introduce $V(t) = \exp(-it\bar{A})$. We are done if we can show $U(t) = V(t)$.

Let $\psi \in \mathfrak{D}(A)$ and abbreviate $\psi(t) = (U(t) - V(t))\psi$. Then

$$\lim_{s \rightarrow 0} \frac{\psi(t+s) - \psi(t)}{s} = i\bar{A}\psi(t) \quad (5.11)$$

and hence $\frac{d}{dt} \|\psi(t)\|^2 = 2\text{Re} \langle \psi(t), iA\psi(t) \rangle = 0$. Since $\psi(0) = 0$ we have $\psi(t) = 0$ and hence $U(t)$ and $V(t)$ coincide on $\mathfrak{D}(A)$. Furthermore, since $\mathfrak{D}(A)$ is dense we have $U(t) = V(t)$ by continuity. \square

As an immediate consequence of the proof we also note the following useful criterion.

Corollary 5.3. *Suppose $\mathfrak{D} \subseteq \mathfrak{D}(A)$ is dense and invariant under $U(t)$. Then A is essentially self-adjoint on \mathfrak{D} .*

Proof. As in the above proof it follows $\langle \varphi, \psi \rangle = 0$ for any $\varphi \in \text{Ker}(A^* - z^*)$ and $\psi \in \mathfrak{D}$. \square

Note that by Lemma 4.8 two strongly continuous one-parameter groups commute

$$[e^{-itA}, e^{-isB}] = 0 \quad (5.12)$$

if and only if the generators commute.

Clearly, for a physicist, one of the goals must be to understand the time evolution of a quantum mechanical system. We have seen that the time evolution is generated by a self-adjoint operator, the Hamiltonian, and is given by a linear first order differential equation, the Schrödinger equation. To understand the dynamics of such a first order differential equation, one must understand the spectrum of the generator. Some general tools for this endeavor will be provided in the following sections.

Problem 5.1. Let $\mathfrak{H} = L^2(0, 2\pi)$ and consider the one parameter unitary group given by $U(t)f(x) = f(x - t \bmod 2\pi)$. What is the generator of U ?

5.2. The RAGE theorem

Now, let us discuss why the decomposition of the spectrum introduced in Section 3.3 is of physical relevance. Let $\|\varphi\| = \|\psi\| = 1$. The vector $\langle\varphi, \psi\rangle\varphi$ is the projection of ψ onto the (one-dimensional) subspace spanned by φ . Hence $|\langle\varphi, \psi\rangle|^2$ can be viewed as the part of ψ which is in the state φ . A first question one might rise is, how does

$$|\langle\varphi, U(t)\psi\rangle|^2, \quad U(t) = e^{-itA}, \quad (5.13)$$

behave as $t \rightarrow \infty$? By the spectral theorem,

$$\hat{\mu}_{\varphi, \psi}(t) = \langle\varphi, U(t)\psi\rangle = \int_{\mathbb{R}} e^{-it\lambda} d\mu_{\varphi, \psi}(\lambda) \quad (5.14)$$

is the **Fourier transform** of the measure $\mu_{\varphi, \psi}$. Thus our question is answered by Wiener's theorem.

Theorem 5.4 (Wiener). *Let μ be a finite complex Borel measure on \mathbb{R} and let*

$$\hat{\mu}(t) = \int_{\mathbb{R}} e^{-it\lambda} d\mu(\lambda) \quad (5.15)$$

be its Fourier transform. Then the Cesàro time average of $\hat{\mu}(t)$ has the following limit

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T |\hat{\mu}(t)|^2 dt = \sum_{\lambda \in \mathbb{R}} |\mu(\{\lambda\})|^2, \quad (5.16)$$

where the sum on the right hand side is finite.

Proof. By Fubini we have

$$\begin{aligned} \frac{1}{T} \int_0^T |\hat{\mu}(t)|^2 dt &= \frac{1}{T} \int_0^T \int_{\mathbb{R}} \int_{\mathbb{R}} e^{-i(x-y)t} d\mu(x) d\mu^*(y) dt \\ &= \int_{\mathbb{R}} \int_{\mathbb{R}} \left(\frac{1}{T} \int_0^T e^{-i(x-y)t} dt \right) d\mu(x) d\mu^*(y). \end{aligned} \quad (5.17)$$

The function in parentheses is bounded by one and converges pointwise to $\chi_{\{0\}}(x-y)$ as $T \rightarrow \infty$. Thus, by the dominated convergence theorem, the limit of the above expression is given by

$$\int_{\mathbb{R}} \int_{\mathbb{R}} \chi_{\{0\}}(x-y) d\mu(x) d\mu^*(y) = \int_{\mathbb{R}} \mu(\{y\}) d\mu^*(y) = \sum_{y \in \mathbb{R}} |\mu(\{y\})|^2. \quad (5.18)$$

□

To apply this result to our situation, observe that the subspaces \mathfrak{H}_{ac} , \mathfrak{H}_{sc} , and \mathfrak{H}_{pp} are invariant with respect to time evolution since $P^{xx}U(t) = \chi_{M_{xx}}(A) \exp(-itA) = \exp(-itA) \chi_{M_{xx}}(A) = U(t)P^{xx}$, $xx \in \{ac, sc, pp\}$. Moreover, if $\psi \in \mathfrak{H}_{xx}$ we have $P^{xx}\psi = \psi$ which shows $\langle \varphi, f(A)\psi \rangle = \langle \varphi, P^{xx}f(A)\psi \rangle = \langle P^{xx}\varphi, f(A)\psi \rangle$ implying $d\mu_{\varphi, \psi} = d\mu_{P^{xx}\varphi, \psi}$. Thus if μ_{ψ} is *ac*, *sc*, or *pp*, so is $\mu_{\varphi, \psi}$ for every $\varphi \in \mathfrak{H}$.

That is, if $\psi \in \mathfrak{H}_c = \mathfrak{H}_{ac} \oplus \mathfrak{H}_{sc}$, then the Cesàro mean of $\langle \varphi, U(t)\psi \rangle$ tends to zero. In other words, the average of the probability of finding the system in any prescribed state tends to zero if we start in the continuous subspace \mathfrak{H}_c of A .

If $\psi \in \mathfrak{H}_{ac}$, then $d\mu_{\varphi, \psi}$ is absolutely continuous with respect to Lebesgue measure and thus $\hat{\mu}_{\varphi, \psi}(t)$ is continuous and tends to zero as $|t| \rightarrow \infty$. In fact, this follows from the Riemann-Lebesgue lemma (see Lemma 7.6 below).

Now we want to draw some additional consequences from Wiener's theorem. This will eventually yield a dynamical characterization of the continuous and pure point spectrum due to Ruelle, Amrein, Gorgescu, and Enß. But first we need a few definitions.

An operator $K \in \mathfrak{L}(\mathfrak{H})$ is called **finite rank** if its range is finite dimensional. The dimension $n = \dim \text{Ran}(K)$ is called the **rank** of K . If $\{\psi_j\}_{j=1}^n$ is an orthonormal basis for $\text{Ran}(K)$ we have

$$K\psi = \sum_{j=1}^n \langle \psi_j, K\psi \rangle \psi_j = \sum_{j=1}^n \langle \varphi_j, \psi \rangle \psi_j, \quad (5.19)$$

where $\varphi_j = K^*\psi_j$. The elements φ_j are linearly independent since $\text{Ran}(K) = \text{Ker}(K^*)^\perp$. Hence every finite rank operator is of the form (5.19). In addition, the adjoint of K is also finite rank and given by

$$K^*\psi = \sum_{j=1}^n \langle \psi_j, \psi \rangle \varphi_j. \quad (5.20)$$

The closure of the set of all finite rank operators in $\mathfrak{L}(\mathfrak{H})$ is called the set of **compact operators** $\mathfrak{C}(\mathfrak{H})$. It is straightforward to verify (Problem 5.2)

Lemma 5.5. *The set of all compact operators $\mathfrak{C}(\mathfrak{H})$ is a closed *-ideal in $\mathfrak{L}(\mathfrak{H})$.*

There is also a weaker version of compactness which is useful for us. The operator K is called **relatively compact** with respect to A if

$$KR_A(z) \in \mathfrak{C}(\mathfrak{H}) \quad (5.21)$$

for one $z \in \rho(A)$. By the first resolvent identity this then follows for all $z \in \rho(A)$. In particular we have $\mathfrak{D}(A) \subseteq \mathfrak{D}(K)$.

Now let us return to our original problem.

Theorem 5.6. *Let A be self-adjoint and suppose K is relatively compact. Then*

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \|Ke^{-itA}P^c\psi\|^2 dt = 0 \quad \text{and} \quad \lim_{t \rightarrow \infty} \|Ke^{-itA}P^{ac}\psi\| = 0 \quad (5.22)$$

for every $\psi \in \mathfrak{D}(A)$. In particular, if K is also bounded, then the result holds for any $\psi \in \mathfrak{H}$.

Proof. Let $\psi \in \mathfrak{H}_c$ respectively $\psi \in \mathfrak{H}_{ac}$ and drop the projectors. Then, if K is a rank one operator (i.e., $K = \langle \varphi_1, \cdot \rangle \varphi_2$), the claim follows from Wiener's theorem respectively the Riemann-Lebesgue lemma. Hence it holds for any finite rank operator K .

If K is compact, there is a sequence K_n of finite rank operators such that $\|K - K_n\| \leq 1/n$ and hence

$$\|Ke^{-itA}\psi\| \leq \|K_n e^{-itA}\psi\| + \frac{1}{n}\|\psi\|. \quad (5.23)$$

Thus the claim holds for any compact operator K .

If $\psi \in \mathfrak{D}(A)$ we can set $\psi = (A - i)^{-1}\varphi$, where $\varphi \in \mathfrak{H}_c$ if and only if $\psi \in \mathfrak{H}_c$ (since \mathfrak{H}_c reduces A). Since $K(A + i)^{-1}$ is compact by assumption, the claim can be reduced to the previous situation. If, in addition, K is bounded, we can find a sequence $\psi_n \in \mathfrak{D}(A)$ such that $\|\psi - \psi_n\| \leq 1/n$ and hence

$$\|Ke^{-itA}\psi\| \leq \|Ke^{-itA}\psi_n\| + \frac{1}{n}\|K\|, \quad (5.24)$$

concluding the proof. \square

With the help of this result we can now prove an abstract version of the RAGE theorem.

Theorem 5.7 (RAGE). *Let A be self-adjoint. Suppose $K_n \in \mathfrak{L}(\mathfrak{H})$ is a sequence of relatively compact operators which converges strongly to the identity. Then*

$$\begin{aligned}\mathfrak{H}_c &= \{\psi \in \mathfrak{H} \mid \lim_{n \rightarrow \infty} \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \|K_n e^{-itA} \psi\| dt = 0\}, \\ \mathfrak{H}_{pp} &= \{\psi \in \mathfrak{H} \mid \lim_{n \rightarrow \infty} \sup_{t \geq 0} \|(\mathbb{I} - K_n) e^{-itA} \psi\| = 0\}.\end{aligned}\quad (5.25)$$

Proof. Abbreviate $\psi(t) = \exp(-itA)\psi$. We begin with the first equation.

Let $\psi \in \mathfrak{H}_c$, then

$$\frac{1}{T} \int_0^T \|K_n \psi(t)\| dt \leq \left(\frac{1}{T} \int_0^T \|K_n \psi(t)\|^2 dt \right)^{1/2} \rightarrow 0 \quad (5.26)$$

by Cauchy-Schwarz and the previous theorem. Conversely, if $\psi \notin \mathfrak{H}_c$ we can write $\psi = \psi^c + \psi^{pp}$. By our previous estimate it suffices to show $\|K_n \psi^{pp}(t)\| \geq \varepsilon > 0$ for n large. In fact, we even claim

$$\lim_{n \rightarrow \infty} \sup_{t \geq 0} \|K_n \psi^{pp}(t) - \psi^{pp}(t)\| = 0. \quad (5.27)$$

By the spectral theorem, we can write $\psi^{pp}(t) = \sum_j \alpha_j(t) \psi_j$, where the ψ_j are orthonormal eigenfunctions and $\alpha_j(t) = \exp(-it\lambda_j) \alpha_j$. Truncate this expansion after N terms, then this part converges uniformly to the desired limit by strong convergence of K_n . Moreover, by Lemma 1.13 we have $\|K_n\| \leq M$, and hence the error can be made arbitrarily small by choosing N large.

Now let us turn to the second equation. If $\psi \in \mathfrak{H}_{pp}$ the claim follows by (5.27). Conversely, if $\psi \notin \mathfrak{H}_{pp}$ we can write $\psi = \psi^c + \psi^{pp}$ and by our previous estimate it suffices to show that $\|(\mathbb{I} - K_n) \psi^c(t)\|$ does not tend to 0 as $n \rightarrow \infty$. If it would, we would have

$$\begin{aligned}0 &= \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \|(\mathbb{I} - K_n) \psi^c(t)\|^2 dt \\ &\geq \|\psi^c(t)\|^2 - \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \|K_n \psi^c(t)\|^2 dt = \|\psi^c(t)\|^2,\end{aligned}\quad (5.28)$$

a contradiction. \square

In summary, regularity properties of spectral measures are related to the long time behavior of the corresponding quantum mechanical system.

However, a more detailed investigation of this topic is beyond the scope of this manuscript. For a survey containing several recent results see [9].

It is often convenient to treat the observables as time dependent rather than the states. We set

$$K(t) = e^{itA} K e^{-itA} \quad (5.29)$$

and note

$$\langle \psi(t), K\psi(t) \rangle = \langle \psi, K(t)\psi \rangle, \quad \psi(t) = e^{-itA}\psi. \quad (5.30)$$

This point of view is often referred to as **Heisenberg picture** in the physics literature. If K is unbounded we will assume $\mathfrak{D}(A) \subseteq \mathfrak{D}(K)$ such that the above equations make sense at least for $\psi \in \mathfrak{D}(A)$. The main interest is the behavior of $K(t)$ for large t . The strong limits are called **asymptotic observables** if they exist.

Theorem 5.8. *Suppose A is self-adjoint and K is relatively compact. Then*

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T e^{itA} K e^{-itA} \psi dt = \sum_{\lambda \in \sigma_p(A)} P_A(\{\lambda\}) K P_A(\{\lambda\}) \psi, \quad \psi \in \mathfrak{D}(A). \quad (5.31)$$

If K is in addition bounded, the result holds for any $\psi \in \mathfrak{H}$.

Proof. We will assume that K is bounded. To obtain the general result, use the same trick as before and replace K by $K R_A(z)$. Write $\psi = \psi^c + \psi^{pp}$. Then

$$\lim_{T \rightarrow \infty} \frac{1}{T} \left\| \int_0^T K(t) \psi^c dt \right\| \leq \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \|K(t) \psi^c\| dt = 0 \quad (5.32)$$

by Theorem 5.6. As in the proof of the previous theorem we can write $\psi^{pp} = \sum_j \alpha_j \psi_j$ and hence

$$\sum_j \alpha_j \frac{1}{T} \int_0^T K(t) \psi_j dt = \sum_j \alpha_j \left(\frac{1}{T} \int_0^T e^{it(A-\lambda_j)} dt \right) K \psi_j. \quad (5.33)$$

As in the proof of Wiener's theorem, we see that the operator in parenthesis tends to $P_A(\{\lambda_j\})$ strongly as $T \rightarrow \infty$. Since this operator is also bounded by 1 for all T , we can interchange the limit with the summation and the claim follows. \square

We also note the following corollary.

Corollary 5.9. *Under the same assumptions as in the RAGE theorem we have*

$$\lim_{n \rightarrow \infty} \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T e^{itA} K_n e^{-itA} \psi dt = P^{pp} \psi \quad (5.34)$$

respectively

$$\lim_{n \rightarrow \infty} \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T e^{-itA} (\mathbb{I} - K_n) e^{-itA} \psi dt = P^c \psi. \quad (5.35)$$

Problem 5.2. Prove Lemma 5.5.

Problem 5.3. Prove Corollary 5.9.

5.3. The Trotter product formula

In many situations the operator is of the form $A + B$, where e^{itA} and e^{itB} can be computed explicitly. Since A and B will not commute in general, we cannot obtain $e^{it(A+B)}$ from $e^{itA}e^{itB}$. However, we at least have:

Theorem 5.10 (Trotter product formula). *Suppose, A , B , and $A + B$ are self-adjoint. Then*

$$e^{it(A+B)} = \text{s-lim}_{n \rightarrow \infty} \left(e^{i\frac{t}{n}A} e^{i\frac{t}{n}B} \right)^n. \quad (5.36)$$

Proof. First of all note that we have

$$\begin{aligned} & (e^{i\tau A} e^{i\tau B})^n - e^{it(A+B)} \\ &= \sum_{j=0}^{n-1} (e^{i\tau A} e^{i\tau B})^{n-1-j} \left(e^{i\tau A} e^{i\tau B} - e^{i\tau(A+B)} \right) \left(e^{i\tau(A+B)} \right)^j, \end{aligned} \quad (5.37)$$

where $\tau = \frac{t}{n}$, and hence

$$\| (e^{i\tau A} e^{i\tau B})^n - e^{it(A+B)} \psi \| \leq |t| \max_{|s| \leq |t|} F_\tau(s), \quad (5.38)$$

where

$$F_\tau(s) = \left\| \frac{1}{\tau} (e^{i\tau A} e^{i\tau B} - e^{i\tau(A+B)}) e^{is(A+B)} \psi \right\|. \quad (5.39)$$

Now for $\psi \in \mathfrak{D}(A + B) = \mathfrak{D}(A) \cap \mathfrak{D}(B)$ we have

$$\frac{1}{\tau} (e^{i\tau A} e^{i\tau B} - e^{i\tau(A+B)}) \psi \rightarrow iA\psi + iB\psi - i(A + B)\psi = 0 \quad (5.40)$$

as $\tau \rightarrow 0$. So $\lim_{\tau \rightarrow 0} F_\tau(s) = 0$ at least pointwise, but we need this uniformly with respect to $s \in [-|t|, |t|]$.

Pointwise convergence implies

$$\left\| \frac{1}{\tau} (e^{i\tau A} e^{i\tau B} - e^{i\tau(A+B)}) \psi \right\| \leq C(\psi) \quad (5.41)$$

and, since $\mathfrak{D}(A + B)$ is a Hilbert space when equipped with the graph norm $\|\psi\|_{\Gamma(A+B)}^2 = \|\psi\|^2 + \|(A + B)\psi\|^2$, we can invoke the uniform boundedness principle to obtain

$$\left\| \frac{1}{\tau} (e^{i\tau A} e^{i\tau B} - e^{i\tau(A+B)}) \psi \right\| \leq C \|\psi\|_{\Gamma(A+B)}. \quad (5.42)$$

Now

$$\begin{aligned} |F_\tau(s) - F_\tau(r)| &\leq \left\| \frac{1}{\tau} (e^{i\tau A} e^{i\tau B} - e^{i\tau(A+B)}) (e^{is(A+B)} - e^{ir(A+B)}) \psi \right\| \\ &\leq C \| (e^{is(A+B)} - e^{ir(A+B)}) \psi \|_{\Gamma(A+B)}. \end{aligned} \quad (5.43)$$

shows that $F_\tau(\cdot)$ is uniformly continuous and the claim follows by a standard $\frac{\varepsilon}{2}$ argument. \square

If the operators are semi-bounded from below the same proof shows

Theorem 5.11 (Trotter product formula). *Suppose, A , B , and $A + B$ are self-adjoint and semi-bounded from below. Then*

$$e^{-t(A+B)} = \text{s-lim}_{n \rightarrow \infty} \left(e^{-\frac{t}{n}A} e^{-\frac{t}{n}B} \right)^n, \quad t \geq 0. \quad (5.44)$$

Problem 5.4. *Proof Theorem 5.11.*

Perturbation theory for self-adjoint operators

The Hamiltonian of a quantum mechanical system is usually the sum of the kinetic energy H_0 (free Schrödinger operator) plus an operator V corresponding to the potential energy. Since H_0 is easy to investigate, one usually tries to consider V as a perturbation of H_0 . This will only work if V is *small* with respect to H_0 . Hence we study such perturbations of self-adjoint operators next.

6.1. Relatively bounded operators and the Kato–Rellich theorem

An operator B is called A **bounded** or **relatively bounded** with respect to A if $\mathfrak{D}(A) \subseteq \mathfrak{D}(B)$ and if there are constants $a, b \geq 0$ such that

$$\|B\psi\| \leq a\|A\psi\| + b\|\psi\|, \quad \psi \in \mathfrak{D}(A). \quad (6.1)$$

The infimum of all constants a for which a corresponding b exists such that (6.1) holds is called the **A -bound** of B .

The triangle inequality implies

Lemma 6.1. *Suppose B_j , $j = 1, 2$, are A bounded with respective A -bounds a_i , $i = 1, 2$. Then $\alpha_1 B_1 + \alpha_2 B_2$ is also A bounded with A -bound less than $|\alpha_1|a_1 + |\alpha_2|a_2$. In particular, the set of all A bounded operators forms a linear space.*

There are also the following equivalent characterizations:

Lemma 6.2. *Suppose A is closed and B is closable. Then the following are equivalent:*

- (i) B is A bounded.
- (ii) $\mathfrak{D}(A) \subseteq \mathfrak{D}(B)$.
- (iii) $BR_A(z)$ is bounded for one (and hence for all) $z \in \rho(A)$.

Moreover, the A -bound of B is no larger than $\inf_{z \in \rho(A)} \|BR_A(z)\|$.

Proof. (i) \Rightarrow (ii) is true by definition. (ii) \Rightarrow (iii) since $BR_A(z)$ is a closed (Problem 2.6) operator defined on all of \mathfrak{H} and hence bounded by the closed graph theorem (Theorem 2.7). To see (iii) \Rightarrow (i) let $\psi \in \mathfrak{D}(A)$, then

$$\|B\psi\| = \|BR_A(z)(A - z)\psi\| \leq a\|(A - z)\psi\| \leq a\|A\psi\| + (a|z|)\|\psi\|, \quad (6.2)$$

where $a = \|BR_A(z)\|$. Finally, note that if $BR_A(z)$ is bounded for one $z \in \rho(A)$, it is bounded for all $z \in \rho(A)$ by the first resolvent formula. \square

We are mainly interested in the situation where A is self-adjoint and B is symmetric. Hence we will restrict our attention to this case.

Lemma 6.3. *Suppose A is self-adjoint and B relatively bounded. The A -bound of B is given by*

$$\lim_{\lambda \rightarrow \infty} \|BR_A(\pm i\lambda)\|. \quad (6.3)$$

If A is bounded from below, we can also replace $\pm i\lambda$ by $-\lambda$.

Proof. Let $\varphi = R_A(\pm i\lambda)\psi$, $\lambda > 0$, and let a_∞ be the A -bound of B . If B is A bounded, then (use the spectral theorem to estimate the norms)

$$\|BR_A(\pm i\lambda)\psi\| \leq a\|AR_A(\pm i\lambda)\psi\| + b\|R_A(\pm i\lambda)\psi\| \leq (a + \frac{b}{\lambda})\|\psi\|. \quad (6.4)$$

Hence $\limsup_{\lambda} \|BR_A(\pm i\lambda)\| \leq a_\infty$ which, together with $a_\infty \leq \inf_{\lambda} \|BR_A(\pm i\lambda)\|$ from the previous lemma, proves the claim.

The case where A is bounded from below is similar. \square

Now we will show the basic perturbation result due to Kato and Rellich.

Theorem 6.4 (Kato–Rellich). *Suppose A is (essentially) self-adjoint and B is symmetric with A -bound less than one. Then $A + B$, $\mathfrak{D}(A + B) = \mathfrak{D}(A)$, is (essentially) self-adjoint. If A is essentially self-adjoint we have $\mathfrak{D}(\overline{A}) \subseteq \mathfrak{D}(\overline{B})$ and $\overline{A + B} = \overline{A} + \overline{B}$.*

If A is bounded from below by γ , then $A + B$ is bounded from below by $\min(\gamma, b/(a - 1))$.

Proof. Since $\mathfrak{D}(\overline{A}) \subseteq \mathfrak{D}(\overline{B})$ and $\mathfrak{D}(\overline{A}) \subseteq \mathfrak{D}(\overline{A+B})$ by (6.1) we can assume that A is closed (i.e., self-adjoint). It suffices to show that $\text{Ran}(A+B \pm i\lambda) = \mathfrak{H}$. By the above lemma we can find a $\lambda > 0$ such that $\|BR_A(\pm i\lambda)\| < 1$. Hence $-1 \in \rho(BR_A(\pm i\lambda))$ and thus $\mathbb{I} + BR_A(\pm i\lambda)$ is onto. Thus

$$(A + B \pm i\lambda) = (\mathbb{I} + BR_A(\pm i\lambda))(A \pm i\lambda) \quad (6.5)$$

is onto and the proof of the first part is complete.

If A is bounded from below we can replace $\pm i\lambda$ by $-\lambda$ and the above equation shows that R_{A+B} exists for λ sufficiently large. By the proof of the previous lemma we can choose $-\lambda < \min(\gamma, b/(a-1))$. \square

Finally, let us show that there is also a connection between the resolvents.

Lemma 6.5. *Suppose A and B are closed and $\mathfrak{D}(A) \subseteq \mathfrak{D}(B)$. Then we have the **second resolvent formula***

$$R_{A+B}(z) - R_A(z) = -R_A(z)BR_{A+B}(z) = -R_{A+B}(z)BR_A(z) \quad (6.6)$$

for $z \in \rho(A) \cap \rho(A+B)$.

Proof. We compute

$$R_{A+B}(z) + R_A(z)BR_{A+B}(z) = R_A(z)(A+B-z)R_{A+B}(z) = R_A(z). \quad (6.7)$$

The second identity is similar. \square

Problem 6.1. *Compute the resolvent of $A + \alpha\langle\psi, \cdot\rangle\psi$. (Hint: Show*

$$(\mathbb{I} + \alpha\langle\varphi, \cdot\rangle\psi)^{-1} = \mathbb{I} - \frac{\alpha}{1 + \alpha\langle\varphi, \psi\rangle}\langle\varphi, \cdot\rangle\psi \quad (6.8)$$

and use the second resolvent formula.)

6.2. More on compact operators

Recall from Section 5.2 that we have introduced the set of compact operators $\mathfrak{C}(\mathfrak{H})$ as the closure of the set of all finite rank operators in $\mathfrak{L}(\mathfrak{H})$. Before we can proceed, we need to establish some further results for such operators. We begin by investigating the spectrum of self-adjoint compact operators and show that the spectral theorem takes a particular simple form in this case.

We introduce some notation first. The **discrete spectrum** $\sigma_d(A)$ is the set of all eigenvalues which are discrete points of the spectrum and whose corresponding eigenspace is finite dimensional. The complement of the discrete spectrum is called the **essential spectrum** $\sigma_{ess}(A) = \sigma(A) \setminus \sigma_d(A)$. If A is self-adjoint we might equivalently set

$$\sigma_d(A) = \{\lambda \in \sigma_p(A) \mid \text{rank}(P_A((\lambda - \varepsilon, \lambda + \varepsilon))) < \infty \text{ for some } \varepsilon > 0\}. \quad (6.9)$$

respectively

$$\sigma_{ess}(A) = \{\lambda \in \mathbb{R} | \text{rank}(P_A((\lambda - \varepsilon, \lambda + \varepsilon))) = \infty \text{ for all } \varepsilon > 0\}. \quad (6.10)$$

Theorem 6.6 (Spectral theorem for compact operators). *Suppose the operator K is self-adjoint and compact. Then the spectrum of K consists of an at most countable number of eigenvalues which can only cluster at 0. Moreover, the eigenspace to each nonzero eigenvalue is finite dimensional. In other words,*

$$\sigma_{ess}(K) \subseteq \{0\}, \quad (6.11)$$

where equality holds if and only if \mathfrak{H} is infinite dimensional.

In addition, we have

$$K = \sum_{\lambda \in \sigma(K)} \lambda P_K(\{\lambda\}). \quad (6.12)$$

Proof. It suffices to show $\text{rank}(P_K((\lambda - \varepsilon, \lambda + \varepsilon))) < \infty$ for $0 < \varepsilon < |\lambda|$.

Let K_n be a sequence of finite rank operators such that $\|K - K_n\| \leq 1/n$. If $\text{Ran}P_K((\lambda - \varepsilon, \lambda + \varepsilon))$ is infinite dimensional we can find a vector ψ_n in this range such that $\|\psi_n\| = 1$ and $K_n\psi_n = 0$. But this yields a contradiction

$$\frac{1}{n} \geq |\langle \psi_n, (K - K_n)\psi_n \rangle| = |\langle \psi_n, K\psi_n \rangle| \geq |\lambda| - \varepsilon > 0 \quad (6.13)$$

by (4.2). \square

As a consequence we obtain the canonical form of a general compact operator.

Theorem 6.7 (Canonical form of compact operators). *Let K be compact. There exists orthonormal sets $\{\hat{\phi}_j\}$, $\{\phi_j\}$ and positive numbers $s_j = s_j(K)$ such that*

$$K = \sum_j s_j \langle \phi_j, \cdot \rangle \hat{\phi}_j, \quad K^* = \sum_j s_j \langle \hat{\phi}_j, \cdot \rangle \phi_j. \quad (6.14)$$

Note $K\phi_j = s_j\hat{\phi}_j$ and $K^*\hat{\phi}_j = s_j\phi_j$, and hence $K^*K\phi_j = s_j^2\phi_j$ and $KK^*\hat{\phi}_j = s_j^2\hat{\phi}_j$.

The numbers $s_j(K)^2 > 0$ are the nonzero eigenvalues of KK^* respectively K^*K (counted with multiplicity) and $s_j(K) = s_j(K^*) = s_j$ are called **singular values** of K . There are either finitely many singular values (if K is finite rank) or they converge to zero.

Proof. By Lemma 5.5 K^*K is compact and hence Theorem 6.6 applies. Let $\{\phi_j\}$ be an orthonormal basis of eigenvectors for $P_{K^*K}((0, \infty))\mathfrak{H}$ and let

s_j^2 be the eigenvalue corresponding to ϕ_j . Then, for any $\psi \in \mathfrak{H}$ we can write

$$\psi = \sum_j \langle \phi_j, \psi \rangle \phi_j + \tilde{\psi} \quad (6.15)$$

with $\tilde{\psi} \in \text{Ker}(K^*K) = \text{Ker}(K)$. Then

$$K\psi = \sum_j s_j \langle \phi_j, \psi \rangle \hat{\phi}_j, \quad (6.16)$$

where $\hat{\phi}_j = s_j^{-1}K\phi_j$, since $\|K\tilde{\psi}\|^2 = \langle \tilde{\psi}, K^*K\tilde{\psi} \rangle = 0$. By $\langle \hat{\phi}_j, \hat{\phi}_k \rangle = (s_j s_k)^{-1} \langle K\phi_j, K\phi_k \rangle = (s_j s_k)^{-1} \langle K^*K\phi_j, \phi_k \rangle = s_j s_k^{-1} \langle \phi_j, \phi_k \rangle$ we see that $\{\hat{\phi}_j\}$ are orthonormal and the formula for K^* follows by taking the adjoint of the formula for K (Problem 6.2). \square

If K is self-adjoint then $\phi_j = \sigma_j \hat{\phi}_j$, $\sigma_j^2 = 1$ are the eigenvectors of K and $\sigma_j s_j$ are the corresponding eigenvalues.

Moreover, note that we have

$$\|K\| = \max_j s_j(K). \quad (6.17)$$

Finally, let me remark that there are a number of other equivalent definitions for compact operators.

Lemma 6.8. *For $K \in \mathfrak{L}(\mathfrak{H})$ the following statements are equivalent:*

- (i) K is compact.
- (i') K^* is compact.
- (ii) $A_n \in \mathfrak{L}(\mathfrak{H})$ and $A_n \xrightarrow{s} A$ strongly implies $A_n K \rightarrow AK$.
- (iii) $\psi_n \rightharpoonup \psi$ weakly implies $K\psi_n \rightarrow K\psi$ in norm.
- (iv) ψ_n bounded implies that $K\psi_n$ has a (norm) convergent subsequence.

Proof. (i) \Leftrightarrow (i'). This is immediate from Theorem 6.7.

(i) \Rightarrow (ii). Translating $A_n \rightarrow A_n - A$ it is no restriction to assume $A = 0$. Since $\|A_n\| \leq M$ it suffices to consider the case where K is finite rank. Then (by (6.14))

$$\|A_n K\|^2 = \sup_{\|\psi\|=1} \sum_{j=1}^N s_j |\langle \phi_j, \psi \rangle|^2 \|A_n \hat{\phi}_j\|^2 \leq \sum_{j=1}^N s_j \|A_n \hat{\phi}_j\|^2 \rightarrow 0. \quad (6.18)$$

(ii) \Rightarrow (iii). Again, replace $\psi_n \rightarrow \psi_n - \psi$ and assume $\psi = 0$. Choose $A_n = \langle \psi_n, \cdot \rangle \varphi$, $\|\varphi\| = 1$, then $\|K\psi_n\|^2 = \|A_n K^*\| \rightarrow 0$.

(iii) \Rightarrow (iv). If ψ_n is bounded it has a weakly convergent subsequence by Lemma 1.12. Now apply (iii) to this subsequence.

(iv) \Rightarrow (i). Let φ_j be an orthonormal basis and set

$$K_n = \sum_{j=1}^n \langle \varphi_j, \cdot \rangle K \varphi_j. \quad (6.19)$$

Then

$$\gamma_n = \|K - K_n\| = \sup_{\psi \in \text{span}\{\varphi_j\}_{j=n}^{\infty}, \|\psi\|=1} \|K\psi\| \quad (6.20)$$

is a decreasing sequence tending to a limit $\varepsilon \geq 0$. Moreover, we can find a sequence of unit vectors $\psi_n \in \text{span}\{\varphi_j\}_{j=n}^{\infty}$ for which $\|K\psi_n\| \geq \varepsilon$. By assumption, $K\psi_n$ has a convergent subsequence which, since ψ_n converges weakly to 0, converges to 0. Hence ε must be 0 and we are done. \square

The last condition explains the name compact. Moreover, note that you cannot replace $A_n K \rightarrow AK$ by $KA_n \rightarrow KA$ unless you additionally require A_n to be normal (then this follows by taking adjoints — recall that only for normal operators taking adjoints is continuous with respect to strong convergence). Without the requirement that A_n is normal the claim is wrong as the following example shows.

Example. Let $\mathfrak{H} = \ell^2(\mathbb{N})$, A_n the operator which shifts each sequence n places to the left, and $K = \langle \delta_1, \cdot \rangle \delta_1$, where $\delta_1 = (1, 0, \dots)$. Then $s\text{-lim } A_n = 0$ but $\|KA_n\| = 1$. \diamond

Problem 6.2. Deduce the formula for K^* from the one for K in (6.14).

6.3. Hilbert–Schmidt and trace class operators

Among the compact operators two special classes of particular importance. The first one are integral operators

$$K\psi(x) = \int_M K(x, y)\psi(y)d\mu(y), \quad \psi \in L^2(M, d\mu), \quad (6.21)$$

where $K(x, y) \in L^2(M \times M, d\mu \oplus d\mu)$. Such an operator is called **Hilbert–Schmidt operator**. Using Cauchy–Schwarz,

$$\begin{aligned} \int_M |K\psi(x)|^2 d\mu(x) &= \int_M \left| \int_M K(x, y)\psi(y)d\mu(y) \right|^2 d\mu(x) \\ &\leq \int_M \left(\int_M |K(x, y)|^2 d\mu(y) \right) \left(\int_M |\psi(y)|^2 d\mu(y) \right) d\mu(x) \\ &= \left(\int_M \int_M |K(x, y)|^2 d\mu(y) d\mu(x) \right) \left(\int_M |\psi(y)|^2 d\mu(y) \right) \end{aligned} \quad (6.22)$$

we see that K is bounded. Next, pick an orthonormal basis $\varphi_j(x)$ for $L^2(M, d\mu)$. Then, by Lemma 1.9, $\varphi_i(x)\varphi_j(y)$ is an orthonormal basis for

$L^2(M \times M, d\mu \oplus d\mu)$ and

$$K(x, y) = \sum_{i,j} c_{i,j} \varphi_i(x) \varphi_j(y), \quad c_{i,j} = \langle \varphi_i, K \varphi_j^* \rangle, \quad (6.23)$$

where

$$\sum_{i,j} |c_{i,j}|^2 = \int_M \int_M |K(x, y)|^2 d\mu(y) d\mu(x) < \infty. \quad (6.24)$$

In particular,

$$K\psi(x) = \sum_{i,j} c_{i,j} \langle \varphi_j^*, \psi \rangle \varphi_i(x) \quad (6.25)$$

shows that K can be approximated by finite rank operators (take finitely many terms in the sum) and is hence compact.

Using (6.14) we can also give a different characterization of Hilbert–Schmidt operators.

Lemma 6.9. *If $\mathfrak{H} = L^2(M, d\mu)$, then a compact operator K is Hilbert–Schmidt if and only if $\sum_j s_j(K)^2 < \infty$ and*

$$\sum_j s_j(K)^2 = \int_M \int_M |K(x, y)|^2 d\mu(x) d\mu(y), \quad (6.26)$$

in this case.

Proof. If K is compact we can define approximating finite rank operators K_n by considering only finitely many terms in (6.14):

$$K_n = \sum_{j=1}^n s_j \langle \phi_j, \cdot \rangle \hat{\phi}_j. \quad (6.27)$$

Then K_n has the kernel $K_n(x, y) = \sum_{j=1}^n s_j \phi_j(y)^* \hat{\phi}_j(x)$ and

$$\int_M \int_M |K_n(x, y)|^2 d\mu(x) d\mu(y) = \sum_{j=1}^n s_j(K)^2 \quad (6.28)$$

Now if one side converges, so does the other and in particular, (6.26) holds in this case. \square

Hence we will call a compact operator Hilbert–Schmidt if its singular values satisfy

$$\sum_j s_j(K)^2 < \infty. \quad (6.29)$$

By our lemma this coincides with our previous definition if $\mathfrak{H} = L^2(M, d\mu)$.

Since every Hilbert space is isomorphic to some $L^2(M, d\mu)$ we see that the Hilbert–Schmidt operators together with the norm

$$\|K\|_2 = \left(\sum_j s_j(K)^2 \right)^{1/2} \quad (6.30)$$

form a Hilbert space (isomorphic to $L^2(M \times M, d\mu \otimes d\mu)$). Note that $\|K\|_2 = \|K^*\|_2$ (since $s_j(K) = s_j(K^*)$). There is another useful characterization for identifying Hilbert–Schmidt operators:

Lemma 6.10. *A compact operator K is Hilbert–Schmidt if and only if*

$$\sum_n \|K\psi_n\|^2 < \infty \quad (6.31)$$

for some orthonormal set and

$$\sum_n \|K\psi_n\|^2 = \|K\|_2^2 \quad (6.32)$$

in this case.

Proof. This follows from

$$\begin{aligned} \sum_n \|K\psi_n\|^2 &= \sum_{n,j} |\langle \hat{\phi}_j, K\psi_n \rangle|^2 = \sum_{n,j} |\langle K^* \hat{\phi}_j, \psi_n \rangle|^2 \\ &= \sum_n \|K^* \hat{\phi}_n\|^2 = \sum_j s_j(K)^2. \end{aligned} \quad (6.33)$$

□

Corollary 6.11. *The set of Hilbert–Schmidt operators forms a $*$ -ideal in $\mathfrak{L}(\mathfrak{H})$ and*

$$\|KA\|_2 \leq \|A\| \|K\|_2 \quad \text{respectively} \quad \|AK\|_2 \leq \|A\| \|K\|_2. \quad (6.34)$$

Proof. Let K be Hilbert–Schmidt and A bounded. Then AK is compact and

$$\|AK\|_2^2 = \sum_n \|AK\psi_n\|^2 \leq \|A\|^2 \sum_n \|K\psi_n\|^2 = \|A\|^2 \|K\|_2^2. \quad (6.35)$$

For KA just consider adjoints. □

This approach can be generalized by defining

$$\|K\|_p = \left(\sum_j s_j(K)^p \right)^{1/p} \quad (6.36)$$

plus corresponding spaces

$$\mathcal{J}_p(\mathfrak{H}) = \{K \in \mathfrak{C}(\mathfrak{H}) \mid \|K\|_p < \infty\}, \quad (6.37)$$

which are known as **Schatten p -class**. Note that

$$\|K\| \leq \|K\|_p. \quad (6.38)$$

and that by $s_j(K) = s_j(K^*)$ we have

$$\|K\|_p = \|K^*\|_p. \quad (6.39)$$

Lemma 6.12. *The spaces $\mathcal{J}_p(\mathfrak{H})$ together with the norm $\|\cdot\|_p$ are Banach spaces. Moreover,*

$$\|K\|_p = \sup \left\{ \left(\sum_j |\langle \psi_j, K\varphi_j \rangle|^p \right)^{1/p} \mid \{\psi_j\}, \{\varphi_j\} \text{ ONS} \right\}, \quad (6.40)$$

where the sup is taken over all orthonormal systems.

