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Mathematical Foundations of Quantum Mechanics

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Contents

Introduction

These lecture notes were created as a companion to the lecture series hold together with Kedar Ranade in the summer term 2015 under the same title. The lecture was aimed at both master students of physics and mathematics. Therefore we required no prior exposure to neither the apparatus of functional analysis nor to quantum physics. The mathematical background was presented in my lectures, whereas the students were introduced to the physics of quantum mechanics in Kedar's part of the lecture.

The aim of the lectures was to present most of the mathematical results and concepts used in an introductory course in quantum mechanics in a rigorous way. Since physics students usually have no background in Lebesgue integration, a short primer on this topic without proofs is contained in the first chapter. Thereafter the fundamentals of the theory of Hilbert and Sobolev spaces and their connection with the Fourier transform are developed from scratch. It follows a detailed study of self-adjoint operators and the self-adjointness of important quantum mechanical observables, such as the Hamiltonian of the hydrogen atom, is shown. Further, the notes contain a careful presentation of the spectral theorem for unbounded self-adjoint operators and a proof of Stone's theorem on unitary groups which is central for the description of the time evolution of quantum mechanical systems. The spectral theory of self-adjoint operators and Hamiltonians is only covered in a very rudimentary manner.

In the last part a short introduction to the theory of distributions is given. Further, we present the nuclear spectral theorem which gives the spectral decomposition of self-adjoint operators in a form very natural for physicists.

The appendix covers precise mathematical statements of the postulates of quantum mechanics presented in the course for further easy reference.

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1 A Crash Course in Measure Theory

In classical quantum mechanics (pure) a quantum mechanical system is described by some complex Hilbert space. For example, the (pure) states of a single one-dimensional particle can be described by elements in the Hilbert space $L^2(\mathbb{R})$ as introduced in introductory courses in quantum mechanics. A natural first attempt to mathematically define this space is the following:

$$L^2(\mathbb{R}) = \left\{ f : \mathbb{R} \to \mathbb{C} : f_{|[-n,n]} \text{ Riemann-int. for } n \in \mathbb{N} \text{ and } \int_{-\infty}^{\infty} |f(x)|^2 \, dx < \infty \right\}.$$

However, there are several issues. First of all, the natural choice

$$\|f\|_2 := \left(\int_{-\infty}^{\infty} |f(x)|^2 \, dx \right)^{1/2}$$

does not define a norm on $L^2(\mathbb{R})$ as there exist functions $0 \neq f \in L^2(\mathbb{R})$ with $\|f\|_2 = 0$. This problem can easily be solved by identifying two functions $f, g \in L^2(\mathbb{R})$ whenever $\|f - g\|_2 = 0$. A more fundamental problem is that the above defined space is not complete, i.e. there exist Cauchy sequences in $L^2(\mathbb{R})$ which do not converge in $L^2(\mathbb{R})$. Therefore one has to replace $L^2(\mathbb{R})$ as defined above by its completion. This is perfectly legitimate from a mathematical point of view. However, this approach has a severe shortcoming: we do not have an explicit description of the elements in the completion. Even worse, we do not even know whether these elements can be represented as functions.

To overcome these issues, we now introduce an alternative way to integration, finally replacing the Riemann-integral by the so-called *Lebesgue-integral*. In order to be able to introduce the Lebesgue-integral we need first a rigorous method to measure the volume of subsets of $\mathbb{R}^n$ or more abstract sets which then can be used to define the Lebesgue integral.

The material covered in this chapter essentially corresponds to the basic definitions and results presented in an introductory course to measure theory. We just give the definitions with some basic examples to illustrate the concepts and then state the main theorems without proofs. More details and the proofs can be learned in any course on measure theory or from the many excellent text books, for example [Bar95] or [Rud87]. For further details we guide the interested reader to the monographs [Bog07].

1.1 Measure Spaces

For $n \in \mathbb{N}$ let $\mathcal{P}(\mathbb{R}^n)$ denote the set of all subsets of $\mathbb{R}^n$. The measurement of volumes can then be described by a mapping $m \colon \mathcal{P}(\mathbb{R}^n) \to \mathbb{R}_{\geq 0} \cup \{\infty\}$. In order to obtain a reasonable notion of volume one should at least require

(i) $m(A \cup B) = m(A) + m(B)$ for all $A, B \subset \mathbb{R}^n$ with $A \cap B = \emptyset$,

(ii) $m(A) = m(B)$ whenever $A, B \subset \mathbb{R}^n$ are congruent, i.e. B can be obtained from B by a finite combination of rigid motions.

Intuitively, this sounds perfectly fine. However, there is the following result published by S. Banach and A. Tarski in 1924.

Theorem 1.1.1 (Banach–Tarski paradox). *Let $n \geq 3$ and $A, B \subset \mathbb{R}^n$ be arbitrary bounded subsets with non-empty interiors. Then A and B can be partitioned into a finite number of disjoints subsets*

$$A = A_1 \cup \ldots \cup A_n \qquad \text{and} \qquad B = B_1 \cup \ldots \cup B_n$$

such that for all $i = 1, \ldots, n$ the sets A_i and B_i are congruent.

Using such paradoxical decompositions we see that m must agree for all bounded subsets of $\mathbb{R}^n$ with non-empty interiors. For example, by splitting a cube Q into two smaller parts, we see that $m(Q) \in (0, \infty)$ leads to a contradiction. Hence, it is impossible to measure the volume of arbitrary subsets of $\mathbb{R}^n$ in a reasonable way!

Remark 1.1.2. Of course, we all know that in physical reality such a paradox does not occur. Indeed, the decompositions given by the Banach–Tarski paradox are not constructive and therefore cannot be realized in the real world. More precisely in mathematical terms, the proof of the Banach–Tarski paradox requires some form of the axiom of choice.

Since we cannot measure the volume of arbitrary subsets of $\mathbb{R}^n$ in a consistent reasonable way, it is necessary to restrict the volume measurement to a subset of $\mathcal{P}(\mathbb{R}^n)$. This subset should be closed under basic set theoretic operations. This leads to the following definition which can be given for arbitrary sets Ω instead of $\mathbb{R}^n$.

Definition 1.1.3 (σ-algebra). Let Ω be a set. A subset $\Sigma \subset \mathcal{P}(\Omega)$ is called a *σ-algebra* if

(a) $\emptyset \in \Sigma$,

(b) $A^c \in \Sigma$ for all $A \in \Sigma$,

(c) $\cup_{n \in \mathbb{N}} A_n \in \Sigma$ whenever $(A_n)_{n \in \mathbb{N}} \subset \Sigma$.

The tuple (Ω, Σ) is called a *measurable space* and the elements of Σ are called *measurable*.

Note that it follows from the definition that for $A, B \in \Sigma$ one also has $A \cap B \in \Sigma$ and $B \setminus A \in \Sigma$. The closedness of Σ under countable unions may be the less intuitive of the above defining properties. It guarantees that σ-algebras behave well under limiting processes which lie at the hearth of analysis. We now give some elementary examples of σ-algebras.

Example 1.1.4. (i) Let Ω be an arbitrary set. Then the power set $\mathcal{P}(\Omega)$ is clearly a σ-algebra.

(ii) Let Ω be an arbitrary set. We define Σ as the set of subsets of Ω which are countable or whose complement is countable. One then can check that Σ is a σ-algebra. Here one has to use the fact that countable unions of countable sets are again countable. Note that Σ does in general not agree with $\mathcal{P}(\Omega)$. For example, if $\Omega = \mathbb{R}$, then the interval $[0,1]$ is not contained in Σ.

We now give an important and non-trivial example of a σ-algebra which will be frequently used in the following.

Example 1.1.5 (Borel σ-algebra). Let Ω be a subset of $\mathbb{R}^n$ for $n \in \mathbb{N}$, or more general a normed, metric or topological space. Then the smallest σ-algebra that contains all open sets $\mathcal{O}$ of Ω

$$\mathcal{B}(\Omega) = \bigcap_{\substack{\Sigma\ \sigma\text{-algebra:} \\ \Sigma \supset \mathcal{O}}} \Sigma$$

is called the *Borel σ-algebra* on Ω. One can show that $\mathcal{B}(\mathbb{R}^n)$ is the smallest σ-algebra that is generated by elements of the form $[a_1, b_1) \times \cdots [a_n, b_n)$ for $a_i < b_i$, i.e. by products of half-open intervals.

Recall that a function $f : \Omega_1 \to \Omega_2$ between two normed or more general metric or topological spaces is continuous if and only if the preimage of every open set under f is again open. This means that f preserves the topological structure. In the same spirit *measurable mappings* are compatible with the measurable structures on the underlying spaces.

Definition 1.1.6 (Measurable mapping). Let (Ω_1, Σ_1) and (Ω_2, Σ_2) be two measurable spaces. A map $f : \Omega_1 \to \Omega_2$ is called *measurable* if

$$f^{-1}(A) \in \Sigma_1 \qquad \text{for all } A \in \Sigma_2.$$

A function $f : \Omega_1 \to \Omega_2$ between two normed spaces (or more generally two metric or topological spaces) is called *measurable* if f is a measurable map between the measurable spaces $(\Omega_1, \mathcal{B}(\Omega_1))$ and $(\Omega_2, \mathcal{B}(\Omega_2))$.

It is often very convenient to consider functions $f\colon \Omega \to \overline{\mathbb{R}}$, where $\overline{\mathbb{R}}$ denotes the extended real line $\overline{\mathbb{R}} = \mathbb{R} \cup \{\infty\} \cup \{-\infty\}$. In this case one calls f measurable if and only if $X_\infty = \{x \in \Omega : f(x) = \infty\}$ and $X_{-\infty} = \{x \in \Omega : f(x) = -\infty\}$ are measurable and the restricted function $f\colon \Omega \setminus (X_\infty \cup X_{-\infty}) \to \mathbb{R}$ is measurable in the sense just defined above. If a real-valued function takes the values ∞ or $-\infty$, we will implicitly always work with this definition. We will often need the following sufficient conditions for a mapping to be measurable.

Proposition 1.1.7. *Let Ω_1 and Ω_2 be two normed vector spaces or more generally metric or topological spaces. Then every continuous mapping $f\colon \Omega_1 \to \Omega_2$ is measurable. Further, every monotone function $f\colon \mathbb{R} \to \mathbb{R}$ is measurable.*

Furthermore, measurable functions are closed under the usual arithmetic operations and under pointwise limits.

Proposition 1.1.8. *Let (Ω, Σ, μ) be a measure space.*

(a) *Let $f, g\colon \Omega \to \mathbb{C}$ be measurable. Then $f+g$, $f-g$, $f \cdot g$ and f/g provided $g(x) \neq 0$ for all $x \in \Omega$ are measurable as well.*

(b) *Let $f_n\colon \Omega \to \mathbb{C}$ be a sequence of measurable functions such that $f(x) := \lim_{n\to\infty} f_n(x)$ exists for all $x \in \Omega$. Then f is measurable.*

We now assign a measure to a measurable space.

Definition 1.1.9 (Measure). Let (Ω, Σ) be a measurable space. A *measure* on (Ω, Σ) is a mapping $\mu\colon \Sigma \to \mathbb{R}_{\geq 0} \cup \{\infty\}$ that satisfies

(i) $\mu(\emptyset) = 0$.

(ii) $\mu(\cup_{n\in\mathbb{N}} A_n) = \sum_{n=1}^{\infty} \mu(A_n)$ for all pairwise disjoint $(A_n)_{n\in\mathbb{N}} \subset \Sigma$.

The triple (Ω, Σ, μ) is a *measure space*. If $\mu(\Omega) < \infty$, then (Ω, Σ, μ) is called a *finite measure space*. If $\mu(\Omega) = 1$, one says that (Ω, Σ, μ) is a *probability space*.

One can deduce from the above definition that a measure satisfies $\mu(A) \leq \mu(B)$ for all measurable $A \subset B$ and $\mu(\cup_{n\in\mathbb{N}} B_n) \leq \sum_{n=1}^{\infty} \mu(B_n)$ for arbitrary $(B_n)_{n\in\mathbb{N}} \subset \Sigma$. Moreover, one has $\mu(A \setminus B) = \mu(A) - \mu(B)$ for measurable $B \subset A$ whenever $\mu(B) < \infty$. We begin with some elementary examples of measure spaces.

Example 1.1.10. (i) Consider $(\Omega, \mathcal{P}(\Omega))$ for an arbitrary set Ω and define $\mu(A)$ as the number of elements in A whenever A is a finite subset and $\mu(A) = \infty$ otherwise. Then μ is a measure on $(\Omega, \mathcal{P}(\Omega))$.

(ii) Let Ω be an arbitrary non-empty set and $a \in \Omega$. Define

$$\delta_a \colon \mathcal{P}(\Omega) \to \mathbb{R}_{\geq 0}$$
$$A \mapsto \begin{cases} 1 & \text{if } a \in A \\ 0 & \text{else} \end{cases}.$$

Then δ_a is a measure on $(\Omega, \mathcal{P}(\Omega))$ and is called the *Dirac measure in a*.

We now come to the most important example for our purposes.

Theorem 1.1.11 (Lebesgue Measure). *Let $n \in \mathbb{N}$. There exists a unique* Borel measure λ, *i.e. a measure defined on* $(\mathbb{R}^n, \mathcal{B}(\mathbb{R}^n))$, *that satisfies*

$$\lambda([a_1, b_1) \times \cdots [a_n, b_n)) = \prod_{k=1}^{n} (b_k - a_k)$$

for all products with $a_i < b_i$. The measure λ is called the Lebesgue measure *on* $\mathbb{R}^n$.

Of course, one can also restrict the Lebesuge measure to $(\Omega, \mathcal{B}(\Omega))$ for subsets $\Omega \subset \mathbb{R}^n$. The uniqueness in the above theorem is not trivial, but essentially follows from the fact that the products of half-open intervals used in the above definition generate the Borel-σ-algebra and are closed under finite intersections. The existence is usually proved via Carathéodory's extension theorem.

1.2 The Lebesgue Integral

Given a measure space (Ω, Σ, μ), one can integrate certain functions $f : \Omega \to \mathbb{C}$ over the measure μ. One extends the integral step by step to more general classes of functions. A function $f : \Omega \to \mathbb{C}$ is a *simple function* if there exist finite measurable sets $A_1, \ldots, A_n \in \Sigma$ and $a_1, \ldots, a_n \in \mathbb{C}$ such that $f = \sum_{k=1}^{n} a_k \mathbb{1}_{A_k}$. Here $\mathbb{1}_{A_k}$ is the function defined by

$$\mathbb{1}_{A_k}(x) = \begin{cases} 1 & \text{if } x \in A_k \\ 0 & \text{if } x \notin A_k \end{cases}.$$

Definition 1.2.1 (Lebesgue integral). Let (Ω, Σ, μ) be a measure space.