Proof. The hard part is to prove (6.40): Choose q such that $\frac{1}{p} + \frac{1}{q} = 1$ and use Hölder's inequality to obtain $(s_j|\dots|^2)^{1/p} = (s_j^p|\dots|^2)^{1/p}|\dots|^{2/q}$

$$\begin{aligned} \sum_j s_j |\langle \varphi_n, \phi_j \rangle|^2 &\leq \left(\sum_j s_j^p |\langle \varphi_n, \phi_j \rangle|^2 \right)^{1/p} \left(\sum_j |\langle \varphi_n, \phi_j \rangle|^2 \right)^{1/q} \\ &\leq \left(\sum_j s_j^p |\langle \varphi_n, \phi_j \rangle|^2 \right)^{1/p}. \end{aligned} \quad (6.41)$$

Clearly the analogous equation holds for $\hat{\phi}_j, \psi_n$. Now using Cauchy-Schwarz we have

$$\begin{aligned} |\langle \psi_n, K\varphi_n \rangle|^p &= \left| \sum_j s_j^{1/2} \langle \varphi_n, \phi_j \rangle s_j^{1/2} \langle \hat{\phi}_j, \psi_n \rangle \right|^p \\ &\leq \left(\sum_j s_j^p |\langle \varphi_n, \phi_j \rangle|^2 \right)^{1/2} \left(\sum_j s_j^p |\langle \psi_n, \hat{\phi}_j \rangle|^2 \right)^{1/2} \end{aligned} \quad (6.42)$$

Summing over n , a second appeal to Cauchy-Schwarz and interchanging the order of summation finally gives

$$\begin{aligned} \sum_n |\langle \psi_n, K\varphi_n \rangle|^p &\leq \left(\sum_{n,j} s_j^p |\langle \varphi_n, \phi_j \rangle|^2 \right)^{1/2} \left(\sum_{n,j} s_j^p |\langle \psi_n, \hat{\phi}_j \rangle|^2 \right)^{1/2} \\ &\leq \left(\sum_j s_j^p \right)^{1/2} \left(\sum_j s_j^p \right)^{1/2} = \sum_j s_j^p. \end{aligned} \quad (6.43)$$

Since equality is attained for $\varphi_n = \phi_n$ and $\psi_n = \hat{\phi}_n$ equation (6.40) holds.

Now the rest is straightforward. From

$$\begin{aligned} & \left(\sum_j |\langle \psi_j, (K_1 + K_2)\varphi_j \rangle|^p \right)^{1/p} \\ & \leq \left(\sum_j |\langle \psi_j, K_1\varphi_j \rangle|^p \right)^{1/p} + \left(\sum_j |\langle \psi_j, K_2\varphi_j \rangle|^p \right)^{1/p} \\ & \leq \|K_1\|_p + \|K_2\|_p \end{aligned} \quad (6.44)$$

we infer that $\mathcal{J}_p(\mathfrak{H})$ is a vector space and the triangle inequality. The other requirements for a norm are obvious and it remains to check completeness. If K_n is a Cauchy sequence with respect to $\|\cdot\|_p$ it is also a Cauchy sequence with respect to $\|\cdot\|$ ($\|K\| \leq \|K\|_p$). Since $\mathfrak{C}(\mathfrak{H})$ is closed, there is a compact K with $\|K - K_n\| \rightarrow 0$ and by $\|K_n\|_p \leq C$ we have

$$\left(\sum_j |\langle \psi_j, K\varphi_j \rangle|^p \right)^{1/p} \leq C \quad (6.45)$$

for any finite ONS. Since the right hand side is independent of the ONS (and in particular on the number of vectors), K is in $\mathcal{J}_p(\mathfrak{H})$. \square

The two most important cases are $p = 1$ and $p = 2$: $\mathcal{J}_2(\mathfrak{H})$ is the space of Hilbert–Schmidt operators investigated in the previous section and $\mathcal{J}_1(\mathfrak{H})$ is the space of **trace class** operators. Since Hilbert–Schmidt operators are easy to identify it is important to relate $\mathcal{J}_1(\mathfrak{H})$ with $\mathcal{J}_2(\mathfrak{H})$:

Lemma 6.13. *An operator is trace class if and only if it can be written as the product of two Hilbert–Schmidt operators, $K = K_1K_2$, and we have*

$$\|K\|_1 \leq \|K_1\|_2 \|K_2\|_2 \quad (6.46)$$

in this case.

Proof. By Cauchy-Schwarz we have

$$\begin{aligned} \sum_n |\langle \varphi_n, K\psi_n \rangle| &= \sum_n |\langle K_1^* \varphi_n, K_2 \psi_n \rangle| \leq \left(\sum_n \|K_1^* \varphi_n\|^2 \sum_n \|K_2 \psi_n\|^2 \right)^{1/2} \\ &= \|K_1\|_2 \|K_2\|_2 \end{aligned} \quad (6.47)$$

and hence $K = K_1K_2$ is trace class if both K_1 and K_2 are Hilbert–Schmidt operators. To see the converse let K be given by (6.14) and choose $K_1 = \sum_j \sqrt{s_j(K)} \langle \phi_j, \cdot \rangle \hat{\phi}_j$ respectively $K_2 = \sum_j \sqrt{s_j(K)} \langle \phi_j, \cdot \rangle \phi_j$. \square

Corollary 6.14. *The set of trace class operators forms a $*$ -ideal in $\mathfrak{L}(\mathfrak{H})$ and*

$$\|KA\|_1 \leq \|A\| \|K\|_1 \quad \text{respectively} \quad \|AK\|_1 \leq \|A\| \|K\|_1. \quad (6.48)$$

Proof. Write $K = K_1K_2$ with K_1, K_2 Hilbert–Schmidt and use Corollary 6.11. \square

Now we can also explain the name trace class:

Lemma 6.15. *If K is trace class, then for any ONB $\{\varphi_n\}$ the trace*

$$\operatorname{tr}(K) = \sum_n \langle \varphi_n, K\varphi_n \rangle \quad (6.49)$$

is finite and independent of the ONB.

Moreover, the trace is linear and if $K_1 \leq K_2$ are both trace class we have $\operatorname{tr}(K_1) \leq \operatorname{tr}(K_2)$.

Proof. Let $\{\psi_n\}$ be another ONB. If we write $K = K_1K_2$ with K_1, K_2 Hilbert–Schmidt we have

$$\begin{aligned} \sum_n \langle \varphi_n, K_1K_2\varphi_n \rangle &= \sum_n \langle K_1^*\varphi_n, K_2\varphi_n \rangle = \sum_{n,m} \langle K_1^*\varphi_n, \psi_m \rangle \langle \psi_m, K_2\varphi_n \rangle \\ &= \sum_{m,n} \langle K_2^*\psi_m, \varphi_n \rangle \langle \varphi_n, K_1\psi_m \rangle = \sum_m \langle K_2^*\psi_m, K_1\psi_m \rangle \\ &= \sum_m \langle \psi_m, K_2K_1\psi_m \rangle. \end{aligned} \quad (6.50)$$

Hence the trace is independent of the ONB and we even have $\operatorname{tr}(K_1K_2) = \operatorname{tr}(K_2K_1)$.

The rest follows from linearity of the scalar product and $K_1 \leq K_2$ if and only if $\langle \varphi, K_1\varphi \rangle \leq \langle \varphi, K_2\varphi \rangle$ for every $\varphi \in \mathfrak{H}$. \square

Clearly for self-adjoint trace class operators, the trace is the sum over all eigenvalues (counted with their multiplicity). To see this you just have to choose the ONB to consist of eigenfunctions. This is even true for all trace class operators and is known as Lidiskij trace theorem (see [17] or [6] for an easy to read introduction).

Problem 6.3. *Let $\mathfrak{H} = \ell^2(\mathbb{N})$ and let A be multiplication by a sequence $a(n)$. Show that $A \in \mathcal{J}_p(\ell^2(\mathbb{N}))$ if and only if $a \in \ell^p(\mathbb{N})$. Furthermore, show that $\|A\|_p = \|a\|_p$ in this case.*

Problem 6.4. *Show that $A \geq 0$ is trace class if (6.49) is finite for one (and hence all) ONB. (Hint A is self-adjoint (why?) and $A = \sqrt{A}\sqrt{A}$.)*

Problem 6.5. *Show that for an orthogonal projection P we have*

$$\dim \operatorname{Ran}(P) = \operatorname{tr}(P),$$

where we set $\operatorname{tr}(P) = \infty$ if (6.49) is infinite (for one and hence all ONB by the previous problem).

Problem 6.6. Show that for $K \in \mathfrak{C}$ we have

$$|K| = \sum_j s_j \langle \phi_j, \cdot \rangle \phi_j,$$

where $|K| = \sqrt{K^*K}$. Conclude that

$$\|K\|_p = (\operatorname{tr}(|A|^p))^{1/p}.$$

Problem 6.7. Show that $K : \ell^2(\mathbb{N}) \rightarrow \ell^2(\mathbb{N})$, $f(n) \mapsto \sum_{j \in \mathbb{N}} k(n+j)f(j)$ is Hilbert–Schmidt if $|k(n)| \leq C(n)$, where $C(n)$ is decreasing and summable.

6.4. Relatively compact operators and Weyl’s theorem

In the previous section we have seen that the sum of a self-adjoint and a symmetric operator is again self-adjoint if the perturbing operator is *small*. In this section we want to study the influence of perturbations on the spectrum. Our hope is that at least some parts of the spectrum remain invariant.

Let A be self-adjoint. Note that if we add a multiple of the identity to A , we shift the entire spectrum. Hence, in general, we cannot expect a (relatively) bounded perturbation to leave any part of the spectrum invariant. Next, if λ_0 is in the discrete spectrum, we can easily remove this eigenvalue with a finite rank perturbation of arbitrary small norm. In fact, consider

$$A + \varepsilon P_A(\{\lambda_0\}). \tag{6.51}$$

Hence our only hope is that the remainder, namely the essential spectrum, is stable under finite rank perturbations. To show this, we first need a good criterion for a point to be in the essential spectrum of A .

Lemma 6.16 (Weyl criterion). *A point λ is in the essential spectrum of a self-adjoint operator A if and only if there is a sequence ψ_n such that $\|\psi_n\| = 1$, ψ_n converges weakly to 0, and $\|(A - \lambda)\psi_n\| \rightarrow 0$. Moreover, the sequence can be chosen to be orthonormal. Such a sequence is called **singular Weyl sequence**.*

Proof. Let ψ_n be a singular Weyl sequence for the point λ_0 . By Lemma 2.12 we have $\lambda_0 \in \sigma(A)$ and hence it suffices to show $\lambda_0 \notin \sigma_d(A)$. If $\lambda_0 \in \sigma_d(A)$ we can find an $\varepsilon > 0$ such that $P_\varepsilon = P_A((\lambda_0 - \varepsilon, \lambda_0 + \varepsilon))$ is finite rank. Consider $\tilde{\psi}_n = P_\varepsilon \psi_n$. Clearly $\tilde{\psi}_n$ converges weakly to zero and $\|(A - \lambda_0)\tilde{\psi}_n\| \rightarrow 0$.

Moreover,

$$\begin{aligned}
\|\psi_n - \tilde{\psi}_n\|^2 &= \int_{\mathbb{R} \setminus (\lambda - \varepsilon, \lambda + \varepsilon)} d\mu_{\psi_n}(\lambda) \\
&\leq \frac{1}{\varepsilon^2} \int_{\mathbb{R} \setminus (\lambda - \varepsilon, \lambda + \varepsilon)} (\lambda - \lambda_0)^2 d\mu_{\psi_n}(\lambda) \\
&\leq \frac{1}{\varepsilon^2} \|(A - \lambda_0)\psi_n\|^2
\end{aligned} \tag{6.52}$$

and hence $\|\tilde{\psi}_n\| \rightarrow 1$. Thus $\varphi_n = \|\tilde{\psi}_n\|^{-1}\tilde{\psi}_n$ is also a singular Weyl sequence. But φ_n is a sequence of unit length vectors which lives in a finite dimensional space and converges to 0 weakly, a contradiction.

Conversely, if $\lambda_0 \in \sigma_{ess}(A)$, consider $P_n = P_A([\lambda - \frac{1}{n}, \lambda - \frac{1}{n+1}] \cup (\lambda + \frac{1}{n+1}, \lambda + \frac{1}{n}])$. Then $\text{rank}(P_{n_j}) > 0$ for an infinite subsequence n_j . Now pick $\psi_j \in \text{Ran}P_{n_j}$. \square

Now let K be a self-adjoint compact operator and ψ_n a singular Weyl sequence for A . Then ψ_n converges weakly to zero and hence

$$\|(A + K - \lambda)\psi_n\| \leq \|(A - \lambda)\psi_n\| + \|K\psi_n\| \rightarrow 0 \tag{6.53}$$

since $\|(A - \lambda)\psi_n\| \rightarrow 0$ by assumption and $\|K\psi_n\| \rightarrow 0$ by Lemma 6.8 (iii). Hence $\sigma_{ess}(A) \subseteq \sigma_{ess}(A + K)$. Reversing the roles of $A + K$ and A shows $\sigma_{ess}(A + K) = \sigma_{ess}(A)$. Since we have shown that we can remove any point in the discrete spectrum by a self-adjoint finite rank operator we obtain the following equivalent characterization of the essential spectrum.

Lemma 6.17. *The essential spectrum of a self-adjoint operator A is precisely the part which is invariant under rank-one perturbations. In particular,*

$$\sigma_{ess}(A) = \bigcap_{K \in \mathfrak{C}(\mathfrak{H}), K^* = K} \sigma(A + K). \tag{6.54}$$

There is even a larger class of operators under which the essential spectrum is invariant.

Theorem 6.18 (Weyl). *Suppose A and B are self-adjoint operators. If*

$$R_A(z) - R_B(z) \in \mathfrak{C}(\mathfrak{H}) \tag{6.55}$$

for one $z \in \rho(A) \cap \rho(B)$, then

$$\sigma_{ess}(A) = \sigma_{ess}(B). \tag{6.56}$$

Proof. In fact, suppose $\lambda \in \sigma_{ess}(A)$ and let ψ_n be a corresponding singular Weyl sequence. Then $(R_A(z) - \frac{1}{\lambda - z})\psi_n = \frac{R_A(z)}{z - \lambda}(A - \lambda)\psi_n$ and thus $\|(R_A(z) - \frac{1}{\lambda - z})\psi_n\| \rightarrow 0$. Moreover, by our assumption we also have $\|(R_B(z) - \frac{1}{\lambda - z})\psi_n\| \rightarrow 0$ and thus $\|(B - \lambda)\varphi_n\| \rightarrow 0$, where $\varphi_n = R_B(z)\psi_n$. Since

$\lim_{n \rightarrow \infty} \|\varphi_n\| = \lim_{n \rightarrow \infty} \|R_A(z)\psi_n\| = |\lambda - z|^{-1} \neq 0$ (since $\|(R_A(z) - \frac{1}{\lambda - z})\psi_n\| = \|\frac{1}{\lambda - z}R_A(z)(A - \lambda)\psi_n\| \rightarrow 0$) we obtain a singular Weyl sequence for B , showing $\lambda \in \sigma_{ess}(B)$. Now interchange the roles of A and B . \square

As a first consequence note the following result

Theorem 6.19. *Suppose A is symmetric with equal finite defect indices, then all self-adjoint extensions have the same essential spectrum.*

Proof. By Lemma 2.27 the resolvent difference of two self-adjoint extensions is a finite rank operator if the defect indices are finite. \square

In addition, the following result is of interest.

Lemma 6.20. *Suppose*

$$R_A(z) - R_B(z) \in \mathfrak{C}(\mathfrak{H}) \quad (6.57)$$

for one $z \in \rho(A) \cap \rho(B)$, then this holds for all $z \in \rho(A) \cap \rho(B)$. In addition, if A and B are self-adjoint, then

$$f(A) - f(B) \in \mathfrak{C}(\mathfrak{H}) \quad (6.58)$$

for any $f \in C_\infty(\mathbb{R})$.

Proof. If the condition holds for one z it holds for all since we have (using both resolvent formulas)

$$\begin{aligned} R_A(z') - R_B(z') \\ = (1 - (z - z')R_B(z'))(R_A(z) - R_B(z))(1 - (z - z')R_A(z')). \end{aligned} \quad (6.59)$$

Let A and B be self-adjoint. The set of all functions f for which the claim holds is a closed $*$ -subalgebra of $C_\infty(\mathbb{R})$ (with sup norm). Hence the claim follows from Lemma 4.4. \square

Remember that we have called K relatively compact with respect to A if $KR_A(z)$ is compact (for one and hence for all z) and note that the the resolvent difference $R_{A+K}(z) - R_A(z)$ is compact if K is relatively compact. In particular, Theorem 6.18 applies if $B = A + K$, where K is relatively compact.

For later use observe that set of all operators which are relatively compact with respect to A forms a linear space (since compact operators do) and relatively compact operators have A -bound zero.

Lemma 6.21. *Let A be self-adjoint and suppose K is relatively compact with respect to A . Then the A -bound of K is zero.*

Proof. Write

$$KR_A(\lambda i) = (KR_A(i))(A + i)R_A(\lambda i) \quad (6.60)$$

and observe that the first operator is compact and the second is normal and converges strongly to 0 (by the spectral theorem). Hence the claim follows from Lemma 6.3 and the discussion after Lemma 6.8 (since R_A is normal). \square

In addition, note the following result which is a straightforward consequence of the second resolvent identity.

Lemma 6.22. *Suppose A is self-adjoint and B is symmetric with A -bound less than one. If K is relatively compact with respect to A then it is also relatively compact with respect to $A + B$.*

Proof. Since B is A bounded with A -bound less than one, we can choose a $z \in \mathbb{C}$ such that $\|BR_A(z)\| < 1$. And hence

$$BR_{A+B}(z) = BR_A(z)(\mathbb{I} + BR_A(z))^{-1} \quad (6.61)$$

shows that B is also $A + B$ bounded and the result follows from

$$KR_{A+B}(z) = KR_A(z)(\mathbb{I} - BR_{A+B}(z)) \quad (6.62)$$

since $KR_A(z)$ is compact and $BR_{A+B}(z)$ is bounded. \square

Problem 6.8. *Show that $A = -\frac{d^2}{dx^2} + q(x)$, $\mathfrak{D}(A) = H^2(\mathbb{R})$ is self-adjoint if $q \in L^\infty(\mathbb{R})$. Show that if $-u''(x) + q(x)u(x) = zu(x)$ has a solution for which u and u' are bounded near $+\infty$ (or $-\infty$) but u is not square integrable near $+\infty$ (or $-\infty$), then $z \in \sigma_{\text{ess}}(A)$. (Hint: Use u to construct a Weyl sequence by restricting it to a compact set. Now modify your construction to get a singular Weyl sequence by observing that functions with disjoint support are orthogonal.)*

6.5. Strong and norm resolvent convergence

Suppose A_n and A are self-adjoint operators. We say that A_n converges to A in **norm** respectively **strong resolvent sense** if

$$\lim_{n \rightarrow \infty} R_{A_n}(z) = R_A(z) \quad \text{respectively} \quad \text{s-lim}_{n \rightarrow \infty} R_{A_n}(z) = R_A(z) \quad (6.63)$$

for one $z \in \Gamma = \mathbb{C} \setminus \Sigma$, $\Sigma = \sigma(A) \cup \bigcup_n \sigma(A_n)$.

Using the Stone–Weierstraß theorem we obtain as a first consequence

Theorem 6.23. *Suppose A_n converges to A in norm resolvent sense, then $f(A_n)$ converges to $f(A)$ in norm for any bounded continuous function $f : \Sigma \rightarrow \mathbb{C}$ with $\lim_{\lambda \rightarrow -\infty} f(\lambda) = \lim_{\lambda \rightarrow \infty} f(\lambda)$. If A_n converges to A in strong resolvent sense, then $f(A_n)$ converges to $f(A)$ strongly for any bounded continuous function $f : \Sigma \rightarrow \mathbb{C}$.*

Proof. The set of functions for which the claim holds clearly forms a $*$ -algebra (since resolvents are normal, taking adjoints is continuous even with respect to strong convergence) and since it contains $f(\lambda) = 1$ and $f(\lambda) = \frac{1}{\lambda - z_0}$ this $*$ -algebra is dense by the Stone–Weierstraß theorem. The usual $\frac{\varepsilon}{3}$ shows that this $*$ -algebra is also closed.

To see the last claim let χ_n be a compactly supported continuous function ($0 \leq \chi_m \leq 1$) which is one on the interval $[-m, m]$. Then $f(A_n)\chi_m(A_n) \xrightarrow{s} f(A)\chi_m(A)$ by the first part and hence

$$\begin{aligned} \|(f(A_n) - f(A))\psi\| &\leq \|f(A_n)\| \|(1 - \chi_m(A_n))\psi\| \\ &\quad + \|f(A_n)\| \|(\chi_m(A_n) - \chi_m(A))\psi\| \\ &\quad + \|(f(A_n)\chi_m(A_n) - f(A)\chi_m(A))\psi\| \\ &\quad + \|f(A)\| \|(1 - \chi_m(A))\psi\| \end{aligned} \quad (6.64)$$

can be made arbitrarily small since $\|f(\cdot)\| \leq \|f\|_\infty$ and $\chi_m(\cdot) \xrightarrow{s} \mathbb{I}$ by Theorem 3.1. \square

As a consequence note that the point $z \in \Gamma$ is of no importance

Corollary 6.24. *Suppose A_n converges to A in norm or strong resolvent sense for one $z_0 \in \Gamma$, then this holds for all $z \in \Gamma$.*

and that we have

Corollary 6.25. *Suppose A_n converges to A in strong resolvent sense, then*

$$e^{itA_n} \xrightarrow{s} e^{itA}, \quad t \in \mathbb{R}, \quad (6.65)$$

and if all operators are semi-bounded

$$e^{-tA_n} \xrightarrow{s} e^{-tA}, \quad t \geq 0. \quad (6.66)$$

Finally we need some good criteria to check for norm respectively strong resolvent convergence.

Lemma 6.26. *Let A_n, A be self-adjoint operators with $\mathfrak{D}(A_n) = \mathfrak{D}(A)$. Then A_n converges to A in norm resolvent sense if there are sequences a_n and b_n converging to zero such that*

$$\|(A_n - A)\psi\| \leq a_n\|\psi\| + b_n\|A\psi\|, \quad \psi \in \mathfrak{D}(A) = \mathfrak{D}(A_n). \quad (6.67)$$

Proof. From the second resolvent identity

$$R_{A_n}(z) - R_A(z) = R_{A_n}(z)(A - A_n)R_A(z) \quad (6.68)$$

we infer

$$\begin{aligned} \|(R_{A_n}(i) - R_A(i))\psi\| &\leq \|R_{A_n}(i)\| \left(a_n \|R_A(i)\psi\| + b_n \|AR_A(i)\psi\| \right) \\ &\leq (a_n + b_n)\|\psi\| \end{aligned} \quad (6.69)$$

and hence $\|R_{A_n}(i) - R_A(i)\| \leq a_n + b_n \rightarrow 0$. \square

In particular, norm convergence implies norm resolvent convergence:

Corollary 6.27. *Let A_n, A be bounded self-adjoint operators with $A_n \rightarrow A$, then A_n converges to A in norm resolvent sense.*

Similarly, if no domain problems get in the way, strong convergence implies strong resolvent convergence:

Lemma 6.28. *Let A_n, A be self-adjoint operators. Then A_n converges to A in strong resolvent sense if there is a core \mathfrak{D}_0 of A such that for any $\psi \in \mathfrak{D}_0$ we have $\psi \in \mathfrak{D}(A_n)$ for n sufficiently large and $A_n\psi \rightarrow A\psi$.*

Proof. Using the second resolvent identity we have

$$\|(R_{A_n}(i) - R_A(i))\psi\| \leq \|(A - A_n)R_A(i)\psi\| \rightarrow 0 \quad (6.70)$$

for $\psi \in (A - i)\mathfrak{D}_0$ which is dense, since \mathfrak{D}_0 is a core. The rest follows from Lemma 1.13. \square

If you wonder why we did not define weak resolvent convergence, here is the answer: it is equivalent to strong resolvent convergence.

Lemma 6.29. *Suppose $w\text{-}\lim_{n \rightarrow \infty} R_{A_n}(z) = R_A(z)$ for some $z \in \Gamma$, then also $s\text{-}\lim_{n \rightarrow \infty} R_{A_n}(z) = R_A(z)$.*

Proof. By $R_{A_n}(z) \rightarrow R_A(z)$ we have also $R_{A_n}(z)^* \rightarrow R_A(z)^*$ and thus by the first resolvent identity

$$\begin{aligned} \|R_{A_n}(z)\psi\|^2 - \|R_A(z)\psi\|^2 &= \langle \psi, R_{A_n}(z^*)R_{A_n}(z)\psi - R_A(z^*)R_A(z)\psi \rangle \\ &= \frac{1}{z - z^*} \langle \psi, (R_{A_n}(z) - R_{A_n}(z^*) + R_A(z) - R_A(z^*))\psi \rangle \rightarrow 0. \end{aligned} \quad (6.71)$$

Together with $R_{A_n}(z)\psi \rightarrow R_A(z)\psi$ we have $R_{A_n}(z)\psi \rightarrow R_A(z)\psi$ by virtue of Lemma 1.11 (iv). \square

Now what can we say about the spectrum?

Theorem 6.30. *Let A_n and A be self-adjoint operators. If A_n converges to A in strong resolvent sense we have $\sigma(A) \subseteq \lim_{n \rightarrow \infty} \sigma(A_n)$. If A_n converges to A in norm resolvent sense we have $\sigma(A) = \lim_{n \rightarrow \infty} \sigma(A_n)$.*

Proof. Suppose the first claim were wrong. Then we can find a $\lambda \in \sigma(A)$ and some $\varepsilon > 0$ such that $\sigma(A_n) \cap (\lambda - \varepsilon, \lambda + \varepsilon) = \emptyset$. Choose a bounded continuous function f which is one on $(\lambda - \frac{\varepsilon}{2}, \lambda + \frac{\varepsilon}{2})$ and vanishes outside $(\lambda - \varepsilon, \lambda + \varepsilon)$. Then $f(A_n) = 0$ and hence $f(A)\psi = \lim f(A_n)\psi = 0$ for every ψ . On the other hand, since $\lambda \in \sigma(A)$ there is a nonzero $\psi \in \text{Ran}P_A((\lambda - \frac{\varepsilon}{2}, \lambda + \frac{\varepsilon}{2}))$ implying $f(A)\psi = \psi$, a contradiction.

To see the second claim, recall that the norm of $R_A(z)$ is just one over the distance from the spectrum. In particular, $\lambda \notin \sigma(A)$ if and only if $\|R_A(\lambda + i)\| < 1$. So $\lambda \notin \sigma(A)$ implies $\|R_A(\lambda + i)\| < 1$, which implies $\|R_{A_n}(\lambda + i)\| < 1$ for n sufficiently large, which implies $\lambda \notin \sigma(A_n)$ for n sufficiently large. \square

Note that the spectrum can contract if we only have strong resolvent sense: Let A_n be multiplication by $\frac{1}{n}x$ in $L^2(\mathbb{R})$. Then A_n converges to 0 in strong resolvent sense, but $\sigma(A_n) = \mathbb{R}$ and $\sigma(0) = \{0\}$.

Lemma 6.31. *Suppose A_n converges in strong resolvent sense to A . If $P_A(\{\lambda\}) = 0$, then*

$$\text{s-lim}_{n \rightarrow \infty} P_{A_n}((-\infty, \lambda)) = \text{s-lim}_{n \rightarrow \infty} P_{A_n}((-\infty, \lambda]) = P_A((-\infty, \lambda)) = P_A((-\infty, \lambda]). \quad (6.72)$$

Proof. The idea is to approximate $\chi_{(-\infty, \lambda)}$ by a continuous function f with $0 \leq f \leq \chi_{(-\infty, \lambda)}$. Then

$$\begin{aligned} \|(P_A((-\infty, \lambda)) - P_{A_n}((-\infty, \lambda)))\psi\| &\leq \|(P_A((-\infty, \lambda)) - f(A))\psi\| \\ &+ \|(f(A) - f(A_n))\psi\| + \|(f(A_n) - P_{A_n}((-\infty, \lambda)))\psi\|. \end{aligned} \quad (6.73)$$

The first term can be made arbitrarily small if we let f converge pointwise to $\chi_{(-\infty, \lambda)}$ (Theorem 3.1) and the same is true for the second if we choose n large (Theorem 6.23). However, the third term can only be made small for fixed n . To overcome this problem let us choose another continuous function g with $\chi_{(-\infty, \lambda]} \leq g \leq 1$. Then

$$\|(f(A_n) - P_{A_n}((-\infty, \lambda)))\psi\| \leq \|(g(A_n) - f(A_n))\psi\| \quad (6.74)$$

since $f \leq \chi_{(-\infty, \lambda)} \leq \chi_{(-\infty, \lambda]} \leq g$. Furthermore,

$$\begin{aligned} \|(g(A_n) - f(A_n))\psi\| &\leq \|(g(A_n) - f(A))\psi\| \\ &+ \|(f(A) - g(A))\psi\| + \|(g(A) - g(A_n))\psi\| \end{aligned} \quad (6.75)$$

and now all terms are under control. Since we can replace $P((-\infty, \lambda))$ by $P((-\infty, \lambda])$ in all calculations we are done. \square

Using $P((\lambda_0, \lambda_1)) = P((-\infty, \lambda_1)) - P((-\infty, \lambda_0])$ we also obtain

Corollary 6.32. *Suppose A_n converges in strong resolvent sense to A . If $P_A(\{\lambda_0\}) = P_A(\{\lambda_1\}) = 0$, then*

$$\text{s-lim}_{n \rightarrow \infty} P_{A_n}((\lambda_0, \lambda_1)) = \text{s-lim}_{n \rightarrow \infty} P_{A_n}([\lambda_0, \lambda_1]) = P_A((\lambda_0, \lambda_1)) = P_A([\lambda_0, \lambda_1]). \quad (6.76)$$

Example. The following example shows that the requirement $P_A(\{\lambda\}) = 0$ is crucial, even if we have bounded operators and norm convergence. In fact, let $\mathfrak{H} = \mathbb{C}^2$ and

$$A_n = \frac{1}{n} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (6.77)$$

Then $A_n \rightarrow 0$ and

$$P_{A_n}((-\infty, 0)) = P_{A_n}((-\infty, 0]) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad (6.78)$$

but $P_0((-\infty, 0)) = 0$ and $P_0((-\infty, 0]) = \mathbb{I}$. \diamond

Problem 6.9. Show that for self-adjoint operators, strong resolvent convergence is equivalent to convergence with respect to the metric

$$d(A, B) = \sum_{n \in \mathbb{N}} \frac{1}{2^n} \|(R_A(i) - R_B(i))\varphi_n\|, \quad (6.79)$$

where $\{\varphi_n\}_{n \in \mathbb{N}}$ is some (fixed) ONB.

Problem 6.10 (Weak convergence of spectral measures). Suppose $A_n \rightarrow A$ in strong resolvent sense and let μ_ψ , $\mu_{\psi, n}$ be the corresponding spectral measures. Show that

$$\int f(\lambda) d\mu_{\psi, n}(\lambda) \rightarrow \int f(\lambda) d\mu_\psi(\lambda) \quad (6.80)$$

for every bounded continuous f . Give a counterexample when f is not continuous.

Part 2

Schrödinger Operators

The free Schrödinger operator

7.1. The Fourier transform

We first review some basic facts concerning the **Fourier transform** which will be needed in the following section.

Let $C^\infty(\mathbb{R}^n)$ be the set of all complex-valued functions which have partial derivatives of arbitrary order. For $f \in C^\infty(\mathbb{R}^n)$ and $\alpha \in \mathbb{N}_0^n$ we set

$$\partial_\alpha f = \frac{\partial^{|\alpha|} f}{\partial x_1^{\alpha_1} \cdots \partial x_n^{\alpha_n}}, \quad x^\alpha = x_1^{\alpha_1} \cdots x_n^{\alpha_n}, \quad |\alpha| = \alpha_1 + \cdots + \alpha_n. \quad (7.1)$$

An element $\alpha \in \mathbb{N}_0^n$ is called **multi-index** and $|\alpha|$ is called its **order**. Recall the Schwarz space

$$\mathcal{S}(\mathbb{R}^n) = \{f \in C^\infty(\mathbb{R}^n) \mid \sup_x |x^\alpha (\partial_\beta f)(x)| < \infty, \alpha, \beta \in \mathbb{N}_0^n\} \quad (7.2)$$

which is dense in $L^2(\mathbb{R}^n)$ (since $C_c^\infty(\mathbb{R}^n) \subset \mathcal{S}(\mathbb{R}^n)$ is). For $f \in \mathcal{S}(\mathbb{R}^n)$ we define

$$\mathcal{F}(f)(p) \equiv \hat{f}(p) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-ipx} f(x) d^n x. \quad (7.3)$$

Then it is an exercise in partial integration to prove

Lemma 7.1. *For any multi-index $\alpha \in \mathbb{N}_0^n$ and any $f \in \mathcal{S}(\mathbb{R}^n)$ we have*

$$(\partial_\alpha f)^\wedge(p) = (ip)^\alpha \hat{f}(p), \quad (x^\alpha f(x))^\wedge(p) = i^{|\alpha|} \partial_\alpha \hat{f}(p). \quad (7.4)$$

Hence we will sometimes write $pf(x)$ for $-i\partial f(x)$, where $\partial = (\partial_1, \dots, \partial_n)$ is the **gradient**.

In particular \mathcal{F} maps $\mathcal{S}(\mathbb{R}^n)$ into itself. Another useful property is the convolution formula.

Lemma 7.2. *The Fourier transform of the convolution*

$$(f * g)(x) = \int_{\mathbb{R}^n} f(y)g(x-y)d^n y = \int_{\mathbb{R}^n} f(x-y)g(y)d^n y \quad (7.5)$$

of two functions $f, g \in \mathcal{S}(\mathbb{R}^n)$ is given by

$$(f * g)^\wedge(p) = (2\pi)^{n/2} \hat{f}(p)\hat{g}(p). \quad (7.6)$$

Proof. We compute

$$\begin{aligned} (f * g)^\wedge(p) &= \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-ipx} \int_{\mathbb{R}^n} f(y)g(x-y)d^n y d^n x \\ &= \int_{\mathbb{R}^n} e^{-ipy} f(y) \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-ip(x-y)} g(x-y)d^n x d^n y \\ &= \int_{\mathbb{R}^n} e^{-ipy} f(y)\hat{g}(p)d^n y = (2\pi)^{n/2} \hat{f}(p)\hat{g}(p), \end{aligned} \quad (7.7)$$

where we have used Fubini's theorem. \square

Next, we want to compute the inverse of the Fourier transform. For this the following lemma will be needed.

Lemma 7.3. *We have $e^{-zx^2/2} \in \mathcal{S}(\mathbb{R}^n)$ for $\operatorname{Re}(z) > 0$ and*

$$\mathcal{F}(e^{-zx^2/2})(p) = \frac{1}{z^{n/2}} e^{-p^2/(2z)}. \quad (7.8)$$

Here $z^{n/2}$ has to be understood as $(\sqrt{z})^n$, where the branch cut of the root is chosen along the negative real axis.

Proof. Due to the product structure of the exponential, one can treat each coordinate separately, reducing the problem to the case $n = 1$.

Let $\phi_z(x) = \exp(-zx^2/2)$. Then $\phi'_z(x) + zx\phi_z(x) = 0$ and hence $i(p\hat{\phi}_z(p) + z\hat{\phi}'_z(p)) = 0$. Thus $\hat{\phi}_z(p) = c\phi_{1/z}(p)$ and (Problem 7.1)

$$c = \hat{\phi}_z(0) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \exp(-zx^2/2) dx = \frac{1}{\sqrt{z}} \quad (7.9)$$

at least for $z > 0$. However, since the integral is holomorphic for $\operatorname{Re}(z) > 0$, this holds for all z with $\operatorname{Re}(z) > 0$ if we choose the branch cut of the root along the negative real axis. \square

Now we can show

Theorem 7.4. *The Fourier transform $\mathcal{F} : \mathcal{S}(\mathbb{R}^n) \rightarrow \mathcal{S}(\mathbb{R}^n)$ is a bijection. Its inverse is given by*

$$\mathcal{F}^{-1}(g)(x) \equiv \check{g}(x) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{ipx} g(p) d^n p. \quad (7.10)$$

We have $\mathcal{F}^2(f)(x) = f(-x)$ and thus $\mathcal{F}^4 = \mathbb{I}$.

Proof. It suffices to show $\mathcal{F}^2(f)(x) = f(-x)$. Consider $\phi_z(x)$ from the proof of the previous lemma and observe $\mathcal{F}^2(\phi_z)(x) = \phi_z(-x)$. Moreover, using Fubini this even implies $\mathcal{F}^2(f_\varepsilon)(x) = f_\varepsilon(-x)$ for any $\varepsilon > 0$, where

$$f_\varepsilon(x) = \frac{1}{\varepsilon^n} \int_{\mathbb{R}^n} \phi_{1/\varepsilon^2}(x-y) f(y) d^n y. \quad (7.11)$$

Since $\lim_{\varepsilon \downarrow 0} f_\varepsilon(x) = f(x)$ for every $x \in \mathbb{R}^n$ (Problem 7.2), we infer from dominated convergence $\mathcal{F}^2(f)(x) = \lim_{\varepsilon \downarrow 0} \mathcal{F}^2(f_\varepsilon)(x) = \lim_{\varepsilon \downarrow 0} f_\varepsilon(-x) = f(-x)$. \square

From Fubini's theorem we also obtain **Parseval's identity**

$$\begin{aligned} \int_{\mathbb{R}^n} |\hat{f}(p)|^2 d^n p &= \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} f(x)^* \hat{f}(p) e^{ipx} d^n p d^n x \\ &= \int_{\mathbb{R}^n} |f(x)|^2 d^n x \end{aligned} \quad (7.12)$$

for $f \in \mathcal{S}(\mathbb{R}^n)$ and thus we can extend \mathcal{F} to a unitary operator:

Theorem 7.5. *The Fourier transform \mathcal{F} extends to a unitary operator $\mathcal{F} : L^2(\mathbb{R}^n) \rightarrow L^2(\mathbb{R}^n)$. Its spectrum satisfies*

$$\sigma(\mathcal{F}) = \{z \in \mathbb{C} | z^4 = 1\} = \{1, -1, i, -i\}. \quad (7.13)$$

Proof. It remains to compute the spectrum. In fact, if ψ_n is a Weyl sequence, then $(\mathcal{F}^2 + z^2)(\mathcal{F} + z)(\mathcal{F} - z)\psi_n = (\mathcal{F}^4 - z^4)\psi_n = (1 - z^4)\psi_n \rightarrow 0$ implies $z^4 = 1$. Hence $\sigma(\mathcal{F}) \subseteq \{z \in \mathbb{C} | z^4 = 1\}$. We defer the proof for equality to Section 8.3, where we will explicitly compute an orthonormal basis of eigenfunctions. \square

Lemma 7.1 also allows us to extend differentiation to a larger class. Let us introduce the Sobolev space

$$H^r(\mathbb{R}^n) = \{f \in L^2(\mathbb{R}^n) | |p|^r \hat{f}(p) \in L^2(\mathbb{R}^n)\}. \quad (7.14)$$

We will abbreviate

$$\partial_\alpha f = ((ip)^\alpha \hat{f}(p))^\vee, \quad f \in H^r(\mathbb{R}^n), |\alpha| \leq r \quad (7.15)$$

which implies

$$\int_{\mathbb{R}^n} g(x) (\partial_\alpha f)(x) d^n x = (-1)^\alpha \int_{\mathbb{R}^n} (\partial_\alpha g)(x) f(x) d^n x, \quad (7.16)$$

for $f \in H^r(\mathbb{R}^n)$ and $g \in \mathcal{S}(\mathbb{R}^n)$. That is, $\partial_\alpha f$ is the derivative of f in the sense of distributions.

Finally, we have the **Riemann-Lebesgue lemma**.

Lemma 7.6 (Riemann-Lebesgue). *Let $C_\infty(\mathbb{R}^n)$ denote the Banach space of all continuous functions $f : \mathbb{R}^n \rightarrow \mathbb{C}$ which vanish at ∞ equipped with the sup norm. Then the Fourier transform is a bounded map from $L^1(\mathbb{R}^n)$ into $C_\infty(\mathbb{R}^n)$ satisfying*

$$\|\hat{f}\|_\infty \leq (2\pi)^{-n/2} \|f\|_1. \quad (7.17)$$

Proof. Clearly we have $\hat{f} \in C_\infty(\mathbb{R}^n)$ if $f \in \mathcal{S}(\mathbb{R}^n)$. Moreover, the estimate

$$\sup_p |\hat{f}(p)| \leq \frac{1}{(2\pi)^{n/2}} \sup_p \int_{\mathbb{R}^n} |e^{-ipx} f(x)| d^n x = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} |f(x)| d^n x \quad (7.18)$$

shows $\hat{f} \in C_\infty(\mathbb{R}^n)$ for arbitrary $f \in L^1(\mathbb{R}^n)$ since $\mathcal{S}(\mathbb{R}^n)$ is dense in $L^1(\mathbb{R}^n)$. \square

Problem 7.1. *Show that $\int_{\mathbb{R}} \exp(-x^2/2) dx = \sqrt{2\pi}$. (Hint: Square the integral and evaluate it using polar coordinates.)*

Problem 7.2. *Extend Lemma 0.32 to the case $u, f \in \mathcal{S}(\mathbb{R}^n)$ (compare Problem 0.17).*

7.2. The free Schrödinger operator

In Section 2.1 we have seen that the Hilbert space corresponding to one particle in \mathbb{R}^3 is $L^2(\mathbb{R}^3)$. More generally, the Hilbert space for N particles in \mathbb{R}^d is $L^2(\mathbb{R}^n)$, $n = Nd$. The corresponding non relativistic Hamilton operator, if the particles do not interact, is given by

$$H_0 = -\Delta, \quad (7.19)$$

where Δ is the Laplace operator

$$\Delta = \sum_{j=1}^n \frac{\partial^2}{\partial x_j^2}. \quad (7.20)$$

Our first task is to find a good domain such that H_0 is a self-adjoint operator.