(i) For a simple function $f : \Omega \to \mathbb{R}_{\geq 0}$ given by $f = \sum_{k=1}^{n} a_k \mathbb{1}_{A_k}$ as above one defines the Lebesgue integral as

$$\int_\Omega f \, d\mu = \sum_{k=1}^{n} a_k \mu(A_k).$$

(ii) For a measurable function $f : \Omega \to \mathbb{R}_{\geq 0}$ the Lebesgue integral is defined as

$$\int_\Omega f \, d\mu = \sup_{\substack{g \text{ simple:} \\ 0 \leq g \leq f}} \int_\Omega g \, d\mu.$$

(iii) A general measurable function $f : \Omega \to \mathbb{C}$ can be uniquely decomposed into for non-negative measurable functions $f : \Omega \to \mathbb{R}_{\geq 0}$ such hat $f = (f_1 - f_2) + i(f_3 - f_4)$. One says that f is *integrable* if $\int_\Omega f_i \, d\mu < \infty$ and writes $f \in \mathcal{L}^1(\Omega, \Sigma, \mu)$. In this case one sets the Lebesgue integral as

$$\int_\Omega f \, d\mu = \int_\Omega f_1 \, d\mu - \int_\Omega f_2 \, d\mu + i\left(\int_\Omega f_3 \, d\mu - \int_\Omega f_4 \, d\mu\right).$$

Moreover, for a measurable set $A \in \Sigma$ we use the short-hand notation

$$\int_A f \, d\mu := \int_\Omega \mathbb{1}_A f \, d\mu$$

whenever the integral on the right hand side exists.

We will often use the following terminology. Let (Ω, Σ, μ) be a measure space and $P(x)$ a property for every $x \in \Omega$. We say that P holds almost everywhere if there exists a set $N \in \Sigma$ with $\mu(N) = 0$ such that $P(x)$ holds for all $x \notin N$. For example, on $(\mathbb{R}, \mathcal{B}(\mathbb{R}), \lambda)$ the function $f(x) = \cos(\pi x)$ satisfies $|f(x)| < 1$ almost everywhere because one can choose $N = \mathbb{Z}$ which has zero Lebesgue measure. In the following we will often make use of that the fact that the integrals over two measurable functions f and g agree whenever $f(x) = g(x)$ almost everywhere.

Notice that we can now integrate a function $f : [a, b] \to \mathbb{C}$ in two different ways by either using the Riemann or the Lebesgue integral. These two integrals however agree as soon as both make sense and the Lebesgue integral can be considered as a true extension of the Riemann integral (except for some minor measurability issues).

Theorem 1.2.2 (Lebesgue integral equals Riemann integral). *The Riemann and Lebesgue integral have the following properties.*

(a) *Let $f : [a, b] \to \mathbb{C}$ be a Riemann integrable function. Then there exists a measurable function $g : [a, b] \to \mathbb{C}$ with $f = g$ almost everywhere and $g \in \mathcal{L}^1([a, b], \mathcal{B}([a, b]), \lambda)$. Moreover, one has*

$$\int_a^b f(x) \, dx = \int_{[a,b]} g \, d\lambda.$$

(b) *Let $f : I \to \mathbb{C}$ for some interval $I \subset \mathbb{R}$ be Riemann integrable in the improper sense. If*

$$\sup_{\substack{K \subset I \\ \text{compact interval}}} \int_K |f(x)|\, dx < \infty,$$

then there exists a measurable function $g\colon I \to \mathbb{C}$ with $f = g$ almost everywhere and $g \in \mathcal{L}^1(I, \mathcal{B}(I), \lambda)$. Moreover, one has

$$\int_I f(x)\, dx = \int_I g\, d\lambda.$$

Moreover, if f is measurable (for example if f is continuous), one can choose g equal to f.

For an example of a Lebesgue-integrable function which is not Riemann-integrable, consider $f(x) = \mathbb{1}_{[0,1]\cap\mathbb{Q}}(x)$. Then f is not Riemann-integrable as on arbitrary fine partitions of $[0,1]$ the function takes both values 0 and 1, whereas the Lebesgue integral can be easily calculated as $\int_{[0,1]} f\, d\lambda = \lambda([0,1] \cap \mathbb{Q}) = 0$.

Now suppose that one has given a sequence $f_n\colon \Omega \to \mathbb{C}$ of measurable functions such that $\lim_{n\to\infty} f_n(x)$ exists almost everywhere. Hence, there exists a measurable set N with $\mu(N) = 0$ such that the limit exists for all $x \notin N$. We now set

$$f(x) = \begin{cases} \lim_{n\to\infty} f_n(x) & \text{if this limit exists,} \\ 0 & \text{else.} \end{cases}$$

One can show that the set C of all $x \in \Omega$ for which the above limit exists is measurable. It follows easily from this fact the function $f\colon \Omega \to \mathbb{C}$ is measurable as well. Note further that because of $C \subset N$ one has $\mu(C) = 0$. Hence, the Lebesgue integral of f is independent of the concrete choice of the values at the non-convergent points and therefore the choice does not matter for almost all considerations. We make the agreement that we will always define the pointwise limit of measurable functions in the above way whenever the limit exists almost everywhere. This is particularly useful for the formulation of the following convergence theorems for the Lebesgue integral.

Theorem 1.2.3 (Monotone convergence theorem). *Let (Ω, Σ, μ) be a measure space and $f_n\colon \Omega \to \mathbb{R}$ a sequence of measurable functions with $f_{n+1}(x) \geq f_n(x) \geq 0$ almost everywhere. Suppose further that $f(x) = \lim_{n\to\infty} f_n(x)$ exists almost everywhere. Then*

$$\lim_{n\to\infty} \int_\Omega f_n\, d\mu = \int_\Omega f\, d\mu.$$

Note that the monotonicity assumption is crucial for the theorem. In fact, in general one cannot switch the order of limits and integrals as the following example shows.

$$\lim_{n\to\infty} \int_{\mathbb{R}} \mathbb{1}_{[n,n+1]}\, d\lambda = 1 \neq 0 = \int_{\Omega} \lim_{n\to\infty} \mathbb{1}_{[n,n+1]}\, d\lambda.$$

However, the following result holds for non-positive and non-monotone sequences of functions.

Theorem 1.2.4 (Dominated convergence theorem). *Let (Ω, Σ, μ) be a measure space and $f_n \colon \Omega \to \mathbb{C}$ a sequence of measurable functions for which there exists an integrable function $g \colon \Omega \to \mathbb{R}$ such that for all $n \in \mathbb{N}$ one has $|f_n(x)| \leq g(x)$ almost everywhere. Further suppose that $f(x) = \lim_{n\to\infty} f_n(x)$ exists almost everywhere. Then*

$$\lim_{n\to\infty} \int_{\Omega} f_n\, d\mu = \int_{\Omega} f\, d\mu.$$

For the next result we need a finiteness condition on the underlying measure space.

Definition 1.2.5 (σ-finite measure space). A measure space (Ω, Σ, μ) is called *σ-finite* if there exists a sequence of measurable sets $(A_n)_{n\in\mathbb{N}} \subset \Sigma$ such that $\mu(A_n) < \infty$ for all $n \in \mathbb{N}$ and

$$\Omega = \bigcup_{n=1}^{\infty} A_n.$$

For example, $(\mathbb{N}, \mathcal{P}(\mathbb{N}))$ together with the counting measure or the measure spaces $(\mathbb{R}^n, \mathcal{B}(\mathbb{R}^n), \lambda)$ for $n \in \mathbb{N}$, where λ denotes the Lebesgue measure, are σ-finite. Moreover, every finite measure space and a fortiori every probability space is σ-finite. For an example of a non-σ-finite measure space consider $(\mathbb{R}, \mathcal{P}(\mathbb{R}))$ with the counting measure.

Definition 1.2.6 (Products of measure spaces). Consider the two measure spaces $(\Omega_1, \Sigma_1, \mu_1)$ and $(\Omega_2, \Sigma_2, \mu_2)$.

(i) The σ-algebra on $\Omega_1 \times \Omega_2$ generated by sets of the form $A_1 \times A_2$ for $A_i \in \Sigma_i$ $(i = 1, 2)$ (i.e. the smallest σ-algebra that contains these sets) is called the *product σ-algebra* of Σ_1 and Σ_2 and is denoted by $\Sigma_1 \otimes \Sigma_2$.