By Lemma 7.1 we have that

$$-\Delta\psi(x) = (p^2 \hat{\psi}(p))^\vee(x), \quad \psi \in H^2(\mathbb{R}^n), \quad (7.21)$$

and hence the operator

$$H_0\psi = -\Delta\psi, \quad \mathfrak{D}(H_0) = H^2(\mathbb{R}^n), \quad (7.22)$$

is unitarily equivalent to the maximally defined multiplication operator

$$(\mathcal{F}H_0\mathcal{F}^{-1})\varphi(p) = p^2\varphi(p), \quad \mathfrak{D}(p^2) = \{\varphi \in L^2(\mathbb{R}^n) | p^2\varphi(p) \in L^2(\mathbb{R}^n)\}. \quad (7.23)$$

Theorem 7.7. *The free Schrödinger operator H_0 is self-adjoint and its spectrum is characterized by*

$$\sigma(H_0) = \sigma_{ac}(H_0) = [0, \infty), \quad \sigma_{sc}(H_0) = \sigma_{pp}(H_0) = \emptyset. \quad (7.24)$$

Proof. It suffices to show that $d\mu_\psi$ is purely absolutely continuous for every ψ . First observe that

$$\langle \psi, R_{H_0}(z)\bar{\psi} \rangle = \langle \hat{\psi}, R_{p^2}(z)\hat{\psi} \rangle = \int_{\mathbb{R}^n} \frac{|\hat{\psi}(p)|^2}{p^2 - z} d^n p = \int_{\mathbb{R}} \frac{1}{r^2 - z} d\tilde{\mu}_\psi(r), \quad (7.25)$$

where

$$d\tilde{\mu}_\psi(r) = \chi_{[0, \infty)}(r) r^{n-1} \left(\int_{S^{n-1}} |\hat{\psi}(r\omega)|^2 d^{n-1}\omega \right) dr. \quad (7.26)$$

Hence, after a change of coordinates, we have

$$\langle \psi, R_{H_0}(z)\bar{\psi} \rangle = \int_{\mathbb{R}} \frac{1}{\lambda - z} d\mu_\psi(\lambda), \quad (7.27)$$

where

$$d\mu_\psi(\lambda) = \frac{1}{2} \chi_{[0, \infty)}(\lambda) \lambda^{n/2-1} \left(\int_{S^{n-1}} |\hat{\psi}(\sqrt{\lambda}\omega)|^2 d^{n-1}\omega \right) d\lambda, \quad (7.28)$$

proving the claim. \square

Finally, we note that the compactly supported smooth functions are a core for H_0 .

Lemma 7.8. *The set $C_c^\infty(\mathbb{R}^n) = \{f \in \mathcal{S}(\mathbb{R}^n) | \text{supp}(f) \text{ is compact}\}$ is a core for H_0 .*

Proof. It is not hard to see that $\mathcal{S}(\mathbb{R}^n)$ is a core (Problem 7.3) and hence it suffices to show that the closure of $H_0|_{C_c^\infty(\mathbb{R}^n)}$ contains $H_0|_{\mathcal{S}(\mathbb{R}^n)}$. To see this, let $\varphi(x) \in C_c^\infty(\mathbb{R}^n)$ which is one for $|x| \leq 1$ and vanishes for $|x| \geq 2$. Set $\varphi_n(x) = \varphi(\frac{1}{n}x)$, then $\psi_n(x) = \varphi_n(x)\psi(x)$ is in $C_c^\infty(\mathbb{R}^n)$ for every $\psi \in \mathcal{S}(\mathbb{R}^n)$ and $\psi_n \rightarrow \psi$ respectively $\Delta\psi_n \rightarrow \Delta\psi$. \square

Note also that the quadratic form of H_0 is given by

$$q_{H_0}(\psi) = \sum_{j=1}^n \int_{\mathbb{R}^n} |\partial_j \psi(x)|^2 d^n x, \quad \psi \in \mathfrak{D}(H_0) = H^1(\mathbb{R}^n). \quad (7.29)$$

Problem 7.3. *Show that $\mathcal{S}(\mathbb{R}^n)$ is a core for H_0 . (Hint: Show that the closure of $H_0|_{\mathcal{S}(\mathbb{R}^n)}$ contains H_0 .)*

Problem 7.4. Show that $\{\psi \in \mathcal{S}(\mathbb{R}) \mid \psi(0) = 0\}$ is dense but not a core for $H_0 = -\frac{d^2}{dx^2}$.

7.3. The time evolution in the free case

Now let us look at the time evolution. We have

$$e^{-itH_0}\psi(x) = \mathcal{F}^{-1}e^{-itp^2}\hat{\psi}(p). \quad (7.30)$$

The right hand side is a product and hence our operator should be expressible as an integral operator via the convolution formula. However, since e^{-itp^2} is not in L^2 , a more careful analysis is needed.

Consider

$$f_\varepsilon(p^2) = e^{-(it+\varepsilon)p^2}, \quad \varepsilon > 0. \quad (7.31)$$

Then $f_\varepsilon(H_0)\psi \rightarrow e^{-itH_0}\psi$ by Theorem 3.1. Moreover, by Lemma 7.3 and the convolution formula we have

$$f_\varepsilon(H_0)\psi(x) = \frac{1}{(4\pi(it+\varepsilon))^{n/2}} \int_{\mathbb{R}^n} e^{-\frac{|x-y|^2}{4(it+\varepsilon)}} \psi(y) d^n y \quad (7.32)$$

and hence

$$e^{-itH_0}\psi(x) = \frac{1}{(4\pi it)^{n/2}} \int_{\mathbb{R}^n} e^{i\frac{|x-y|^2}{4t}} \psi(y) d^n y \quad (7.33)$$

for $t \neq 0$ and $\psi \in L^1 \cap L^2$. For general $\psi \in L^2$ the integral has to be understood as a limit.

Using this explicit form, it is not hard to draw some immediate consequences. For example, if $\psi \in L^2(\mathbb{R}^n) \cap L^1(\mathbb{R}^n)$, then $\psi(t) \in C(\mathbb{R}^n)$ for $t \neq 0$ (use dominated convergence and continuity of the exponential) and satisfies

$$\|\psi(t)\|_\infty \leq \frac{1}{|4\pi t|^{n/2}} \|\psi(0)\|_1 \quad (7.34)$$

by the Riemann-Lebesgue lemma. Thus we have spreading of wave functions in this case. Moreover, it is even possible to determine the asymptotic form of the wave function for large t as follows. Observe

$$\begin{aligned} e^{-itH_0}\psi(x) &= \frac{e^{i\frac{x^2}{4t}}}{(4\pi it)^{n/2}} \int_{\mathbb{R}^n} e^{i\frac{y^2}{4t}} \psi(y) e^{i\frac{xy}{2t}} d^n y \\ &= \left(\frac{1}{2it}\right)^{n/2} e^{i\frac{x^2}{4t}} \left(e^{i\frac{y^2}{4t}} \psi(y)\right)^\wedge \left(\frac{x}{2t}\right). \end{aligned} \quad (7.35)$$

Moreover, since $\exp(i\frac{y^2}{4t})\psi(y) \rightarrow \psi(y)$ in L^2 as $|t| \rightarrow \infty$ (dominated convergence) we obtain

Lemma 7.9. For any $\psi \in L^2(\mathbb{R}^n)$ we have

$$e^{-itH_0}\psi(x) - \left(\frac{1}{2it}\right)^{n/2} e^{i\frac{x^2}{4t}} \hat{\psi}\left(\frac{x}{2t}\right) \rightarrow 0 \quad (7.36)$$

in L^2 as $|t| \rightarrow \infty$.

Next we want to apply the RAGE theorem in order to show that for any initial condition, a particle will escape to infinity.

Lemma 7.10. Let $g(x)$ be the multiplication operator by g and let $f(p)$ be the operator given by $f(p)\psi(x) = \mathcal{F}^{-1}(f(p)\hat{\psi}(p))(x)$. Denote by $L^\infty(\mathbb{R}^n)$ the bounded Borel functions which vanish at infinity. Then

$$f(p)g(x) \quad \text{and} \quad g(x)f(p) \quad (7.37)$$

are compact if $f, g \in L^\infty(\mathbb{R}^n)$ and (extend to) Hilbert–Schmidt operators if $f, g \in L^2(\mathbb{R}^n)$.

Proof. By symmetry it suffices to consider $g(x)f(p)$. Let $f, g \in L^2$, then

$$g(x)f(p)\psi(x) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} g(x)\check{f}(x-y)\psi(y)d^n y \quad (7.38)$$

shows that $g(x)f(p)$ is Hilbert–Schmidt since $g(x)\check{f}(x-y) \in L^2(\mathbb{R}^n \times \mathbb{R}^n)$.

If f, g are bounded then the functions $f_R(p) = \chi_{\{p|p^2 \leq R\}}(p)f(p)$ and $g_R(x) = \chi_{\{x|x^2 \leq R\}}(x)g(x)$ are in L^2 . Thus $g_R(x)f_R(p)$ is compact and tends to $g(x)f(p)$ in norm since f, g vanish at infinity. \square

In particular, this lemma implies that

$$\chi_\Omega(H_0 + i)^{-1} \quad (7.39)$$

is compact if $\Omega \subseteq \mathbb{R}^n$ is bounded and hence

$$\lim_{t \rightarrow \infty} \|\chi_\Omega e^{-itH_0}\psi\|^2 = 0 \quad (7.40)$$

for any $\psi \in L^2(\mathbb{R}^n)$ and any bounded subset Ω of \mathbb{R}^n . In other words, the particle will eventually escape to infinity since the probability of finding the particle in any bounded set tends to zero. (If $\psi \in L^1(\mathbb{R}^n)$ this of course also follows from (7.34).)

7.4. The resolvent and Green's function

Now let us compute the resolvent of H_0 . We will try to use a similar approach as for the time evolution in the previous section. However, since it is highly nontrivial to compute the inverse Fourier transform of $\exp(-\varepsilon p^2)(p^2 - z)^{-1}$ directly, we will use a small ruse.

Note that

$$R_{H_0}(z) = \int_0^\infty e^{zt} e^{-tH_0} dt, \quad \operatorname{Re}(z) < 0 \quad (7.41)$$

by Lemma 4.1. Moreover,

$$e^{-tH_0}\psi(x) = \frac{1}{(4\pi t)^{n/2}} \int_{\mathbb{R}^n} e^{-\frac{|x-y|^2}{4t}} \psi(y) d^n y, \quad t > 0, \quad (7.42)$$

by the same analysis as in the previous section. Hence, by Fubini, we have

$$R_{H_0}(z)\psi(x) = \int_{\mathbb{R}^n} G_0(z, |x-y|) \psi(y) d^n y, \quad (7.43)$$

where

$$G_0(z, r) = \int_0^\infty \frac{1}{(4\pi t)^{n/2}} e^{-\frac{r^2}{4t} + zt} dt, \quad r > 0, \operatorname{Re}(z) < 0. \quad (7.44)$$

The function $G_0(z, r)$ is called **Green's function** of H_0 . The integral can be evaluated in terms of modified Bessel functions of the second kind

$$G_0(z, r) = \frac{1}{2\pi} \left(\frac{-z}{4\pi^2 r^2} \right)^{\frac{n-2}{4}} K_{\frac{n}{2}-1}(\sqrt{-z}r). \quad (7.45)$$

The functions $K_\nu(x)$ satisfy the following differential equation

$$\left(\frac{d^2}{dx^2} + \frac{1}{x} \frac{d}{dx} - 1 - \frac{\nu^2}{x^2} \right) K_\nu(x) = 0 \quad (7.46)$$

and have the following asymptotics

$$K_\nu(x) = \begin{cases} \frac{\Gamma(\nu)}{2} \left(\frac{x}{2}\right)^{-\nu} + O(x^{-\nu+1}) & \nu \neq 0 \\ -\ln\left(\frac{x}{2}\right) + O(1) & \nu = 0 \end{cases} \quad (7.47)$$

for $|x| \rightarrow 0$ and

$$K_\nu(x) = \sqrt{\frac{\pi}{2x}} e^{-x} (1 + O(x^{-1})) \quad (7.48)$$

for $|x| \rightarrow \infty$. For more information see for example [22]. In particular, $G_0(z, r)$ has an analytic continuation for $z \in \mathbb{C} \setminus [0, \infty) = \rho(H_0)$. Hence we can define the right hand side of (7.43) for all $z \in \rho(H_0)$ such that

$$\int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \varphi(x) G_0(z, |x-y|) \psi(y) d^n y d^n x \quad (7.49)$$

is analytic for $z \in \rho(H_0)$ and $\varphi, \psi \in \mathcal{S}(\mathbb{R}^n)$ (by Morea's theorem). Since it is equal to $\langle \varphi, R_{H_0}(z)\psi \rangle$ for $\operatorname{Re}(z) < 0$ it is equal to this function for all $z \in \rho(H_0)$, since both functions are analytic in this domain. In particular, (7.43) holds for all $z \in \rho(H_0)$.

If n is odd, we have the case of spherical Bessel functions which can be expressed in terms of elementary functions. For example, we have

$$G_0(z, r) = \frac{1}{2\sqrt{-z}} e^{-\sqrt{-z}r}, \quad n = 1, \quad (7.50)$$

and

$$G_0(z, r) = \frac{1}{4\pi r} e^{-\sqrt{-z}r}, \quad n = 3. \quad (7.51)$$

Problem 7.5. Verify (7.43) directly in the case $n = 1$.

Algebraic methods

8.1. Position and momentum

Apart from the Hamiltonian H_0 , which corresponds to the kinetic energy, there are several other important observables associated with a single particle in three dimensions. Using commutation relation between these observables, many important consequences about these observables can be derived.

First consider the one-parameter unitary group

$$(U_j(t)\psi)(x) = e^{-itx_j}\psi(x), \quad 1 \leq j \leq 3. \quad (8.1)$$

For $\psi \in \mathcal{S}(\mathbb{R}^3)$ we compute

$$\lim_{t \rightarrow 0} i \frac{e^{-itx_j}\psi(x) - \psi(x)}{t} = x_j\psi(x) \quad (8.2)$$

and hence the generator is the multiplication operator by the j -th coordinate function. By Corollary 5.3 it is essentially self-adjoint on $\psi \in \mathcal{S}(\mathbb{R}^3)$. It is custom to combine all three operators to one vector valued operator x , which is known as **position operator**. Moreover, it is not hard to see that the spectrum of x_j is purely absolutely continuous and given by $\sigma(x_j) = \mathbb{R}$. In fact, let $\varphi(x)$ be an orthonormal basis for $L^2(\mathbb{R})$. Then $\varphi_i(x_1)\varphi_j(x_2)\varphi_k(x_3)$ is an orthonormal basis for $L^2(\mathbb{R}^3)$ and x_1 can be written as a orthogonal sum of operators restricted to the subspaces spanned by $\varphi_j(x_2)\varphi_k(x_3)$. Each subspace is unitarily equivalent to $L^2(\mathbb{R})$ and x_1 is given by multiplication with the identity. Hence the claim follows (or use Theorem 4.12).

Next, consider the one-parameter unitary group of translations

$$(U_j(t)\psi)(x) = \psi(x - te_j), \quad 1 \leq j \leq 3, \quad (8.3)$$

where e_j is the unit vector in the j -th coordinate direction. For $\psi \in \mathcal{S}(\mathbb{R}^3)$ we compute

$$\lim_{t \rightarrow 0} i \frac{\psi(x - te_j) - \psi(x)}{t} = \frac{1}{i} \frac{\partial}{\partial x_j} \psi(x) \quad (8.4)$$

and hence the generator is $p_j = \frac{1}{i} \frac{\partial}{\partial x_j}$. Again it is essentially self-adjoint on $\psi \in \mathcal{S}(\mathbb{R}^3)$. Moreover, since it is unitarily equivalent to x_j by virtue of the Fourier transform we conclude that the spectrum of p_j is again purely absolutely continuous and given by $\sigma(p_j) = \mathbb{R}$. The operator p is known as **momentum operator**. Note that since

$$[H_0, p_j] \psi(x) = 0, \quad \psi \in \mathcal{S}(\mathbb{R}^3) \quad (8.5)$$

we have

$$\frac{d}{dt} \langle \psi(t), p_j \psi(t) \rangle = 0, \quad \psi(t) = e^{-itH_0} \psi(0) \in \mathcal{S}(\mathbb{R}^3), \quad (8.6)$$

that is, the momentum is a conserved quantity for the free motion. Similarly one has

$$[p_j, x_k] \psi(x) = \delta_{jk} \psi(x), \quad \psi \in \mathcal{S}(\mathbb{R}^3), \quad (8.7)$$

which is known as the **Weyl relation**.

The Weyl relations also imply that the mean-square deviation of position and momentum cannot be made arbitrarily small simultaneously:

Theorem 8.1 (Heisenberg Uncertainty Principle). *Suppose A and B are two symmetric operators, then for any $\psi \in \mathfrak{D}(A) \cap \mathfrak{D}(B)$ we have*

$$\Delta_\psi(A) \Delta_\psi(B) \geq \frac{1}{2} |\mathbb{E}_\psi([A, B])| \quad (8.8)$$

with equality if

$$(B - \mathbb{E}_\psi(B))\psi = i\lambda(A - \mathbb{E}_\psi(A))\psi, \quad \lambda \in \mathbb{R} \setminus \{0\}, \quad (8.9)$$

or if ψ is an eigenstate of A or B .

Proof. Let us fix $\psi \in \mathfrak{D}(A) \cap \mathfrak{D}(B)$ and abbreviate

$$\hat{A} = A - \mathbb{E}_\psi(A), \quad \hat{B} = B - \mathbb{E}_\psi(B). \quad (8.10)$$

Then $\Delta_\psi(A) = \|\hat{A}\psi\|$, $\Delta_\psi(B) = \|\hat{B}\psi\|$ and hence by Cauchy-Schwarz

$$|\langle \hat{A}\psi, \hat{B}\psi \rangle| \leq \Delta_\psi(A) \Delta_\psi(B). \quad (8.11)$$

Now note that

$$\hat{A}\hat{B} = \frac{1}{2} \{\hat{A}, \hat{B}\} + \frac{1}{2} [A, B], \quad \{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A} \quad (8.12)$$

where $\{\hat{A}, \hat{B}\}$ and $i[A, B]$ are symmetric. So

$$|\langle \hat{A}\psi, \hat{B}\psi \rangle|^2 = |\langle \psi, \hat{A}\hat{B}\psi \rangle|^2 = \frac{1}{2} |\langle \psi, \{\hat{A}, \hat{B}\}\psi \rangle|^2 + \frac{1}{2} |\langle \psi, [A, B]\psi \rangle|^2 \quad (8.13)$$

which proves (8.8).

To have equality if ψ is not an eigenstate we need $\hat{B}\psi = z\hat{A}\psi$ for equality in Cauchy-Schwarz and $\langle \psi, \{\hat{A}, \hat{B}\}\psi \rangle = 0$. Inserting the first into the second requirement gives $0 = (z - z^*)\|\hat{A}\psi\|^2$ and shows $\text{Re}(z) = 0$. \square

In case of position and momentum we have ($\|\psi\| = 1$)

$$\Delta_\psi(p_j)\Delta_\psi(x_k) \geq \frac{\delta_{jk}}{2} \quad (8.14)$$

and the minimum is attained for the **Gaussian wave packets**

$$\psi(x) = \left(\frac{\lambda}{\pi}\right)^{n/4} e^{-\frac{\lambda}{2}|x-x_0|^2 - ip_0x}, \quad (8.15)$$

which satisfy $\mathbb{E}_\psi(x) = x_0$ and $\mathbb{E}_\psi(p) = p_0$ respectively $\Delta_\psi(p_j)^2 = \frac{\lambda}{2}$ and $\Delta_\psi(x_k)^2 = \frac{1}{2\lambda}$.

Problem 8.1. Check that (8.15) realizes the minimum.

8.2. Angular momentum

Now consider the one-parameter unitary group of rotations

$$(U_j(t)\psi)(x) = \psi(M_j(t)x), \quad 1 \leq j \leq 3, \quad (8.16)$$

where $M_j(t)$ is the matrix of rotation around e_j by an angle of t . For $\psi \in \mathcal{S}(\mathbb{R}^3)$ we compute

$$\lim_{t \rightarrow 0} i \frac{\psi(M_i(t)x) - \psi(x)}{t} = \sum_{j,k=1}^3 \varepsilon_{ijk} x_j p_k \psi(x), \quad (8.17)$$

where

$$\varepsilon_{ijk} = \begin{cases} 1 & \text{if } ijk \text{ is an even permutation of } 123 \\ -1 & \text{if } ijk \text{ is an odd permutation of } 123 \\ 0 & \text{else} \end{cases} \quad (8.18)$$

Again one combines the three components to one vector valued operator $L = x \wedge p$, which is known as **angular momentum operator**. Since $e^{i2\pi L_j} = \mathbb{I}$, we see that the spectrum is a subset of \mathbb{Z} . In particular, the continuous spectrum is empty. We will show below that we have $\sigma(L_j) = \mathbb{Z}$. Note that since

$$[H_0, L_j]\psi(x) = 0, \quad \psi \in \mathcal{S}(\mathbb{R}^3), \quad (8.19)$$

we have again

$$\frac{d}{dt} \langle \psi(t), L_j \psi(t) \rangle = 0, \quad \psi(t) = e^{-itH_0} \psi(0) \in \mathcal{S}(\mathbb{R}^3), \quad (8.20)$$

that is, the angular momentum is a conserved quantity for the free motion as well.

Moreover, we even have

$$[L_i, K_j]\psi(x) = i \sum_{k=1}^3 \varepsilon_{ijk} K_k \psi(x), \quad \psi \in \mathcal{S}(\mathbb{R}^3), K_j \in \{L_j, p_j, x_j\}, \quad (8.21)$$

and these algebraic commutation relations are often used to derive information on the point spectra of these operators. In this respect the following domain

$$\mathfrak{D} = \text{span}\{x^\alpha e^{-\frac{x^2}{2}} \mid \alpha \in \mathbb{N}_0^n\} \subset \mathcal{S}(\mathbb{R}^n) \quad (8.22)$$

is often used. It has the nice property that the finite dimensional subspaces

$$\mathfrak{D}_k = \text{span}\{x^\alpha e^{-\frac{x^2}{2}} \mid |\alpha| \leq k\} \quad (8.23)$$

are invariant under L_j (and hence they reduce L_j).

Lemma 8.2. *The subspace $\mathfrak{D} \subset L^2(\mathbb{R}^n)$ defined in (8.22) is dense.*

Proof. By Lemma 1.9 it suffices to consider the case $n = 1$. Suppose $\langle \varphi, \psi \rangle = 0$ for every $\psi \in \mathfrak{D}$. Then

$$\frac{1}{\sqrt{2\pi}} \int \overline{\varphi(x)} e^{-\frac{x^2}{2}} \sum_{j=1}^k \frac{(ix)^j}{j!} = 0 \quad (8.24)$$

for any finite k and hence also in the limit $k \rightarrow \infty$ by the dominated convergence theorem. But the limit is the Fourier transform of $\overline{\varphi(x)} e^{-\frac{x^2}{2}}$, which shows that this function is zero. Hence $\varphi(x) = 0$. \square

Since it is invariant under the unitary groups generated by L_j , the operators L_j are essentially self-adjoint on \mathfrak{D} by Corollary 5.3.

Introducing $L^2 = L_1^2 + L_2^2 + L_3^2$ it is straightforward to check

$$[L^2, L_j]\psi(x) = 0, \quad \psi \in \mathcal{S}(\mathbb{R}^3). \quad (8.25)$$

Moreover, \mathfrak{D}_k is invariant under L^2 and L_3 and hence \mathfrak{D}_k reduces L^2 and L_3 . In particular, L^2 and L_3 are given by finite matrices on \mathfrak{D}_k . Now let $\mathfrak{H}_m = \text{Ker}(L_3 - m)$ and denote by P_k the projector onto \mathfrak{D}_k . Since L^2 and L_3 commute on \mathfrak{D}_k , the space $P_k \mathfrak{H}_m$ is invariant under L^2 which shows that we can choose an orthonormal basis consisting of eigenfunctions of L^2 for $P_k \mathfrak{H}_m$. Increasing k we get an orthonormal set of simultaneous eigenfunctions whose span is equal to \mathfrak{D} . Hence there is an orthonormal basis of simultaneous eigenfunctions of L^2 and L_3 .

Now let us try to draw some further consequences by using the commutation relations (8.21). (All commutation relations below hold for $\psi \in \mathcal{S}(\mathbb{R}^3)$.) Denote by $\mathfrak{H}_{l,m}$ the set of all functions in \mathfrak{D} satisfying

$$L_3 \psi = m \psi, \quad L^2 \psi = l(l+1) \psi. \quad (8.26)$$

By $L^2 \geq 0$ and $\sigma(L_3) \subseteq \mathbb{Z}$ we can restrict our attention to the case $l \geq 0$ and $m \in \mathbb{Z}$.

First introduce two new operators

$$L_{\pm} = L_1 \pm iL_2, \quad [L_3, L_{\pm}] = \pm L_{\pm}. \quad (8.27)$$

Then, for every $\psi \in \mathfrak{H}_{l,m}$ we have

$$L_3(L_{\pm}\psi) = (m \pm 1)(L_{\pm}\psi), \quad L^2(L_{\pm}\psi) = l(l+1)(L_{\pm}\psi), \quad (8.28)$$

that is, $L_{\pm}\mathfrak{H}_{l,m} \rightarrow \mathfrak{H}_{l,m \pm 1}$. Moreover, since

$$L^2 = L_3^2 \pm L_3 + L_{\mp}L_{\pm} \quad (8.29)$$

we obtain

$$\|L_{\pm}\psi\|^2 = \langle \psi, L_{\mp}L_{\pm}\psi \rangle = (l(l+1) - m(m \pm 1))\|\psi\|^2 \quad (8.30)$$

for every $\psi \in \mathfrak{H}_{l,m}$. If $\psi \neq 0$ we must have $l(l+1) - m(m \pm 1) \geq 0$ which shows $\mathfrak{H}_{l,m} = \{0\}$ for $|m| > l$. Moreover, $L_{\pm}\mathfrak{H}_{l,m} \rightarrow \mathfrak{H}_{l,m \pm 1}$ is injective unless $|m| = l$. Hence we must have $\mathfrak{H}_{l,m} = \{0\}$ for $l \notin \mathbb{N}_0$.

Up to this point we know $\sigma(L^2) \subseteq \{l(l+1) | l \in \mathbb{N}_0\}$, $\sigma(L_3) \subseteq \mathbb{Z}$. In order to show that equality holds in both cases, we need to show that $\mathfrak{H}_{l,m} \neq \{0\}$ for $l \in \mathbb{N}_0$, $m = -l, -l+1, \dots, l-1, l$. First of all we observe

$$\psi_{0,0}(x) = \frac{1}{\pi^{3/2}} e^{-\frac{x^2}{2}} \in \mathfrak{H}_{0,0}. \quad (8.31)$$

Next, we note that (8.21) implies

$$\begin{aligned} [L_3, x_{\pm}] &= \pm x_{\pm}, & x_{\pm} &= x_1 \pm ix_2, \\ [L_{\pm}, x_{\pm}] &= 0, & [L_{\pm}, x_{\mp}] &= \pm 2x_3, \\ [L^2, x_{\pm}] &= 2x_{\pm}(1 \pm L_3) \mp 2x_3L_{\pm}. \end{aligned} \quad (8.32)$$

Hence if $\psi \in \mathfrak{H}_{l,l}$, then $(x_1 \pm ix_2)\psi \in \mathfrak{H}_{l \pm 1, l \pm 1}$. And thus

$$\psi_{l,l}(x) = \frac{1}{\sqrt{l!}} (x_1 \pm ix_2)^l \psi_{0,0}(x) \in \mathfrak{H}_{l,l}, \quad (8.33)$$

respectively

$$\psi_{l,m}(x) = \sqrt{\frac{(l+m)!}{(l-m)!(2l)!}} L_-^{l-m} \psi_{l,l}(x) \in \mathfrak{H}_{l,m}. \quad (8.34)$$

The constants are chosen such that $\|\psi_{l,m}\| = 1$.

In summary,

Theorem 8.3. *There exists an orthonormal basis of simultaneous eigenvectors for the operators L^2 and L_j . Moreover, their spectra are given by*

$$\sigma(L^2) = \{l(l+1) | l \in \mathbb{N}_0\}, \quad \sigma(L_3) = \mathbb{Z}. \quad (8.35)$$

We will rederive this result using different methods in Section 10.3.

8.3. The harmonic oscillator

Finally, let us consider another important model whose algebraic structure is similar to those of the angular momentum, the **harmonic oscillator**

$$H = H_0 + \omega^2 x^2, \quad \omega > 0. \quad (8.36)$$

As domain we will choose

$$\mathfrak{D}(H) = \mathfrak{D} = \text{span}\{x^\alpha e^{-\frac{x^2}{2}} \mid \alpha \in \mathbb{N}_0^3\} \subseteq L^2(\mathbb{R}^3) \quad (8.37)$$

from our previous section.

We will first consider the one-dimensional case. Introducing

$$A_\pm = \frac{1}{\sqrt{2}} \left(\sqrt{\omega} x \mp \frac{1}{\sqrt{\omega}} \frac{d}{dx} \right) \quad (8.38)$$

we have

$$[A_-, A_+] = 1 \quad (8.39)$$

and

$$H = \omega(2N + 1), \quad N = A_+ A_-, \quad (8.40)$$

for any function in \mathfrak{D} .

Moreover, since

$$[N, A_\pm] = \pm A_\pm, \quad (8.41)$$

we see that $N\psi = n\psi$ implies $NA_\pm\psi = (n \pm 1)A_\pm\psi$. Moreover, $\|A_+\psi\|^2 = \langle \psi, A_-A_+\psi \rangle = (n+1)\|\psi\|^2$ respectively $\|A_-\psi\|^2 = n\|\psi\|^2$ in this case and hence we conclude that $\sigma(N) \subseteq \mathbb{N}_0$

If $N\psi_0 = 0$, then we must have $A_-\psi_0 = 0$ and the normalized solution of this last equation is given by

$$\psi_0(x) = \left(\frac{\omega}{\pi}\right)^{1/4} e^{-\frac{\omega x^2}{2}} \in \mathfrak{D}. \quad (8.42)$$

Hence

$$\psi_n(x) = \frac{1}{\sqrt{n!}} A_+^n \psi_0(x) \quad (8.43)$$

is a normalized eigenfunction of N corresponding to the eigenvalue n . Moreover, since

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}} \left(\frac{\omega}{\pi}\right)^{1/4} H_n(\sqrt{\omega}x) e^{-\frac{\omega x^2}{2}} \quad (8.44)$$

where $H_n(x)$ is a polynomial of degree n given by

$$H_n(x) = e^{\frac{x^2}{2}} \left(x - \frac{d}{dx}\right)^n e^{-\frac{x^2}{2}} = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}, \quad (8.45)$$

we conclude $\text{span}\{\psi_n\} = \mathfrak{D}$. The polynomials $H_n(x)$ are called **Hermite polynomials**.

In summary,

Theorem 8.4. *The harmonic oscillator H is essentially self adjoint on \mathfrak{D} and has an orthonormal basis of eigenfunctions*

$$\psi_{n_1, n_2, n_3}(x) = \psi_{n_1}(x_1)\psi_{n_2}(x_2)\psi_{n_3}(x_3), \quad (8.46)$$

with $\psi_{n_j}(x_j)$ from (8.44). The spectrum is given by

$$\sigma(H) = \{(2n + 3)\omega \mid n \in \mathbb{N}_0\}. \quad (8.47)$$

Finally, there is also a close connection with the Fourier transformation. without restriction we choose $\omega = 1$ and consider only one dimension. Then it easy to verify that H commutes with the Fourier transformation

$$\mathcal{F}H = H\mathcal{F}. \quad (8.48)$$

Moreover, by $\mathcal{F}A_{\pm} = \mp iA_{\pm}\mathcal{F}$ we even infer

$$\mathcal{F}\psi_n = \frac{1}{\sqrt{n!}}\mathcal{F}A_+^n\psi_0 = \frac{(-i)^n}{\sqrt{n!}}A_+^n\mathcal{F}\psi_0 = (-i)^n\psi_n, \quad (8.49)$$

since $\mathcal{F}\psi_0 = \psi_0$ by Lemma 7.3. In particular,

$$\sigma(\mathcal{F}) = \{z \in \mathbb{C} \mid z^4 = 1\}. \quad (8.50)$$

Problem 8.2. *Show that $H = -\frac{d^2}{dx^2} + q$ can be written as $H = AA^*$, where $A = -\frac{d}{dx} + \phi$, if the differential equation $\psi'' + q\psi = 0$ has a positive solution. Compute $\tilde{H} = A^*A$. (Hint: $\phi = \frac{\psi'}{\psi}$.)*

One dimensional Schrödinger operators

9.1. Sturm-Liouville operators

In this section we want to illustrate some of the results obtained thus far by investigating a specific example, the **Sturm-Liouville equations**.

$$\tau f(x) = \frac{1}{r(x)} \left(-\frac{d}{dx} p(x) \frac{d}{dx} f(x) + q(x) f(x) \right), \quad f, pf' \in AC_{loc}(I) \quad (9.1)$$

The case $p = r = 1$ can be viewed as the model of a particle in one dimension in the external potential q . Moreover, the case of a particle in three dimensions can in some situations be reduced to the investigation of Sturm-Liouville equations. In particular, we will see how this works when explicitly solving the hydrogen atom.

The suitable Hilbert space is

$$L^2((a, b), r(x)dx), \quad \langle f, g \rangle = \int_a^b f(x)^* g(x) r(x) dx, \quad (9.2)$$

where $I = (a, b) \subset \mathbb{R}$ is an arbitrary open interval.

We require

- (i) $p^{-1} \in L^1_{loc}(I)$, real-valued
- (ii) $q \in L^1_{loc}(I)$, real-valued
- (iii) $r \in L^1_{loc}(I)$, positive

If a is finite and if $p^{-1}, q, r \in L^1((a, c))$ ($c \in I$), then the Sturm-Liouville equation (9.1) is called regular at a . Similarly for b . If it is both regular at a and b it is called **regular**.

The maximal domain of definition for τ in $L^2(I, r dx)$ is given by

$$\mathfrak{D}(\tau) = \{f \in L^2(I, r dx) \mid f, pf' \in AC_{loc}(I), \tau f \in L^2(I, r dx)\}. \quad (9.3)$$

It is not clear that $\mathfrak{D}(\tau)$ is dense unless (e.g.) $p \in AC_{loc}(I)$, $p', q \in L^2_{loc}(I)$, $r^{-1} \in L^\infty_{loc}(I)$ since $C^\infty_0(I) \subset \mathfrak{D}(\tau)$ in this case. We will defer the general case to Lemma 9.4 below.

Since we are interested in self-adjoint operators H associated with (9.1), we perform a little calculation. Using integration by parts (twice) we obtain ($a < c < d < b$):

$$\int_c^d g^*(\tau f) r dy = W_d(g^*, f) - W_c(g^*, f) + \int_c^d (\tau g)^* f r dy, \quad (9.4)$$

for $f, g, pf', pg' \in AC_{loc}(I)$ where

$$W_x(f_1, f_2) = \left(p(f_1 f'_2 - f'_1 f_2) \right)(x) \quad (9.5)$$

is called the **modified Wronskian**.

Equation (9.4) also shows that the Wronskian of two solutions of $\tau u = zu$ is constant

$$W_x(u_1, u_2) = W(u_1, u_2), \quad \tau u_{1,2} = zu_{1,2}. \quad (9.6)$$

Moreover, it is nonzero if and only if u_1 and u_2 are linearly independent (compare Theorem 9.1 below).

If we choose $f, g \in \mathfrak{D}(\tau)$ in (9.4), then we can take the limits $c \rightarrow a$ and $d \rightarrow b$, which results in

$$\langle g, \tau f \rangle = W_b(g^*, f) - W_a(g^*, f) + \langle \tau g, f \rangle, \quad f, g \in \mathfrak{D}(\tau). \quad (9.7)$$

Here $W_{a,b}(g^*, f)$ has to be understood as limit.

Finally, we recall the following well-known result from ordinary differential equations.

Theorem 9.1. *Suppose $rg \in L^1_{loc}(I)$, then there exists a unique solution $f, pf' \in AC_{loc}(I)$ of the differential equation*

$$(\tau - z)f = g, \quad z \in \mathbb{C}, \quad (9.8)$$

satisfying the initial condition

$$f(c) = \alpha, \quad (pf')(c) = \beta, \quad \alpha, \beta \in \mathbb{C}, \quad c \in I. \quad (9.9)$$

In addition, f is holomorphic with respect to z .

Note that f, pf' can be extended continuously to a regular end point.

Lemma 9.2. *Suppose u_1, u_2 are two solutions of $(\tau - z)u = 0$ with $W(u_1, u_2) = 1$. Then any other solution of (9.8) can be written as $(\alpha, \beta \in \mathbb{C})$*

$$\begin{aligned} f(x) &= u_1(x) \left(\alpha + \int_c^x u_2 g r \, dy \right) + u_2(x) \left(\beta - \int_c^x u_1 g r \, dy \right), \\ f'(x) &= u_1'(x) \left(\alpha + \int_c^x u_2 g r \, dy \right) + u_2'(x) \left(\beta - \int_c^x u_1 g r \, dy \right). \end{aligned} \quad (9.10)$$

Note that the constants α, β coincide with those from Theorem 9.1 if $u_1(c) = (pu_2')(c) = 1$ and $(pu_1')(c) = u_2(c) = 0$.

Proof. It suffices to check $\tau f - z f = g$. Differentiating the first equation of (9.10) gives the second. Next we compute

$$\begin{aligned} (pf')' &= (pu_1')' \left(\alpha + \int u_2 g r \, dy \right) + (pu_2')' \left(\beta - \int u_1 g r \, dy \right) - W(u_1, u_2) g r \\ &= (q - z)u_1 \left(\alpha + \int u_2 g r \, dy \right) + (q - z)u_2 \left(\beta - \int u_1 g r \, dy \right) - g r \\ &= (q - z)f - g r \end{aligned} \quad (9.11)$$

which proves the claim. \square

Now we want to obtain a symmetric operator and hence we choose

$$A_0 f = \tau f, \quad \mathfrak{D}(A_0) = \mathfrak{D}(\tau) \cap AC_c(I), \quad (9.12)$$

where $AC_c(I)$ are the functions in $AC(I)$ with compact support. This definition clearly ensures that the Wronskian of two such functions vanishes on the boundary, implying that A_0 is symmetric. Our first task is to compute the closure of A_0 and its adjoint. For this the following elementary fact will be needed.

Lemma 9.3. *Suppose V is a vector space and l, l_1, \dots, l_n are linear functionals (defined on all of V) such that $\bigcap_{j=1}^n \text{Ker}(l_j) \subseteq \text{Ker}(l)$. Then $l = \sum_{j=1}^n \alpha_j l_j$ for some constants $\alpha_j \in \mathbb{C}$.*

Proof. First of all it is no restriction to assume that the functionals l_j are linearly independent. Then the map $L : V \rightarrow \mathbb{C}^n, f \mapsto (l_1(f), \dots, l_n(f))$ is surjective (since $x \in \text{Ran}(L)^\perp$ implies $\sum_{j=1}^n x_j l_j(f) = 0$ for all f). Hence there are vectors $f_k \in V$ such that $l_j(f_k) = 0$ for $j \neq k$ and $l_j(f_j) = 1$. Then $f - \sum_{j=1}^n l_j(f) f_j \in \bigcap_{j=1}^n \text{Ker}(l_j)$ and hence $l(f) - \sum_{j=1}^n l_j(f) l(f_j) = 0$. Thus we can choose $\alpha_j = l(f_j)$. \square

Now we are ready to prove

Lemma 9.4. *The operator A_0 is densely defined and its closure is given by*

$$\overline{A_0} f = \tau f, \quad \mathfrak{D}(\overline{A_0}) = \{f \in \mathfrak{D}(\tau) \mid W_a(f, g) = W_b(f, g) = 0, \forall g \in \mathfrak{D}(\tau)\}. \quad (9.13)$$

Its adjoint is given by

$$A_0^* f = \tau f, \quad \mathfrak{D}(A_0^*) = \mathfrak{D}(\tau). \quad (9.14)$$

Proof. We start by computing A_0^* and ignore the fact that we don't know whether $\mathfrak{D}(A_0)$ is dense for now.

By (9.7) we have $\mathfrak{D}(\tau) \subseteq \mathfrak{D}(A_0^*)$ and it remains to show $\mathfrak{D}(A_0^*) \subseteq \mathfrak{D}(\tau)$. If $h \in \mathfrak{D}(A_0^*)$ we must have

$$\langle h, A_0 f \rangle = \langle k, f \rangle, \quad \forall f \in \mathfrak{D}(A_0) \quad (9.15)$$

for some $k \in L^2(I, r dx)$. Using (9.10) we can find a \tilde{h} such that $\tau \tilde{h} = k$ and from integration by parts we obtain

$$\int_a^b (h(x) - \tilde{h}(x))^* (\tau f)(x) r(x) dx = 0, \quad \forall f \in \mathfrak{D}(A_0). \quad (9.16)$$

Clearly we expect that $h - \tilde{h}$ will be a solution of the $\tau u = 0$ and to prove this we will invoke Lemma 9.3. Therefore we consider the linear functionals

$$l(g) = \int_a^b (h(x) - \tilde{h}(x))^* g(x) r(x) dx, \quad l_j(g) = \int_a^b u_j(x)^* g(x) r(x) dx, \quad (9.17)$$

on $L_c^2(I, r dx)$, where u_j are two solutions of $\tau u = 0$ with $W(u_1, u_2) \neq 0$. We have $\text{Ker}(l_1) \cap \text{Ker}(l_2) \subseteq \text{Ker}(l)$. In fact, if $g \in \text{Ker}(l_1) \cap \text{Ker}(l_2)$, then

$$f(x) = u_1(x) \int_a^x u_2(y) g(y) r(y) dy + u_2(x) \int_x^b u_1(y) g(y) r(y) dy \quad (9.18)$$

is in $\mathfrak{D}(A_0)$ and $g = \tau f \in \text{Ker}(l)$ by (9.16). Now Lemma 9.3 implies

$$\int_a^b (h(x) - \tilde{h}(x) + \alpha_1 u_1(x) + \alpha_2 u_2(x))^* g(x) r(x) dx = 0, \quad \forall g \in L_c^2(I, r dx) \quad (9.19)$$

and hence $h = \tilde{h} + \alpha_1 u_1 + \alpha_2 u_2 \in \mathfrak{D}(\tau)$.

Now what if $\mathfrak{D}(A_0)$ were not dense? Then there would be some freedom in choice of k since we could always add a component in $\mathfrak{D}(A_0)^\perp$. So suppose we have two choices $k_1 \neq k_2$. Then by the above calculation, there are corresponding functions \tilde{h}_1 and \tilde{h}_2 such that $h = \tilde{h}_1 + \alpha_{1,1} u_1 + \alpha_{1,2} u_2 = \tilde{h}_2 + \alpha_{2,1} u_1 + \alpha_{2,2} u_2$. In particular, $\tilde{h}_1 - \tilde{h}_2$ is in the kernel of τ and hence $k_1 = \tau \tilde{h}_1 = \tau \tilde{h}_2 = k_2$ contradiction our assumption.

Next we turn to $\overline{A_0}$. Denote the set on the right hand side of (9.13) by \mathfrak{D} . Then we have $\mathfrak{D} \subseteq \mathfrak{D}(A_0^{**}) = \overline{A_0}$ by (9.7). Conversely, since $\overline{A_0} \subseteq A_0^*$ we can use (9.7) to conclude

$$W_a(f, h) + W_b(f, h) = 0, \quad f \in \mathfrak{D}(\overline{A_0}), h \in \mathfrak{D}(A_0^*). \quad (9.20)$$

Now replace h by a $\tilde{h} \in \mathfrak{D}(A_0^*)$ which coincides with h near a and vanishes identically near b (Problem 9.1). Then $W_a(f, h) = W_a(f, \tilde{h}) + W_b(f, \tilde{h}) = 0$. Finally, $W_b(f, h) = -W_a(f, h) = 0$ shows $f \in \mathfrak{D}$. \square

Example. If τ is regular at a , then $f \in \mathfrak{D}(\overline{A_0})$ if and only if $f(a) = (pf')(a) = 0$. This follows since we can prescribe the values of $g(a)$, $(pg')(a)$ for $g \in \mathfrak{D}(\tau)$ arbitrarily. \diamond

This result shows that any self-adjoint extension of A_0 must lie between $\overline{A_0}$ and A_0^* . Moreover, self-adjointness seems to be related to the Wronskian of two functions at the boundary. Hence we collect a few properties first.

Lemma 9.5. *Suppose $v \in \mathfrak{D}(\tau)$ with $W_a(v^*, v) = 0$ and there is a $\hat{f} \in \mathfrak{D}(\tau)$ with $W(v^*, \hat{f})_a \neq 0$. then we have*

$$W_a(v, f) = 0 \quad \Leftrightarrow \quad W_a(v, f^*) = 0 \quad \forall f \in \mathfrak{D}(\tau) \quad (9.21)$$

and

$$W_a(v, f) = W_a(v, g) = 0 \quad \Rightarrow \quad W_a(g^*, f) = 0 \quad \forall f, g \in \mathfrak{D}(\tau) \quad (9.22)$$

Proof. For all $f_1, \dots, f_4 \in \mathfrak{D}(\tau)$ we have the Plücker identity

$$W_x(f_1, f_2)W_x(f_3, f_4) + W_x(f_1, f_3)W_x(f_4, f_2) + W_x(f_1, f_4)W_x(f_2, f_3) = 0 \quad (9.23)$$

which remains valid in the limit $x \rightarrow a$. Choosing $f_1 = v$, $f_2 = f$, $f_3 = v^*$, $f_4 = \hat{f}$ we infer (9.21). Choosing $f_1 = f$, $f_2 = g^*$, $f_3 = v$, $f_4 = \hat{f}$ we infer (9.22). \square

Problem 9.1. *Given $\alpha, \beta, \gamma, \delta$, show that there is a function $f \in \mathfrak{D}(\tau)$ restricted to $[c, d] \subseteq (a, b)$ such that $f(c) = \alpha$, $(pf)(c) = \beta$ and $f(d) = \gamma$, $(pf)(d) = \delta$. (Hint: Lemma 9.2)*

Problem 9.2. *Let $A_0 = -\frac{d^2}{dx^2}$, $\mathfrak{D}(A_0) = \{f \in H^2[0, 1] | f(0) = f(1) = 0\}$. and $B = q$, $\mathfrak{D}(B) = \{f \in L^2(0, 1) | qf \in L^2(0, 1)\}$. Find a $q \in L^1(0, 1)$ such that $\mathfrak{D}(A_0) \cap \mathfrak{D}(B) = \{0\}$. (Hint: Problem 0.18)*

9.2. Weyl's limit circle, limit point alternative

We call τ **limit circle** (l.c.) at a if there is a $v \in \mathfrak{D}(\tau)$ with $W_a(v^*, v) = 0$ such that $W_a(v, f) \neq 0$ for at least one $f \in \mathfrak{D}(\tau)$. Otherwise τ is called **limit point** (l.p.) at a . Similarly for b .

Example. If τ is regular at a , it is limit circle at a . Since

$$W_a(v, f) = (pf')(a)v(a) - (pv')(a)f(a) \quad (9.24)$$

any real-valued v with $(v(a), (pv')(a)) \neq (0, 0)$ works. \diamond

Note that if $W_a(f, v) \neq 0$, then $W_a(f, \operatorname{Re}(v)) \neq 0$ or $W_a(f, \operatorname{Im}(v)) \neq 0$. Hence it is no restriction to assume that v is real and $W_a(v^*, v) = 0$ is trivially satisfied in this case. In particular, τ is limit point if and only if $W_a(f, g) = 0$ for all $f, g \in \mathfrak{D}(\tau)$.

Theorem 9.6. *If τ is l.c. at a , then let $v \in \mathfrak{D}(\tau)$ with $W(v^*, v)_a = 0$ and $W(v, f)_a \neq 0$ for some $f \in \mathfrak{D}(\tau)$. Similarly, if τ is l.c. at b , let w be an analogous function. Then the operator*

$$\begin{aligned} A : \mathfrak{D}(A) &\rightarrow L^2(I, r dx) \\ f &\mapsto \tau f \end{aligned} \quad (9.25)$$

with

$$\mathfrak{D}(A) = \{f \in \mathfrak{D}(\tau) \mid \begin{array}{l} W_a(v, f) = 0 \text{ if l.c. at } a \\ W_b(w, f) = 0 \text{ if l.c. at } b \end{array}\} \quad (9.26)$$

is self-adjoint.

Proof. Clearly $A \subseteq A^* \subseteq A_0^*$. Let $g \in \mathfrak{D}(A^*)$. As in the computation of $\overline{A_0}$ we conclude $W_a(f, g) = 0$ for all $f \in \mathfrak{D}(A)$. Moreover, we can choose f such that it coincides with v near a and hence $W_a(v, g) = 0$, that is $g \in \mathfrak{D}(A)$. \square

The name limit circle respectively limit point stems from the original approach of Weyl, who considered the set of solutions $\tau u = zu$, $z \in \mathbb{C} \setminus \mathbb{R}$ which satisfy $W_c(u^*, u) = 0$. They can be shown to lie on a circle which converges to a circle respectively point as $c \rightarrow a$ (or $c \rightarrow b$).

Example. If τ is regular at a we can choose v such that $(v(a), (pv')(a)) = (\sin(\alpha), -\cos(\alpha))$, $\alpha \in [0, \pi)$, such that

$$W_a(v, f) = \cos(\alpha)f(a) + \sin(\alpha)(pf')(a). \quad (9.27)$$

The most common choice $\alpha = 0$ is known as **Dirichlet boundary condition** $f(a) = 0$. \diamond

Next we want to compute the resolvent of A .

Lemma 9.7. *Suppose $z \in \rho(A)$, then there exists a solution $u_a(z, x)$ which is in $L^2((a, c), r dx)$ and which satisfies the boundary condition at a if τ is l.c. at a . Similarly, there exists a solution $u_b(z, x)$ with the analogous properties near b .*

The resolvent of A is given by

$$(A - z)^{-1}g(x) = \int_a^b G(z, x, y)g(y)r(y)dy, \quad (9.28)$$

where

$$G(z, x, y) = \frac{1}{W(u_b(z), u_a(z))} \begin{cases} u_b(z, x)u_a(z, y) & x \geq y \\ u_a(z, x)u_b(z, y) & x \leq y \end{cases}. \quad (9.29)$$

Proof. Let $g \in L_c^2(I, r dx)$ be real-valued and consider $f = (A - z)^{-1}g \in \mathfrak{D}(A)$. Since $(\tau - z)f = 0$ near a respectively b , we obtain $u_a(z, x)$ by setting it equal to f near a and using the differential equation to extend it to the rest of I . Similarly we obtain u_b . The only problem is that u_a or u_b might be identically zero. Hence we need to show that this can be avoided by choosing g properly.

Fix z and let g be supported in $(c, d) \subset I$. Since $(\tau - z)f = g$ we have

$$f(x) = u_1(x) \left(\alpha + \int_a^x u_2 gr dy \right) + u_2(x) \left(\beta + \int_x^b u_1 gr dy \right). \quad (9.30)$$

Near a ($x < c$) we have $f(x) = \alpha u_1(x) + \tilde{\beta} u_2(x)$ and near b ($x > d$) we have $f(x) = \tilde{\alpha} u_1(x) + \beta u_2(x)$, where $\tilde{\alpha} = \alpha + \int_a^b u_2 gr dy$ and $\tilde{\beta} = \beta + \int_a^b u_1 gr dy$. If f vanishes identically near both a and b we must have $\alpha = \beta = \tilde{\alpha} = \tilde{\beta} = 0$ and thus $\alpha = \beta = 0$ and $\int_a^b u_j(y)g(y)r(y)dy = 0$, $j = 1, 2$. This case can be avoided choosing g suitable and hence there is at least one solution, say $u_b(z)$.

Now choose $u_1 = u_b$ and consider the behavior near b . If u_2 is not square integrable on (d, b) , we must have $\beta = 0$ since $\beta u_2 = f - \tilde{\alpha} u_b$ is. If u_2 is square integrable, we can find two functions in $\mathfrak{D}(\tau)$ which coincide with u_b and u_2 near b . Since $W(u_b, u_2) = 1$ we see that τ is l.c. at a and hence $0 = W_b(u_b, f) = W_b(u_b, \tilde{\alpha} u_b + \beta u_2) = \beta$. Thus $\beta = 0$ in both cases and we have

$$f(x) = u_b(x) \left(\alpha + \int_a^x u_2 gr dy \right) + u_2(x) \int_x^b u_b gr dy. \quad (9.31)$$

Now choosing g such that $\int_a^b u_b gr dy \neq 0$ we infer existence of $u_a(z)$. Choosing $u_2 = u_a$ and arguing as before we see $\alpha = 0$ and hence

$$\begin{aligned} f(x) &= u_b(x) \int_a^x u_a(y)g(y)r(y)dy + u_a(x) \int_x^b u_b(y)g(y)r(y)dy \\ &= \int_a^b G(z, x, y)g(y)r(y)dy \end{aligned} \quad (9.32)$$

for any $g \in L_c^2(I, r dx)$. Since this set is dense the claim follows. \square

Example. If τ is regular at a with a boundary condition as in the previous example, we can choose $u_a(z, x)$ to be the solution corresponding to the initial conditions $(u_a(z, a), (pu'_a)(z, a)) = (\sin(\alpha), -\cos(\alpha))$. In particular, $u_a(z, x)$ exists for all $z \in \mathbb{C}$.

If τ is regular at both a and b there is a corresponding solution $u_b(z, x)$, again for all z . So the only values of z for which $(A - z)^{-1}$ does not exist must be those with $W(u_b(z), u_a(z)) = 0$. However, in this case $u_a(z, x)$

and $u_b(z, x)$ are linearly dependent and $u_a(z, x) = \gamma u_b(z, x)$ satisfies both boundary conditions. That is, z is an eigenvalue in this case.

In particular, regular operators have pure point spectrum. We will see in Theorem 9.10 below, that this holds for any operator which is *l.c.* at both end points. \diamond

In the previous example $u_a(z, x)$ is holomorphic with respect to z and satisfies $u_a(z, x)^* = u_a(z^*, x)$ (since it corresponds to real initial conditions and our differential equation has real coefficients). In general we have:

Lemma 9.8. *Suppose $z \in \rho(A)$, then $u_a(z, x)$ from the previous lemma can be chosen locally holomorphic with respect to z such that*

$$u_a(z, x)^* = u_a(z^*, x). \quad (9.33)$$

Similarly, for $u_b(z, x)$.

Proof. Since this is a local property near a we can suppose b is regular and choose $u_b(z, x)$ such that $(u_b(z, b), (pu'_b)(z, b)) = (\sin(\beta), -\cos(\beta))$ as in the example above. In addition, choose a second solution $v_b(z, x)$ such that $(v_b(z, b), (pv'_b)(z, b)) = (\cos(\beta), \sin(\beta))$ and observe $W(u_b(z), v_b(z)) = 1$. If $z \in \rho(A)$, z is no eigenvalue and hence $u_a(z, x)$ cannot be a multiple of $u_b(z, x)$. Thus we can set

$$u_a(z, x) = v_b(z, x) + m(z)u_b(z, x) \quad (9.34)$$

and it remains to show that $m(z)$ is holomorphic with $m(z)^* = m(z^*)$.

Choosing h with compact support in (a, c) and g with support in (c, b) we have

$$\begin{aligned} \langle h, (A - z)^{-1}g \rangle &= \langle h, u_a(z) \rangle \langle g^*, u_b(z) \rangle \\ &= (\langle h, v_b(z) \rangle + m(z) \langle h, u_b(z) \rangle) \langle g^*, u_b(z) \rangle \end{aligned} \quad (9.35)$$

(with a slight abuse of notation since u_b, v_b might not be square integrable). Choosing (real-valued) functions h and g such that $\langle h, u_b(z) \rangle \langle g^*, u_b(z) \rangle \neq 0$ we can solve for $m(z)$:

$$m(z) = \frac{\langle h, (A - z)^{-1}g \rangle - \langle h, v_b(z) \rangle \langle g^*, u_b(z) \rangle}{\langle h, u_b(z) \rangle \langle g^*, u_b(z) \rangle}. \quad (9.36)$$

This finishes the proof. \square

Example. We already know that $\tau = -\frac{d^2}{dx^2}$ on $I = (-\infty, \infty)$ gives rise to the free Schrödinger operator H_0 . Furthermore,

$$u_{\pm}(z, x) = e^{\mp\sqrt{-z}x}, \quad z \in \mathbb{C}, \quad (9.37)$$

are two linearly independent solutions (for $z \neq 0$) and since $\operatorname{Re}(\sqrt{-z}) > 0$ for $z \in \mathbb{C} \setminus [0, \infty)$, there is precisely one solution (up to a constant multiple)

which is square integrable near $\pm\infty$, namely u_{\pm} . In particular, the only choice for u_a is u_- and for u_b is u_+ and we get

$$G(z, x, y) = \frac{1}{2\sqrt{-z}} e^{-\sqrt{-z}|x-y|} \quad (9.38)$$

which we already found in Section 7.4. \diamond

If, as in the previous example, there is only one square integrable solution, there is no choice for $G(z, x, y)$. But since different boundary conditions must give rise to different resolvents, there is no room for boundary conditions in this case. This indicates a connection between our l.c., l.p. distinction and square integrability of solutions.

Theorem 9.9 (Weyl alternative). *The operator τ is l.c. at a if and only if for one $z_0 \in \mathbb{C}$ all solutions of $(\tau - z_0)u = 0$ are square integrable near a . This then holds for all $z \in \mathbb{C}$. Similarly for b .*

Proof. If all solutions are square integrable near a , τ is l.c. at a since the Wronskian of two linearly independent solutions does not vanish.

Conversely, take two functions $v, \tilde{v} \in \mathfrak{D}(\tau)$ with $W_a(v, \tilde{v}) \neq 0$. By considering real and imaginary parts it is no restriction to assume that v and \tilde{v} are real-valued. Thus they give rise to two different self-adjoint operators A and \tilde{A} (choose any fixed w for the other endpoint). Let u_a and \tilde{u}_a be the corresponding solutions from above, then $W(u_a, \tilde{u}_a) \neq 0$ (since otherwise $A = \tilde{A}$ by Lemma 9.5) and thus there are two linearly independent solutions which are square integrable near a . Since any other solution can be written as a linear combination of those two, every solution is square integrable near a .

It remains to show that all solutions of $(\tau - z)u = 0$ for all $z \in \mathbb{C}$ are square integrable near a if τ is l.c. at a . In fact, the above argument ensures this for every $z \in \rho(A) \cap \rho(\tilde{A})$, that is, at least for all $z \in \mathbb{C} \setminus \mathbb{R}$.

Suppose $(\tau - z)u = 0$. and choose two linearly independent solutions u_j , $j = 1, 2$, of $(\tau - z_0)u = 0$ with $W(u_1, u_2) = 1$. Using $(\tau - z_0)u = (z - z_0)u$ and (9.10) we have ($a < c < x < b$)

$$u(x) = \alpha u_1(x) + \beta u_2(x) + (z - z_0) \int_c^x (u_1(x)u_2(y) - u_1(y)u_2(x))u(y)r(y) dy. \quad (9.39)$$

Since $u_j \in L^2((c, b), r dx)$ we can find a constant $M \geq 0$ such that

$$\int_c^b |u_{1,2}(y)|^2 r(y) dy \leq M. \quad (9.40)$$

Now choose c close to b such that $|z - z_0|M^2 \leq 1/4$. Next, estimating the integral using Cauchy–Schwarz gives

$$\begin{aligned} & \left| \int_c^x (u_1(x)u_2(y) - u_1(y)u_2(x))u(y)r(y) dy \right|^2 \\ & \leq \int_c^x |u_1(x)u_2(y) - u_1(y)u_2(x)|^2 r(y) dy \int_c^x |u(y)|^2 r(y) dy \\ & \leq M \left(|u_1(x)|^2 + |u_2(x)|^2 \right) \int_c^x |u(y)|^2 r(y) dy \end{aligned} \quad (9.41)$$

and hence

$$\begin{aligned} \int_c^x |u(y)|^2 r(y) dy & \leq (|\alpha|^2 + |\beta|^2)M + 2|z - z_0|M^2 \int_c^x |u(y)|^2 r(y) dy \\ & \leq (|\alpha|^2 + |\beta|^2)M + \frac{1}{2} \int_c^x |u(y)|^2 r(y) dy. \end{aligned} \quad (9.42)$$

Thus

$$\int_c^x |u(y)|^2 r(y) dy \leq 2(|\alpha|^2 + |\beta|^2)M \quad (9.43)$$

and since $u \in AC_{loc}(I)$ we have $u \in L^2((c, b), r dx)$ for every $c \in (a, b)$. \square

Note that all eigenvalues are simple. If τ is l.p. at one endpoint this is clear, since there is at most one solution of $(\tau - \lambda)u = 0$ which is square integrable near this end point. If τ is l.c. this also follows since the fact that two solutions of $(\tau - \lambda)u = 0$ satisfy the same boundary condition implies that their Wronskian vanishes.

Finally, let us shed some additional light on the number of possible boundary conditions. Suppose τ is l.c. at a and let u_1, u_2 be two solutions of $\tau u = 0$ with $W(u_1, u_2) = 1$. Abbreviate

$$BC_x^j(f) = W_x(u_j, f), \quad f \in \mathfrak{D}(\tau). \quad (9.44)$$

Let v be as in Theorem 9.6, then, using Lemma 9.5 it is not hard to see that

$$W_a(v, f) = 0 \Leftrightarrow \cos(\alpha)BC_a^1(f) + \sin(\alpha)BC_a^2(f) = 0, \quad (9.45)$$

where $\tan(\alpha) = -\frac{BC_a^1(v)}{BC_a^2(v)}$. Hence all possible boundary conditions can be parametrized by $\alpha \in [0, \pi)$. If τ is regular at a and if we choose $u_1(a) = p(a)u_2'(a) = 1$ and $p(a)u_1'(a) = u_2(a) = 0$, then

$$BC_a^1(f) = f(a), \quad BC_a^2(f) = p(a)f'(a) \quad (9.46)$$

and the boundary condition takes the simple form

$$\cos(\alpha)f(a) + \sin(\alpha)p(a)f'(a) = 0. \quad (9.47)$$

Finally, note that if τ is l.c. at both a and b , then Theorem 9.6 does not give all possible self-adjoint extensions. For example, one could also choose

$$BC_a^1(f) = e^{i\alpha}BC_b^1(f), \quad BC_a^2(f) = e^{i\alpha}BC_b^2(f). \quad (9.48)$$

The case $\alpha = 0$ gives rise to periodic boundary conditions in the regular case.

Now we turn to the investigation of the spectrum of A . If τ is l.c. at both endpoints, then the spectrum of A is very simple

Theorem 9.10. *If τ is l.c. at both end points, then the resolvent is a Hilbert–Schmidt operator, that is,*

$$\int_a^b \int_a^b |G(z, x, y)|^2 r(y) dy r(x) dx < \infty. \quad (9.49)$$

In particular, the spectrum of any self adjoint extensions is purely discrete and the eigenfunctions (which are simple) form an orthonormal basis.

Proof. This follows from the estimate

$$\begin{aligned} & \int_a^b \left(\int_a^x |u_b(x)u_a(y)|^2 r(y) dy + \int_x^b |u_b(y)u_a(x)|^2 r(y) dy \right) r(x) dx \\ & \leq 2 \int_a^b |u_a(y)|^2 r(y) dy \int_a^b |u_b(y)|^2 r(y) dy, \end{aligned} \quad (9.50)$$

which shows that the resolvent is Hilbert–Schmidt and hence compact. \square

If τ is not l.c. the situation is more complicated and we can only say something about the essential spectrum.

Theorem 9.11. *All self adjoint extensions have the same essential spectrum. Moreover, if A_{ac} and A_{cb} are self-adjoint extensions of τ restricted to (a, c) and (c, b) (for any $c \in I$), then*

$$\sigma_{ess}(A) = \sigma_{ess}(A_{ac}) \cup \sigma_{ess}(A_{cb}). \quad (9.51)$$

Proof. Since $(\tau - i)u = 0$ has two linearly independent solutions, the defect indices are at most two (they are zero if τ is l.p. at both end points, one if τ is l.c. at one and l.p. at the other end point, and two if τ is l.c. at both endpoints). Hence the first claim follows from Theorem 6.19.

For the second claim restrict τ to the functions with compact support in $(a, c) \cup (c, d)$. Then, this operator is the orthogonal sum of the operators $A_{0,ac}$ and $A_{0,cb}$. Hence the same is true for the adjoints and hence the defect indices of $A_{0,ac} \oplus A_{0,cb}$ are at most four. Now note that A and $A_{ac} \oplus A_{cb}$ are both self-adjoint extensions of this operator. Thus the second claim also follows from Theorem 6.19. \square

Problem 9.3. *Compute the spectrum and the resolvent of $\tau = -\frac{d^2}{dx^2}$, $I = (0, \infty)$ defined on $\mathfrak{D}(A) = \{f \in \mathfrak{D}(\tau) | f(0) = 0\}$.*

9.3. Spectral transformations

In this section we want to provide some fundamental tools for investigating the spectra of Sturm-Liouville operators and, at the same time, give some nice illustrations of the spectral theorem.

Example. Consider again $\tau = -\frac{d^2}{dx^2}$ on $I = (-\infty, \infty)$. From Section 7.2 we know that the Fourier transform maps the associated operator H_0 to the multiplication operator with p^2 in $L^2(\mathbb{R})$. To get multiplication by λ , as in the spectral theorem, we set $p = \sqrt{\lambda}$ and split the Fourier integral into a positive and negative part

$$(Uf)(\lambda) = \begin{pmatrix} \int_{\mathbb{R}} e^{i\sqrt{\lambda}x} f(x) dx \\ \int_{\mathbb{R}} e^{-i\sqrt{\lambda}x} f(x) dx \end{pmatrix}, \quad \lambda \in \sigma(H_0) = [0, \infty). \quad (9.52)$$

Then

$$U : L^2(\mathbb{R}) \rightarrow \bigoplus_{j=1}^2 L^2(\mathbb{R}, \frac{\chi_{[0,\infty)}(\lambda)}{2\sqrt{\lambda}} d\lambda) \quad (9.53)$$

is the spectral transformation whose existence is guaranteed by the spectral theorem (Lemma 3.3). \diamond

Note that in the previous example the kernel $e^{\pm i\sqrt{\lambda}x}$ of the integral transform U is just a pair of linearly independent solutions of the underlying differential equation (though no eigenfunctions, since they are not square integrable).

More general, if

$$U : L^2(I, r dx) \rightarrow L^2(\mathbb{R}, d\mu), \quad f(x) \mapsto \int_{\mathbb{R}} u(\lambda, x) f(x) r(x) dx \quad (9.54)$$

is an integral transformation which maps a self-adjoint Sturm-Liouville operator A to multiplication by λ , then its kernel $u(\lambda, x)$ is a solution of the underlying differential equation. This formally follows from $UAf = \lambda Uf$ which implies

$$\int_{\mathbb{R}} u(\lambda, x) (\tau - \lambda) f(x) r(x) dx = \int_{\mathbb{R}} (\tau - \lambda) u(\lambda, x) f(x) r(x) dx \quad (9.55)$$

and hence $(\tau - \lambda)u(\lambda, \cdot) = 0$.

Lemma 9.12. *Suppose*

$$U : L^2(I, r dx) \rightarrow \bigoplus_{j=1}^k L^2(\mathbb{R}, d\mu_j) \quad (9.56)$$

is a spectral mapping as in Lemma 3.3. Then U is of the form

$$Uf(x) = \int_a^b u(\lambda, x) f(x) r(x) dx, \quad (9.57)$$

where $u(\lambda, x) = (u_1(\lambda, x), \dots, u_k(\lambda, x))$ and each $u_j(\lambda, \cdot)$ is a solution of $\tau u_j = \lambda u_j$ for a.e. λ (with respect to μ_j). The inverse is given by

$$U^{-1}F(\lambda) = \sum_{j=1}^k \int_{\mathbb{R}} u_j(\lambda, x)^* F_j(\lambda) d\mu_j(\lambda). \quad (9.58)$$

Moreover, the solutions $u_j(\lambda)$ are linearly independent if the spectral measures are ordered and, if τ is l.c. at some endpoint, they satisfy the boundary condition. In particular, for ordered spectral measures we have always $k \leq 2$ and even $k = 1$ if τ is l.c. at one endpoint.

Proof. Using $U_j R_A(z) = \frac{1}{\lambda - z} U_j$ we have

$$U_j f(x) = (\lambda - z) U_j \int_a^b G(z, x, y) f(y) r(y) dy. \quad (9.59)$$

If we restrict $R_A(z)$ to a compact interval $[c, d] \subset (a, b)$, then $R_A(z)\chi_{[c, d]}$ is Hilbert–Schmidt since $G(z, x, y)\chi_{[c, d]}(y)$ is square integrable over $(a, b) \times (a, b)$. Hence $U_j \chi_{[c, d]} = (\lambda - z) U_j R_A(z)\chi_{[c, d]}$ is Hilbert–Schmidt as well and by Lemma 6.9 there is a corresponding kernel $u_j^{[c, d]}(\lambda, y)$ such that

$$(U_j \chi_{[c, d]} f)(\lambda) = \int_a^b u_j^{[c, d]}(\lambda, x) f(x) r(x) dx. \quad (9.60)$$

Now take a larger compact interval $[\hat{c}, \hat{d}] \supseteq [c, d]$, then the kernels coincide on $[c, d]$, $u_j^{[c, d]}(\lambda, \cdot) = u_j^{[\hat{c}, \hat{d}]}(\lambda, \cdot)\chi_{[c, d]}$, since we have $U_j \chi_{[c, d]} = U_j \chi_{[\hat{c}, \hat{d}]} \chi_{[c, d]}$. In particular, there is a kernel $u_j(\lambda, x)$ such that

$$U_j f(x) = \int_a^b u_j(\lambda, x) f(x) r(x) dx \quad (9.61)$$

for every f with compact support in (a, b) . Since functions with compact support are dense and U_j is continuous, this formula holds for any f (provided the integral is understood as the corresponding limit).

Using the fact that U is unitary, $\langle F, U g \rangle = \langle U^{-1} F, g \rangle$, we see

$$\sum_j \int_{\mathbb{R}} F_j(\lambda)^* \int_a^b u_j(\lambda, x) g(x) r(x) dx = \int_a^b (U^{-1} F)(x)^* g(x) r(x) dx. \quad (9.62)$$

Interchanging integrals on the right hand side (which is permitted at least for g, F with compact support), the formula for the inverse follows.

Next, from $U_j A f = \lambda U_j f$ we have

$$\int_a^b u_j(\lambda, x) (\tau f)(x) r(x) dx = \lambda \int_a^b u_j(\lambda, x) f(x) r(x) dx \quad (9.63)$$

for a.e. λ and every $f \in \mathfrak{D}(A_0)$. Restricting everything to $[c, d] \subset (a, b)$ the above equation implies $u_j(\lambda, \cdot)|_{[c, d]} \in \mathfrak{D}(A_{cd,0}^*)$ and $A_{ab,0}^* u_j(\lambda, \cdot)|_{[c, d]} = \lambda u_j(\lambda, \cdot)|_{[c, d]}$. In particular, $u_j(\lambda, \cdot)$ is a solution of $\tau u_j = \lambda u_j$. Moreover, if $u_j(\lambda, \cdot)$ is τ is l.c. near a , we can choose $\alpha = a$ and f to satisfy the boundary condition.

Finally, fix $l \leq k$. If we assume the μ_j are ordered, there is a set Ω_l such that $\mu_j(\Omega_l) \neq 0$ for $1 \leq j \leq l$. Suppose

$$\sum_{j=1}^l c_j(\lambda) u_j(\lambda, x) = 0 \quad (9.64)$$

then we have

$$\sum_{j=1}^l c_j(\lambda) F_j(\lambda) = 0, \quad F_j = U_j f, \quad (9.65)$$

for every f . Since U is surjective, we can prescribe F_j arbitrarily, e.g., $F_j(\lambda) = 1$ for $j = j_0$ and $F_j(\lambda) = 0$ else which shows $c_{j_0}(\lambda) = 0$. Hence $u_j(\lambda, x)$, $1 \leq j \leq l$, are linearly independent for $\lambda \in \Omega_l$ which shows $k \leq 2$ since there are at most two linearly independent solutions. If τ is l.c. and $u_j(\lambda, x)$ must satisfy the boundary condition, there is only one linearly independent solution and thus $k = 1$. \square

Please note that the integral in (9.57) has to be understood as

$$U_j f(x) = \lim_{\alpha \downarrow a, \beta \uparrow b} \int_{\alpha}^{\beta} u_j(\lambda, x) f(x) r(x) dx, \quad (9.66)$$

where the limit is taken in $L^2(\mathbb{R}, d\mu_j)$. Similarly for (9.58).

For simplicity we will only pursue the case where one endpoint, say a , is regular. The general case can usually be reduced to this case by choosing $c \in (a, b)$ and splitting A as in Theorem 9.11.

We choose a boundary condition

$$\cos(\alpha) f(a) + \sin(\alpha) p(a) f'(a) = 0 \quad (9.67)$$

and introduce two solution $s(z, x)$ and $c(z, x)$ of $\tau u = zu$ satisfying the initial conditions

$$\begin{aligned} s(z, a) &= -\sin(\alpha), & p(a) s'(z, a) &= \cos(\alpha), \\ c(z, a) &= \cos(\alpha), & p(a) c'(z, a) &= \sin(\alpha). \end{aligned} \quad (9.68)$$

Note that $s(z, x)$ is the solution which satisfies the boundary condition at a , that is, we can choose $u_a(z, x) = s(z, x)$. Moreover, in our previous lemma we have $u_1(\lambda, x) = \gamma_a(\lambda) s(\lambda, x)$ and using the rescaling $d\mu(\lambda) =$

$|\gamma_a(\lambda)|^2 d\mu_a(\lambda)$ and $(U_1 f)(\lambda) = \gamma_a(\lambda)(Uf)(\lambda)$ we obtain a unitary map

$$U : L^2(I, r dx) \rightarrow L^2(\mathbb{R}, d\mu), \quad (Uf)(\lambda) = \int_a^b s(\lambda, x)f(x)r(x)dx \quad (9.69)$$

with inverse

$$(U^{-1}F)(x) = \int_{\mathbb{R}} s(\lambda, x)F(\lambda)d\mu(\lambda). \quad (9.70)$$

Note however, that while this rescaling gets rid of the unknown factor $\gamma_a(\lambda)$, it destroys the normalization of the measure μ . For μ_1 we know $\mu_1(\mathbb{R}) = 1$, but μ might not even be bounded! In fact, it turns out that μ is indeed unbounded.

So up to this point we have our spectral transformation U which maps A to multiplication by λ , but we know nothing about the measure μ . Furthermore, the measure μ is the object of desire since it contains all the spectral information of A . So our next aim must be to compute μ . If A has only pure point spectrum (i.e., only eigenvalues) this is straightforward as the following example shows.

Example. Suppose $E \in \sigma_p(A)$ is an eigenvalue. Then $s(E, x)$ is the corresponding eigenfunction and hence the same is true for $S_E(\lambda) = (Us(E))(\lambda)$. In particular, $S_E(\lambda) = 0$ for a.e. $\lambda \neq E$, that is

$$S_E(\lambda) = \begin{cases} \|s(E)\|^2, & \lambda = E \\ 0, & \lambda \neq E \end{cases}. \quad (9.71)$$

Moreover, since U is unitary we have

$$\|s(E)\|^2 = \int_a^b s(E, x)^2 r(x) dx = \int_{\mathbb{R}} S_E(\lambda)^2 d\mu(\lambda) = \|s(E)\|^4 \mu(\{E\}), \quad (9.72)$$

that is $\mu(\{E\}) = \|s(E)\|^{-2}$. In particular, if A has pure point spectrum (e.g., if τ is limit circle at both endpoints), we have

$$d\mu(\lambda) = \sum_{j=1}^{\infty} \frac{1}{\|s(E_j)\|^2} d\Theta(\lambda - E_j), \quad \sigma_p(A) = \{E_j\}_{j=1}^{\infty}, \quad (9.73)$$

where $d\Theta$ is the Dirac measure centered at 0. For arbitrary A , the above formula holds at least for the pure point part μ_{pp} . \diamond

In the general case we have to work a bit harder. Since $c(z, x)$ and $s(z, x)$ are linearly independent solutions,

$$W(c(z), s(z)) = 1, \quad (9.74)$$

we can write $u_b(z, x) = \gamma_b(z)(c(z, x) + m_b(z)s(z, x))$, where

$$m_b(z) = \frac{\cos(\alpha)p(a)u'_b(z, a) - \sin(\alpha)u_b(z, a)}{\cos(\alpha)u_b(z, a) + \sin(\alpha)p(a)u'_b(z, a)}, \quad z \in \rho(A), \quad (9.75)$$

is known as **Weyl-Titchmarsh m -function**. Note that $m_b(z)$ is holomorphic in $\rho(A)$ and that

$$m_b(z)^* = m_b(z^*) \quad (9.76)$$

since the same is true for $u_b(z, x)$ (the denominator in (9.75) only vanishes if $u_b(z, x)$ satisfies the boundary condition at a , that is, if z is an eigenvalue). Moreover, the constant $\gamma_b(z)$ is of no importance and can be chosen equal to one,

$$u_b(z, x) = c(z, x) + m_b(z)s(z, x). \quad (9.77)$$

Lemma 9.13. *The Weyl m -function is a Herglotz function and satisfies*

$$\operatorname{Im}(m_b(z)) = \operatorname{Im}(z) \int_a^b |u_b(z, x)|^2 r(x) dx, \quad (9.78)$$

where $u_b(z, x)$ is normalized as in (9.77).

Proof. Given two solutions $u(x)$, $v(x)$ of $\tau u = zu$, $\tau v = \hat{z}v$ it is straightforward to check

$$(\hat{z} - z) \int_a^x u(y)v(y)r(y) dy = W_x(u, v) - W_a(u, v) \quad (9.79)$$

(clearly it is true for $x = a$, now differentiate with respect to x). Now choose $u(x) = u_b(z, x)$ and $v(x) = u_b(z, x)^* = u_b(z^*, x)$,

$$-2\operatorname{Im}(z) \int_a^x |u_b(z, y)|^2 r(y) dy = W_x(u_b(z), u_b(z)^*) - 2\operatorname{Im}(m_b(z)), \quad (9.80)$$

and observe that $W_x(u_b, u_b^*)$ vanishes as $x \uparrow b$, since both u_b and u_b^* are in $\mathfrak{D}(\tau)$ near b . \square

Lemma 9.14. *We have*

$$(Uu_b(z))(\lambda) = \frac{1}{\lambda - z}, \quad (9.81)$$

where $u_b(z, x)$ is normalized as in (9.77).

Proof. First of all note that from $R_A(z)f = U^{-1} \frac{1}{\lambda - z} Uf$ we have

$$\int_a^b G(z, x, y)f(y)r(y) dy = \int_{\mathbb{R}} \frac{s(\lambda, x)F(\lambda)}{\lambda - z} d\mu(\lambda), \quad (9.82)$$

where $F = Uf$. Here equality is to be understood in L^2 , that is for a.e. x . However, the right hand side is continuous with respect to x and so is the left hand side, at least if F has compact support. Hence in this case the formula holds for all x and we can choose $x = a$ to obtain

$$\sin(\alpha) \int_a^b u_b(z, y)f(y)r(y) dy = \sin(\alpha) \int_{\mathbb{R}} \frac{F(\lambda)}{\lambda - z} d\mu(\lambda), \quad (9.83)$$

for all f , where F has compact support. Since these functions are dense, the claim follows if we can cancel $\sin(\alpha)$, that is, $\alpha \neq 0$. To see the case $\alpha = 0$, first differentiate (9.82) with respect to x before setting $x = a$. \square

Now combining the last two lemmas we infer from unitarity of U that

$$\operatorname{Im}(m_b(z)) = \operatorname{Im}(z) \int_a^b |u_b(z, x)|^2 r(x) dx = \operatorname{Im}(z) \int_{\mathbb{R}} \frac{1}{|\lambda - z|^2} d\mu(\lambda) \quad (9.84)$$

and since a holomorphic function is determined up to a real constant by its imaginary part we obtain

Theorem 9.15. *The Weyl m -function is given by*

$$m_b(z) = d + \int_{\mathbb{R}} \left(\frac{1}{\lambda - z} - \frac{\lambda}{1 + \lambda^2} \right) d\mu(\lambda), \quad d \in \mathbb{R}, \quad (9.85)$$

and

$$d = \operatorname{Re}(m_b(i)), \quad \int_{\mathbb{R}} \frac{1}{1 + \lambda^2} d\mu(\lambda) = \operatorname{Im}(m_b(i)) < \infty. \quad (9.86)$$

Moreover, μ is given by Stieltjes inversion formula

$$\mu(\lambda) = \lim_{\delta \downarrow 0} \lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \int_{\delta}^{\lambda + \delta} \operatorname{Im}(m_b(\lambda + i\varepsilon)) d\lambda, \quad (9.87)$$

where

$$\operatorname{Im}(m_b(\lambda + i\varepsilon)) = \varepsilon \int_a^b |u_b(\lambda + i\varepsilon, x)|^2 r(x) dx. \quad (9.88)$$

Proof. Choosing $z = i$ in (9.84) shows (9.86) and hence the right hand side of (9.85) is a well-defined holomorphic function in $\mathbb{C} \setminus \mathbb{R}$. By $\operatorname{Im}\left(\frac{1}{\lambda - z} - \frac{\lambda}{1 + \lambda^2}\right) = \frac{\operatorname{Im}(z)}{|\lambda - z|^2}$ its imaginary part coincides with that of $m_b(z)$ and hence equality follows. Stieltjes inversion formula follows as in the case where the measure is bounded. \square

Example. Consider $\tau = -\frac{d^2}{dx^2}$ on $I = (0, \infty)$. Then

$$c(z, x) = \cos(\alpha) \cos(\sqrt{z}x) + \frac{\sin(\alpha)}{\sqrt{z}} \sin(\sqrt{z}x) \quad (9.89)$$

and

$$s(z, x) = -\sin(\alpha) \cos(\sqrt{z}x) + \frac{\cos(\alpha)}{\sqrt{z}} \sin(\sqrt{z}x). \quad (9.90)$$

Moreover,

$$u_b(z, x) = u_b(z, 0) e^{-\sqrt{-z}x} \quad (9.91)$$

and thus

$$m_b(z) = \frac{\sqrt{-z} \cos(\alpha) + \sin(\alpha)}{\sqrt{-z} \sin(\alpha) - \cos(\alpha)} \quad (9.92)$$

respectively

$$d\mu(\lambda) = \frac{\sqrt{\lambda}}{\pi(\cos(\alpha)^2 + \lambda \sin(\alpha)^2)} d\lambda. \quad (9.93)$$

◇

Note that if $\alpha \neq 0$ we even have $\int \frac{1}{|\lambda-z|} d\mu(\lambda) < 0$ in the previous example and hence

$$m_b(z) = \cot(\alpha) + \int_{\mathbb{R}} \frac{1}{\lambda - z} d\mu(\lambda) \quad (9.94)$$

in this case (the factor $-\cot(\alpha)$ follows by considering the limit $|z| \rightarrow \infty$ of both sides). One can show that this remains true in the general case. Formally it follows by choosing $x = a$ in $u_b(z, x) = (U^{-1} \frac{1}{\lambda-z})(x)$, however, since we know equality only for a.e. x , a more careful analysis is needed.