(ii) A measure μ on the measurable space $(\Omega_1 \times \Omega_2, \Sigma_1 \otimes \Sigma_2)$ is called a *product measure* of μ_1 and μ_2 if

$$\mu(A_1 \times A_2) = \mu_1(A_1) \cdot \mu_2(A_2) \qquad \text{for all } A_1 \in \Sigma_1, A_2 \in \Sigma_2.$$

Here we use the convention that $0 \cdot \infty = \infty \cdot 0 = 0$.

For example, one has $\mathcal{B}(\mathbb{R}^n)\otimes\mathcal{B}(\mathbb{R}^m) = \mathcal{B}(\mathbb{R}^{n+m})$ which can be easily verified using the fact that products of half-open intervals generate $\mathcal{B}(\mathbb{R}^n)$. It follows from the characterizing property of the Lebesgue measure λ_n on $(\mathbb{R}^n, \mathcal{B}(\mathbb{R}^n))$ that for all $n, m \in \mathbb{N}$ the measure λ_{n+m} is a product measure of λ_n and λ_m. One can show that there always exists a product measure for two arbitrary measure spaces. In most concrete situations there exists a uniquely determined product measure as the following theorem shows.

Theorem 1.2.7. *Let $(\Omega_1, \Sigma_1, \mu_1)$ and $(\Omega_2, \Sigma_2, \mu_2)$ be two σ-finite measure spaces. Then there exists a unique product measure on $(\Omega_1 \times \Omega_2, \Sigma_1 \otimes \Sigma_2)$ which is denoted by $\mu_1 \otimes \mu_2$.*

It is now a natural question how integration over product measures is related to integration over the single measures. An answer is given by Fubini's theorem.

Theorem 1.2.8 (Fubini–Tonelli theorem). *Let $(\Omega_1, \Sigma_1, \mu_1)$ and $(\Omega_2, \Sigma_2, \mu_2)$ be two σ-finite measure spaces and $f : (\Omega_1 \times \Omega_2, \Sigma_1 \otimes \Sigma_2) \to \mathbb{C}$ a measurable function. Then the functions*

$$y \mapsto \int_{\Omega_1} f(x,y)\, d\mu_1(x) \qquad \text{and} \qquad x \mapsto \int_{\Omega_2} f(x,y)\, d\mu_2(y)$$

are measurable functions $\Omega_2 \to \mathbb{C}$ respectively $\Omega_1 \to \mathbb{C}$. If one of the three integrals

$$\int_{\Omega_1}\int_{\Omega_2} |f(x,y)|\, d\mu_2(y)\, d\mu_1(x), \quad \int_{\Omega_2}\int_{\Omega_1} |f(x,y)|\, d\mu_1(x)\, d\mu_2(y) \quad \text{or}$$
$$\int_{\Omega_1\times\Omega_2} |f(x,y)|\, d\mu_1 \otimes \mu_2(x,y)$$

is finite, then one has for the product and iterated integrals

$$\begin{aligned}\int_{\Omega_1\times\Omega_2} f(x,y)\, d(\mu_1\otimes\mu_2)(x,y) &= \int_{\Omega_1}\int_{\Omega_2} f(x,y)\, d\mu_2(y)\, d\mu_1(x) \\ &= \int_{\Omega_2}\int_{\Omega_1} f(x,y)\, d\mu_1(x)\, d\mu_2(y).\end{aligned}$$

Moreover, if f is a non-negative function, one can omit the finiteness assumption on the integrals and the conclusion is still valid (in this case all integrals can be infinite).

Note that there are also variants of Fubini's theorem (not in the above generality) for non σ-finite measure spaces. However, this case is more technical and rarely used in practice and therefore we omit it.

1.3 Lebesgue Spaces

We now come back to the motivation at the beginning of this chapter. After our preliminary work we can now define $L^2(\mathbb{R})$ or more generally $L^p(\Omega)$ over an arbitrary measure space (Ω, Σ, μ).

Definition 1.3.1 ($\mathcal{L}^p$-spaces). Let (Ω, Σ, μ) be a measure space. For $p \in [1, \infty)$ we set

$$\mathcal{L}^p(\Omega, \Sigma, \mu) := \left\{ f : \Omega \to \mathbb{K} \text{ measurable} : \int_\Omega |f|^p \, d\mu < \infty \right\},$$
$$\|f\|_p := \left(\int_\Omega |f|^p \, d\mu \right)^{1/p}.$$

For $p = \infty$ we set

$$\mathcal{L}^\infty(\Omega, \Sigma, \mu) := \{ f : \Omega \to \mathbb{K} \text{ measurable} : \exists C \geq 0 : |f(x)| \leq C \text{ alm. everywhere} \}.$$
$$\|f\|_\infty := \inf\{ C \geq 0 : |f(x)| \leq C \text{ almost everywhere} \}.$$

Note that the space $\mathcal{L}^1(\Omega, \Sigma, \mu)$ agrees with the space $\mathcal{L}^1(\Omega, \Sigma, \mu)$ previously defined in Definition 1.2.1. One can show that $(\mathcal{L}^p(\Omega, \Sigma, \mu), \|\cdot\|_p)$ is a semi-normed vector space, i.e. $\|\cdot\|_p$ satisfies all axioms of a norm except for definiteness. Here, the validity of the triangle inequality, the so-called *Minkowski inequality*, is a non-trivial fact. If one identifies two functions whenever they agree almost everywhere, one obtains a normed space.

Definition 1.3.2 (L^p-spaces). Let (Ω, Σ, μ) be a measure space and $p \in [1, \infty]$. The space $L^p(\Omega, \Sigma, \mu)$ is defined as the space $\mathcal{L}^p(\Omega, \Sigma, \mu)$ with the additional agreement that two functions $f, g : \Omega \to \mathbb{K}$ are identified with each other whenever $f - g = 0$ almost everywhere.

As a consequence of the above identification $(L^p(\Omega, \Sigma, \mu), \|\cdot\|_p)$ is a normed vector space. In contrast to the variant using the Riemann integral these spaces are complete.

Definition 1.3.3 (Banach space). A normed vector space which is complete with respect to the given norm is called a *Banach space*.

Recall that a normed vector space or more generally a metric space is called *complete* if every Cauchy sequence converges to an element in the space. A sequence $(x_n)_{n \in \mathbb{N}}$ in a normed vector space $(V, \|\cdot\|)$ is called a *Cauchy sequence* if for all $\varepsilon > 0$ there exists $n_0 \in \mathbb{N}$ such that $\|x_n - x_m\| \leq \varepsilon$ for all $n, m \geq n_0$. Using this terminology we have

Theorem 1.3.4 (Riesz–Fischer). *Let (Ω, Σ, μ) be a measure space and $p \in [1, \infty]$. Then $L^p(\Omega, \Sigma, \mu)$ is a Banach space.*

Let $(f_n)_{n\in\mathbb{N}}$ be a sequence in $L^p(\Omega,\Sigma,\mu)$ with $f_n \to f$ in L^p. One often says that f_n converges to f in the *p-th mean* which gives the right visual interpretation for convergence in L^p-spaces. Note that the sequence $\mathbb{1}_{[0,1]}$, $\mathbb{1}_{[0,1/2]}$, $\mathbb{1}_{[1/2,1]}$, $\mathbb{1}_{[0,1/4]}$, $\mathbb{1}_{[1/4,1/2]}$ and so on converges in $L^p([0,1])$ for all $p \in [1,\infty)$ to the zero function although $f_n(x)$ diverges for all $x \in [0,1]$. Conversely, pointwise convergence in general does not imply convergence in L^p. For example, the sequence $f_n = \mathbb{1}_{[n,n+1]}$ does not converge in $L^p(\mathbb{R})$ although $f_n(x) \to 0$ for all $x \in \mathbb{R}$. In concrete situations one can often infer L^p-convergence from pointwise convergence with the help of the dominated convergence theorem. In the opposite direction one has the following useful result which actually follows directly from the proof of the Riesz–Fischer theorem.