We conclude this section with some asymptotics for large z away from the spectrum. For simplicity we only consider the case $p = k \equiv 1$. We first observe (Problem 9.4):

Lemma 9.16. *We have*

$$\begin{aligned} c(z, x) &= \frac{1}{2} \left(\cos(\alpha) + \frac{\sin(\alpha)}{\sqrt{-z}} \right) e^{\sqrt{-z}(x-a)} \left(1 + O\left(\frac{1}{\sqrt{-z}}\right) \right) \\ s(z, x) &= \frac{1}{2} \left(-\sin(\alpha) + \frac{\cos(\alpha)}{\sqrt{-z}} \right) e^{\sqrt{-z}(x-a)} \left(1 + O\left(\frac{1}{\sqrt{-z}}\right) \right) \end{aligned} \quad (9.95)$$

for fixed $x \in (a, b)$ as $\text{Im}(z) \rightarrow \infty$.

Furthermore we have

Lemma 9.17. *The Green's function of A*

$$G(z, x, y) = s(z, x)u_b(z, y), \quad x \leq y, \quad (9.96)$$

satisfies

$$\lim_{\text{Im}(z) \rightarrow \infty} G(z, x, y) = 0 \quad (9.97)$$

for every $x, y \in (a, b)$.

Proof. Let φ be some continuous positive function supported in $[-1, 1]$ with $\int \varphi(x) dx = 1$ and set $\varphi_k(x) = k \varphi(kx)$. Then, by $\|R_A(z)\| \leq \text{Im}(z)^{-1}$ (see Theorem 2.14),

$$\begin{aligned} |G(z, x, y)| &\leq |G_k(z, x, y)| + |G(z, x, y) - G_k(z, x, y)| \\ &\leq \frac{k \|\varphi\|^2}{\text{Im}(z)} + |G(z, x, y) - G_k(z, x, y)|, \end{aligned} \quad (9.98)$$

where

$$G_k(z, x, y) = \langle \varphi_k(\cdot - x), R_A(z) \varphi_k(\cdot - y) \rangle. \quad (9.99)$$

Since $G(z, x, y) = \lim_{k \rightarrow \infty} G_k(z, x, y)$ we can first choose k sufficiently large such that $|G(z, x, y) - G_k(z, x, y)| \leq \frac{\varepsilon}{2}$ and then $\text{Im}(z)$ so large such that $\frac{k\|\varphi\|^2}{\text{Im}(z)} \leq \frac{\varepsilon}{2}$. Hence $|G(z, x, y)| \leq \varepsilon$ and the claim follows. \square

Combining the last two lemmas we also obtain

Lemma 9.18. *The Weyl m -function satisfies*

$$m_b(z) = \begin{cases} \cot(\alpha) + O\left(\frac{1}{\sqrt{-z}}\right), & \alpha \neq 0 \\ -\sqrt{-z} + O\left(\frac{1}{\sqrt{-z}}\right), & \alpha = 0 \end{cases} \quad (9.100)$$

as $\text{Im}(z) \rightarrow \infty$.

Proof. Plugging the asymptotic expansions from Lemma 9.16 into Lemma 9.17 we see

$$m_b(z) = -\frac{c(z, x)}{s(z, x)} + o(e^{-2\sqrt{-z}(x-a)}) \quad (9.101)$$

from which the claim follows. \square

Note that assuming $q \in C^k([a, b])$ one can obtain further asymptotic terms in Lemma 9.16 and hence also in the expansion of $m_b(z)$.

Problem 9.4. *Prove the asymptotics for $c(z, x)$ and $s(z, x)$ from Lemma 9.16. (Hint: Use that*

$$\begin{aligned} c(z, x) &= \cos(\alpha) \cosh(\sqrt{-z}x) + \frac{\sin(\alpha)}{\sqrt{-z}} \sinh(\sqrt{-z}x) \\ &\quad - \frac{1}{\sqrt{-z}} \int_a^x \sinh(\sqrt{-z}(x-y))q(y)c(z, y)dy \end{aligned}$$

by Lemma 9.2 and consider $\tilde{c}(z, x) = e^{-\sqrt{-z}x}c(z, x)$.)

One-particle Schrödinger operators

10.1. Self-adjointness and spectrum

Our next goal is to apply these results to Schrödinger operators. The Hamiltonian of one particle in d dimensions is given by

$$H = H_0 + V, \tag{10.1}$$

where $V : \mathbb{R}^d \rightarrow \mathbb{R}$ is the potential energy of the particle. We are mainly interested in the case $1 \leq d \leq 3$ and want to find classes of potentials which are relatively bounded respectively relatively compact. To do this we need a better understanding of the functions in the domain of H_0 .

Lemma 10.1. *Suppose $n \leq 3$ and $\psi \in H^2(\mathbb{R}^n)$. Then $\psi \in C_\infty(\mathbb{R}^n)$ and for any $a > 0$ there is a $b > 0$ such that*

$$\|\psi\|_\infty \leq a\|H_0\psi\| + b\|\psi\|. \tag{10.2}$$

Proof. The important observation is that $(p^2 + \gamma^2)^{-1} \in L^2(\mathbb{R}^n)$ if $n \leq 3$. Hence, since $(p^2 + \gamma^2)\hat{\psi} \in L^2(\mathbb{R}^n)$, the Cauchy-Schwarz inequality

$$\begin{aligned} \|\hat{\psi}\|_1 &= \|(p^2 + \gamma^2)^{-1}(p^2 + \gamma^2)\hat{\psi}(p)\|_1 \\ &\leq \|(p^2 + \gamma^2)^{-1}\| \|(p^2 + \gamma^2)\hat{\psi}(p)\|. \end{aligned} \tag{10.3}$$

shows $\hat{\psi} \in L^1(\mathbb{R}^n)$. But now everything follows from the Riemann-Lebesgue lemma

$$\begin{aligned} \|\psi\|_\infty &\leq (2\pi)^{-n/2} \|(p^2 + \gamma^2)^{-1}\| (\|p^2\hat{\psi}(p)\| + \gamma^2\|\hat{\psi}(p)\|) \\ &= (\gamma/2\pi)^{n/2} \|(p^2 + 1)^{-1}\| (\gamma^{-2}\|H_0\psi\| + \|\psi\|) \end{aligned} \tag{10.4}$$

finishes the proof. \square

Now we come to our first result.

Theorem 10.2. *Let V be real-valued and $V \in L^\infty(\mathbb{R}^n)$ if $n > 3$ and $V \in L^\infty(\mathbb{R}^n) + L^2(\mathbb{R}^n)$ if $n \leq 3$. Then V is relatively compact with respect to H_0 . In particular,*

$$H = H_0 + V, \quad \mathfrak{D}(H) = H^2(\mathbb{R}^n), \quad (10.5)$$

is self-adjoint, bounded from below and

$$\sigma_{\text{ess}}(H) = [0, \infty). \quad (10.6)$$

Moreover, $C_0^\infty(\mathbb{R}^n)$ is a core for H .

Proof. Our previous lemma shows $\mathfrak{D}(H_0) \subseteq \mathfrak{D}(V)$ and the rest follows from Lemma 7.10 using $f(p) = (p^2 - z)^{-1}$ and $g(x) = V(x)$. Note that $f \in L^\infty(\mathbb{R}^n) \cap L^2(\mathbb{R}^n)$ for $n \leq 3$. \square

Observe that since $C_c^\infty(\mathbb{R}^n) \subseteq \mathfrak{D}(H_0)$, we must have $V \in L_{\text{loc}}^2(\mathbb{R}^n)$ if $\mathfrak{D}(V) \subseteq \mathfrak{D}(H_0)$.

10.2. The hydrogen atom

We begin with the simple model of a single electron in \mathbb{R}^3 moving in the external potential V generated by a nucleus (which is assumed to be fixed at the origin). If one takes only the electrostatic force into account, then V is given by the Coulomb potential and the corresponding Hamiltonian is given by

$$H^{(1)} = -\Delta - \frac{\gamma}{|x|}, \quad \mathfrak{D}(H^{(1)}) = H^2(\mathbb{R}^3). \quad (10.7)$$

If the potential is attracting, that is, if $\gamma > 0$, then it describes the hydrogen atom and is probably the most famous model in quantum mechanics.

As domain we have chosen $\mathfrak{D}(H^{(1)}) = \mathfrak{D}(H_0) \cap \mathfrak{D}(\frac{1}{|x|}) = \mathfrak{D}(H_0)$ and by Theorem 10.2 we conclude that $H^{(1)}$ is self-adjoint. Moreover, Theorem 10.2 also tells us

$$\sigma_{\text{ess}}(H^{(1)}) = [0, \infty) \quad (10.8)$$

and that $H^{(1)}$ is bounded from below

$$E_0 = \inf \sigma(H^{(1)}) > -\infty. \quad (10.9)$$

If $\gamma \leq 0$ we have $H^{(1)} \geq 0$ and hence $E_0 = 0$, but if $\gamma > 0$, we might have $E_0 < 0$ and there might be some discrete eigenvalues below the essential spectrum.

In order to say more about the eigenvalues of $H^{(1)}$ we will use the fact that both H_0 and $V^{(1)} = -\gamma/|x|$ have a simple behavior with respect to scaling. Consider the **dilation group**

$$U(s)\psi(x) = e^{-ns/2}\psi(e^{-s}x), \quad s \in \mathbb{R}, \quad (10.10)$$

which is a strongly continuous one-parameter unitary group. The generator can be easily computed

$$D\psi(x) = \frac{1}{2}(xp + px)\psi(x) = (xp - \frac{in}{2})\psi(x), \quad \psi \in \mathcal{S}(\mathbb{R}^n). \quad (10.11)$$

Now let us investigate the action of $U(s)$ on $H^{(1)}$

$$H^{(1)}(s) = U(-s)H^{(1)}U(s) = e^{-2s}H_0 + e^{-s}V^{(1)}, \quad \mathfrak{D}(H^{(1)}(s)) = \mathfrak{D}(H^{(1)}). \quad (10.12)$$

Now suppose $H\psi = \lambda\psi$, then

$$\langle \psi, [U(s), H]\psi \rangle = \langle U(-s)\psi, H\psi \rangle - \langle H\psi, U(s)\psi \rangle = 0 \quad (10.13)$$

and hence

$$\begin{aligned} 0 &= \lim_{s \rightarrow 0} \frac{1}{s} \langle \psi, [U(s), H]\psi \rangle = \lim_{s \rightarrow 0} \langle U(-s)\psi, \frac{H - H(s)}{s}\psi \rangle \\ &= \langle \psi, (2H_0 + V^{(1)})\psi \rangle. \end{aligned} \quad (10.14)$$

Thus we have proven the **virial theorem**.

Theorem 10.3. *Suppose $H = H_0 + V$ with $U(-s)VU(s) = e^{-s}V$. Then any normalized eigenfunction ψ corresponding to an eigenvalue λ satisfies*

$$\lambda = -\langle \psi, H_0\psi \rangle = \frac{1}{2}\langle \psi, V\psi \rangle. \quad (10.15)$$

In particular, all eigenvalues must be negative.

This result even has some further consequences for the point spectrum of $H^{(1)}$.

Corollary 10.4. *Suppose $\gamma > 0$. Then*

$$\sigma_p(H^{(1)}) = \sigma_d(H^{(1)}) = \{E_{j-1}\}_{j \in \mathbb{N}_0}, \quad E_0 < E_j < E_{j+1} < 0, \quad (10.16)$$

with $\lim_{j \rightarrow \infty} E_j = 0$.

Proof. Choose $\psi \in C_c^\infty(\mathbb{R} \setminus \{0\})$ and set $\psi(s) = U(-s)\psi$. Then

$$\langle \psi(s), H^{(1)}\psi(s) \rangle = e^{-2s}\langle \psi, H_0\psi \rangle + e^{-s}\langle \psi, V^{(1)}\psi \rangle \quad (10.17)$$

which is negative for s large. Now choose a sequence $s_n \rightarrow \infty$ such that we have $\text{supp}(\psi(s_n)) \cap \text{supp}(\psi(s_m)) = \emptyset$ for $n \neq m$. Then Theorem 4.11 (i) shows that $\text{rank}(P_{H^{(1)}}((-\infty, 0))) = \infty$. Since each eigenvalue E_j has finite multiplicity (it lies in the discrete spectrum) there must be an infinite number of eigenvalues which accumulate at 0. \square

If $\gamma \leq 0$ we have $\sigma_d(H^{(1)}) = \emptyset$ since $H^{(1)} \geq 0$ in this case.

Hence we have gotten a quite complete picture of the spectrum of $H^{(1)}$. Next, we could try to compute the eigenvalues of $H^{(1)}$ (in the case $\gamma > 0$) by solving the corresponding eigenvalue equation, which is given by the partial differential equation

$$-\Delta\psi(x) - \frac{\gamma}{|x|}\psi(x) = \lambda\psi(x). \quad (10.18)$$

For a general potential this is hopeless, but in our case we can use the rotational symmetry of our operator to reduce our partial differential equation to ordinary ones.

First of all, it suggests itself to switch to spherical coordinates $(x_1, x_2, x_3) \mapsto (r, \theta, \varphi)$

$$x_1 = r \sin(\theta) \cos(\varphi), \quad x_2 = r \sin(\theta) \sin(\varphi), \quad x_3 = r \cos(\theta), \quad (10.19)$$

which correspond to a unitary transform

$$L^2(\mathbb{R}^3) \rightarrow L^2((0, \infty), r^2 dr) \otimes L^2((0, \pi), \sin(\theta) d\theta) \otimes L^2((0, 2\pi), d\varphi). \quad (10.20)$$

In these new coordinates (r, θ, φ) our operator reads

$$H^{(1)} = -\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2} L^2 + V(r), \quad V(r) = -\frac{\gamma}{r}, \quad (10.21)$$

where

$$L^2 = L_1^2 + L_2^2 + L_3^2 = -\frac{1}{\sin(\theta)} \frac{\partial}{\partial \theta} \sin(\theta) \frac{\partial}{\partial \theta} - \frac{1}{\sin(\theta)^2} \frac{\partial^2}{\partial \varphi^2}. \quad (10.22)$$

(Recall the angular momentum operators L_j from Section 8.2.)

Making the product ansatz (separation of variables)

$$\psi(r, \theta, \varphi) = R(r)\Theta(\theta)\Phi(\varphi) \quad (10.23)$$

we obtain the following three Sturm-Liouville equations

$$\begin{aligned} \left(-\frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} + \frac{l(l+1)}{r^2} + V(r) \right) R(r) &= \lambda R(r) \\ \frac{1}{\sin(\theta)} \left(-\frac{d}{d\theta} \sin(\theta) \frac{d}{d\theta} + \frac{m^2}{\sin(\theta)^2} \right) \Theta(\theta) &= l(l+1)\Theta(\theta) \\ -\frac{d^2}{d\varphi^2} \Phi(\varphi) &= m^2 \Phi(\varphi) \end{aligned} \quad (10.24)$$

The form chosen for the constants $l(l+1)$ and m^2 is for convenience later on. These equations will be investigated in the following sections.

10.3. Angular momentum

We start by investigating the equation for $\Phi(\varphi)$ which associated with the Sturm-Liouville equation

$$\tau\Phi = -\Phi'', \quad I = (0, 2\pi). \quad (10.25)$$

since we want ψ defined via (10.23) to be in the domain of H_0 (in particular continuous), we choose periodic boundary conditions the Sturm-Liouville equation

$$A\Phi = \tau\Phi, \quad \mathfrak{D}(A) = \{\Phi \in L^2(0, 2\pi) \mid \Phi \in AC^1[0, 2\pi], \\ \Phi(0) = \Phi(2\pi), \Phi'(0) = \Phi'(2\pi)\} \quad (10.26)$$

From our analysis in Section 9.1 we immediately obtain

Theorem 10.5. *The operator A defined via (10.25) is self-adjoint. Its spectrum is purely discrete*

$$\sigma(A) = \sigma_d(A) = \{m^2 \mid m \in \mathbb{Z}\} \quad (10.27)$$

and the corresponding eigenfunctions

$$\Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi}, \quad m \in \mathbb{Z}, \quad (10.28)$$

form an orthonormal basis for $L^2(0, 2\pi)$.

Note that except for the lowest eigenvalue, all eigenvalues are twice degenerate.

We note that this operator is essentially the square of the angular momentum in the third coordinate direction, since in polar coordinates

$$L_3 = \frac{1}{i} \frac{\partial}{\partial \varphi}. \quad (10.29)$$

Now we turn to the equation for $\Theta(\theta)$

$$\tau_m \Theta(\theta) = \frac{1}{\sin(\theta)} \left(-\frac{d}{d\theta} \sin(\theta) \frac{d}{d\theta} + \frac{m^2}{\sin(\theta)} \right) \Theta(\theta), \quad I = (0, \pi), m \in \mathbb{N}_0. \quad (10.30)$$

For the investigation of the corresponding operator we use the unitary transform

$$L^2((0, \pi), \sin(\theta)d\theta) \rightarrow L^2((-1, 1), dx), \quad \Theta(\theta) \mapsto f(x) = \Theta(\arccos(x)). \quad (10.31)$$

The operator τ transforms to the somewhat simpler form

$$\tau_m = -\frac{d}{dx} (1-x^2) \frac{d}{dx} - \frac{m^2}{1-x^2}. \quad (10.32)$$

The corresponding eigenvalue equation

$$\tau_m u = l(l+1)u \quad (10.33)$$

is the **associated Legendre equation**. For $l \in \mathbb{N}_0$ it is solved by the **associated Legendre functions**

$$P_{lm}(x) = (1-x^2)^{m/2} \frac{d^m}{dx^m} P_l(x), \quad (10.34)$$

where

$$P_l(x) = \frac{1}{2^l l!} \frac{d^l}{dx^l} (x^2-1)^l \quad (10.35)$$

are the **Legendre polynomials**. This is straightforward to check. Moreover, note that $P_l(x)$ are (nonzero) polynomials of degree l . A second, linearly independent solution is given by

$$Q_{lm}(x) = P_{lm}(x) \int_0^x \frac{dt}{(1-t^2)P_{lm}(t)^2}. \quad (10.36)$$

In fact, for every Sturm-Liouville equation $v(x) = u(x) \int^x \frac{dt}{p(t)u(t)^2}$ satisfies $\tau v = 0$ whenever $\tau u = 0$. Now fix $l = 0$ and note $P_0(x) = 1$. For $m = 0$ we have $Q_{00} = \operatorname{arctanh}(x) \in L^2$ and so τ_0 is l.c. at both end points. For $m > 0$ we have $Q_{0m} = (x \pm 1)^{-m/2}(C + O(x \pm 1))$ which shows that it is not square integrable. Thus τ_m is l.c. for $m = 0$ and l.p. for $m > 0$ at both endpoints. In order to make sure that the eigenfunctions for $m = 0$ are continuous (such that ψ defined via (10.23) is continuous) we choose the boundary condition generated by $P_0(x) = 1$ in this case

$$A_m f = \tau f, \quad \mathfrak{D}(A_m) = \{f \in L^2(-1, 1) \mid f \in AC^1(0, \pi), \tau f \in L^2(-1, 1), \lim_{x \rightarrow \pm 1} (1-x^2)f'(x) = 0\} \quad (10.37)$$

Theorem 10.6. *The operator A_m , $m \in \mathbb{N}_0$, defined via (10.37) is self-adjoint. Its spectrum is purely discrete*

$$\sigma(A_m) = \sigma_d(A_m) = \{l(l+1) \mid l \in \mathbb{N}_0, l \geq m\} \quad (10.38)$$

and the corresponding eigenfunctions

$$u_{lm}(x) = \sqrt{\frac{2l+1}{2} \frac{(l+m)!}{(l-m)!}} P_{lm}(x), \quad l \in \mathbb{N}_0, l \geq m, \quad (10.39)$$

form an orthonormal basis for $L^2(-1, 1)$.

Proof. By Theorem 9.6, A_m is self-adjoint. Moreover, P_{lm} is an eigenfunction corresponding to the eigenvalue $l(l+1)$ and it suffices to show that P_{lm} form a basis. To prove this, it suffices to show that the functions $P_{lm}(x)$ are dense. Since $(1-x^2) > 0$ for $x \in (-1, 1)$ it suffices to show that the functions $(1-x^2)^{-m/2} P_{lm}(x)$ are dense. But the span of these functions

contains every polynomial. Every continuous function can be approximated by polynomials (in the sup norm and hence in the L^2 norm) and since the continuous functions are dense, so are the polynomials.

The only thing remaining is the normalization of the eigenfunctions, which can be found in any book on special functions. \square

Returning to our original setting we conclude that

$$\Theta_{lm}(\theta) = \sqrt{\frac{2l+1}{2} \frac{(l+m)!}{(l-m)!}} P_{lm}(\cos(\theta)), \quad l = m, m+1, \dots \quad (10.40)$$

form an orthonormal basis for $L^2((0, \pi), \sin(\theta)d\theta)$ for any fixed $m \in \mathbb{N}_0$.

Theorem 10.7. *The operator L^2 on $L^2((0, \pi), \sin(\theta)d\theta) \otimes L^2((0, 2\pi))$ has a purely discrete spectrum given*

$$\sigma(L^2) = \{l(l+1) | l \in \mathbb{N}_0\}. \quad (10.41)$$

The spherical harmonics

$$Y_{lm}(\theta, \varphi) = \Theta_{l|m|}(\theta) \Phi_m(\varphi) = \sqrt{\frac{2l+1}{4\pi} \frac{(l+|m|)!}{(l-|m|)!}} P_{l|m|}(\cos(\theta)) e^{im\varphi}, \quad |m| \leq l, \quad (10.42)$$

form an orthonormal basis and satisfy $L^2 Y_{lm} = l(l+1) Y_{lm}$ and $L_3 Y_{lm} = m Y_{lm}$.

Proof. Everything follows from our construction, if we can show that Y_{lm} form a basis. But this follows as in the proof of Lemma 1.9. \square

Note that transforming Y_{lm} back to cartesian coordinates gives

$$Y_{l,\pm m}(x) = \sqrt{\frac{2l+1}{4\pi} \frac{(l+m)!}{(l-m)!}} \tilde{P}_{lm}\left(\frac{x_3}{r}\right) \left(\frac{x_1 \pm ix_2}{r}\right)^m, \quad r = |x|, \quad (10.43)$$

where \tilde{P}_{lm} is a polynomial of degree $l-m$ given by

$$\tilde{P}_{lm}(x) = (1-x^2)^{-m/2} P_{lm}(x) = \frac{d^{l+m}}{dx^{l+m}} (1-x^2)^l. \quad (10.44)$$

In particular, Y_{lm} are smooth away from the origin and by construction they satisfy

$$-\Delta Y_{lm} = \frac{l(l+1)}{r^2} Y_{lm}. \quad (10.45)$$

10.4. The eigenvalues of the hydrogen atom

Now we want to use the considerations from the previous section to decompose the Hamiltonian of the hydrogen atom. In fact, we can even admit any spherically symmetric potential $V(x) = V(|x|)$ with

$$V(r) \in L^\infty(\mathbb{R}) + L^2((0, \infty), r^2 dr). \quad (10.46)$$

The important observation is that the spaces

$$\mathfrak{H}_{lm} = \{\psi(x) = R(r)Y_{lm}(\theta, \varphi) \mid R(r) \in L^2((0, \infty), r^2 dr)\} \quad (10.47)$$

reduce our operator $H = H_0 + V$. Hence

$$H = H_0 + V = \bigoplus_{l,m} \tilde{H}_l, \quad (10.48)$$

where

$$\begin{aligned} \tilde{H}_l R(r) &= \tilde{\tau}_l R(r), \quad \tilde{\tau}_l = -\frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} + \frac{l(l+1)}{r^2} + V(r) \\ \mathfrak{D}(H_l) &\subseteq L^2((0, \infty), r^2 dr). \end{aligned} \quad (10.49)$$

Using the unitary transformation

$$L^2((0, \infty), r^2 dr) \rightarrow L^2((0, \infty)), \quad R(r) \mapsto u(r) = rR(r), \quad (10.50)$$

our operator transforms to

$$\begin{aligned} A_l f &= \tau_l f, \quad \tau_l = -\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + V(r) \\ \mathfrak{D}(A_l) &\subseteq L^2((0, \infty)). \end{aligned} \quad (10.51)$$

It remains to investigate this operator.

Theorem 10.8. *The domain of the operator A_l is given by*

$$\begin{aligned} \mathfrak{D}(A_l) &= \{f \in L^2(I) \mid f, f' \in AC(I), \tau f \in L^2(I), \\ &\quad \lim_{r \rightarrow 0} (f(r) - r f'(r)) = 0 \text{ if } l = 0\}, \end{aligned} \quad (10.52)$$

where $I = (0, \infty)$. Moreover, $\sigma_{ess}(A_l) = [0, \infty)$.

Proof. By construction of A_l we know that it is self-adjoint and satisfies $\sigma_{ess}(A_l) = [0, \infty)$. Hence it remains to compute the domain. We know at least $\mathfrak{D}(A_l) \subseteq \mathfrak{D}(\tau)$ and since $\mathfrak{D}(H) = \mathfrak{D}(H_0)$ it suffices to consider the case $V = 0$. In this case the solutions of $-u''(r) + \frac{l(l+1)}{r^2}u(r) = 0$ are given by $u(r) = \alpha r^{l+1} + \beta r^{-l}$. Thus we are in the l.p. case at ∞ for any $l \in \mathbb{N}_0$. However, at 0 we are in the l.p. case only if $l > 0$, that is, we need an additional boundary condition at 0 if $l = 0$. Since we need $R(r) = \frac{u(r)}{r}$ to be bounded (such that (10.23) is in the domain of H_0), we have to take the boundary condition generated by $u(r) = r$. \square

Finally let us turn to some explicit choices for V , where the corresponding differential equation can be explicitly solved. The simplest case is $V = 0$ in this case the solutions of

$$-u''(r) + \frac{l(l+1)}{r^2}u(r) = zu(r) \quad (10.53)$$

are given by the **spherical Bessel** respectively **spherical Neumann** functions

$$u(r) = \alpha j_l(\sqrt{z}r) + \beta n_l(\sqrt{z}r), \quad (10.54)$$

where

$$j_l(r) = (-r)^l \left(\frac{1}{r} \frac{d}{dr} \right)^l \frac{\sin(r)}{r}. \quad (10.55)$$

In particular,

$$u_a(z, r) = j_l(\sqrt{z}r) \quad \text{and} \quad u_b(z, r) = j_l(\sqrt{z}r) + in_l(\sqrt{z}r) \quad (10.56)$$

are the functions which are square integrable and satisfy the boundary condition (if any) near $a = 0$ and $b = \infty$, respectively.

The second case is that of our Coulomb potential

$$V(r) = -\frac{\gamma}{r}, \quad \gamma > 0, \quad (10.57)$$

where we will try to compute the eigenvalues plus corresponding eigenfunctions. It turns out that they can be expressed in terms of the **Laguerre polynomials**

$$L_j(r) = e^r \frac{d^j}{dr^j} e^{-r} r^j \quad (10.58)$$

and the **associated Laguerre polynomials**

$$L_j^k(r) = \frac{d^k}{dr^k} L_j(r). \quad (10.59)$$

Note that L_j^k is a polynomial of degree $j - k$.

Theorem 10.9. *The eigenvalues of $H^{(1)}$ are explicitly given by*

$$E_n = -\left(\frac{\gamma}{2(n+1)} \right)^2, \quad n \in \mathbb{N}_0. \quad (10.60)$$

An orthonormal basis for the corresponding eigenspace is given by

$$\psi_{nlm}(x) = R_{nl}(r)Y_{lm}(x), \quad (10.61)$$

where

$$R_{nl}(r) = \sqrt{\frac{\gamma^3(n-l)!}{2n^3((n+l+1)!)^3}} \left(\frac{\gamma r}{n+1} \right)^l e^{-\frac{\gamma r}{2(n+1)}} L_{n+l+1}^{2l+1}\left(\frac{\gamma r}{n+1}\right). \quad (10.62)$$

In particular, the lowest eigenvalue $E_0 = -\frac{\gamma^2}{4}$ is simple and the corresponding eigenfunction $\psi_{000}(x) = \sqrt{\frac{\gamma^3}{4^3\pi}} e^{-\gamma r/2}$ is positive.

Proof. It is a straightforward calculation to check that R_{nl} are indeed eigenfunctions of A_l corresponding to the eigenvalue $-(\frac{\gamma}{2(n+1)})^2$ and for the norming constants we refer to any book on special functions. The only problem is to show that we have found *all* eigenvalues.

Since all eigenvalues are negative, we need to look at the equation

$$-u''(r) + \left(\frac{l(l+1)}{r^2} - \frac{\gamma}{r}\right)u(r) = \lambda u(r) \quad (10.63)$$

for $\lambda < 0$. Introducing new variables $x = \sqrt{-\lambda}r$ and $v(x) = \frac{e^x}{x^{l+1}}u(\frac{x}{\sqrt{-\lambda}})$ this equation transforms into

$$xv''(x) + 2(l+1-x)v'(x) + 2nv(x) = 0, \quad n = \frac{\gamma}{2\sqrt{-\lambda}} - (l+1). \quad (10.64)$$

Now let us search for a solution which can be expanded into a convergent power series

$$v(x) = \sum_{j=0}^{\infty} v_j x^j, \quad v_0 = 1. \quad (10.65)$$

The corresponding $u(r)$ is square integrable near 0 and satisfies the boundary condition (if any). Thus we need to find those values of λ for which it is square integrable near $+\infty$.

Substituting the ansatz (10.65) into our differential equation and comparing powers of x gives the following recursion for the coefficients

$$v_{j+1} = \frac{2(j-n)}{(j+1)(j+2(l+1))}v_j \quad (10.66)$$

and thus

$$v_j = \frac{1}{j!} \prod_{k=0}^{j-1} \frac{2(k-n)}{k+2(l+1)}. \quad (10.67)$$

Now there are two cases to distinguish. If $n \in \mathbb{N}_0$, then $v_j = 0$ for $j > n$ and $v(x)$ is a polynomial. In this case $u(r)$ is square integrable and hence an eigenfunction corresponding to the eigenvalue $\lambda_n = -(\frac{\gamma}{2(n+l+1)})^2$. Otherwise we have $v_j \geq \frac{(2-\varepsilon)^j}{j!}$ for j sufficiently large. Hence by adding a polynomial to $v(x)$ we can get a function $\tilde{v}(x)$ such that $\tilde{v}_j \geq \frac{(2-\varepsilon)^j}{j!}$ for all j . But then $\tilde{v}(x) \geq \exp((2-\varepsilon)x)$ and thus the corresponding $u(r)$ is not square integrable near $-\infty$. \square

10.5. Nondegeneracy of the ground state

The lowest eigenvalue (below the essential spectrum) of a Schrödinger operator is called **ground state**. Since the laws of physics state that a quantum system will transfer energy to its surroundings (e.g., an atom emits radiation) until it eventually reaches its ground state, this state is in some sense

the most important state. We have seen that the hydrogen atom has a nondegenerate (simple) ground state with a corresponding positive eigenfunction. In particular, the hydrogen atom is stable in the sense that there is a lowest possible energy. This is quite surprising since the corresponding classical mechanical system is not, the electron could fall into the nucleus!

Our aim in this section is to show that the ground state is simple with a corresponding positive eigenfunction. Note that it suffices to show that any ground state eigenfunction is positive since nondegeneracy then follows for free: two positive functions cannot be orthogonal.

To set the stage let us introduce some notation. Let $\mathfrak{H} = L^2(\mathbb{R}^n)$. We call $f \in L^2(\mathbb{R}^n)$ **positive** if $f \geq 0$ a.e. and $f \neq 0$. We call f **strictly positive** if $f > 0$ a.e.. A bounded operator A is called **positivity preserving** if $f \geq 0$ implies $Af \geq 0$ and **positivity improving** if $f \geq 0$ implies $Af > 0$. Clearly A is positivity preserving (improving) if and only if $\langle f, Ag \rangle \geq 0$ (> 0) for $f, g \geq 0$.

Example. Multiplication by a positive function is positivity preserving (but not improving). Convolution with a strictly positive function is positivity improving. \diamond

We first show that positivity improving operators have positive eigenfunctions.

Theorem 10.10. *Suppose $A \in \mathfrak{L}(L^2(\mathbb{R}^n))$ is a self-adjoint, positivity improving and real (i.e., it maps real functions to real functions) operator. If $\|A\|$ is an eigenvalue, then it is simple and the corresponding eigenfunction is strictly positive.*

Proof. Let ψ be an eigenfunction, then it is no restriction to assume that ψ is real (since A is real both real and imaginary part of ψ are eigenfunctions as well). We assume $\|\psi\| = 1$ and denote by $\psi_{\pm} = \frac{f \pm |f|}{2}$ the positive and negative parts of ψ . Then by $|A\psi| = |A\psi_+ - A\psi_-| \leq A\psi_+ + A\psi_- = A|\psi|$ we have

$$\|A\| = \langle \psi, A\psi \rangle \leq \langle |\psi|, |A\psi| \rangle \leq \langle |\psi|, A|\psi| \rangle \leq \|A\|, \quad (10.68)$$

that is, $\langle \psi, A\psi \rangle = \langle |\psi|, A|\psi| \rangle$ and thus

$$\langle \psi_+, A\psi_- \rangle = \frac{1}{4}(\langle |\psi|, A|\psi| \rangle - \langle \psi, A\psi \rangle) = 0. \quad (10.69)$$

Consequently $\psi_- = 0$ or $\psi_+ = 0$ since otherwise $A\psi_- > 0$ and hence also $\langle \psi_+, A\psi_- \rangle > 0$. Without restriction $\psi = \psi_+ \geq 0$ and since A is positivity increasing we even have $\psi = \|A\|^{-1}A\psi > 0$. \square

So we need a positivity improving operator. By (7.42) and (7.43) both E^{-tH_0} , $t > 0$ and $R_{\lambda}(H_0)$, $\lambda < 0$ are since they are given by convolution

with a strictly positive function. Our hope is that this property carries over to $H = H_0 + V$.

Theorem 10.11. *Suppose $H = H_0 + V$ is self-adjoint and bounded from below with $C_c^\infty(\mathbb{R}^n)$ as a core. If $E_0 = \min \sigma(H)$ is an eigenvalue, it is simple and the corresponding eigenfunction is strictly positive.*

Proof. We first show that e^{-tH} , $t > 0$, is positivity preserving. If we set $V_n = V\chi_{\{|x| \leq n\}}$, then V_n is bounded and $H_n = H_0 + V_n$ is positivity preserving by the Trotter product formula since both e^{-tH_0} and e^{-tV} are. Moreover, we have $H_n\psi \rightarrow H\psi$ for $\psi \in C_c^\infty(\mathbb{R}^n)$ (note that necessarily $V \in L_{loc}^2$) and hence $H_n \xrightarrow{sr} H$ in strong resolvent sense by Lemma 6.28. Hence $e^{-tH_n} \xrightarrow{s} e^{-tH}$ by Theorem 6.23, which shows that e^{-tH} is at least positivity preserving (since 0 cannot be an eigenvalue of e^{-tH} it cannot map a positive function to 0).

Next I claim that for ψ positive the closed set

$$N(\psi) = \{\varphi \in L^2(\mathbb{R}^n) \mid \varphi \geq 0, \langle \varphi, e^{-sH}\psi \rangle = 0 \forall s \geq 0\} \quad (10.70)$$

is just $\{0\}$. If $\varphi \in N(\psi)$ we have by $e^{-sH}\psi \geq 0$ that $\varphi e^{-sH}\psi = 0$. Hence $e^{tV_n}\varphi e^{-sH}\psi = 0$, that is $e^{tV_n}\varphi \in N(\psi)$. In other words, both e^{tV_n} and e^{-tH} leave $N(\psi)$ invariant and invoking again Trotter's formula the same is true for

$$e^{-t(H-V_n)} = \text{s-lim}_{k \rightarrow \infty} \left(e^{-\frac{t}{k}H} e^{\frac{t}{k}V_n} \right)^k. \quad (10.71)$$

Since $e^{-t(H-V_n)} \xrightarrow{s} e^{-tH_0}$ we finally obtain that e^{-tH_0} leaves $N(\psi)$ invariant, but this operator is positivity increasing and thus $N(\psi) = \{0\}$.

Now it remains to use (7.41) which shows

$$\langle \varphi, R_H(\lambda)\psi \rangle = \int_0^\infty e^{\lambda t} \langle \varphi, e^{-tH}\psi \rangle dt > 0, \quad \lambda < E_0, \quad (10.72)$$

for φ, ψ positive. So $R_H(\lambda)$ is positivity increasing for $\lambda < E_0$.

If ψ is an eigenfunction of H corresponding to E_0 it is an eigenfunction of $R_H(\lambda)$ corresponding to $\frac{1}{E_0 - \lambda}$ and the claim follows since $\|R_H(\lambda)\| = \frac{1}{E_0 - \lambda}$. \square

Atomic Schrödinger operators

11.1. Self-adjointness

In this section we want to have a look at the Hamiltonian corresponding to more than one interacting particle. It is given by

$$H = -\sum_{j=1}^N \Delta_j + \sum_{j < k}^N V_{j,k}(x_j - x_k). \quad (11.1)$$

We first consider the case of two particles, which will give us a feeling for how the many particle case differs from the one particle case and how the difficulties can be overcome.

We denote the coordinates corresponding to the first particle by $x_1 = (x_{1,1}, x_{1,2}, x_{1,3})$ and those corresponding to the second particle by $x_2 = (x_{2,1}, x_{2,2}, x_{2,3})$. If we assume that the interaction is again of the Coulomb type, the Hamiltonian is given by

$$H = -\Delta_1 - \Delta_2 - \frac{\gamma}{|x_1 - x_2|}, \quad \mathfrak{D}(H) = H^2(\mathbb{R}^6). \quad (11.2)$$

Since Theorem 10.2 does not allow singularities for $n \geq 3$, it does *not* tell us whether H is self-adjoint or not. Let

$$(y_1, y_2) = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbb{I} & \mathbb{I} \\ -\mathbb{I} & \mathbb{I} \end{pmatrix} (x_1, x_2), \quad (11.3)$$

then H reads in this new coordinates

$$H = (-\Delta_1) + \left(-\Delta_2 - \frac{\gamma/\sqrt{2}}{|y_2|}\right). \quad (11.4)$$

In particular, it is the sum of a free particle plus a particle in an external Coulomb field. From a physics point of view, the first part corresponds to the center of mass motion and the second part to the relative motion.

Using that $\gamma/(\sqrt{2}|y_2|)$ has $(-\Delta_2)$ -bound 0 in $L^2(\mathbb{R}^3)$ it is not hard to see that the same is true for the $(-\Delta_1 - \Delta_2)$ -bound in $L^2(\mathbb{R}^6)$ (details will follow in the next section). In particular, H is self-adjoint and semi-bounded for any $\gamma \in \mathbb{R}$. Moreover, you might suspect that $\gamma/(\sqrt{2}|y_2|)$ is relatively compact with respect to $-\Delta_1 - \Delta_2$ in $L^2(\mathbb{R}^6)$ since it is with respect to $-\Delta_2$ in $L^2(\mathbb{R}^3)$. However, this is *not* true! This is due to the fact that $\gamma/(\sqrt{2}|y_2|)$ does not vanish as $|y| \rightarrow \infty$.

Let us look at this problem from the physical view point. If $\lambda \in \sigma_{ess}(H)$, this means that the movement of the whole system is somehow unbounded. There are two possibilities for this.

Firstly, both particles are far away from each other (such that we can neglect the interaction) and the energy corresponds to the sum of the kinetic energies of both particles. Since both can be arbitrarily small (but positive), we expect $[0, \infty) \subseteq \sigma_{ess}(H)$.

Secondly, both particles remain close to each other and move together. In the last coordinates this corresponds to a bound state of the second operator. Hence we expect $[\lambda_0, \infty) \subseteq \sigma_{ess}(H)$, where $\lambda_0 = -\gamma^2/8$ is the smallest eigenvalue of the second operator if the forces are attracting ($\gamma \geq 0$) and $\lambda_0 = 0$ if they are repelling ($\gamma \leq 0$).

It is not hard to translate this intuitive ideas into a rigorous proof. Let $\psi_1(y_1)$ be a Weyl sequence corresponding to $\lambda \in [0, \infty)$ for $-\Delta_1$ and $\psi_2(y_2)$ be a Weyl sequence corresponding to λ_0 for $-\Delta_2 - \gamma/(\sqrt{2}|y_2|)$. Then, $\psi_1(y_1)\psi_2(y_2)$ is a Weyl sequence corresponding to $\lambda + \lambda_0$ for H and thus $[\lambda_0, \infty) \subseteq \sigma_{ess}(H)$. Conversely, we have $-\Delta_1 \geq 0$ respectively $-\Delta_2 - \gamma/(\sqrt{2}|y_2|) \geq \lambda_0$ and hence $H \geq \lambda_0$. Thus we obtain

$$\sigma(H) = \sigma_{ess}(H) = [\lambda_0, \infty), \quad \lambda_0 = \begin{cases} -\gamma^2/8, & \gamma \geq 0 \\ 0, & \gamma \leq 0 \end{cases}. \quad (11.5)$$

Clearly, the physically relevant information is the spectrum of the operator $-\Delta_2 - \gamma/(\sqrt{2}|y_2|)$ which is hidden by the spectrum of $-\Delta_1$. Hence, in order to reveal the physics, one first has to *remove* the center of mass motion.

To avoid clumsy notation, we will restrict ourselves to the case of one atom with N electrons whose nucleus is fixed at the origin. In particular, this implies that we do not have to deal with the center of mass motion

encountered in our example above. The Hamiltonian is given by

$$\begin{aligned} H^{(N)} &= -\sum_{j=1}^N \Delta_j - \sum_{j=1}^N V_{ne}(x_j) + \sum_{j=1}^N \sum_{j < k}^N V_{ee}(x_j - x_k), \\ \mathfrak{D}(H^{(N)}) &= H^2(\mathbb{R}^{3N}), \end{aligned} \quad (11.6)$$

where V_{ne} describes the interaction of one electron with the nucleus and V_{ee} describes the interaction of two electrons. Explicitly we have

$$V_j(x) = \frac{\gamma_j}{|x|}, \quad \gamma_j > 0, \quad j = ne, ee. \quad (11.7)$$

We first need to establish self-adjointness of $H^{(N)}$. This will follow from Kato's theorem.

Theorem 11.1 (Kato). *Let $V_k \in L^\infty(\mathbb{R}^d) + L^2(\mathbb{R}^d)$, $d \leq 3$, be real-valued and let $V_k(y^{(k)})$ be the multiplication operator in $L^2(\mathbb{R}^n)$, $n = Nd$, obtained by letting $y^{(k)}$ be the first d coordinates of a unitary transform of \mathbb{R}^n . Then V_k is H_0 bounded with H_0 -bound 0. In particular,*

$$H = H_0 + \sum_k V_k(y^{(k)}), \quad \mathfrak{D}(H) = H^2(\mathbb{R}^n), \quad (11.8)$$

is self-adjoint and $C_0^\infty(\mathbb{R}^n)$ is a core.

Proof. It suffices to consider one k . After a unitary transform of \mathbb{R}^n we can assume $y^{(1)} = (x_1, \dots, x_d)$ since such transformations leave both the scalar product of $L^2(\mathbb{R}^n)$ and H_0 invariant. Now let $\psi \in \mathcal{S}(\mathbb{R}^n)$, then

$$\|V_k \psi\|^2 \leq a^2 \int_{\mathbb{R}^n} |\Delta_1 \psi(x)|^2 d^n x + b^2 \int_{\mathbb{R}^n} |\psi(x)|^2 d^n x, \quad (11.9)$$

where $\Delta_1 = \sum_{j=1}^d \partial^2 / \partial^2 x_j$, by our previous lemma. Hence we obtain

$$\begin{aligned} \|V_k \psi\|^2 &\leq a^2 \int_{\mathbb{R}^n} \left| \sum_{j=1}^d p_j^2 \hat{\psi}(p) \right|^2 d^n p + b^2 \|\psi\|^2 \\ &\leq a^2 \int_{\mathbb{R}^n} \left| \sum_{j=1}^n p_j^2 \hat{\psi}(p) \right|^2 d^n p + b^2 \|\psi\|^2 \\ &= a^2 \|H_0 \psi\|^2 + b^2 \|\psi\|^2, \end{aligned} \quad (11.10)$$

which implies that V_k is relatively bounded with bound 0. \square

11.2. The HVZ theorem

The considerations of the beginning of this section show that it is not so easy to determine the essential spectrum of $H^{(N)}$ since the potential does not decay in all directions as $|x| \rightarrow \infty$. However, there is still something we

can do. Denote the infimum of the spectrum of $H^{(N)}$ by λ^N . Then, let us split the system into $H^{(N-1)}$ plus a single electron. If the single electron is far away from the remaining system such that there is little interaction, the energy should be the sum of the kinetic energy of the single electron and the energy of the remaining system. Hence arguing as in the two electron example of the previous section we expect

Theorem 11.2 (HVZ). *Let $H^{(N)}$ be the self-adjoint operator given in (11.6). Then $H^{(N)}$ is bounded from below and*

$$\sigma_{ess}(H^{(N)}) = [\lambda^{N-1}, \infty), \quad (11.11)$$

where $\lambda^{N-1} = \min \sigma(H^{(N-1)}) < 0$.

In particular, the ionization energy (i.e., the energy needed to remove one electron from the atom in its ground state) of an atom with N electrons is given by $\lambda^N - \lambda^{N-1}$.

Our goal for the rest of this section is to prove this result which is due to Zhislin, van Winter and Hunziker and known as HVZ theorem. In fact there is a version which holds for general N -body systems. The proof is similar but involves some additional notation.

The idea of proof is the following. To prove $[\lambda^{N-1}, \infty) \subseteq \sigma_{ess}(H^{(N)})$ we choose Weyl sequences for $H^{(N-1)}$ and $-\Delta_N$ and proceed according to our intuitive picture from above. To prove $\sigma_{ess}(H^{(N)}) \subseteq [\lambda^{N-1}, \infty)$ we will *localize* $H^{(N)}$ on sets where either one electron is far away from the others or all electrons are far away from the nucleus. Since the error turns out relatively compact, it remains to consider the infimum of the spectra of these operators. For all cases where one electron is far away it is λ^{N-1} and for the case where all electrons are far away from the nucleus it is 0 (since the electrons repel each other).

We begin with the first inclusion. Let $\psi^{N-1}(x_1, \dots, x_{N-1}) \in H^2(\mathbb{R}^{3(N-1)})$ such that $\|\psi^{N-1}\| = 1$, $\|(H^{(N-1)} - \lambda^{N-1})\psi^{N-1}\| \leq \varepsilon$ and $\psi^1 \in H^2(\mathbb{R}^3)$ such that $\|\psi^1\| = 1$, $\|(-\Delta_N - \lambda)\psi^1\| \leq \varepsilon$ for some $\lambda \geq 0$. Now consider $\psi_r(x_1, \dots, x_N) = \psi^{N-1}(x_1, \dots, x_{N-1})\psi_r^1(x_N)$, $\psi_r^1(x_N) = \psi^1(x_N - r)$, then

$$\begin{aligned} \|(H^{(N)} - \lambda - \lambda^{N-1})\psi_r\| &\leq \|(H^{(N-1)} - \lambda^{N-1})\psi^{N-1}\| \|\psi_r^1\| \\ &\quad + \|\psi^{N-1}\| \|(-\Delta_N - \lambda)\psi_r^1\| \\ &\quad + \|(V_N - \sum_{j=1}^{N-1} V_{N,j})\psi_r\|, \end{aligned} \quad (11.12)$$

where $V_N = V_{ne}(x_N)$ and $V_{N,j} = V_{ee}(x_N - x_j)$. Since $(V_N - \sum_{j=1}^{N-1} V_{N,j})\psi^{N-1} \in L^2(\mathbb{R}^{3N})$ and $|\psi_r^1| \rightarrow 0$ pointwise as $|r| \rightarrow \infty$ (by Lemma 10.1), the third

term can be made smaller than ε by choosing $|r|$ large (dominated convergence). In summary,

$$\|(H^{(N)} - \lambda - \lambda^{N-1})\psi_r\| \leq 3\varepsilon \quad (11.13)$$

proving $[\lambda^{N-1}, \infty) \subseteq \sigma_{\text{ess}}(H^{(N)})$.

The second inclusion is more involved. We begin with a **localization formula**, which can be verified by a straightforward computation

Lemma 11.3 (IMS localization formula). *Suppose $\phi_j \in C^\infty(\mathbb{R}^n)$, $0 \leq j \leq N$, is such that*

$$\sum_{j=0}^N \phi_j(x)^2 = 1, \quad x \in \mathbb{R}^n, \quad (11.14)$$

then

$$\Delta\psi = \sum_{j=0}^N \phi_j \Delta\phi_j \psi - |\partial\phi_j|^2 \psi, \quad \psi \in H^2(\mathbb{R}^n). \quad (11.15)$$

Abbreviate $B = \{x \in \mathbb{R}^{3N} \mid |x| \geq 1\}$. Now we will choose ϕ_j , $1 \leq j \leq N$, in such a way that $x \in \text{supp}(\phi_j) \cap B$ implies that the j -th particle is far away from all the others and from the nucleus. Similarly, we will choose ϕ_0 in such a way that $x \in \text{supp}(\phi_0) \cap B$ implies that all particle are far away from the nucleus.

Lemma 11.4. *There exists functions $\phi_j \in C^\infty(\mathbb{R}^n, [0, 1])$, $0 \leq j \leq N$, is such that (11.14) holds,*

$$\begin{aligned} \text{supp}(\phi_j) \cap B &\subseteq \{x \in B \mid |x_j - x_\ell| \geq C|x| \text{ for all } \ell \neq j, \text{ and } |x_j| \geq C|x|\}, \\ \text{supp}(\phi_0) \cap B &\subseteq \{x \in B \mid |x_\ell| \geq C|x| \text{ for all } \ell\} \end{aligned} \quad (11.16)$$

for some $C \in [0, 1]$, and $|\partial\phi_j(x)| \rightarrow 0$ as $|x| \rightarrow \infty$.

Proof. Consider the sets

$$\begin{aligned} U_j^n &= \{x \in S^{3N-1} \mid |x_j - x_\ell| > n^{-1} \text{ for all } \ell \neq j, \text{ and } |x_j| > n^{-1}\}, \\ U_0^n &= \{x \in S^{3N-1} \mid |x_\ell| > n^{-1} \text{ for all } \ell\}. \end{aligned} \quad (11.17)$$

We claim that

$$\bigcup_{n=1}^{\infty} \bigcup_{j=0}^N U_j^n = S^{3N-1}. \quad (11.18)$$

Indeed, suppose there is an $x \in S^{3N-1}$ which is not an element of this union. Then $x \notin U_0^n$ for all n implies $0 = |x_j|$ for some j , say $j = 1$. Next, since $x \notin U_1^n$ for all n implies $0 = |x_j - x_1| = |x_j|$ for some $j > 1$, say $j = 2$.

Proceeding like this we end up with $x = 0$, a contradiction. By compactness of S^{3N-1} we even have

$$\bigcup_{j=0}^N U_j^n = S^{3N-1} \quad (11.19)$$

for n sufficiently large. It is well-known that there is a partition of unity $\tilde{\phi}_j(x)$ subordinate to this cover. Extend $\tilde{\phi}_j(x)$ to a smooth function from $\mathbb{R}^{3N} \setminus \{0\}$ to $[0, 1]$ by

$$\tilde{\phi}_j(\lambda x) = \tilde{\phi}_j(x), \quad x \in S^{3N-1}, \lambda > 0, \quad (11.20)$$

and pick a function $\tilde{\phi} \in C^\infty(\mathbb{R}^{3N}, [0, 1])$ with support inside the unit ball which is 1 in a neighborhood of the origin. Then

$$\phi_j = \frac{\tilde{\phi} + (1 - \tilde{\phi})\tilde{\phi}_j}{\sqrt{\sum_{\ell=0}^N \tilde{\phi} + (1 - \tilde{\phi})\tilde{\phi}_\ell}} \quad (11.21)$$

are the desired functions. The gradient tends to zero since $\phi_j(\lambda x) = \phi_j(x)$ for $\lambda \geq 1$ and $|x| \geq 1$ which implies $(\partial\phi_j)(\lambda x) = \lambda^{-1}(\partial\phi_j)(x)$. \square

By our localization formula we have

$$H^{(N)} = \sum_{j=0}^N \phi_j H^{(N,j)} \phi_j + K, \quad K = \sum_{j=0}^N \phi_j^2 V^{(N,j)} + |\partial\phi_j|^2, \quad (11.22)$$

where

$$\begin{aligned} H^{(N,j)} &= -\sum_{\ell=1}^N \Delta_\ell - \sum_{\ell \neq j}^N V_\ell + \sum_{k < \ell, k, \ell \neq j}^N V_{k,\ell}, & H^{(N,0)} &= -\sum_{\ell=1}^N \Delta_\ell + \sum_{k < \ell}^N V_{k,\ell} \\ V^{(N,j)} &= V_j + \sum_{\ell \neq j}^N V_{j,\ell}, & V^{(N,0)} &= \sum_{\ell=1}^N V_\ell \end{aligned} \quad (11.23)$$

To show that our choice of the functions ϕ_j implies that K is relatively compact with respect to H we need the following

Lemma 11.5. *Let V be H_0 bounded with H_0 -bound 0 and suppose that $\|\chi_{\{|x| \geq R\}} V R_{H_0}(z)\| \rightarrow 0$ as $R \rightarrow \infty$. Then V is relatively compact with respect to H_0 .*

Proof. Let ψ_n converge to 0 weakly. Note that $\|\psi_n\| \leq M$ for some $M > 0$. It suffices to show that $\|V R_{H_0}(z) \psi_n\|$ converges to 0. Choose $\phi \in C_0^\infty(\mathbb{R}^n, [0, 1])$ such that it is one for $|x| \leq R$. Then

$$\begin{aligned} \|V R_{H_0}(z) \psi_n\| &\leq \|(1 - \phi) V R_{H_0}(z) \psi_n\| + \|\phi V R_{H_0}(z) \psi_n\| \\ &\leq \|(1 - \phi) V R_{H_0}(z)\|_\infty \|\psi_n\| + \\ &\quad a \|H_0 \phi R_{H_0}(z) \psi_n\| + b \|\phi R_{H_0}(z) \psi_n\|. \end{aligned} \quad (11.24)$$

By assumption, the first term can be made smaller than ε by choosing R large. Next, the same is true for the second term choosing a small. Finally, the last term can also be made smaller than ε by choosing n large since ϕ is H_0 compact. \square

The terms $|\partial\phi_j|^2$ are bounded and vanish at ∞ , hence they are H_0 compact by Lemma 7.10. The terms $\phi_j V^{(N,j)}$ are relatively compact by the lemma and hence K is relatively compact with respect to H_0 . By Lemma 6.22, K is also relatively compact with respect to $H^{(N)}$ since $V^{(N)}$ is relatively bounded with respect to H_0 .

In particular $H^{(N)} - K$ is self-adjoint on $H^2(\mathbb{R}^{3N})$ and $\sigma_{ess}(H^{(N)}) = \sigma_{ess}(H^{(N)} - K)$. Since the operators $H^{(N,j)}$, $1 \leq j \leq N$, are all of the form $H^{(N-1)}$ plus one particle which does not interact with the others and the nucleus, we have $H^{(N,j)} - \lambda^{N-1} \geq 0$, $1 \leq j \leq N$. Moreover, we have $H^{(0)} \geq 0$ since $V_{j,k} \geq 0$ and hence

$$\langle \psi, (H^{(N)} - K - \lambda^{N-1})\psi \rangle = \sum_{j=0}^N \langle \phi_j \psi, (H^{(N,j)} - \lambda^{N-1})\phi_j \psi \rangle \geq 0. \quad (11.25)$$

Thus we obtain the remaining inclusion

$$\sigma_{ess}(H^{(N)}) = \sigma_{ess}(H^{(N)} - K) \subseteq \sigma(H^{(N)} - K) \subseteq [\lambda^{N-1}, \infty) \quad (11.26)$$

which finishes the proof of the HVZ theorem.

Note that the same proof works if we add additional nuclei at fixed locations. That is, we can also treat molecules if we assume that the nuclei are fixed in space.

Finally, let us consider the example of Helium like atoms ($N = 2$). By the HVZ theorem and the considerations of the previous section we have

$$\sigma_{ess}(H^{(2)}) = [-\frac{\gamma_{ne}^2}{4}, \infty). \quad (11.27)$$

Moreover, if $\gamma_{ee} = 0$ (no electron interaction), we can take products of one particle eigenfunctions to show that

$$-\gamma_{ne}^2 \left(\frac{1}{4n^2} + \frac{1}{4m^2} \right) \in \sigma_p(H^{(2)}(\gamma_{ee} = 0)), \quad n, m \in \mathbb{N}. \quad (11.28)$$

In particular, there are eigenvalues embedded in the essential spectrum in this case. Moreover, since the electron interaction term is positive, we see

$$H^{(2)} \geq -\frac{\gamma_{ne}^2}{2}. \quad (11.29)$$

Note that there can be no positive eigenvalues by the virial theorem. This even holds for arbitrary N ,

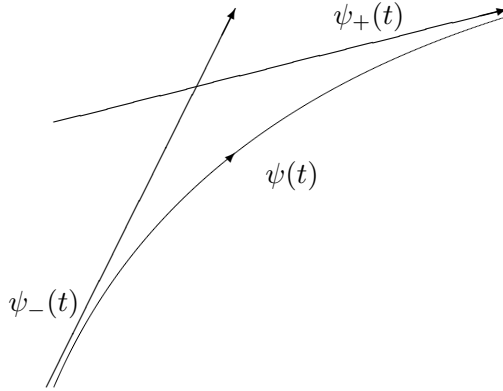
$$\sigma_p(H^{(N)}) \subset (-\infty, 0). \quad (11.30)$$

Scattering theory

12.1. Abstract theory

In physical measurements one often has the following situation. A particle is shot into a region where it interacts with some forces and then leaves the region again. Outside this region the forces are negligible and hence the time evolution should be asymptotically free. Hence one expects asymptotic states $\psi_{\pm}(t) = \exp(-itH_0)\psi_{\pm}(0)$ to exist such that

$$\|\psi(t) - \psi_{\pm}(t)\| \rightarrow 0 \quad \text{as } t \rightarrow \pm\infty. \quad (12.1)$$



Rewriting this condition we see

$$0 = \lim_{t \rightarrow \pm\infty} \|e^{-itH}\psi(0) - e^{-itH_0}\psi_{\pm}(0)\| = \lim_{t \rightarrow \pm\infty} \|\psi(0) - e^{itH}e^{-itH_0}\psi_{\pm}(0)\| \quad (12.2)$$

and motivated by this we define the **wave operators** by

$$\begin{aligned} \mathfrak{D}(\Omega_{\pm}) &= \{\psi \in \mathfrak{H} | \exists \lim_{t \rightarrow \pm\infty} e^{itH}e^{-itH_0}\psi\} \\ \Omega_{\pm}\psi &= \lim_{t \rightarrow \pm\infty} e^{itH}e^{-itH_0}\psi \end{aligned} \quad (12.3)$$

The set $\mathfrak{D}(\Omega_{\pm})$ is the set of all incoming/outgoing asymptotic states ψ_{\pm} and $\text{Ran}(\Omega_{\pm})$ is the set of all states which have an incoming/outgoing asymptotic state. If a state ψ has both, that is, $\psi \in \text{Ran}(\Omega_{+}) \cap \text{Ran}(\Omega_{-})$, it is called a **scattering state**.

By construction we have

$$\|\Omega_{\pm}\psi\| = \lim_{t \rightarrow \pm\infty} \|e^{itH}e^{-itH_0}\psi\| = \lim_{t \rightarrow \pm\infty} \|\psi\| = \|\psi\| \quad (12.4)$$

and it is not hard to see that $\mathfrak{D}(\Omega_{\pm})$ is closed. Moreover, interchanging the roles of H_0 and H amounts to replacing Ω_{\pm} by Ω_{\pm}^{-1} and hence $\text{Ran}(\Omega_{\pm})$ is also closed. In summary,

Lemma 12.1. *The sets $\mathfrak{D}(\Omega_{\pm})$ and $\text{Ran}(\Omega_{\pm})$ are closed and $\Omega_{\pm} : \mathfrak{D}(\Omega_{\pm}) \rightarrow \text{Ran}(\Omega_{\pm})$ is unitary.*

Next, observe that

$$\lim_{t \rightarrow \pm\infty} e^{itH}e^{-itH_0}(e^{-isH_0}\psi) = \lim_{t \rightarrow \pm\infty} e^{-isH}(e^{i(t+s)H}e^{-i(t+s)H_0}\psi) \quad (12.5)$$

and hence

$$\Omega_{\pm}e^{-itH_0}\psi = e^{-itH}\Omega_{\pm}\psi, \quad \psi \in \mathfrak{D}(\Omega_{\pm}). \quad (12.6)$$

In addition, $\mathfrak{D}(\Omega_{\pm})$ is invariant under $\exp(-itH_0)$ and $\text{Ran}(\Omega_{\pm})$ is invariant under $\exp(-itH)$. Moreover, if $\psi \in \mathfrak{D}(\Omega_{\pm})^{\perp}$ then

$$\langle \varphi, \exp(-itH_0)\psi \rangle = \langle \exp(itH_0)\varphi, \psi \rangle = 0, \quad \varphi \in \mathfrak{D}(\Omega_{\pm}). \quad (12.7)$$

Hence $\mathfrak{D}(\Omega_{\pm})^{\perp}$ is invariant under $\exp(-itH_0)$ and $\text{Ran}(\Omega_{\pm})^{\perp}$ is invariant under $\exp(-itH)$. Consequently, $\mathfrak{D}(\Omega_{\pm})$ reduces $\exp(-itH_0)$ and $\text{Ran}(\Omega_{\pm})$ reduces $\exp(-itH)$. Moreover, differentiating (12.6) with respect to t we obtain from Theorem 5.1 the **intertwining property** of the wave operators.

Theorem 12.2. *The subspaces $\mathfrak{D}(\Omega_{\pm})$ respectively $\text{Ran}(\Omega_{\pm})$ reduce H_0 respectively H and the operators restricted to these subspaces are unitarily equivalent*

$$\Omega_{\pm}H_0\psi = H\Omega_{\pm}\psi, \quad \psi \in \mathfrak{D}(\Omega_{\pm}) \cap \mathfrak{D}(H_0). \quad (12.8)$$

It is interesting to know the correspondence between incoming and outgoing states. Hence we define the **scattering operator**

$$S = \Omega_{+}^{-1}\Omega_{-}, \quad \mathfrak{D}(S) = \{\psi \in \mathfrak{D}(\Omega_{-}) \mid \Omega_{-}\psi \in \text{Ran}(\Omega_{+})\}. \quad (12.9)$$

Note that we have $\mathfrak{D}(S) = \mathfrak{D}(\Omega_{-})$ if and only if $\text{Ran}(\Omega_{-}) \subseteq \text{Ran}(\Omega_{+})$ and $\text{Ran}(S) = \mathfrak{D}(\Omega_{+})$ if and only if $\text{Ran}(\Omega_{+}) \subseteq \text{Ran}(\Omega_{-})$. Moreover, S is unitary from $\mathfrak{D}(S)$ onto $\text{Ran}(S)$ and we have

$$H_0S\psi = SH_0\psi, \quad \mathfrak{D}(H_0) \cap \mathfrak{D}(S). \quad (12.10)$$

However, note that this whole theory is meaningless until we can show that $\mathfrak{D}(\Omega_{\pm})$ are nontrivial. We first show a criterion due to Cook.

Lemma 12.3 (Cook). *Suppose $\mathfrak{D}(H) \subseteq \mathfrak{D}(H_0)$. If*

$$\int_0^\infty \|(H - H_0) \exp(\mp itH_0)\psi\| dt < \infty, \quad \psi \in \mathfrak{D}(H_0), \quad (12.11)$$

then $\psi \in \mathfrak{D}(\Omega_\pm)$, respectively. Moreover, we even have

$$\|(\Omega_\pm - \mathbb{I})\psi\| \leq \int_0^\infty \|(H - H_0) \exp(\mp itH_0)\psi\| dt \quad (12.12)$$

in this case.

Proof. The result follows from

$$e^{itH} e^{-itH_0} \psi = \psi + i \int_0^t \exp(isH)(H - H_0) \exp(-isH_0) \psi ds \quad (12.13)$$

which holds for $\psi \in \mathfrak{D}(H_0)$. \square

As a simple consequence we obtain the following result for Schrödinger operators in \mathbb{R}^3

Theorem 12.4. *Suppose H_0 is the free Schrödinger operator and $H = H_0 + V$ with $V \in L^2(\mathbb{R}^3)$, then the wave operators exist and $\mathfrak{D}(\Omega_\pm) = \mathfrak{H}$.*

Proof. Since we want to use Cook's lemma, we need to estimate

$$\|V\psi(s)\|^2 = \int_{\mathbb{R}^3} |V(x)\psi(s, x)|^2 dx, \quad \psi(s) = \exp(isH_0)\psi, \quad (12.14)$$

for given $\psi \in \mathfrak{D}(H_0)$. Invoking (7.34) we get

$$\|V\psi(s)\| \leq \|\psi(s)\|_\infty \|V\| \leq \frac{1}{(4\pi s)^{3/2}} \|\psi\|_1 \|V\|, \quad s > 0, \quad (12.15)$$

at least for $\psi \in L^1(\mathbb{R}^3)$. Moreover, this implies

$$\int_1^\infty \|V\psi(s)\| ds \leq \frac{1}{4\pi^{3/2}} \|\psi\|_1 \|V\| \quad (12.16)$$

and thus any such ψ is in $\mathfrak{D}(\Omega_+)$. Since such functions are dense, we obtain $\mathfrak{D}(\Omega_+) = \mathfrak{H}$. Similarly for Ω_- . \square

By the intertwining property ψ is an eigenfunction of H_0 if and only if it is an eigenfunction of H . Hence for $\psi \in \mathfrak{H}_{pp}(H_0)$ it is easy to check whether it is in $\mathfrak{D}(\Omega_\pm)$ or not and only the continuous subspace is of interest. We will say that the **wave operators exist** if all elements of $\mathfrak{H}_{ac}(H_0)$ are asymptotic states, that is,

$$\mathfrak{H}_{ac}(H_0) \subseteq \mathfrak{D}(\Omega_\pm) \quad (12.17)$$

and that they are **complete** if, in addition, all elements of $\mathfrak{H}_{ac}(H)$ are scattering states, that is,

$$\mathfrak{H}_{ac}(H) \subseteq \text{Ran}(\Omega_\pm). \quad (12.18)$$

If we even have

$$\mathfrak{H}_c(H) \subseteq \text{Ran}(\Omega_\pm), \quad (12.19)$$

they are called **asymptotically complete**. We will be mainly interested in the case where H_0 is the free Schrödinger operator and hence $\mathfrak{H}_{ac}(H_0) = \mathfrak{H}$. In this later case the wave operators exist if $\mathfrak{D}(\Omega_\pm) = \mathfrak{H}$, they are complete if $\mathfrak{H}_{ac}(H) = \text{Ran}(\Omega_\pm)$, and asymptotically complete if $\mathfrak{H}_c(H) = \text{Ran}(\Omega_\pm)$. In particular asymptotic completeness implies $\mathfrak{H}_{sc}(H) = \emptyset$ since H restricted to $\text{Ran}(\Omega_\pm)$ is unitarily equivalent to H_0 .

12.2. Incoming and outgoing states

In the remaining sections we want to apply this theory to Schrödinger operators. Our first goal is to give a precise meaning to some terms in the intuitive picture of scattering theory introduced in the previous section.

This physical picture suggests that we should be able to decompose $\psi \in \mathfrak{H}$ into an incoming and an outgoing part. But how should incoming respectively outgoing be defined for $\psi \in \mathfrak{H}$? Well incoming (outgoing) means that the expectation of x^2 should decrease (increase). Set $x(t)^2 = \exp(iH_0 t)x^2 \exp(-iH_0 t)$, then, abbreviating $\psi(t) = e^{-itH_0}\psi$,

$$\frac{d}{dt} \mathbb{E}_\psi(x(t)^2) = \langle \psi(t), i[H_0, x^2]\psi(t) \rangle = 4\langle \psi(t), D\psi(t) \rangle, \quad \psi \in \mathcal{S}(\mathbb{R}^n), \quad (12.20)$$

where D is the dilation operator introduced in (10.11). Hence it is natural to consider $\psi \in \text{Ran}(P_\pm)$,

$$P_\pm = P_D((0, \pm\infty)), \quad (12.21)$$

as outgoing respectively incoming states. If we project a state in $\text{Ran}(P_\pm)$ to energies in the interval (a^2, b^2) , we expect that it cannot be found in a ball of radius proportional to $a|t|$ as $t \rightarrow \pm\infty$ (a is the minimal velocity of the particle, since we have assumed the mass to be two). In fact, we will show below that the tail decays faster than any inverse power of $|t|$.

We first collect some properties of D which will be needed later on. Note

$$\mathcal{F}D = -D\mathcal{F} \quad (12.22)$$

and hence $\mathcal{F}f(D) = f(-D)\mathcal{F}$. To say more we will look for a transformation which maps D to a multiplication operator.

Since the dilation group acts on $|x|$ only, it seems reasonable to switch to polar coordinates $x = r\omega$, $(t, \omega) \in \mathbb{R}^+ \times S^{n-1}$. Since $U(s)$ essentially transforms r into $r \exp(s)$ we will replace r by $\rho = \ln(r)$. In these coordinates we have

$$U(s)\psi(e^\rho\omega) = e^{-ns/2}\psi(e^{\rho-s}\omega) \quad (12.23)$$

and hence $U(s)$ corresponds to a shift of ρ (the constant in front is absorbed by the volume element). Thus D corresponds to differentiation with respect to this coordinate and all we have to do to make it a multiplication operator is to take the Fourier transform with respect to ρ .

This leads us to the **Mellin transform**

$$\begin{aligned} \mathcal{M} : L^2(\mathbb{R}^n) &\rightarrow L^2(\mathbb{R} \times S^{n-1}) \\ \psi(r\omega) &\rightarrow (\mathcal{M}\psi)(\lambda, \omega) = \frac{1}{\sqrt{2\pi}} \int_0^\infty r^{-i\lambda} \psi(r\omega) r^{\frac{n}{2}-1} dr \end{aligned} \quad (12.24)$$

By construction, \mathcal{M} is unitary, that is,

$$\int_{\mathbb{R}} \int_{S^{n-1}} |(\mathcal{M}\psi)(\lambda, \omega)|^2 d\lambda d^{n-1}\omega = \int_{\mathbb{R}^+} \int_{S^{n-1}} |\psi(r\omega)|^2 r^{n-1} dr d^{n-1}\omega, \quad (12.25)$$

where $d^{n-1}\omega$ is the normalized surface measure on S^{n-1} . Moreover,

$$\mathcal{M}^{-1}U(s)\mathcal{M} = e^{-is\lambda} \quad (12.26)$$

and hence

$$\mathcal{M}^{-1}D\mathcal{M} = \lambda. \quad (12.27)$$

From this it is straightforward to show that

$$\sigma(D) = \sigma_{ac}(D) = \mathbb{R}, \quad \sigma_{sc}(D) = \sigma_{pp}(D) = \emptyset \quad (12.28)$$

and that $\mathcal{S}(\mathbb{R}^n)$ is a core for D . In particular we have $P_+ + P_- = \mathbb{I}$.

Using the Mellin transform we can now prove Perry's estimate [11].

Lemma 12.5. *Suppose $f \in C_c^\infty(\mathbb{R})$ with $\text{supp}(f) \subset (a^2, b^2)$ for some $a, b > 0$. For any $R \in \mathbb{R}$, $N \in \mathbb{N}$ there is a constant C such that*

$$\|\chi_{\{|x| < 2a|t|\}} e^{-itH_0} f(H_0) P_D((\pm R, \pm\infty))\| \leq \frac{C}{(1 + |t|)^N}, \quad \pm t \geq 0, \quad (12.29)$$

respectively.

Proof. We prove only the + case, the remaining one being similar. Consider $\psi \in \mathcal{S}(\mathbb{R}^n)$. Introducing

$$\begin{aligned} \psi(t, x) &= e^{-itH_0} f(H_0) P_D((R, \infty)) \psi(x) = \langle K_{t,x}, \mathcal{F}P_D((R, \infty)) \psi \rangle \\ &= \langle K_{t,x}, P_D((-\infty, -R)) \hat{\psi} \rangle, \end{aligned} \quad (12.30)$$

where

$$K_{t,x}(p) = \frac{1}{(2\pi)^{n/2}} e^{i(tp^2 - px)} f(p^2)^*, \quad (12.31)$$

we see that it suffices to show

$$\|P_D((-\infty, -R)) K_{t,x}\|^2 \leq \frac{\text{const}}{(1 + |t|)^{2N}}, \quad \text{for } |x| < 2a|t|, t > 0. \quad (12.32)$$

Now we invoke the Mellin transform to estimate this norm

$$\|P_D((-\infty, -R))K_{t,x}\|^2 = \int_{-\infty}^R \int_{S^{n-1}} |(\mathcal{M}K_{t,x})(\lambda, \omega)|^2 d\lambda d^{n-1}\omega. \quad (12.33)$$

Since

$$(\mathcal{M}K_{t,x})(\lambda, \omega) = \frac{1}{(2\pi)^{(n+1)/2}} \int_0^\infty \tilde{f}(r) e^{i\alpha(r)} dr \quad (12.34)$$

with $\tilde{f}(r) = f(r^2) * r^{n/2-1} \in C_c^\infty((a^2, b^2))$, $\alpha(r) = tr^2 + r\omega x - \lambda \ln(r)$. Estimating the derivative of α we see

$$\alpha'(r) = 2tr + \omega x - \lambda/r > 0, \quad r \in (a, b), \quad (12.35)$$

for $\lambda \leq -R$ and $t > R(2\varepsilon a)^{-1}$, where ε is the distance of a to the support of \tilde{f} . Hence we can find a constant such that

$$\frac{1}{|\alpha'(r)|} \leq \frac{\text{const}}{1 + |\lambda| + |t|}, \quad r \in (a, b), \quad (12.36)$$

and λ, t as above. Using this we can estimate the integral in (12.34)

$$\left| \int_0^\infty \tilde{f}(r) \frac{1}{\alpha'(r)} \frac{d}{dr} e^{i\alpha(r)} dr \right| \leq \frac{\text{const}}{1 + |\lambda| + |t|} \left| \int_0^\infty \tilde{f}'(r) e^{i\alpha(r)} dr \right|, \quad (12.37)$$

(the last step uses integration by parts) for λ, t as above. By increasing the constant we can even assume that it holds for $t \geq 0$ and $\lambda \leq -R$. Moreover, by iterating the last estimate we see

$$|(\mathcal{M}K_{t,x})(\lambda, \omega)| \leq \frac{\text{const}}{(1 + |\lambda| + |t|)^N} \quad (12.38)$$

for any $N \in \mathbb{N}$ and $t \geq 0$ and $\lambda \leq -R$. This finishes the proof. \square

Corollary 12.6. *Suppose that $f \in C_c^\infty((0, \infty))$ and $R \in \mathbb{R}$. Then the operator $P_D((\pm R, \pm\infty))f(H_0) \exp(-itH_0)$ converges strongly to 0 as $t \rightarrow \mp\infty$.*

Proof. Abbreviating $P_D = P_D((\pm R, \pm\infty))$ and $\chi = \chi_{\{|x| < 2a|t|\}}$ we have

$$\|P_D f(H_0) e^{-itH_0} \psi\| \leq \|\chi e^{itH_0} f(H_0) * P_D\| \|\psi\| + \|f(H_0)\| \|(\mathbb{I} - \chi)\psi\|. \quad (12.39)$$

since $\|A\| = \|A^*\|$. Taking $t \rightarrow \mp\infty$ the first term goes to zero by our lemma and the second goes to zero since $\chi\psi \rightarrow \psi$. \square

12.3. Schrödinger operators with short range potentials

By the RAGE theorem we know that for $\psi \in \mathfrak{H}_c$, $\psi(t)$ will eventually leave every compact ball (at least on the average). Hence we expect that the time evolution will asymptotically look like the free one for $\psi \in \mathfrak{H}_c$ if the potential decays sufficiently fast. In other words, we expect such potentials to be asymptotically complete.

Suppose V is relatively bounded with bound less than one. Introduce

$$h_1(r) = \|VR_{H_0}(z)\chi_r\|, \quad h_2(r) = \|\chi_rVR_{H_0}(z)\|, \quad r \geq 0, \quad (12.40)$$

where

$$\chi_r = \chi_{\{|x| \geq r\}}. \quad (12.41)$$

The potential V will be called **short range** if these quantities are integrable. We first note that it suffices to check this for h_1 or h_2 and for one $z \in \rho(H_0)$.

Lemma 12.7. *The function h_1 is integrable if and only if h_2 is. Moreover, h_j integrable for one $z_0 \in \rho(H_0)$ implies h_j integrable for all $z \in \rho(H_0)$.*

Proof. Pick $\phi \in C_c^\infty(\mathbb{R}^n, [0, 1])$ such that $\phi(x) = 0$ for $0 \leq |x| \leq 1/2$ and $\phi(x) = 0$ for $1 \leq |x|$. Then it is not hard to see that h_j is integrable if and only if \tilde{h}_j is integrable, where

$$\tilde{h}_1(r) = \|VR_{H_0}(z)\phi_r\|, \quad \tilde{h}_2(r) = \|\phi_rVR_{H_0}(z)\|, \quad r \geq 1, \quad (12.42)$$

and $\phi_r(x) = \phi(x/r)$. Using

$$\begin{aligned} [R_{H_0}(z), \phi_r] &= -R_{H_0}(z)[H_0(z), \phi_r]R_{H_0}(z) \\ &= R_{H_0}(z)(\Delta\phi_r + (\partial\phi_r)\partial)R_{H_0}(z) \end{aligned} \quad (12.43)$$

and $\Delta\phi_r = \phi_{r/2}\Delta\phi_r$, $\|\Delta\phi_r\|_\infty \leq \|\Delta\phi\|_\infty/r^2$ respectively $(\partial\phi_r) = \phi_{r/2}(\partial\phi_r)$, $\|\partial\phi_r\|_\infty \leq \|\partial\phi\|_\infty/r^2$ we see

$$|\tilde{h}_1(r) - \tilde{h}_2(r)| \leq \frac{c}{r}\tilde{h}_1(r/2), \quad r \geq 1. \quad (12.44)$$

Hence \tilde{h}_2 is integrable if \tilde{h}_1 is. Conversely,

$$\tilde{h}_1(r) \leq \tilde{h}_2(r) + \frac{c}{r}\tilde{h}_1(r/2) \leq \tilde{h}_2(r) + \frac{c}{r}\tilde{h}_2(r/2) + \frac{2c}{r^2}\tilde{h}_1(r/4) \quad (12.45)$$

shows that \tilde{h}_2 is integrable if \tilde{h}_1 is.

Invoking the first resolvent formula

$$\|\phi_rVR_{H_0}(z)\| \leq \|\phi_rVR_{H_0}(z_0)\| \|\mathbb{I} - (z - z_0)R_{H_0}(z)\| \quad (12.46)$$

finishes the proof. \square

As a first consequence note

Lemma 12.8. *If V is short range, then $R_H(z) - R_{H_0}(z)$ is compact.*

Proof. The operator $R_H(z)V(\mathbb{I} - \chi_r)R_{H_0}(z)$ is compact since $(\mathbb{I} - \chi_r)R_{H_0}(z)$ is by Lemma 7.10 and $R_H(z)V$ is bounded by Lemma 6.22. Moreover, by our short range condition it converges in norm to

$$R_H(z)V R_{H_0}(z) = R_H(z) - R_{H_0}(z) \quad (12.47)$$

as $r \rightarrow \infty$ (at least for some subsequence). \square

In particular, by Weyl's theorem we have $\sigma_{ess}(H) = [0, \infty)$. Moreover, V short range implies that H and H_0 look alike far outside.

Lemma 12.9. *Suppose $R_H(z) - R_{H_0}(z)$ is compact, then so is $f(H) - f(H_0)$ for any $f \in C_\infty(\mathbb{R})$ and*

$$\lim_{r \rightarrow \infty} \|(f(H) - f(H_0))\chi_r\| = 0. \quad (12.48)$$

Proof. The first part is Lemma 6.20 and the second part follows from part (ii) of Lemma 6.8 since χ_r converges strongly to 0. \square

However, this is clearly not enough to prove asymptotic completeness and we need a more careful analysis. The main ideas are due to Enß [4].