Proposition 1.3.5. *Let (Ω,Σ,μ) be a measure space and $p \in [1,\infty)$. Further suppose that $f_n \to f$ in $L^p(\Omega,\Sigma,\mu)$. Then there exist a subsequence $(f_{n_k})_{k\in\mathbb{N}}$ and $g \in L^p(\Omega,\Sigma,\mu)$ such that*

(a) *$f_{n_k}(x) \to f(x)$ almost everywhere;*

(b) *$|f_{n_k}(x)| \le |g(x)|$ for all $n \in \mathbb{N}$ almost everywhere.*

We will later need some further properties of L^p-spaces. The following result is natural, but needs some effort to be proven rigorously.

Proposition 1.3.6. *Let $\Omega \subset \mathbb{R}^n$ be open and $p \in [1,\infty)$. Then $C_c(\Omega)$, the space of all continuous functions on Ω with compact support (in Ω), is a dense subspace of $L^p(\Omega)$.*

The Cauchy–Schwarz inequality for L^2-spaces generalizes to Hölder's inequality in the L^p-setting. In the following we use the agreement $1/\infty = 0$.

Proposition 1.3.7 (Hölder's inequality). *Let (Ω,Σ,μ) be a measure space. Further let $p \in [1,\infty]$ and $q \in [1,\infty]$ be its dual index given by $\frac{1}{p} + \frac{1}{q} = 1$. Then for $f \in L^p(\Omega,\Sigma,\mu)$ and $g \in L^q(\Omega,\Sigma,\mu)$ the product $f \cdot g$ lies in $L^1(\Omega,\Sigma,\mu)$ and satisfies*

$$\int_\Omega |f\,g|\,d\mu \le \left(\int_\Omega |f|^p\,d\mu\right)^{1/p} \left(\int_\Omega |g|^q\,d\mu\right)^{1/q}.$$

As an important and direct consequence of Hölder's inequality one has the following inclusions between L^p-spaces.

Proposition 1.3.8. *Let (Ω,Σ,μ) be a finite measure space, i.e. $\mu(\Omega) < \infty$. Then for $p \ge q \in [1,\infty]$ one has the inclusion*

$$L^p(\Omega,\Sigma,\mu) \subset L^q(\Omega,\Sigma,\mu).$$

Proof. We only deal with the case $p \in (1,\infty)$ (the other cases are easy to show). It follows from Hölder's inequality because of $p/q \geq 1$ that

$$\left(\int_\Omega |f|^q \, d\mu\right)^{1/q} = \left(\int_\Omega |f|^q \, \mathbb{1} \, d\mu\right)^{1/q} \leq \left(\int_\Omega |f|^p \, d\mu\right)^{1/p} \left(\int_\Omega \mathbb{1} \, d\mu\right)^{(1-q/p)\cdot 1/q}$$
$$= \mu(\Omega)^{1/q-1/p} \left(\int_\Omega |f|^p \, d\mu\right)^{1/p}. \qquad \square$$

A second application of Hölder's inequality is the next important estimate on convolutions of two functions.

Definition 1.3.9. Let $f, g \in L^1(\mathbb{R}^n)$. We define the *convolution* of f and g by

$$(f * g)(x) = \int_{\mathbb{R}^n} f(y) g(x-y) \, dy.$$

Note that it is not clear that $f * g$ exists under the above assumptions. This is indeed the case as the following argument shows. Note that the function $(x,y) \mapsto f(y)g(x-y)$ is measurable as a map $\mathbb{R}^{2n} \to \mathbb{R}$ by the definition of product σ-algebras and the fact that the product and the composition of measurable functions is measurable. It follows from Fubini's theorem that the function $x \mapsto (f * g)(x)$ is measurable and satisfies

$$\int_{\mathbb{R}^n} |f * g|(x) \, dx \leq \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} |f(y)||g(x-y)| \, dy \, dx = \int_{\mathbb{R}^n} |f(y)| \int_{\mathbb{R}^n} |g(x-y)| \, dx \, dy$$
$$= \int_{\mathbb{R}^n} |f(y)| \int_{\mathbb{R}^n} |g(x)| \, dx \, dy = \|f\|_1 \, \|g\|_1 .$$

Hence, the function $f * g$ is finite almost everywhere. Moreover, we have shown that $f * g \in L^1(\mathbb{R}^n)$ and that the pointwise formula in the definition holds with finite values almost everywhere after taking representatives. It follows from the next inequality that the convolution also exists as an L^p-integrable function if one function is assumed to be in L^p.

Proposition 1.3.10 (Minkowski's inequality for convolutions). *For some $p \in [1,\infty]$ let $g \in L^p(\mathbb{R}^n)$ and $f \in L^1(\mathbb{R}^n)$. Then one has*

$$\|f * g\|_p \leq \|f\|_1 \, \|g\|_p .$$

Proof. We only deal with the cases $p \in (1,\infty)$ as the boundary cases are simple to prove. We apply Hölder's inequality to the functions $|g(x-y)|$ and $\mathbb{1}$ for the measure $\mu = |f(y)| \, dy$ (i.e. $\mu(A) = \int_A |f(y)| \, dy$) and obtain

$$|(f * g)(x)| \leq \left(\int_{\mathbb{R}^n} |g(x-y)|^p |f(y)| \, dy\right)^{1/p} \left(\int_{\mathbb{R}^n} |f(y)| \, dy\right)^{1/q},$$

where $1/p + 1/q = 1$. Taking the L^p-norm in the above inequality, we obtain the desired inequality

$$\begin{aligned}\|f * g\|_p &\leq \left(\int_{\mathbb{R}^n} \int_{\mathbb{R}^n} |g(x-y)|^p |f(y)|\, dy\, \|f\|_1^{p/q}\, dx \right)^{1/p} \\ &= \|f\|_1^{1/q} \left(\int_{\mathbb{R}^n} |f(y)| \int_{\mathbb{R}^n} |g(x-y)|^p\, dx\, dy \right)^{1/p} = \|f\|_1^{1/q} \|f\|_1^{1/p} \|g\|_p \\ &= \|f\|_1 \|g\|_p . \end{aligned}$$

□

2

The Theory of Self-Adjoint Operators in Hilbert Spaces

2.1 Basic Hilbert Space Theory

By the postulates of quantum mechanics a quantum mechanical system is described by some complex Hilbert space. Before going any further, we therefore need some basic results from Hilbert space theory. In this section we introduce Hilbert spaces and bounded operators between these spaces. As important examples for the further development, we introduce Fourier transforms and Sobolev spaces.

We follow the typical physical convention that an inner product on some complex vector space is linear in the second and anti-linear in the first component.

Definition 2.1.1. A *Hilbert space* $\mathcal{H}$ is a $\mathbb{K}$-vector space endowed with an inner product $\langle\cdot|\cdot\rangle$ such that $\mathcal{H}$ is complete with respect to the norm $\|\cdot\|_{\mathcal{H}} \coloneqq \sqrt{\langle\cdot|\cdot\rangle}$ induced by the inner product (i.e. every Cauchy sequence in $\mathcal{H}$ converges to an element in $\mathcal{H}$).

Recall that a sequence $(x_n)_{n\in\mathbb{N}}$ in a normed space $(N, \|\cdot\|)$ is called a *Cauchy sequence* if for every $\varepsilon > 0$ there exists $N \in \mathbb{N}$ with $\|x_n - x_m\| \leq \varepsilon$ for all $n, m \geq N$. Note that the spaces $\mathbb{C}^n$ for $n \in \mathbb{N}$ are finite-dimensional Hilbert spaces with respect to the inner product $\langle x|y\rangle = \sum_{k=1}^{n} \overline{x_k} y_k$. We now give a first important infinite-dimensional example.

Example 2.1.2. Let (Ω, Σ, μ) be an arbitrary measure space. Then $L^2(\Omega, \Sigma, \mu)$ as defined in Definition 1.3.2 is a Hilbert space with respect to the inner product

$$\langle f|g\rangle_{L^2} \coloneqq \int_\Omega \overline{f}(x) g(x)\, d\mu(x).$$

Note that the space $L^2(\Omega, \Sigma, \mu)$ is complete by the Riesz–Fischer Theorem 1.3.4. Further, the finiteness of the scalar product is a consequence of Hölder's inequality. As a special case one can take for an open set $\Omega \subset \mathbb{R}^n$ the measure space $(\Omega, \mathcal{B}(\Omega), \lambda)$ and obtains the L^2-space $L^2(\Omega) = L^2(\Omega, \mathcal{B}(\Omega), \lambda_{|\mathcal{B}(\Omega)})$.

We now state some elementary concepts and properties of Hilbert spaces.

Proposition 2.1.3. *Let $\mathcal{H}$ be a Hilbert space and $x, y \in \mathcal{H}$. Then the* Cauchy–Schwarz *inequality*

$$|\langle x|y\rangle| \leq \|x\|_{\mathcal{H}} \|y\|_{\mathcal{H}} \tag{CS}$$

holds. In particular, the scalar product seen as a mapping $\mathcal{H}\times\mathcal{H} \to \mathbb{K}$ is continuous, i.e. $x_n \to x$ and $y_n \to y$ in $\mathcal{H}$ imply $\langle x_n|y_n\rangle \to \langle x|y\rangle$.

2.1.1 Orthonormal Bases

Orthonormal bases are one of the most fundamental concepts in Hilbert space theory and we will meet such bases in abundance while studying concrete quantum mechanical systems.

Definition 2.1.4. A family $(e_i)_{i\in I}$ of elements in some Hilbert space $\mathcal{H}$ is called *orthogonal* if $\langle e_i|e_j\rangle = 0$ for all $i \neq j \in I$. If one additionally has $\|e_i\| = 1$ for all $i \in I$, one says that $(e_i)_{i\in I}$ is *orthonormal*. If moreover the linear span of $(e_i)_{i\in I}$ is dense in $\mathcal{H}$, the family $(e_i)_{i\in I}$ is called an *orthonormal basis* of $\mathcal{H}$.

As a simple example, consider the Hilbert space $\mathbb{C}^n$ for some $n \in \mathbb{N}$. Then the n unit vectors form an orthonormal basis of $\mathbb{C}^n$, whereas every subset of the unit vectors is orthonormal. Here the linear span of $e_1,\dots,e_n$ clearly is not only dense in $\mathbb{C}^n$, but even spans $\mathbb{C}^n$ completely. This changes in the infinite-dimensional setting. Consider ℓ^2, the space of all square summable sequences. Then the unit vectors $(e_n)_{n\in\mathbb{N}}$ again form an orthonormal basis as one can directly verify. However, the span of $(e_n)_{n\in\mathbb{N}}$ consists exactly of the sequences with finite support which is a dense proper subspace of ℓ^2. Let us now consider the space $L^2([0,1])$ for which it is slightly more difficult to give an example of an orthonormal basis.

Example 2.1.5 (Trigonometric system). Consider $e_n(x) = e^{2\pi inx}$ for $n \in \mathbb{Z}$. Then $(e_n)_{n\in\mathbb{Z}}$ forms an orthonormal set in $L^2([0,1])$ as one can verify by a direct computation. Moreover, if one consider the Fréchet kernel defined by

$$F_N(x) = \frac{1}{2N+1} \sum_{n=-N}^{N} \sum_{k=-n}^{n} e^{2\pi ikx},$$

it follows from a standard theorem in analysis that for every continuous periodic function $f \in C_{\text{per}}([0,1])$ the convolution $F_n * f$ converges uniformly to f (we will study the convolution of functions on the real line more closely in some later section). Note that it follows from

$$\int_0^1 |F_N * f - f|^2 \, dx \leq \|F_N - f\|_\infty^2 \xrightarrow[N\to\infty]{} 0$$

that the convergence $F_N * f \to f$ also holds in L^2. Since $F_N * f$ is explicitly given by

$$(F_N * f)(x) = \frac{1}{2N+1} \sum_{n=-N}^{N} \sum_{k=-n}^{n} \hat{f}(k) e^{2\pi ikx},$$

where $\hat{f}(k)$ for $k \in \mathbb{Z}$ denotes the k-th *Fourier coefficient* of f given by

$$\hat{f}(k) = \int_0^1 f(x) e^{-2\pi i k x}\, dx = \langle e_k | f \rangle,$$

one sees immediately that $F_N \circ f$ lies in the span of $(e_n)_{|n|\leq N}$. Hence, the span of $(e_n)_{n\in\mathbb{Z}}$ is dense in $C([0,1])$ and therefore also dense in $L^2([0,1])$ by a variant of Proposition 1.3.6 (note that $L^2((0,1)) = L^2([0,1])$) and we have shown that $(e_n)_{n\in\mathbb{Z}}$ forms an orthonormal basis of $L^2([0,1])$.

We have constructed orthonormal bases of fundamental examples of Hilbert spaces. In fact, this is no coincidence as every Hilbert space has an orthonormal basis. The most important infinite-dimensional case is when the index set of an orthonormal bases can be chosen as the natural numbers

Definition 2.1.6. A normed space $(N, \|\cdot\|)$ is called *separable* if there exists a countable dense subset of N.

Theorem 2.1.7. *Every Hilbert space $\mathcal{H}$ has an orthonormal basis. Moreover and more concretely, if $\mathcal{H}$ is infinite dimensional and separable, then there exists an orthonormal basis $(e_n)_{n\in\mathbb{N}}$ of $\mathcal{H}$.*

The proof of the above theorem in the separable case usually uses the well-known Gram–Schmidt orthonormalization process known from linear algebra applied to a dense countable subset of $\mathcal{H}$. Orthonormal bases are a fundamental tool in the study of Hilbert spaces as we see in the following.

Lemma 2.1.8. *Let $\mathcal{H}$ be a Hilbert space and $x, y \in \mathcal{H}$. Then*

$$\|x+y\|^2 = \|x\|^2 + \|y\|^2 + 2\,\mathrm{Re}\langle x|y\rangle.$$

Proof. This follows by a direct computation from the relation between the scalar product and the norm on a Hilbert space. Indeed, we have

$$\begin{aligned}\|x+y\|^2 = \langle x+y|x+y\rangle &= \langle x|x\rangle + \langle x|y\rangle + \langle y|x\rangle + \langle y|y\rangle = \|x\|^2 + \|y\|^2 + \langle x|y\rangle + \overline{\langle x|y\rangle} \\ &= \|x\|^2 + \|y\|^2 + 2\,\mathrm{Re}\langle x|y\rangle.\end{aligned}$$

□

Note that in particular if x and y are orthogonal, i.e. $\langle x|y\rangle = 0$, then $\|x+y\|^2 = \|x\|^2 + \|y\|^2$. As a direct application we can study the expansion of Hilbert space elements with respect to orthonormal bases. All what follows can be extended to arbitrary Hilbert spaces. However, for the sake of simplicity we will only deal with the separable infinite-dimensional case.

Theorem 2.1.9. *Let $\mathcal{H}$ be an infinite-dimensional separable Hilbert space and $(e_n)_{n\in\mathbb{N}}$ an orthonormal basis of $\mathcal{H}$.*

(a) *For every $x \in \mathcal{H}$ one has*

$$x = \sum_{n=1}^{\infty} \langle e_n | x \rangle e_n,$$

where the convergence of the series is understood in the norm of $\mathcal{H}$. Moreover, the above expansion is unique.