We begin by showing that the wave operators exist. By Cook's criterion (Lemma 12.3) we need to show that

$$\begin{aligned} \|V \exp(\mp itH_0)\psi\| &\leq \|VR_{H_0}(-1)\| \|(\mathbb{I} - \chi_{2a|t|}) \exp(\mp itH_0)(H_0 + \mathbb{I})\psi\| \\ &\quad + \|VR_{H_0}(-1)\chi_{2a|t|}\| \|(H_0 + \mathbb{I})\psi\| \end{aligned} \quad (12.49)$$

is integrable for a dense set of vectors ψ . The second term is integrable by our short range assumption. The same is true by Perry's estimate (Lemma 12.5) for the first term if we choose $\psi = f(H_0)P_D((\pm R, \pm\infty))\varphi$. Since vectors of this form are dense, we see that the wave operators exist,

$$\mathfrak{D}(\Omega_\pm) = \mathfrak{H}. \quad (12.50)$$

Since H restricted to $\text{Ran}(\Omega_\pm^*)$ is unitarily equivalent to H_0 , we obtain $[0, \infty) = \sigma_{ac}(H_0) \subseteq \sigma_{ac}(H)$. And by $\sigma_{ac}(H) \subseteq \sigma_{ess}(H) = [0, \infty)$ we even have $\sigma_{ac}(H) = [0, \infty)$.

To prove asymptotic completeness of the wave operators we will need that $(\Omega_\pm - \mathbb{I})f(H_0)P_\pm$ are compact.

Lemma 12.10. *Let $f \in C_c^\infty((0, \infty))$ and suppose ψ_n converges weakly to 0. Then*

$$\lim_{n \rightarrow \infty} \|(\Omega_\pm - \mathbb{I})f(H_0)P_\pm\psi_n\| = 0, \quad (12.51)$$

that is, $(\Omega_\pm - \mathbb{I})f(H_0)P_\pm$ is compact.

Proof. By (12.13) we see

$$\|R_H(z)(\Omega_\pm - \mathbb{I})f(H_0)P_\pm\psi_n\| \leq \int_0^\infty \|R_H(z)V \exp(-isH_0)f(H_0)P_\pm\psi_n\| dt. \quad (12.52)$$

Since $R_H(z)VR_{H_0}$ is compact we see that the integrand

$$\begin{aligned} R_H(z)V \exp(-isH_0)f(H_0)P_\pm\psi_n &= \\ R_H(z)VR_{H_0} \exp(-isH_0)(H_0 + 1)f(H_0)P_\pm\psi_n & \end{aligned} \quad (12.53)$$

converges pointwise to 0. Moreover, arguing as in (12.49) the integrand is bounded by an L^1 function depending only on $\|\psi_n\|$. Thus $R_H(z)(\Omega_\pm - \mathbb{I})f(H_0)P_\pm$ is compact by the dominated convergence theorem. Furthermore, using the intertwining property we see that

$$\begin{aligned} (\Omega_\pm - \mathbb{I})\tilde{f}(H_0)P_\pm &= R_H(z)(\Omega_\pm - \mathbb{I})f(H_0)P_\pm \\ &\quad - (R_H(z) - R_{H_0}(z))f(H_0)P_\pm \end{aligned} \quad (12.54)$$

is compact by Lemma 6.20, where $\tilde{f}(\lambda) = (\lambda + 1)f(\lambda)$. \square

Now we have gathered enough information to tackle the problem of asymptotic completeness.

We first show that the singular continuous spectrum is absent. This is not really necessary, but avoids the use of Cesàro means in our main argument.

Abbreviate $P = P_H^{sc}P_H((a, b))$, $0 < a < b$. Since H restricted to $\text{Ran}(\Omega_\pm)$ is unitarily equivalent to H_0 (which has purely absolutely continuous spectrum), the singular part must live on $\text{Ran}(\Omega_\pm)^\perp$, that is, $P_H^{sc}\Omega_\pm = 0$. Thus $Pf(H_0) = P(\mathbb{I} - \Omega_+)f(H_0)P_+ + P(\mathbb{I} - \Omega_-)f(H_0)P_-$ is compact. Since $f(H) - f(H_0)$ is compact, it follows that $Pf(H)$ is also compact. Choosing f such that $f(\lambda) = 1$ for $\lambda \in [a, b]$ we see that $P = Pf(H)$ is compact and hence finite dimensional. In particular $\sigma_{sc}(H) \cap (a, b)$ is a finite set. But a continuous measure cannot be supported on a finite set, showing $\sigma_{sc}(H) \cap (a, b) = \emptyset$. Since $0 < a < b$ are arbitrary we even have $\sigma_{sc}(H) \cap (0, \infty) = \emptyset$ and by $\sigma_{sc}(H) \subseteq \sigma_{ess}(H) = [0, \infty)$ we obtain $\sigma_{sc}(H) = \emptyset$.

Observe that replacing P_H^{sc} by P_H^{pp} the same argument shows that all nonzero eigenvalues are finite dimensional and cannot accumulate in $(0, \infty)$.

In summary we have shown

Theorem 12.11. *Suppose V is short range. Then*

$$\sigma_{ac}(H) = \sigma_{ess}(H) = [0, \infty), \quad \sigma_{sc}(H) = \emptyset. \quad (12.55)$$

All nonzero eigenvalues have finite multiplicity and cannot accumulate in $(0, \infty)$.

Now we come to the anticipated asymptotic completeness result of Enß. Choose

$$\psi \in \mathfrak{H}_c(H) = \mathfrak{H}_{ac}(H) \quad \text{such that} \quad \psi = f(H)\psi \quad (12.56)$$

for some $f \in C_c^\infty((0, \infty))$. By the RAGE theorem the sequence $\psi(t)$ converges weakly to zero as $t \rightarrow \pm\infty$. Abbreviate $\psi(t) = \exp(-itH)\psi$. Introduce

$$\varphi_\pm(t) = f(H_0)P_\pm\psi(t). \quad (12.57)$$

which satisfy

$$\lim_{t \rightarrow \pm\infty} \|\psi(t) - \varphi_+(t) - \varphi_-(t)\| = 0. \quad (12.58)$$

Indeed this follows from

$$\psi(t) = \varphi_+(t) + \varphi_-(t) + (f(H) - f(H_0))\psi(t) \quad (12.59)$$

and Lemma 6.20. Moreover, we even have

$$\lim_{t \rightarrow \pm\infty} \|(\Omega_\pm - \mathbb{I})\varphi_\pm(t)\| = 0 \quad (12.60)$$

by Lemma 12.10. Now suppose $\psi \in \text{Ran}(\Omega_\pm)^\perp$, then

$$\begin{aligned} \|\psi\|^2 &= \lim_{t \rightarrow \pm\infty} \langle \psi(t), \psi(t) \rangle \\ &= \lim_{t \rightarrow \pm\infty} \langle \psi(t), \varphi_+(t) + \varphi_-(t) \rangle \\ &= \lim_{t \rightarrow \pm\infty} \langle \psi(t), \Omega_+\varphi_+(t) + \Omega_-\varphi_-(t) \rangle. \end{aligned} \quad (12.61)$$

By Theorem 12.2, $\text{Ran}(\Omega_\pm)^\perp$ is invariant under H and hence $\psi(t) \in \text{Ran}(\Omega_\pm)^\perp$ implying

$$\begin{aligned} \|\psi\|^2 &= \lim_{t \rightarrow \pm\infty} \langle \psi(t), \Omega_\mp \varphi_\mp(t) \rangle \\ &= \lim_{t \rightarrow \pm\infty} \langle P_\mp f(H_0)^* \Omega_\mp^* \psi(t), \psi(t) \rangle. \end{aligned} \quad (12.62)$$

Invoking the intertwining property we see

$$\|\psi\|^2 = \lim_{t \rightarrow \pm\infty} \langle P_\mp f(H_0)^* e^{-itH_0} \Omega_\mp^* \psi, \psi(t) \rangle = 0 \quad (12.63)$$

by Corollary 12.6. Hence $\text{Ran}(\Omega_\pm) = \mathfrak{H}_{ac}(H) = \mathfrak{H}_c(H)$ and we thus have shown

Theorem 12.12 (Enß). *Suppose V is short range, then the wave operators are asymptotically complete.*

For further results and references see for example [3].

Part 3

Appendix

Almost everything about Lebesgue integration

In this appendix I give a brief introduction to measure theory. Good references are [2] or [18].

A.1. Borel measures in a nut shell

The first step in defining the Lebesgue integral is extending the notion of size from intervals to arbitrary sets. Unfortunately, this turns out to be too much, since a classical paradox by Banach and Tarski shows that one can break the unit ball in \mathbb{R}^3 into a finite number of (wild – choosing the pieces uses the Axiom of Choice and cannot be done with a jigsaw;-) pieces, rotate and translate them, and reassemble them to get two copies of the unit ball (compare Problem A.1). Hence any reasonable notion of size (i.e., one which is translation and rotation invariant) cannot be defined for all sets!

A collection of subsets \mathcal{A} of a given set X such that

- $X \in \mathcal{A}$,
- \mathcal{A} is closed under finite unions,
- \mathcal{A} is closed under complements.

is called an **algebra**. Note that $\emptyset \in \mathcal{A}$ and that, by de Morgan, \mathcal{A} is also closed under finite intersections. If an algebra is closed under countable unions (and hence also countable intersections), it is called a **σ -algebra**.

Moreover, the intersection of any family of (σ) -algebras $\{\mathcal{A}_\alpha\}$ is again a (σ) -algebra and for any collection S of subsets there is a unique smallest (σ) -algebra $\Sigma(S)$ containing S (namely the intersection of all (σ) -algebra containing S). It is called the (σ) -algebra generated by S .

If X is a topological space, the **Borel σ -algebra** of X is defined to be the σ -algebra generated by all open (respectively all closed) sets. Sets in the Borel σ -algebra are called **Borel sets**.

Example. In the case $X = \mathbb{R}^n$ the Borel σ -algebra will be denoted by \mathfrak{B}^n and we will abbreviate $\mathfrak{B} = \mathfrak{B}^1$. \diamond

Now let us turn to the definition of a measure: A set X together with a σ -algebra Σ is called a **measure space**. A **measure** μ is a map $\mu : \Sigma \rightarrow [0, \infty]$ on a σ -algebra Σ such that

- $\mu(\emptyset) = 0$,
- $\mu(\bigcup_{j=1}^{\infty} A_j) = \sum_{j=1}^{\infty} \mu(A_j)$ if $A_j \cap A_k = \emptyset$ for all j, k (σ -additivity).

It is called **σ -finite** if there is a countable cover $\{X_j\}_{j=1}^{\infty}$ of X with $\mu(X_j) < \infty$ for all j . (Note that it is no restriction to assume $X_j \nearrow X$.) It is called **finite** if $\mu(X) < \infty$. The sets in Σ are called **measurable sets**.

If we replace the σ -algebra by an algebra \mathcal{A} , then μ is called a **premeasure**. In this case σ -additivity clearly only needs to hold for disjoint sets A_n for which $\bigcup_n A_n \in \mathcal{A}$.

We will write $A_n \nearrow A$ if $A_n \subseteq A_{n+1}$ (note $A = \bigcup_n A_n$) and $A_n \searrow A$ if $A_{n+1} \subseteq A_n$ (note $A = \bigcap_n A_n$).

Theorem A.1. *Any measure μ satisfies the following properties:*

- (i) $A \subseteq B$ implies $\mu(A) \leq \mu(B)$ (*monotonicity*).
- (ii) $\mu(A_n) \rightarrow \mu(A)$ if $A_n \nearrow A$ (*continuity from below*).
- (iii) $\mu(A_n) \rightarrow \mu(A)$ if $A_n \searrow A$ and $\mu(A_1) < \infty$ (*continuity from above*).

Proof. The first claim is obvious. The second follows using $\tilde{A}_n = A_n \setminus A_{n-1}$ and σ -additivity. The third follows from the second using $\tilde{A}_n = A_1 \setminus A_n$ and $\mu(\tilde{A}_n) = \mu(A_1) - \mu(A_n)$. \square

Example. Let $A \in \mathfrak{P}(M)$ and set $\mu(A)$ to be the number of elements of A (respectively ∞ if A is infinite). This is the so called **counting measure**.

Note that if $X = \mathbb{N}$ and $A_n = \{j \in \mathbb{N} | j \geq n\}$, then $\mu(A_n) = \infty$, but $\mu(\bigcap_n A_n) = \mu(\emptyset) = 0$ which shows that the requirement $\mu(A_1) < \infty$ in the last claim of Theorem A.1 is not superfluous. \diamond

A measure on the Borel σ -algebra is called a **Borel measure** if $\mu(C) < \infty$ for any compact set C . A Borel measure is called **outer regular** if

$$\mu(A) = \inf_{A \subseteq O, O \text{ open}} \mu(O) \quad (\text{A.1})$$

and **inner regular** if

$$\mu(A) = \sup_{C \subseteq A, C \text{ compact}} \mu(C). \quad (\text{A.2})$$

It is called **regular** if it is both outer and inner regular.

But how can we obtain some more interesting Borel measures? We will restrict ourselves to the case of $X = \mathbb{R}$ for simplicity. Then the strategy is as follows: Start with the algebra of finite unions of disjoint intervals and define μ for those sets (as the sum over the intervals). This yields a premeasure. Extend this to an *outer measure* for all subsets of \mathbb{R} . Show that the restriction to the Borel sets is a measure.

Let us first show how we should define μ for intervals: To every Borel measure on \mathfrak{B} we can assign its **distribution function**

$$\mu(x) = \begin{cases} -\mu((x, 0]), & x < 0 \\ 0, & x = 0 \\ \mu((0, x]), & x > 0 \end{cases} \quad (\text{A.3})$$

which is right continuous and non-decreasing. Conversely, given a right continuous non-decreasing function $\mu : \mathbb{R} \rightarrow \mathbb{R}$ we can set

$$\mu(A) = \begin{cases} \mu(b) - \mu(a), & A = (a, b] \\ \mu(b) - \mu(a-), & A = [a, b] \\ \mu(b-) - \mu(a), & A = (a, b) \\ \mu(b-) - \mu(a-), & A = [a, b) \end{cases}, \quad (\text{A.4})$$

where $\mu(a-) = \lim_{\varepsilon \downarrow 0} \mu(a - \varepsilon)$. In particular, this gives a premeasure on the algebra of finite unions of intervals which can be extended to a measure:

Theorem A.2. *For every right continuous non-decreasing function $\mu : \mathbb{R} \rightarrow \mathbb{R}$ there exists a unique regular Borel measure μ which extends (A.4). Two different functions generate the same measure if and only if they differ by a constant.*

Since the proof of this theorem is rather involved, we defer it to the next section and look at some examples first.

Example. Suppose $\Theta(x) = 0$ for $x < 0$ and $\Theta(x) = 1$ for $x \geq 0$. Then we obtain the so-called **Dirac measure** at 0, which is given by $\Theta(A) = 1$ if $0 \in A$ and $\Theta(A) = 0$ if $0 \notin A$. \diamond

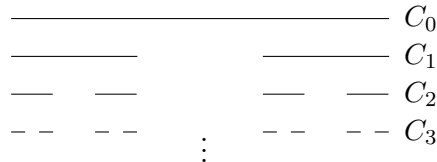
Example. Suppose $\lambda(x) = x$, then the associated measure is the ordinary **Lebesgue measure** on \mathbb{R} . We will abbreviate the Lebesgue measure of a Borel set A by $\lambda(A) = |A|$. \diamond

It can be shown that Borel measures on a separable metric space are always regular.

A set $A \in \Sigma$ is called a **support** for μ if $\mu(X \setminus A) = 0$. A property is said to hold **μ -almost everywhere** (a.e.) if it holds on a support for μ or, equivalently, if the set where it does not hold is contained in a set of measure zero.

Example. The set of rational numbers has Lebesgue measure zero: $\lambda(\mathbb{Q}) = 0$. In fact, any single point has Lebesgue measure zero, and so has any countable union of points (by countable additivity). \diamond

Example. The **Cantor set** is an example of a closed uncountable set of Lebesgue measure zero. It is constructed as follows: Start with $C_0 = [0, 1]$ and remove the middle third to obtain $C_1 = [0, \frac{1}{3}] \cup [\frac{2}{3}, 1]$. Next, again remove the middle third's of the remaining sets to obtain $C_2 = [0, \frac{1}{9}] \cup [\frac{2}{9}, \frac{1}{3}] \cup [\frac{2}{3}, \frac{7}{9}] \cup [\frac{8}{9}, 1]$.



Proceeding like this we obtain a sequence of nesting sets C_n and the limit $C = \bigcap_n C_n$ is the Cantor set. Since C_n is compact, so is C . Moreover, C_n consists of 2^n intervals of length 3^{-n} , and thus its Lebesgue measure is $\lambda(C_n) = (2/3)^n$. In particular, $\lambda(C) = \lim_{n \rightarrow \infty} \lambda(C_n) = 0$. Using the ternary expansion it is extremely simple to describe: C is the set of all $x \in [0, 1]$ whose ternary expansion contains no one's, which shows that C is uncountable (why?). It has some further interesting properties: it is totally disconnected (i.e., it contains no subintervals) and perfect (it has no isolated points). \diamond

Problem A.1 (Vitali set). *Call two numbers $x, y \in [0, 1]$ equivalent if $x - y$ is rational. Construct the set V by choosing one representative from each equivalence class. Show that V cannot be measurable with respect to any finite translation invariant measure on $[0, 1]$. (Hint: How can you build up $[0, 1]$ from V ?)*

A.2. Extending a premeasure to a measure

The purpose of this section is to prove Theorem A.2. It is rather technical and should be skipped on first reading.

In order to prove Theorem A.2 we need to show how a premeasure can be extended to a measure. As a prerequisite we first establish that it suffices to check increasing (or decreasing) sequences of sets when checking whether a given algebra is in fact a σ -algebra:

A collection of sets \mathcal{M} is called a **monotone class** if $A_n \nearrow A$ implies $A \in \mathcal{M}$ whenever $A_n \in \mathcal{M}$ and $A_n \searrow A$ implies $A \in \mathcal{M}$ whenever $A_n \in \mathcal{M}$. Every σ -algebra is a monotone class and the intersection of monotone classes is a monotone class. Hence every collection of sets S generates a smallest monotone class $\mathcal{M}(S)$.

Theorem A.3. *Let \mathcal{A} be an algebra. Then $\mathcal{M}(\mathcal{A}) = \Sigma(\mathcal{A})$.*

Proof. We first show that $\mathcal{M} = \mathcal{M}(\mathcal{A})$ is an algebra.

Put $M(A) = \{B \in \mathcal{M} \mid A \cup B \in \mathcal{M}\}$. If B_n is an increasing sequence of sets in $M(A)$ then $A \cup B_n$ is an increasing sequence in \mathcal{M} and hence $\bigcup_n (A \cup B_n) \in \mathcal{M}$. Now

$$A \cup \left(\bigcup_n B_n \right) = \bigcup_n (A \cup B_n) \quad (\text{A.5})$$

shows that $M(A)$ is closed under increasing sequences. Similarly, $M(A)$ is closed under decreasing sequences and hence it is a monotone class. But does it contain any elements? Well if $A \in \mathcal{A}$ we have $\mathcal{A} \subseteq M(A)$ implying $M(A) = \mathcal{M}$. Hence $A \cup B \in \mathcal{M}$ if at least one of the sets is in \mathcal{A} . But this shows $\mathcal{A} \subseteq M(A)$ and hence $M(A) = \mathcal{M}$ for any $A \in \mathcal{M}$. So \mathcal{M} is closed under finite unions.

To show that we are closed under complements consider $M = \{A \in \mathcal{M} \mid X \setminus A \in \mathcal{M}\}$. If A_n is an increasing sequence then $X \setminus A_n$ is a decreasing sequence and $X \setminus \bigcup_n A_n = \bigcap_n X \setminus A_n \in \mathcal{M}$ if $A_n \in M$. Similarly for decreasing sequences. Hence M is a monotone class and must be equal to \mathcal{M} since it contains \mathcal{A} .

So we know that \mathcal{M} is an algebra. To show that it is a σ -algebra let A_n be given and put $\tilde{A}_n = \bigcup_{k \leq n} A_k$. Then \tilde{A}_n is increasing and $\bigcup_n \tilde{A}_n = \bigcup_n A_n \in \mathcal{A}$. \square

The typical use of this theorem is as follows: First verify some property for sets in an algebra \mathcal{A} . In order to show that it holds for any set in $\Sigma(\mathcal{A})$, it suffices to show that the sets for which it holds is closed under countable increasing and decreasing sequences (i.e., is a monotone class).

Now we start by proving that (A.4) indeed gives rise to a premeasure.

Lemma A.4. μ as defined in (A.4) gives rise to a unique σ -finite regular premeasure on the algebra \mathcal{A} of finite unions of disjoint intervals.

Proof. First of all, (A.4) can be extended to finite unions of disjoint intervals by summing over all intervals. It is straightforward to verify that μ is well defined (one set can be represented by different unions of intervals) and by construction additive.

To show regularity, we can assume any such union to consist of open intervals and points only. To show outer regularity replace each point $\{x\}$ by a small open interval $(x + \varepsilon, x - \varepsilon)$ and use that $\mu(\{x\}) = \lim_{\varepsilon \downarrow} \mu(x + \varepsilon) - \mu(x - \varepsilon)$. Similarly, to show inner regularity, replace each open interval (a, b) by a compact one $[a_n, b_n] \subseteq (a, b)$ and use $\mu((a, b)) = \lim_{n \rightarrow \infty} \mu(b_n) - \mu(a_n)$ if $a_n \downarrow a$ and $b_n \uparrow b$.

It remains to verify σ -additivity. We need to show

$$\mu\left(\bigcup_k I_k\right) = \sum_k \mu(I_k) \quad (\text{A.6})$$

whenever $I_n \in \mathcal{A}$ and $I = \bigcup_k I_k \in \mathcal{A}$. Since each I_n is a finite union of intervals, we can as well assume each I_n is just one interval (just split I_n into its subintervals and note that the sum does not change by additivity). Similarly, we can assume that I is just one interval (just treat each subinterval separately).

By additivity μ is monotone and hence

$$\sum_{k=1}^n \mu(I_k) = \mu\left(\bigcup_{k=1}^n I_k\right) \leq \mu(I) \quad (\text{A.7})$$

which shows

$$\sum_{k=1}^{\infty} \mu(I_k) \leq \mu(I). \quad (\text{A.8})$$

To get the converse inequality we need to work harder.

By outer regularity we can cover each I_k by open interval J_k such that $\mu(J_k) \leq \mu(I_k) + \frac{\varepsilon}{2^k}$. Suppose I is compact first. Then finitely many of the J_k , say the first n , cover I and we have

$$\mu(I) \leq \mu\left(\bigcup_{k=1}^n J_k\right) \leq \sum_{k=1}^n \mu(J_k) \leq \sum_{k=1}^{\infty} \mu(I_k) + \varepsilon. \quad (\text{A.9})$$

Since $\varepsilon > 0$ is arbitrary, this shows σ -additivity for compact intervals. By additivity we can always add/subtract the end points of I and hence σ -additivity holds for any bounded interval. If I is unbounded, say $I = [a, \infty)$,

then given $x > 0$ we can find an n such that J_n cover at least $[0, x]$ and hence

$$\sum_{k=1}^n \mu(I_k) \geq \sum_{k=1}^n \mu(J_k) - \varepsilon \geq \mu([a, x]) - \varepsilon. \quad (\text{A.10})$$

Since $x > a$ and $\varepsilon > 0$ are arbitrary we are done. \square

This premeasure determines the corresponding measure μ uniquely (if there is one at all):

Theorem A.5 (Uniqueness of measures). *Let μ be a σ -finite premeasure on an algebra \mathcal{A} . Then there is at most one extension to $\Sigma(\mathcal{A})$.*

Proof. We first assume that $\mu(X) < \infty$. Suppose there is another extension $\tilde{\mu}$ and consider the set

$$S = \{A \in \Sigma(\mathcal{A}) \mid \mu(A) = \tilde{\mu}(A)\}. \quad (\text{A.11})$$

I claim S is a monotone class and hence $S = \Sigma(\mathcal{A})$ since $\mathcal{A} \subseteq S$ by assumption (Theorem A.3).

Let $A_n \nearrow A$. If $A_n \in S$ we have $\mu(A_n) = \tilde{\mu}(A_n)$ and taking limits (Theorem A.1 (ii)) we conclude $\mu(A) = \tilde{\mu}(A)$. Next let $A_n \searrow A$ and take again limits. This finishes the finite case. To extend our result to the σ -finite case let $X_j \nearrow X$ be an increasing sequence such that $\mu(X_j) < \infty$. By the finite case $\mu(A \cap X_j) = \tilde{\mu}(A \cap X_j)$ (just restrict $\mu, \tilde{\mu}$ to X_j). Hence

$$\mu(A) = \lim_{j \rightarrow \infty} \mu(A \cap X_j) = \lim_{j \rightarrow \infty} \tilde{\mu}(A \cap X_j) = \tilde{\mu}(A) \quad (\text{A.12})$$

and we are done. \square

Note that if our premeasure is regular, so will be the extension:

Lemma A.6. *Suppose μ is a σ -finite premeasure on some algebra \mathcal{A} generating the Borel sets \mathfrak{B} . Then outer (inner) regularity holds for all Borel sets if it holds for all sets in \mathcal{A} .*

Proof. We first assume that $\mu(X) < \infty$. Set

$$\mu^\circ(A) = \inf_{A \subseteq O, O \text{ open}} \mu(O) \geq \mu(A) \quad (\text{A.13})$$

and let $M = \{A \in \mathfrak{B} \mid \mu^\circ(A) = \mu(A)\}$. Since by assumption M contains some algebra generating \mathfrak{B} it suffices to prove that M is a monotone class.

Let $A_n \in M$ be a monotone sequence and let $O_n \supseteq A_n$ be open sets such that $\mu(O_n) \leq \mu(A_n) + \frac{1}{n}$. Then

$$\mu(A_n) \leq \mu^\circ(A_n) \leq \mu(O_n) \leq \mu(A_n) + \frac{1}{n}. \quad (\text{A.14})$$

Now if $A_n \nearrow A$ just take limits and use continuity from below of μ . Similarly if $A_n \searrow A$.

Now let μ be arbitrary. Given A we can split it into disjoint sets A_j such that $A_j \subseteq X_j$ ($A_1 = A \cap X_1$, $A_2 = (A \setminus A_1) \cap X_2$, etc.). Let X_j be a cover with $\mu(X_j) < \infty$. By regularity, we can assume X_j open. Thus there are open (in X) sets O_j covering A_j such that $\mu(O_j) \leq \mu(A_j) + \frac{\varepsilon}{2^j}$. Then $O = \bigcup_j O_j$ is open, covers A , and satisfies

$$\mu(A) \leq \mu(O) \leq \sum_j \mu(O_j) \leq \mu(A) + \varepsilon. \quad (\text{A.15})$$

This settles outer regularity.

Next let us turn to inner regularity. If $\mu(X) < \infty$ one can show as before that $M = \{A \in \mathfrak{B} \mid \mu_\circ(A) = \mu(A)\}$, where

$$\mu_\circ(A) = \sup_{C \subseteq A, C \text{ compact}} \mu(C) \leq \mu(A) \quad (\text{A.16})$$

is a monotone class. This settles the finite case.

For the σ -finite case split again A as before. Since X_j has finite measure, there are compact subsets K_j of A_j such that $\mu(A_j) \leq \mu(K_j) + \frac{\varepsilon}{2^j}$. Now we need to distinguish two cases: If $\mu(A) = \infty$, the sum $\sum_j \mu(A_j)$ will diverge and so will $\sum_j \mu(K_j)$. Hence $\tilde{K}_n = \bigcup_{j=1}^n K_j \subseteq A$ is compact with $\mu(\tilde{K}_n) \rightarrow \infty = \mu(A)$. If $\mu(A) < \infty$, the sum $\sum_j \mu(A_j)$ will converge and choosing n sufficiently large we will have

$$\mu(\tilde{K}_n) \leq \mu(A) \leq \mu(\tilde{K}_n) + 2\varepsilon. \quad (\text{A.17})$$

This finishes the proof. \square

So it remains to ensure that there is an extension at all. For any pre-measure μ we define

$$\mu^*(A) = \inf \left\{ \sum_{n=1}^{\infty} \mu(A_n) \mid A \subseteq \bigcup_{n=1}^{\infty} A_n, A_n \in \mathcal{A} \right\} \quad (\text{A.18})$$

where the infimum extends over all countable covers from \mathcal{A} . Then the function $\mu^* : \mathfrak{P}(X) \rightarrow [0, \infty]$ is an **outer measure**, that is, it has the properties (Problem A.2)

- $\mu^*(\emptyset) = 0$,
- $A_1 \subseteq A_2 \Rightarrow \mu^*(A_1) \leq \mu^*(A_2)$, and
- $\mu^*(\bigcup_{n=1}^{\infty} A_n) \leq \sum_{n=1}^{\infty} \mu^*(A_n)$ (subadditivity).

Note that $\mu^*(A) = \mu(A)$ for $A \in \mathcal{A}$ (Problem A.3).

Theorem A.7 (Extensions via outer measures). *Let μ^* be an outer measure. Then the set Σ of all sets A satisfying the Carathéodory condition*

$$\mu^*(E) = \mu^*(A \cap E) + \mu^*(A' \cap E) \quad \forall E \subseteq X \quad (\text{A.19})$$

(where $A' = X \setminus A$ is the complement of A) form a σ -algebra and μ^* restricted to this σ -algebra is a measure.

Proof. We first show that Σ is an algebra. It clearly contains X and is closed under complements. Let $A, B \in \Sigma$. Applying Carathéodory's condition twice finally shows

$$\begin{aligned} \mu^*(E) &= \mu^*(A \cap B \cap E) + \mu^*(A' \cap B \cap E) + \mu^*(A \cap B' \cap E) \\ &\quad + \mu^*(A' \cap B' \cap E) \\ &\geq \mu^*((A \cup B) \cap E) + \mu^*((A \cup B)' \cap E), \end{aligned} \quad (\text{A.20})$$

where we have used De Morgan and

$$\mu^*(A \cap B \cap E) + \mu^*(A' \cap B \cap E) + \mu^*(A \cap B' \cap E) \geq \mu^*((A \cup B) \cap E) \quad (\text{A.21})$$

which follows from subadditivity and $(A \cup B) \cap E = (A \cap B \cap E) \cup (A' \cap B \cap E) \cup (A \cap B' \cap E)$. Since the reverse inequality is just subadditivity, we conclude that Σ is an algebra.

Next, let A_n be a sequence of sets from Σ . Without restriction we can assume that they are disjoint (compare the last argument in proof of Theorem A.3). Abbreviate $\tilde{A}_n = \bigcup_{k \leq n} A_k$, $A = \bigcup_n A_n$. Then for any set E we have

$$\begin{aligned} \mu^*(\tilde{A}_n \cap E) &= \mu^*(A_n \cap \tilde{A}_n \cap E) + \mu^*(A'_n \cap \tilde{A}_n \cap E) \\ &= \mu^*(A_n \cap E) + \mu^*(\tilde{A}_{n-1} \cap E) \\ &= \dots = \sum_{k=1}^n \mu^*(A_k \cap E). \end{aligned} \quad (\text{A.22})$$

Using $\tilde{A}_n \in \Sigma$ and monotonicity of μ^* , we infer

$$\begin{aligned} \mu^*(E) &= \mu^*(\tilde{A}_n \cap E) + \mu^*(\tilde{A}'_n \cap E) \\ &\geq \sum_{k=1}^n \mu^*(A_k \cap E) + \mu^*(A' \cap E). \end{aligned} \quad (\text{A.23})$$

Letting $n \rightarrow \infty$ and using subadditivity finally gives

$$\begin{aligned} \mu^*(E) &\geq \sum_{k=1}^{\infty} \mu^*(A_k \cap E) + \mu^*(A' \cap E) \\ &\geq \mu^*(A \cap E) + \mu^*(B' \cap E) \geq \mu^*(E) \end{aligned} \quad (\text{A.24})$$

and we infer that Σ is a σ -algebra.

Finally, setting $E = A$ in (A.24) we have

$$\mu^*(A) = \sum_{k=1}^{\infty} \mu^*(A_k \cap A) + \mu^*(A' \cap A) = \sum_{k=1}^{\infty} \mu^*(A_k) \quad (\text{A.25})$$

and we are done. \square

Remark: The constructed measure μ is **complete**, that is, for any measurable set A of measure zero, any subset of A is again measurable (Problem A.4).

The only remaining question is whether there are any nontrivial sets satisfying the Carathéodory condition.

Lemma A.8. *Let μ be a premeasure on \mathcal{A} and let μ^* be the associated outer measure. Then every set in \mathcal{A} satisfies the Carathéodory condition.*

Proof. Let $A_n \in \mathcal{A}$ be a countable cover for E . Then for any $A \in \mathcal{A}$ we have

$$\sum_{n=1}^{\infty} \mu(A_n) = \sum_{n=1}^{\infty} \mu(A_n \cap A) + \sum_{n=1}^{\infty} \mu(A_n \cap A') \geq \mu^*(E \cap A) + \mu^*(E \cap A') \quad (\text{A.26})$$

since $A_n \cap A \in \mathcal{A}$ is a cover for $E \cap A$ and $A_n \cap A' \in \mathcal{A}$ is a cover for $E \cap A'$. Taking the infimum we have $\mu^*(E) \geq \mu^*(E \cap A) + \mu^*(E \cap A')$ which finishes the proof. \square

Thus, as a consequence we obtain Theorem A.2.

Problem A.2. *Show that μ^* defined in (A.18) is an outer measure. (Hint for the last property: Take a cover $\{B_{nk}\}_{k=1}^{\infty}$ for A_n such that $\mu^*(A_n) = \frac{\varepsilon}{2^n} + \sum_{k=1}^{\infty} \mu(B_{nk})$ and note that $\{B_{nk}\}_{n,k=1}^{\infty}$ is a cover for $\bigcup_n A_n$.)*

Problem A.3. *Show that μ^* defined in (A.18) extends μ . (Hint: For the cover A_n it is no restriction to assume $A_n \cap A_m = \emptyset$ and $A_n \subseteq A$.)*

Problem A.4. *Show that the measure constructed in Theorem A.7 is complete.*

A.3. Measurable functions

The Riemann integral works by splitting the x coordinate into small intervals and approximating $f(x)$ on each interval by its minimum and maximum. The problem with this approach is that the difference between maximum and minimum will only tend to zero (as the intervals get smaller) if $f(x)$ is sufficiently nice. To avoid this problem we can force the difference to go to zero by considering, instead of an interval, the set of x for which $f(x)$ lies between two given numbers $a < b$. Now we need the size of the set of these x , that is, the size of the preimage $f^{-1}((a, b))$. For this to work, preimages of intervals must be measurable.

A function $f : X \rightarrow \mathbb{R}^n$ is called **measurable** if $f^{-1}(A) \in \Sigma$ for every $A \in \mathfrak{B}^n$. A complex-valued function is called measurable if both its real and imaginary parts are. Clearly it suffices to check this condition for every

set A in a collection of sets which generate \mathfrak{B}^n , say for all open intervals or even for open intervals which are products of (a, ∞) :

Lemma A.9. *A function $f : X \rightarrow \mathbb{R}^n$ is measurable if and only if*

$$f^{-1}(I) \in \Sigma \quad \forall I = \prod_{j=1}^n (a_j, \infty). \quad (\text{A.27})$$

In particular, a function $f : X \rightarrow \mathbb{R}^n$ is measurable if and only if every component is measurable.

Proof. All you have to use is $f^{-1}(\mathbb{R}^n \setminus A) = X \setminus f^{-1}(A)$, $f^{-1}(\bigcup_j A_j) = \bigcup_j f^{-1}(A_j)$ and the fact that any open set is a countable union of open intervals. \square

If Σ is the Borel σ -algebra, we will call a measurable function also **Borel function**. Note that, in particular,

Lemma A.10. *Any continuous function is measurable and the composition of two measurable functions is again measurable.*

Moreover, sometimes it is also convenient to allow $\pm\infty$ as possible values for f , that is, functions $f : X \rightarrow \overline{\mathbb{R}}$, $\overline{\mathbb{R}} = \mathbb{R} \cup \{-\infty, \infty\}$. In this case $A \subseteq \overline{\mathbb{R}}$ is called Borel if $A \cap \mathbb{R}$ is.

The set of all measurable functions forms an algebra.

Lemma A.11. *Suppose $f, g : X \rightarrow \mathbb{R}$ are measurable functions. Then the sum $f + g$ and the product fg is measurable.*

Proof. Note that addition and multiplication are continuous functions from $\mathbb{R}^2 \rightarrow \mathbb{R}$ and hence the claim follows from the previous lemma. \square

Moreover, the set of all measurable functions is closed under all important limiting operations.

Lemma A.12. *Suppose $f_n : X \rightarrow \mathbb{R}$ is a sequence of measurable functions, then*

$$\inf_{n \in \mathbb{N}} f_n, \quad \sup_{n \in \mathbb{N}} f_n, \quad \liminf_{n \rightarrow \infty} f_n, \quad \limsup_{n \rightarrow \infty} f_n \quad (\text{A.28})$$

are measurable as well.

Proof. It suffices to proof that $\sup f_n$ is measurable since the rest follows from $\inf f_n = -\sup(-f_n)$, $\liminf f_n = \sup_k \inf_{n \geq k} f_n$, and $\limsup f_n = \inf_k \sup_{n \geq k} f_n$. But $(\sup f_n)^{-1}((a, \infty)) = \bigcup_n f_n^{-1}((a, \infty))$ and we are done. \square

It follows that if f and g are measurable functions, so are $\min(f, g)$, $\max(f, g)$, $|f| = \max(f, -f)$, $f^\pm = \max(\pm f, 0)$.

A.4. The Lebesgue integral

Now we can define the integral for measurable functions as follows. A measurable function $s : X \rightarrow \mathbb{R}$ is called **simple** if its range is finite $s(X) = \{\alpha_j\}_{j=1}^p$, that is, if

$$s = \sum_{j=1}^p \alpha_j \chi_{A_j}, \quad A_j = s^{-1}(\alpha_j) \in \Sigma. \quad (\text{A.29})$$

Here χ_A is the **characteristic function** of A , that is, $\chi_A(x) = 1$ if $x \in A$ and $\chi_A(x) = 0$ else.

For a positive simple function we define its **integral** as

$$\int_A s \, d\mu = \sum_{j=1}^n \alpha_j \mu(A_j \cap A). \quad (\text{A.30})$$

Here we use the convention $0 \cdot \infty = 0$.

Lemma A.13. *The integral has the following properties:*

- (i) $\int_A s \, d\mu = \int_X \chi_A s \, d\mu$.
- (ii) $\int_{\bigcup_{j=1}^{\infty} A_j} s \, d\mu = \sum_{j=1}^{\infty} \int_{A_j} s \, d\mu$.
- (iii) $\int_A \alpha s \, d\mu = \alpha \int_A s \, d\mu$.
- (iv) $\int_A (s + t) \, d\mu = \int_A s \, d\mu + \int_A t \, d\mu$.
- (v) $A \subseteq B \Rightarrow \int_A s \, d\mu \leq \int_B s \, d\mu$.
- (vi) $s \leq t \Rightarrow \int_A s \, d\mu \leq \int_A t \, d\mu$.

Proof. (i) is clear from the definition. (ii) follows from σ -additivity of μ . (iii) is obvious. (iv) Let $s = \sum_j \alpha_j \chi_{A_j}$, $t = \sum_j \beta_j \chi_{B_j}$ and abbreviate $C_{jk} = (A_j \cap B_k) \cap A$. Then

$$\begin{aligned} \int_A (s + t) \, d\mu &= \sum_{j,k} \int_{C_{jk}} (s + t) \, d\mu = \sum_{j,k} (\alpha_j + \beta_k) \mu(C_{jk}) \\ &= \sum_{j,k} \left(\int_{C_{jk}} s \, d\mu + \int_{C_{jk}} t \, d\mu \right) = \int_A s \, d\mu + \int_A t \, d\mu \end{aligned} \quad (\text{A.31})$$

(v) follows from monotonicity of μ . (vi) follows using $t - s \geq 0$ and arguing as in (iii). \square

Our next task is to extend this definition to arbitrary positive functions by

$$\int_A f \, d\mu = \sup_{s \leq f} \int_A s \, d\mu, \quad (\text{A.32})$$

where the supremum is taken over all simple functions $s \leq f$. Note that, except for possibly (ii) and (iv), Lemma A.13 still holds for this extension.