(b) *For every $x, y \in \mathcal{H}$ Parseval's identity holds:*

$$\langle x | y \rangle = \sum_{n=1}^{\infty} \langle x | e_n \rangle \langle e_n | y \rangle.$$

In particular one has

$$\|x\|^2 = \sum_{n=1}^{\infty} |\langle e_n | x \rangle|^2 .$$

Proof. We start with (a). Suppose that $x = \sum_{n=1}^{\infty} a_n e_n$ is an arbitrary expansion of x. Then it follows from the continuity of the scalar product that for every $k \in \mathbb{N}$ one has

$$\langle e_k | x \rangle = \left\langle e_k \middle| \sum_{n=1}^{\infty} a_n e_n \right\rangle = \lim_{N \to \infty} \left\langle e_k \middle| \sum_{n=1}^{N} a_n e_n \right\rangle = \lim_{N \to \infty} \sum_{n=1}^{N} a_n \langle e_k | e_n \rangle = a_k.$$

The uniqueness of the expansion follows directly from the above equation. For the existence of the expansion we have to show that the partial sums $\sum_{n=1}^{N} \langle e_n | x \rangle e_n$ converge to x in $\mathcal{H}$. By orthogonality we have

$$\begin{aligned} \|x\|^2 &= \left\| x - \sum_{n=1}^{N} \langle e_n | x \rangle e_n + \sum_{n=1}^{N} \langle e_n | x \rangle e_n \right\|^2 = \left\| x - \sum_{n=1}^{N} \langle e_n | x \rangle e_n \right\|^2 + \left\| \sum_{n=1}^{N} \langle e_n | x \rangle e_n \right\|^2 \\ &= \left\| x - \sum_{n=1}^{N} \langle e_n | x \rangle e_n \right\|^2 + \sum_{n=1}^{N} |\langle e_n | x \rangle|^2 \geq \sum_{n=1}^{N} |\langle e_n | x \rangle|^2 . \end{aligned}$$

This shows that the sequence $(\langle e_n | x \rangle)_{n \in \mathbb{N}}$ is square summable and that

$$\sum_{n=1}^{\infty} |\langle e_n | x \rangle|^2 \leq \|x\|^2 . \tag{2.1}$$

In particular it follows that for $m \geq n$ one has by orthogonality

$$\left\| \sum_{k=1}^{m} \langle e_k | x \rangle e_k - \sum_{k=1}^{n} \langle e_k | x \rangle e_k \right\|^2 = \left\| \sum_{k=n}^{m} \langle e_k | x \rangle e_k \right\|^2 = \sum_{k=n}^{m} |\langle e_k | x \rangle|^2 \leq \sum_{k=n}^{\infty} |\langle e_k | x \rangle|^2 ,$$

which goes to zero as $n \to \infty$. This shows that the sequence of partial sums forms a Cauchy sequence in $\mathcal{H}$. By the completeness of $\mathcal{H}$ the sequence of

partial sums converges. Hence, $\sum_{n=1}^{\infty}\langle e_n|x\rangle e_n \in \mathcal{H}$. It remains to show that this series is indeed x. In order to show this define for $N \in \mathbb{N}$

$$P_N : x \mapsto \sum_{n=1}^{N}\langle e_n|x\rangle.$$

We have just shown that for every $x \in \mathcal{H}$ the limit of $P_N x$ as $N \to \infty$ exists. Moreover, it follows from the estimate (2.1) that P_N is a contraction, i.e. $\|P_N x\| \leq \|x\|$ for all $x \in \mathcal{H}$. Moreover, if x is in the span of $(e_n)_{n\in\mathbb{N}}$, then $P_N x = x$ for N large enough. In particular, one has $\lim_{N\to\infty} P_N x = x$ for all x in the span of $(e_n)_{n\in\mathbb{N}}$ which is a dense subset of $\mathcal{H}$ by the definition of an orthonormal basis. In other words, we have $\lim_{N\to\infty} P_N = \mathrm{Id}$ pointwise on a dense subset. It now follows from Lemma 2.1.10 applied to $P_N - \mathrm{Id}$ because of $\|P_N\| \leq 1$ that this convergence indeed holds for all $x \in \mathcal{H}$, i.e. one has the desired expansion

$$x = \sum_{n=1}^{\infty}\langle e_n|x\rangle e_n$$

for all $x \in \mathcal{H}$. This finishes the proof of (a). Now Parseval's identity in (b) is an immediate consequence. Indeed, we have for $x, y \in \mathcal{H}$

$$\begin{aligned}\langle x|y\rangle &= \left\|\sum_{n=1}^{\infty}|\langle e_n|x\rangle e_n|\right\|^2 = \lim_{N\to\infty}\lim_{M\to\infty}\sum_{n=1}^{N}\sum_{k=1}^{M}\overline{\langle e_n|x\rangle}\langle e_k|y\rangle\langle e_n|e_k\rangle \\ &= \sum_{n=1}^{\infty}\langle x|e_n\rangle\langle e_n|y\rangle.\end{aligned}$$

□

We now prove the lemma left open in the previous proof.

Lemma 2.1.10. *Let $T_n : X \to X$ be a sequence of uniformly bounded linear operators on some Banach space X, i.e. $\|T_n x\| \leq C\|x\|$ for some $C \geq 0$ and all $n \in \mathbb{N}$ and $x \in X$. Further suppose that $\lim_{n\to\infty} T_n x = 0$ for all x in a dense subset $M \subset X$. Then*

$$\lim_{n\to\infty} T_n x = 0 \qquad \text{for all } x \in X.$$

Proof. Let $x \in X$ and $\varepsilon > 0$. Choose $y \in M$ with $\|x - y\| \leq \varepsilon$. Then we have

$$\limsup_{n\to\infty}\|T_n x\| \leq \limsup_{n\to\infty}\|T_n(x-y)\| + \|T_n y\| \leq C\|x-y\|.$$

Since $\varepsilon > 0$ is arbitrary, it follows that $\lim_{n\to\infty}\|T_n x\| = 0$. □

If we apply Parseval's identity to the trigonometric basis considered in Example 2.1.5, we obtain Plancherel's identity from Fourier analysis.

Corollary 2.1.11 (Plancherel's identity). *Let $f \in L^2([0,1])$ and let $\hat{f}(n)$ for $n \in \mathbb{Z}$ denote its n-th Fourier coefficient. Then*

$$\int_0^1 |f(x)|^2 \, dx = \sum_{n \in \mathbb{Z}} |\hat{f}(n)|^2.$$

2.1.2 Bounded Operators on Hilbert Spaces

We have already encountered bounded linear operators in Lemma 2.1.10. This subsection is devoted to a closer study of such operators. Recall that by the postulates of quantum mechanics a physical observable is modeled by a self-adjoint operator on some Hilbert space. Such operators are often unbounded in important examples. Nevertheless it is important as a first step to understand the easier case of bounded self- and non-self-adjoint operators. Moreover, the evolution operators of quantum mechanical systems that we will consider in the study of the Schrödinger equation and orthogonal projections which are fundamental in the mathematical description of the measurement process in quantum mechanics are important examples of bounded operators.

Definition 2.1.12. A linear operator $T\colon X \to Y$ between two Banach spaces is *bounded* if there exists a constant $C \geq 0$ such that

$$\|Tx\|_Y \leq C \|x\|_X \qquad \text{for all } x \in \mathcal{X}.$$

The smallest constant $C \geq 0$ such that the above inequality holds is called the *operator norm* of T and is denoted by $\|T\|$. The space of all bounded linear operators between X and Y is denoted by $\mathcal{B}(X,Y)$. It is a Banach space with respect to the operator norm.