Theorem A.14 (monotone convergence). *Let f_n be a monotone non-decreasing sequence of positive measurable functions, $f_n \nearrow f$. Then*

$$\int_A f_n d\mu \rightarrow \int_A f d\mu. \quad (\text{A.33})$$

Proof. By property (v) $\int_A f_n d\mu$ is monotone and converges to some number α . By $f_n \leq f$ and again (v) we have

$$\alpha \leq \int_A f d\mu. \quad (\text{A.34})$$

To show the converse let s be simple such that $s \leq f$ and let $\theta \in (0, 1)$. Put $A_n = \{x \in A \mid f_n(x) \geq \theta s(x)\}$ and note $A_n \nearrow X$ (show this). Then

$$\int_A f_n d\mu \geq \int_{A_n} f_n d\mu \geq \theta \int_{A_n} s d\mu. \quad (\text{A.35})$$

Letting $n \rightarrow \infty$ we see

$$\alpha \geq \theta \int_A s d\mu. \quad (\text{A.36})$$

Since this is valid for any $\theta < 1$, it still holds for $\theta = 1$. Finally, since $s \leq f$ is arbitrary, the claim follows. \square

In particular

$$\int_A f d\mu = \lim_{n \rightarrow \infty} \int_A s_n d\mu, \quad (\text{A.37})$$

for any monotone sequence $s_n \nearrow f$ of simple functions. Note that there is always such a sequence, for example,

$$s_n(x) = \sum_{k=0}^{n^2} \frac{k}{n} \chi_{f^{-1}(A_k)}(x), \quad A_k = \left[\frac{k}{n}, \frac{k+1}{n^2}\right), \quad A_{n^2} = [n, \infty). \quad (\text{A.38})$$

By construction s_n converges uniformly if f is bounded, since $s_n(x) = n$ if $f(x) = \infty$ and $f(x) - s_n(x) < \frac{1}{n}$ if $f(x) < n + 1$.

Now what about the missing items (ii) and (iv) from Lemma A.13? Since limits can be spread over sums, the extension is linear (i.e., item (iv) holds) and (ii) also follows directly from the monotone convergence theorem. We even have the following result:

Lemma A.15. *If $f \geq 0$ is measurable, then $d\nu = f d\mu$ defined via*

$$\nu(A) = \int_A f d\mu \quad (\text{A.39})$$

is a measure such that

$$\int g \, d\nu = \int gf \, d\mu. \quad (\text{A.40})$$

Proof. As already mentioned, additivity of μ is equivalent to linearity of the integral and σ -additivity follows from the monotone convergence theorem

$$\nu\left(\bigcup_{n=1}^{\infty} A_n\right) = \int \left(\sum_{n=1}^{\infty} \chi_{A_n}\right) f \, d\mu = \sum_{n=1}^{\infty} \int \chi_{A_n} f \, d\mu = \sum_{n=1}^{\infty} \nu(A_n). \quad (\text{A.41})$$

The second claim holds for simple functions and hence for all functions by construction of the integral. \square

If f_n is not necessarily monotone we have at least

Theorem A.16 (Fatou's Lemma). *If f_n is a sequence of nonnegative measurable function, then*

$$\int_A \liminf_{n \rightarrow \infty} f_n \, d\mu \leq \liminf_{n \rightarrow \infty} \int_A f_n \, d\mu, \quad (\text{A.42})$$

Proof. Set $g_n = \inf_{k \geq n} f_k$. Then $g_n \leq f_n$ implying

$$\int_A g_n \, d\mu \leq \int_A f_n \, d\mu. \quad (\text{A.43})$$

Now take the \liminf on both sides and note that by the monotone convergence theorem

$$\liminf_{n \rightarrow \infty} \int_A g_n \, d\mu = \lim_{n \rightarrow \infty} \int_A g_n \, d\mu = \int_A \lim_{n \rightarrow \infty} g_n \, d\mu = \int_A \liminf_{n \rightarrow \infty} f_n \, d\mu, \quad (\text{A.44})$$

proving the claim. \square

If the integral is finite for both the positive and negative part f^{\pm} of an arbitrary measurable function f , we call f **integrable** and set

$$\int_A f \, d\mu = \int_A f^+ \, d\mu - \int_A f^- \, d\mu. \quad (\text{A.45})$$

The set of all integrable functions is denoted by $\mathcal{L}^1(X, d\mu)$.

Lemma A.17. *Lemma A.13 holds for integrable functions s, t .*

Similarly, we handle the case where f is complex-valued by calling f integrable if both the real and imaginary part are and setting

$$\int_A f \, d\mu = \int_A \operatorname{Re}(f) \, d\mu + i \int_A \operatorname{Im}(f) \, d\mu. \quad (\text{A.46})$$

Clearly f is integrable if and only if $|f|$ is.

Lemma A.18. For any integrable functions f, g we have

$$\left| \int_A f d\mu \right| \leq \int_A |f| d\mu \quad (\text{A.47})$$

and (triangle inequality)

$$\int_A |f + g| d\mu \leq \int_A |f| d\mu + \int_A |g| d\mu. \quad (\text{A.48})$$

Proof. Put $\alpha = \frac{z^*}{|z|}$, where $z = \int_A f d\mu$ (without restriction $z \neq 0$). Then

$$\left| \int_A f d\mu \right| = \alpha \int_A f d\mu = \int_A \alpha f d\mu = \int_A \operatorname{Re}(\alpha f) d\mu \leq \int_A |f| d\mu. \quad (\text{A.49})$$

proving the first claim. The second follows from $|f + g| \leq |f| + |g|$. \square

In addition, our integral is well behaved with respect to limiting operations.

Theorem A.19 (dominated convergence). Let f_n be a convergent sequence of measurable functions and set $f = \lim_{n \rightarrow \infty} f_n$. Suppose there is an integrable function g such that $|f_n| \leq g$. Then f is integrable and

$$\lim_{n \rightarrow \infty} \int_A f_n d\mu = \int_A f d\mu. \quad (\text{A.50})$$

Proof. The real and imaginary parts satisfy the same assumptions and so do the positive and negative parts. Hence it suffices to prove the case where f_n and f are nonnegative.

By Fatou's lemma

$$\liminf_{n \rightarrow \infty} \int_A f_n d\mu \geq \int_A f d\mu \quad (\text{A.51})$$

and

$$\liminf_{n \rightarrow \infty} \int_A (g - f_n) d\mu \geq \int_A (g - f) d\mu. \quad (\text{A.52})$$

Subtracting $\int_A g d\mu$ on both sides of the last inequality finishes the proof since $\liminf(-f_n) = -\limsup f_n$. \square

Remark: Since sets of measure zero do not contribute to the value of the integral, it clearly suffices if the requirements of the dominated convergence theorem are satisfied almost everywhere (with respect to μ).

Note that the existence of g is crucial, as the example $f_n(x) = \frac{1}{n} \chi_{[-n,n]}(x)$ on \mathbb{R} with Lebesgue measure shows.

Example. If $\mu(x) = \sum_n \alpha_n \Theta(x - x_n)$ is a sum of Dirac measures $\Theta(x)$ centered at $x = 0$, then

$$\int f(x) d\mu(x) = \sum_n \alpha_n f(x_n). \quad (\text{A.53})$$

Hence our integral contains sums as special cases. \diamond

Problem A.5. Show that the set $B(X)$ of bounded measurable functions is a Banach space. Show that the set $S(X)$ of simple functions is dense in $B(X)$. Show that the integral is a bounded linear functional on $B(X)$. (Hence Theorem 0.24 could be used to extend the integral from simple to bounded measurable functions.)

Problem A.6. Show that the dominated convergence theorem implies (under the same assumptions)

$$\lim_{n \rightarrow \infty} \int |f_n - f| d\mu = 0. \quad (\text{A.54})$$

Problem A.7. Suppose $y \mapsto f(x, y)$ is measurable for every x and $x \mapsto f(x, y)$ is continuous for every y . Show that

$$F(x) = \int_A f(x, y) d\mu(y) \quad (\text{A.55})$$

is continuous if there is an integrable function $g(y)$ such that $|f(x, y)| \leq g(y)$.

Problem A.8. Suppose $y \mapsto f(x, y)$ is measurable for fixed x and $x \mapsto f(x, y)$ is differentiable for fixed y . Show that

$$F(x) = \int_A f(x, y) d\mu(y) \quad (\text{A.56})$$

is differentiable if there is an integrable function $g(y)$ such that $|\frac{\partial}{\partial x} f(x, y)| \leq g(y)$. Moreover, $x \mapsto \frac{\partial}{\partial x} f(x, y)$ is measurable and

$$F'(x) = \int_A \frac{\partial}{\partial x} f(x, y) d\mu(y) \quad (\text{A.57})$$

in this case.

A.5. Product measures

Let μ_1 and μ_2 be two measures on Σ_1 and Σ_2 , respectively. Let $\Sigma_1 \otimes \Sigma_2$ be the σ -algebra generated by **rectangles** of the form $A_1 \times A_2$.

Example. Let \mathfrak{B} be the Borel sets in \mathbb{R} then $\mathfrak{B}^2 = \mathfrak{B} \otimes \mathfrak{B}$ are the Borel sets in \mathbb{R}^2 (since the rectangles are a basis for the product topology). \diamond

Any set in $\Sigma_1 \otimes \Sigma_2$ has the **section property**, that is,

Lemma A.20. *Suppose $A \in \Sigma_1 \otimes \Sigma_2$ then its sections*

$$A_1(x_2) = \{x_1 | (x_1, x_2) \in A\} \quad \text{and} \quad A_2(x_1) = \{x_2 | (x_1, x_2) \in A\} \quad (\text{A.58})$$

are measurable.

Proof. Denote all sets $A \in \Sigma_1 \otimes \Sigma_2$ in with the property that $A_1(x_2) \in \Sigma_1$ by S . Clearly all rectangles are in S and it suffices to show that S is a σ -algebra. Moreover, if $A \in S$, then $(A')_1(x_2) = (A_1(x_2))' \in \Sigma_2$ and thus S is closed under complements. Similarly, if $A_n \in S$, then $(\bigcup_n A_n)_1(x_2) = \bigcup_n (A_n)_1(x_2)$ shows that S is closed under countable unions. \square

This implies that if f is a measurable function on $X_1 \times X_2$, then $f(\cdot, x_2)$ is measurable on X_1 for every x_2 and $f(x_1, \cdot)$ is measurable on X_2 for every x_1 (observe $A_1(x_2) = \{x_1 | f(x_1, x_2) \in B\}$, where $A = \{(x_1, x_2) | f(x_1, x_2) \in B\}$). In fact, this is even equivalent since $\chi_{A_1(x_2)}(x_1) = \chi_{A_2(x_1)}(x_2) = \chi_A(x_1, x_2)$.

Given two measures μ_1 on Σ_1 and μ_2 on Σ_2 we now want to construct the **product measure**, $\mu_1 \otimes \mu_2$ on $\Sigma_1 \otimes \Sigma_2$ such that

$$\mu_1 \otimes \mu_2(A_1 \times A_2) = \mu_1(A_1)\mu_2(A_2), \quad A_j \in \Sigma_j, j = 1, 2. \quad (\text{A.59})$$

Theorem A.21. *Let μ_1 and μ_2 be two σ -finite measures on Σ_1 and Σ_2 , respectively. Let $A \in \Sigma_1 \otimes \Sigma_2$. Then $\mu_2(A_2(x_1))$ and $\mu_1(A_1(x_2))$ are measurable and*

$$\int_{X_1} \mu_2(A_2(x_1)) d\mu_1(x_1) = \int_{X_2} \mu_1(A_1(x_2)) d\mu_2(x_2). \quad (\text{A.60})$$

Proof. Let S be the set of all subsets for which our claim holds. Note that S contains at least all rectangles. It even contains the algebra of finite disjoint unions of rectangles. Thus it suffices to show that S is a monotone class. If μ_1 and μ_2 are finite, this follows from continuity from above and below of measures. The case if μ_1 and μ_2 are σ -finite can be handled as in Theorem A.5. \square

Hence we can define

$$\mu_1 \otimes \mu_2(A) = \int_{X_1} \mu_2(A_2(x_1)) d\mu_1(x_1) = \int_{X_2} \mu_1(A_1(x_2)) d\mu_2(x_2) \quad (\text{A.61})$$

or equivalently

$$\begin{aligned} \mu_1 \otimes \mu_2(A) &= \int_{X_1} \left(\int_{X_2} \chi_A(x_1, x_2) d\mu_2(x_2) \right) d\mu_1(x_1) \\ &= \int_{X_2} \left(\int_{X_1} \chi_A(x_1, x_2) d\mu_1(x_1) \right) d\mu_2(x_2). \end{aligned} \quad (\text{A.62})$$

Additivity of $\mu_1 \otimes \mu_2$ follows from the monotone convergence theorem.

Note that (A.59) uniquely defines $\mu_1 \otimes \mu_2$ as a σ -finite premeasure on the algebra of finite disjoint unions of rectangles. Hence by Theorem A.5 it is the only measure on $\Sigma_1 \otimes \Sigma_2$ satisfying (A.59).

Finally we have:

Theorem A.22 (Fubini). *Let f be a measurable function on $X_1 \times X_2$ and let μ_1, μ_2 be σ -finite measures on X_1, X_2 , respectively.*

(i) *If $f \geq 0$ then $\int f(\cdot, x_2) d\mu_2(x_2)$ and $\int f(x_1, \cdot) d\mu_1(x_1)$ are both measurable and*

$$\begin{aligned} \iint f(x_1, x_2) d\mu_1 \otimes \mu_2(x_1, x_2) &= \int \left(\int f(x_1, x_2) d\mu_1(x_1) \right) d\mu_2(x_2) \\ &= \int \left(\int f(x_1, x_2) d\mu_2(x_2) \right) d\mu_1(x_1). \end{aligned} \quad (\text{A.63})$$

(ii) *If f is complex then*

$$\int |f(x_1, x_2)| d\mu_1(x_1) \in \mathcal{L}^1(X_2, d\mu_2) \quad (\text{A.64})$$

respectively

$$\int |f(x_1, x_2)| d\mu_2(x_2) \in \mathcal{L}^1(X_1, d\mu_1) \quad (\text{A.65})$$

if and only if $f \in \mathcal{L}^1(X_1 \times X_2, d\mu_1 \otimes d\mu_2)$. In this case (A.63) holds.

Proof. By Theorem A.21 the claim holds for simple functions. Now (i) follows from the monotone convergence theorem and (ii) from the dominated convergence theorem. \square

In particular, if $f(x_1, x_2)$ is either nonnegative or integrable, then the order of integration can be interchanged.

Lemma A.23. *If μ_1 and μ_2 are σ -finite regular Borel measures with, so is $\mu_1 \otimes \mu_2$.*

Proof. Regularity holds for every rectangle and hence also for the algebra of finite disjoint unions of rectangles. Thus the claim follows from Lemma A.6. \square

Note that we can iterate this procedure.

Lemma A.24. *Suppose $\mu_j, j = 1, 2, 3$ are σ -finite measures. Then*

$$(\mu_1 \otimes \mu_2) \otimes \mu_3 = \mu_1 \otimes (\mu_2 \otimes \mu_3). \quad (\text{A.66})$$

Proof. First of all note that $(\Sigma_1 \otimes \Sigma_2) \otimes \Sigma_3 = \Sigma_1 \otimes (\Sigma_2 \otimes \Sigma_3)$ is the sigma algebra generated by the cuboids $A_1 \times A_2 \times A_3$ in $X_1 \times X_2 \times X_3$. Moreover, since

$$\begin{aligned} ((\mu_1 \otimes \mu_2) \otimes \mu_3)(A_1 \times A_2 \times A_3) &= \mu_1(A_1)\mu_2(A_2)\mu_3(A_3) \\ &= (\mu_1 \otimes (\mu_2 \otimes \mu_3))(A_1 \times A_2 \times A_3) \end{aligned} \quad (\text{A.67})$$

the two measures coincide on the algebra of finite disjoint unions of cuboids. Hence they coincide everywhere by Theorem A.5. \square

Example. If λ is Lebesgue measure on \mathbb{R} , then $\lambda^n = \lambda \otimes \cdots \otimes \lambda$ is Lebesgue measure on \mathbb{R}^n . Since λ is regular, so is λ^n . \diamond

A.6. Decomposition of measures

Let μ, ν be two measures on a measure space (X, Σ) . They are called **mutually singular** (in symbols $\mu \perp \nu$) if they are supported on disjoint sets. That is, there is a measurable set N such that $\mu(N) = 0$ and $\nu(X \setminus N) = 0$.

Example. Let λ be the Lebesgue measure and Θ the Dirac measure (centered at 0), then $\lambda \perp \Theta$: Just take $N = \{0\}$, then $\lambda(\{0\}) = 0$ and $\Theta(\mathbb{R} \setminus \{0\}) = 0$. \diamond

On the other hand, ν is called **absolutely continuous** with respect to μ (in symbols $\nu \ll \mu$) if $\mu(A) = 0$ implies $\nu(A) = 0$.

Example. The prototypical example is the measure $d\nu = f d\mu$ (compare Lemma A.15). Indeed $\mu(A) = 0$ implies

$$\nu(A) = \int_A f d\mu = 0 \quad (\text{A.68})$$

and shows that ν is absolutely continuous with respect to μ . In fact, we will show below that every absolutely continuous measure is of this form. \diamond

The two main results will follow as simple consequence of the following result:

Theorem A.25. *Let μ, ν be σ -finite measures. Then there exists a unique (a.e.) nonnegative function f and a set N of μ measure zero, such that*

$$\nu(A) = \nu(A \cap N) + \int_A f d\mu. \quad (\text{A.69})$$

Proof. We first assume μ, ν to be finite measures. Let $\alpha = \mu + \nu$ and consider the Hilbert space $L^2(X, d\alpha)$. Then

$$\ell(h) = \int_X h d\nu \quad (\text{A.70})$$

is a bounded linear functional by Cauchy-Schwarz:

$$\begin{aligned} |\ell(h)|^2 &= \left| \int_X 1 \cdot h \, d\nu \right|^2 \leq \left(\int |1|^2 \, d\nu \right) \left(\int |h|^2 \, d\nu \right) \\ &\leq \nu(X) \left(\int |h|^2 \, d\alpha \right) = \nu(X) \|h\|^2. \end{aligned} \quad (\text{A.71})$$

Hence by the Riesz lemma (Theorem 1.7) there exists an $g \in L^2(X, d\alpha)$ such that

$$\ell(h) = \int_X hg \, d\alpha. \quad (\text{A.72})$$

By construction

$$\nu(A) = \int \chi_A \, d\nu = \int \chi_A g \, d\alpha = \int_A g \, d\alpha. \quad (\text{A.73})$$

In particular, g must be positive a.e. (take A the set where g is negative). Furthermore, let $N = \{x | g(x) \geq 1\}$, then

$$\nu(N) = \int_N g \, d\alpha \geq \alpha(N) = \mu(N) + \nu(N), \quad (\text{A.74})$$

which shows $\mu(N) = 0$. Now set

$$f = \frac{g}{1-g} \chi_{N'}, \quad N' = X \setminus N. \quad (\text{A.75})$$

Then, since (A.73) implies $d\nu = g \, d\alpha$ respectively $d\mu = (1-g)d\alpha$, we have

$$\begin{aligned} \int_A f \, d\mu &= \int \chi_A \frac{g}{1-g} \chi_{N'} \, d\mu \\ &= \int \chi_{A \cap N'} g \, d\alpha \\ &= \nu(A \cap N') \end{aligned} \quad (\text{A.76})$$

as desired. Clearly f is unique, since if there is a second function \tilde{f} , then $\int_A (f - \tilde{f}) \, d\mu = 0$ for every A shows $f - \tilde{f} = 0$ a.e..

To see the σ -finite case, observe that $X_n \nearrow X$, $\mu(X_n) < \infty$ and $Y_n \nearrow X$, $\nu(Y_n) < \infty$ implies $X_n \cap Y_n \nearrow X$ and $\alpha(X_n \cap Y_n) < \infty$. Hence when restricted to $X_n \cap Y_n$ we have sets N_n and functions f_n . Now take $N = \bigcup N_n$ and choose f such that $f|_{X_n} = f_n$ (this is possible since $f_{n+1}|_{X_n} = f_n$ a.e.). Then $\mu(N) = 0$ and

$$\nu(A \cap N') = \lim_{n \rightarrow \infty} \nu(A \cap (X_n \setminus N)) = \lim_{n \rightarrow \infty} \int_{A \cap X_n} f \, d\mu = \int_A f \, d\mu, \quad (\text{A.77})$$

which finishes the proof. \square

Now the anticipated results follow with no effort:

Theorem A.26 (Lebesgue decomposition). *Let μ, ν be two σ -finite measures on a measure space (X, Σ) . Then ν can be uniquely decomposed as $\nu = \nu_{ac} + \nu_{sing}$, where ν_{ac} and ν_{sing} are mutually singular and ν_{ac} is absolutely continuous with respect to μ .*

Proof. Taking $\nu_{sing}(A) = \nu(A \cap N)$ and $d\nu_{ac} = f d\mu$ there is at least one such decomposition. To show uniqueness, let ν be finite first. If there is another one $\nu = \tilde{\nu}_{ac} + \tilde{\nu}_{sing}$, then let \tilde{N} be such that $\mu(\tilde{N}) = 0$ and $\tilde{\nu}_{sing}(\tilde{N}') = 0$. Then $\tilde{\nu}_{sing}(A) - \nu_{sing}(A) = \int_A (\tilde{f} - f) d\mu$. In particular, $\int_{A \cap N' \cap \tilde{N}'} (\tilde{f} - f) d\mu = 0$ and hence $\tilde{f} = f$ a.e. away from $N \cup \tilde{N}$. Since $\mu(N \cup \tilde{N}) = 0$, we have $\tilde{f} = f$ a.e. and hence $\tilde{\nu}_{ac} = \nu_{ac}$ as well as $\tilde{\nu}_{sing} = \nu - \tilde{\nu}_{ac} = \nu - \nu_{ac} = \nu_{sing}$. The σ -finite case follows as usual. \square

Theorem A.27 (Radon-Nikodym). *Let μ, ν be two σ -finite measures on a measure space (X, Σ) . Then ν is absolutely continuous with respect to μ if and only if there is a positive measurable function f such that*

$$\nu(A) = \int_A f d\mu \quad (\text{A.78})$$

for every $A \in \Sigma$. The function f is determined uniquely a.e. with respect to μ and is called the **Radon-Nikodym derivative** $\frac{d\nu}{d\mu}$ of ν with respect to μ .

Proof. Just observe that in this case $\nu(A \cap N) = 0$ for every A , that is $\nu_{sing} = 0$. \square

Problem A.9. *Let μ is a Borel measure on \mathfrak{B} and suppose its distribution function $\mu(x)$ is differentiable. Show that the Radon-Nikodym derivative equals the ordinary derivative $\mu'(x)$.*

Problem A.10 (Chain rule). *Show that $\nu \ll \mu$ is a transitive relation. In particular, if $\omega \ll \nu \ll \mu$ show that*

$$\frac{d\omega}{d\mu} = \frac{d\omega}{d\nu} \frac{d\nu}{d\mu}.$$

Problem A.11. *Suppose $\nu \ll \mu$. Show that*

$$\frac{d\omega}{d\mu} d\mu = \frac{d\omega}{d\nu} d\nu + d\zeta,$$

where ζ is a positive measure which is singular with respect to ν . Show that $\zeta = 0$ if and only if $\mu \ll \nu$.

A.7. Derivatives of measures

If μ is a Borel measure on \mathfrak{B} and its distribution function $\mu(x)$ is differentiable, then the Radon-Nikodym derivative is just the ordinary derivative

$\mu'(x)$. Our aim in this section is to generalize this result to arbitrary measures on \mathfrak{B}^n .

We call

$$(D\mu)(x) = \lim_{\varepsilon \downarrow 0} \frac{\mu(B_\varepsilon(x))}{|B_\varepsilon(x)|}, \quad (\text{A.79})$$

the derivative of μ at $x \in \mathbb{R}^n$ provided the above limit exists. (Here $B_r(x) \subset \mathbb{R}^n$ is a ball of radius r centered at $x \in \mathbb{R}^n$ and $|A|$ denotes the Lebesgue measure of $A \in \mathfrak{B}^n$).

Note that for a Borel measure on \mathfrak{B} , $(D\mu)(x)$ exists if and only if $\mu(x)$ (as defined in (A.3)) is differentiable at x and $(D\mu)(x) = \mu'(x)$ in this case.

We will assume that μ is regular throughout this section. It can be shown that every Borel

To compute the derivative of μ we introduce the **upper** and **lower derivative**

$$(\overline{D}\mu)(x) = \limsup_{\varepsilon \downarrow 0} \frac{\mu(B_\varepsilon(x))}{|B_\varepsilon(x)|} \quad \text{and} \quad (\underline{D}\mu)(x) = \liminf_{\varepsilon \downarrow 0} \frac{\mu(B_\varepsilon(x))}{|B_\varepsilon(x)|}. \quad (\text{A.80})$$

Clearly μ is differentiable if $(\overline{D}\mu)(x) = (\underline{D}\mu)(x) < \infty$. First of all note that they are measurable:

Lemma A.28. *The upper derivative is lower semicontinuous, that is the set $\{x | (\overline{D}\mu)(x) > \alpha\}$ is open for every $\alpha \in \mathbb{R}$. Similarly, the lower derivative is upper semicontinuous, that is $\{x | (\underline{D}\mu)(x) < \alpha\}$ is open.*

Proof. We only prove the claim for $\overline{D}\mu$, the case $\underline{D}\mu$ being similar. Abbreviate,

$$M_r(x) = \sup_{0 < \varepsilon < r} \frac{\mu(B_\varepsilon(x))}{|B_\varepsilon(x)|} \quad (\text{A.81})$$

and note that it suffices to show that $O_r = \{x | M_r(x) > \alpha\}$ is open.

If $x \in O_r$, there is some $\varepsilon < r$ such that

$$\frac{\mu(B_\varepsilon(x))}{|B_\varepsilon(x)|} > \alpha. \quad (\text{A.82})$$

Let $\delta > 0$ and $y \in B_\delta(x)$. Then $B_\varepsilon(x) \subseteq B_{\varepsilon+\delta}(y)$ implying

$$\frac{\mu(B_{\varepsilon+\delta}(y))}{|B_{\varepsilon+\delta}(y)|} \geq \left(\frac{\varepsilon}{\varepsilon+\delta}\right)^n \frac{\mu(B_\varepsilon(x))}{|B_\varepsilon(x)|} > \alpha \quad (\text{A.83})$$

for δ sufficiently small. That is, $B_\delta(x) \subseteq O$. \square

In particular, both the upper and lower derivative are measurable. Next, the following geometric fact of \mathbb{R}^n will be needed.

Lemma A.29. *Given open balls B_1, \dots, B_m in \mathbb{R}^n , there is a subset of disjoint balls B_{j_1}, \dots, B_{j_k} such that*

$$\left| \bigcup_{i=1}^m B_i \right| \leq 3^n \sum_{i=1}^k |B_{j_i}|. \quad (\text{A.84})$$

Proof. Start with $B_{j_1} = B_1 = B_{r_1}(x_1)$ and remove all balls from our list which intersect B_{j_1} . Observe that the removed balls are all contained in $3B_1 = B_{3r_1}(x_1)$. Proceeding like this we obtain B_{j_1}, \dots, B_{j_k} such that

$$\bigcup_{i=1}^m B_i \subseteq \bigcup_{i=1}^k B_{3r_{j_i}}(x_{j_i}) \quad (\text{A.85})$$

and the claim follows since $|B_{3r}(x)| = 3^n |B_r(x)|$. \square

Now we can show

Lemma A.30. *Let $\alpha > 0$. For any Borel set A we have*

$$|\{x \in A \mid (\overline{D}\mu)(x) > \alpha\}| \leq 3^n \frac{\mu(A)}{\alpha} \quad (\text{A.86})$$

and

$$|\{x \in A \mid (\overline{D}\mu)(x) > 0\}| = 0, \text{ whenever } \mu(A) = 0. \quad (\text{A.87})$$

Proof. Let $A_\alpha = \{x \mid (\overline{D}\mu)(x) > \alpha\}$. We will show

$$|K| \leq 3^n \frac{\mu(O)}{\alpha} \quad (\text{A.88})$$

for any compact set K and open set O with $K \subseteq E \subseteq O$. The first claim then follows from regularity of μ and the Lebesgue measure.

Given fixed K, O , for every $x \in K$ there is some r_x such that $B_{r_x}(x) \subseteq O$ and $|B_{r_x}(x)| < \alpha^{-1} \mu(B_{r_x}(x))$. Since K is compact, we can choose a finite subcover of K . Moreover, by Lemma A.29 we can refine our set of balls such that

$$|K| \leq 3^n \sum_{i=1}^k |B_{r_i}(x_i)| < \frac{3^n}{\alpha} \sum_{i=1}^k \mu(B_{r_i}(x_i)) \leq 3^n \frac{\mu(O)}{\alpha}. \quad (\text{A.89})$$

To see the second claim, observe that

$$\{x \in A \mid (\overline{D}\mu)(x) > 0\} = \bigcup_{j=1}^{\infty} \{x \in A \mid (\overline{D}\mu)(x) > \frac{1}{j}\} \quad (\text{A.90})$$

and by the first part $|\{x \in A \mid (\overline{D}\mu)(x) > \frac{1}{j}\}| = 0$ for any j if $\mu(A) = 0$. \square

Theorem A.31 (Lebesgue). *Let f be (locally) integrable, then for a.e. $x \in \mathbb{R}^n$ we have*

$$\lim_{r \downarrow 0} \frac{1}{|B_r(x)|} \int_{B_r(x)} |f(y) - f(x)| dy = 0. \quad (\text{A.91})$$

Proof. Decompose f as $f = g + h$, where g is continuous and $\|h\|_1 < \varepsilon$ (Theorem 0.31) and abbreviate

$$D_r(f)(x) = \frac{1}{|B_r(x)|} \int_{B_r(x)} |f(y) - f(x)| dy. \quad (\text{A.92})$$

Then, since $\lim F_r(g)(x) = 0$ (for every x) and $D_r(f) \leq D_r(g) + D_r(h)$ we have

$$\limsup_{r \downarrow 0} D_r(f) \leq \limsup_{r \downarrow 0} D_r(h) \leq (\overline{D}\mu)(x) + |h(x)|, \quad (\text{A.93})$$

where $d\mu = |h|dx$. Using $|\{x \mid |h(x)| \geq \alpha\}| \leq \alpha^{-1} \|h\|_1$ and the first part of Lemma A.30 we see

$$|\{x \mid \limsup_{r \downarrow 0} D_r(f)(x) \geq \alpha\}| \leq (3^n + 1) \frac{\varepsilon}{\alpha} \quad (\text{A.94})$$

Since ε is arbitrary, the Lebesgue measure of this set must be zero for every α . That is, the set where the limsup is positive has Lebesgue measure zero. \square

The points where (A.91) holds are called **Lebesgue points** of f .

Note that the balls can be replaced by more general sets: A sequence of sets $A_j(x)$ is said to shrink to x nicely if there are balls $B_{r_j}(x)$ with $r_j \rightarrow 0$ and a constant $\varepsilon > 0$ such that $A_j(x) \subseteq B_{r_j}(x)$ and $|A_j| \geq \varepsilon |B_{r_j}(x)|$. For example $A_j(x)$ could be some balls or cubes (not necessarily containing x). However, the portion of $B_{r_j}(x)$ which they occupy must not go to zero! For example the rectangles $(0, \frac{1}{j}) \times (0, \frac{2}{j}) \subset \mathbb{R}^2$ do shrink nicely to 0, but the rectangles $(0, \frac{1}{j}) \times (0, \frac{2}{j^2})$ don't.

Lemma A.32. *Let f be (locally) integrable, then at every Lebesgue point we have*

$$f(x) = \lim_{j \rightarrow \infty} \frac{1}{|A_j(x)|} \int_{A_j(x)} f(y) dy. \quad (\text{A.95})$$

whenever $A_j(x)$ shrinks to x nicely.

Proof. Let x be a Lebesgue point and choose some nicely shrinking sets $A_j(x)$ with corresponding $B_{r_j}(x)$ and ε . Then

$$\frac{1}{|A_j(x)|} \int_{A_j(x)} |f(y) - f(x)| dy \leq \frac{1}{\varepsilon |B_{r_j}(x)|} \int_{B_{r_j}(x)} |f(y) - f(x)| dy \quad (\text{A.96})$$

and the claim follows. \square

Corollary A.33. *Suppose μ is an absolutely continuous Borel measure on \mathbb{R} , then its distribution function is differentiable a.e. and $d\mu(x) = \mu'(x)dx$.*

As another consequence we obtain

Theorem A.34. *Let μ be a Borel measure on \mathbb{R}^n . The derivative $D\mu$ exists a.e. with respect to Lebesgue measure and equals the Radon-Nikodym derivative of the absolutely continuous part of μ with respect to Lebesgue measure, that is,*

$$\mu_{ac}(A) = \int_A (D\mu)(x)dx. \quad (\text{A.97})$$

Proof. If $d\mu = f dx$ is absolutely continuous with respect to Lebesgue measure the claim follows from Theorem A.31. To see the general case use the Lebesgue decomposition of μ and let N be a support for the singular part with $|N| = 0$. Then $(\overline{D}\mu_{sing})(x) = 0$ for a.e. $x \in N'$ by the second part of Lemma A.30. \square

In particular, μ is singular with respect to Lebesgue measure if and only if $D\mu = 0$ a.e. with respect to Lebesgue measure.

Using the upper and lower derivatives we can also give supports for the absolutely and singularly continuous parts.

Theorem A.35. *The set $\{x | (D\mu)(x) = \infty\}$ is a support for the singular and $\{x | 0 < (D\mu)(x) < \infty\}$ is a support for the absolutely continuous part.*

Proof. Suppose μ is purely singular first. Let us show that the set $O_k = \{x | (\underline{D}\mu)(x) < k\}$ satisfies $\mu(O_k) = 0$ for every $k \in \mathbb{N}$.

Let $K \subset O_k$ be compact, let $V_j \supset K$ be some open set such that $|V_j \setminus K| \leq \frac{1}{j}$. For every $x \in K$ there is some $\varepsilon = \varepsilon(x)$ such that $B_\varepsilon(x) \subseteq V_j$ and $\mu(B_\varepsilon(x)) \leq k|B_\varepsilon(x)|$. By compactness, finitely many of these balls cover K and hence

$$\mu(K) \leq \sum_i \mu(B_{\varepsilon_i}(x_i)) \leq k \sum_i |B_{\varepsilon_i}(x_i)|. \quad (\text{A.98})$$

Selecting disjoint balls as in Lemma A.29 further shows

$$\mu(K) \leq k3^n \sum_\ell |B_{\varepsilon_{i_\ell}}(x_{i_\ell})| \leq k3^n |V_j|. \quad (\text{A.99})$$

Letting $j \rightarrow \infty$ we see $\mu(K) \leq k3^n |K|$ and by regularity we even have $\mu(A) \leq k3^n |A|$ for every $A \subseteq O_k$. Hence μ is absolutely continuous on O_k and since we assumed μ to be singular we must have $\mu(O_k) = 0$.

Thus $(\underline{D}\mu_{sing})(x) = \infty$ for a.e. x with respect to μ_{sing} and we are done. \square

Example. The **Cantor function** is constructed as follows: Take the sets C_n used in the construction of the Cantor set C : C_n is the union of 2^n closed intervals with $2^n - 1$ open gaps in between. Set f_n equal to $j/2^n$ on the j 'th gap of C_n and extend it to $[0, 1]$ by linear interpolation. Note that, since we are creating precisely one new gap between every old gap when going from C_n to C_{n+1} , the value of f_{n+1} is the same as the value of f_n on the gaps of C_n . In particular, $\|f_n - f_m\|_\infty \leq 2^{-\min(n,m)}$ and hence we can define the Cantor function as $f = \lim_{n \rightarrow \infty} f_n$. By construction f is a continuous function which is constant on every subinterval of $[0, 1] \setminus C$. Since C is of Lebesgue measure zero, this set is of full Lebesgue measure and hence $f' = 0$ a.e. in $[0, 1]$. In particular, the corresponding measure, the **Cantor measure**, is supported on C and purely singular with respect to Lebesgue measure. \diamond

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Glossary of notations

$AC(I)$... absolutely continuous functions, 72
\mathfrak{B}	$= \mathfrak{B}^1$
\mathfrak{B}^n	... Borel σ -field of \mathbb{R}^n , 210 .
$\mathfrak{C}(\mathfrak{H})$... set of compact operators, 112 .
$C(U)$... set of continuous functions from U to \mathbb{C} .
$C_\infty(U)$... set of functions in $C(U)$ which vanish at ∞ .
$C(U, V)$... set of continuous functions from U to V .
$C_c^\infty(U, V)$... set of compactly supported smooth functions
$\chi_\Omega(\cdot)$... characteristic function of the set Ω
\dim	... dimension of a linear space
$\text{dist}(x, Y)$	$= \inf_{y \in Y} \ x - y\ $, distance between x and Y
$\mathfrak{D}(\cdot)$... domain of an operator
e	... exponential function, $e^z = \exp(z)$
$\mathbb{E}(A)$... expectation of an operator A , 47
\mathcal{F}	... Fourier transform, 139
H	... Schrödinger operator, 177
H_0	... free Schrödinger operator, 142
$H^m(a, b)$... Sobolev space, 72
$H^m(\mathbb{R}^n)$... Sobolev space, 141
$\text{hull}(\cdot)$... convex hull
\mathfrak{H}	... a separable Hilbert space
i	... complex unity, $i^2 = -1$
$\text{Im}(\cdot)$... imaginary part of a complex number
\inf	... infimum
$\text{Ker}(A)$... kernel of an operator A
$\mathfrak{L}(X, Y)$... set of all bounded linear operators from X to Y , 20

$\mathfrak{L}(X)$	$= \mathfrak{L}(X, X)$
$L^p(M, d\mu)$... Lebesgue space of p integrable functions, 22
$L^p_{loc}(M, d\mu)$... locally p integrable functions
$L^p_c(M, d\mu)$... compactly supported p integrable functions
$L^\infty(M, d\mu)$... Lebesgue space of bounded functions, 23
$L^\infty(\mathbb{R}^n)$... Lebesgue space of bounded functions vanishing at ∞
λ	... a real number
\max	... maximum
\mathcal{M}	... Mellin transform, 201
μ_ψ	... spectral measure, 82
\mathbb{N}	... the set of positive integers
\mathbb{N}_0	$= \mathbb{N} \cup \{0\}$
Ω	... a Borel set
Ω_\pm	... wave operators, 197
$P_A(\cdot)$... family of spectral projections of an operator A
P_\pm	... projector onto outgoing/incoming states, 200
\mathbb{Q}	... the set of rational numbers
$\mathfrak{D}(\cdot)$... form domain of an operator, 84
$R(I, X)$... set of regulated functions, 98
$R_A(z)$... resolvent of A , 62
$\text{Ran}(A)$... range of an operator A
$\text{rank}(A)$	$= \dim \text{Ran}(A)$, rank of an operator A , 111
$\text{Re}(\cdot)$... real part of a complex number
$\rho(A)$... resolvent set of A , 61
\mathbb{R}	... the set of real numbers
$S(I, X)$... set of simple functions, 98
$\mathcal{S}(\mathbb{R}^n)$... set of smooth functions with rapid decay, 139
\sup	... supremum
supp	... support of a function
$\sigma(A)$... spectrum of an operator A , 61
$\sigma_{ac}(A)$... absolutely continuous spectrum of A , 91
$\sigma_{sc}(A)$... singular continuous spectrum of A , 91
$\sigma_{pp}(A)$... pure point spectrum of A , 91
$\sigma_p(A)$... point spectrum (set of eigenvalues) of A , 88
$\sigma_d(A)$... discrete spectrum of A , 119
$\sigma_{ess}(A)$... essential spectrum of A , 119
$\text{span}(M)$... set of finite linear combinations from M , 12
\mathbb{Z}	... the set of integers
z	... a complex number

\mathbb{I}	... identity operator
\sqrt{z}	... square root of z with branch cut along $(-\infty, 0)$
z^*	... complex conjugation
A^*	... adjoint of A , 51
\overline{A}	... closure of A , 55
\hat{f}	$= \mathcal{F}f$, Fourier transform of f
\check{f}	$= \mathcal{F}^{-1}f$, inverse Fourier transform of f
$\ \cdot\ $... norm in the Hilbert space \mathfrak{H}
$\ \cdot\ _p$... norm in the Banach space L^p , 22
$\langle \cdot, \cdot \rangle$... scalar product in \mathfrak{H}
$\mathbb{E}_\psi(A)$	$= \langle \psi, A\psi \rangle$ expectation value
$\Delta_\psi(A)$	$= \mathbb{E}_\psi(A^2) - \mathbb{E}_\psi(A)^2$ variance
\oplus	... orthogonal sum of linear spaces or operators, 38
Δ	... Laplace operator, 142
∂	... gradient, 139
∂_α	... derivative, 139
M^\perp	... orthogonal complement, 36
(λ_1, λ_2)	$= \{\lambda \in \mathbb{R} \mid \lambda_1 < \lambda < \lambda_2\}$, open interval
$[\lambda_1, \lambda_2]$	$= \{\lambda \in \mathbb{R} \mid \lambda_1 \leq \lambda \leq \lambda_2\}$, closed interval
$\psi_n \rightarrow \psi$... norm convergence
$\psi_n \rightharpoonup \psi$... weak convergence, 41
$A_n \rightarrow A$... norm convergence
$A_n \xrightarrow{s} A$... strong convergence, 43
$A_n \rightharpoonup A$... weak convergence, 43
$A_n \xrightarrow{nr} A$... norm resolvent convergence, 131
$A_n \xrightarrow{sr} A$... strong resolvent convergence, 131

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