The last fact is left as an exercise to the reader. Notice that a linear operator T is bounded if and only if it is continuous, i.e. $x_n \to x$ in X implies $Tx_n \to Tx$ in X. This is also left as an exercise to the reader. Finally, the reader should verify that

$$\|T\| = \sup_{\|x\| \leq 1} \|Tx\|.$$

Suppose one has given two bounded linear operators $T\colon X \to Y$ and $S\colon Y \to Z$ between Banach spaces X, Y and Z. Then one has for all $x \in X$

$$\|STx\| \leq \|S\| \|Tx\| \leq \|S\| \|T\| \|x\|.$$

This shows by definition the fundamental operator inequality $\|ST\| \leq \|T\| \|S\|$, the so-called submultiplicativity of the norm. As a consequence the composition operation $\mathcal{B}(X) \times \mathcal{B}(X) \to \mathcal{B}(X)$ is continuous, i.e. $S_n \to S$ and $T_n \to T$ in $\mathcal{B}(X)$ implies $S_n T_n \to ST$.

We continue with a fundamental class of examples of bounded operators.

Example 2.1.13 (Multipliers for orthonormal bases). We choose the Hilbert space $\mathcal{H} = \ell^2 = \ell^2(\mathbb{N})$. Further let $e_n = (\delta_{nm})_{m\in\mathbb{N}}$ denote the n-th unit vector. We have seen in the discussion before Example 2.1.5 that $(e_n)_{n\in\mathbb{N}}$ is an orthonormal basis of $\ell^2(\mathbb{N})$. Let $x = (x_n)_{n\in\mathbb{N}}$ be a sequence in $\ell^2(\mathbb{N})$. Then one has the unique representation $x = \sum_{n=1}^{\infty} x_n e_n$ with respect to the unit vector basis. Hence, for a bounded sequence $(a_n)_{n\in\mathbb{N}} \in \ell^\infty(\mathbb{N})$ we obtain a well-defined linear operator by setting

$$T\left(\sum_{n=1}^{\infty} x_n e_n\right) = \sum_{n=1}^{\infty} a_n x_n e_n.$$

This follows from the fact that $(a_n x_n)_{n\in\mathbb{N}} \in \ell^2(\mathbb{N})$ whenever $(x_n)_{n\in\mathbb{N}} \in \ell^2(\mathbb{N})$. Moreover, with the help of the Parseval's identity one obtains

$$\left\|\sum_{n=1}^{\infty} a_n x_n e_n\right\|^2 = \sum_{n=1}^{\infty} |a_n x_n|^2 \leq (\sup_{n\in\mathbb{N}} |a_n|)^2 \sum_{n=1}^{\infty} |x_n|^2 = (\sup_{n\in\mathbb{N}} |a_n|)^2 \left\|\sum_{n=1}^{\infty} x_n e_n\right\|^2.$$

This shows that T is bounded with $\|T\| \leq \sup_{n\in\mathbb{N}} |a_n|$. Conversely, for all $\varepsilon > 0$ there exists $n_0 \in \mathbb{N}$ such that $|a_{n_0}| > \sup_{n\in\mathbb{N}} |a_n| - \varepsilon$. Let $\varphi \in [0, 2\pi)$ be such that $e^{i\varphi} a_{n_0} = |a_{n_0}|$. Then one has $\|e^{i\varphi} e_{n_0}\| = 1$ and

$$\|T(e^{i\varphi} e_{n_0})\| = e^{i\varphi} a_{n_0} = |a_{n_0}| \geq \sup_{n\in\mathbb{N}} |a_n| - \varepsilon.$$

Hence, $\|T\| \geq \sup_{n\in\mathbb{N}} |a_n| - \varepsilon$ for all $\varepsilon > 0$. Since $\varepsilon > 0$ is arbitrary, the equality $\|T\| = \sup_{n\in\mathbb{N}} |a_n|$ follows. Notice that the same reasoning applies if one replaces ℓ^2 by an arbitrary infinite-dimensional separable Hilbert space and $(e_n)_{n\in\mathbb{N}}$ by an arbitrary orthonormal basis of $\mathcal{H}$.

Notice that the above example in particular shows that in general there is no x in the unit ball of $\mathcal{H}$ such that $\|Tx\| = \|T\|$, i.e. T does not attain its norm. We now turn our attention to dual spaces, a concept fundamental for the Dirac formulation of quantum mechanics.

Example 2.1.14 (Orthogonal projection). Let $\mathcal{H}$ be a separable Hilbert space of infinite dimension and $(e_n)_{n\in\mathbb{N}}$ an orthonormal basis of $\mathcal{H}$. Using the expansion with respect to $(e_n)_{n\in\mathbb{N}}$ we define for $N \in \mathbb{N}$ the operator

$$P_N\left(\sum_{n=1}^{\infty} a_n e_n\right) = \sum_{n=1}^{N} a_n e_n.$$

Clearly, P_N is linear and we have implicitly shown in estimate (2.1) in the proof of Theorem 2.1.9 that P_N is a bounded operator with $\|P_N\| \leq 1$. Because of $P_N e_1 = e_1$ one directly sees that $\|P_N\| = 1$. Note that $P_N^2 = P_N$. Hence, P_N is a

projection onto $\operatorname{span}\{e_1,\dots,e_N\}$. Moreover, one has $\langle P_N x|(\mathrm{Id}-P_N)y\rangle = 0$ for all $x, y \in \mathcal{H}$. Indeed, one has

$$\begin{aligned}\left\langle \sum_{n=1}^{N} \langle e_n|x\rangle e_n | y - \sum_{k=1}^{N} \langle e_k|y\rangle e_k \right\rangle &= \sum_{n=1}^{N} \langle x|e_n\rangle \left\langle e_n | y - \sum_{k=1}^{N} \langle e_k|y\rangle e_k \right\rangle \\ &= \sum_{n=1}^{N} \langle x|e_n\rangle (\langle e_n|y\rangle - \langle e_n|y\rangle) = 0.\end{aligned}$$

Hence, the kernel and the image of P_N are orthogonal subspaces. Such a projection is called an *orthogonal projection*.

More generally, let $M \subset \mathcal{H}$ be a closed subspace of $\mathcal{H}$. Since M is closed, M is complete with respect to the norm induced by the inherited scalar product of $\mathcal{H}$. Hence, M is a Hilbert space as well. We assume that M is infinite-dimensional. The finite dimensional case is simpler and can be treated as above. Then M has an orthonormal basis $(e_n)_{n\in\mathbb{N}}$ by Theorem 2.1.7. Now define the linear operator

$$P_M \colon x \mapsto \sum_{n=1}^{\infty} \langle e_n|x\rangle e_n.$$

By estimate (2.1) used in the proof of Theorem 2.1.9 one has $\|P_M x\| \leq \|x\|$. Moreover, taking again $x = e_1$ we see that $P_M e_1 = e_1$. Hence, $\|P_M\| = 1$. More generally, one has $P_M x = x$ for all $x \in M$ as in this case one has $x = \sum_{n=1}^{\infty} \langle e_n|x\rangle e_n$ by Theorem 2.1.9. Furthermore, $P_M^2 = P_M$ holds and P_M is orthogonal. This can be shown as in the first part of the example. Hence, P_M is an orthogonal projection onto the closed subspace M.

Definition 2.1.15 (Dual space). Let $\mathcal{H}$ be a Hilbert space. Then its *(topological) dual space* is defined as

$$\mathcal{H}' := \{\varphi \colon \mathcal{H} \to \mathbb{K} : \varphi \text{ linear and continuous}\}.$$

Example 2.1.16. Let $\mathcal{H}$ be a Hilbert space. For $y \in \mathcal{H}$ one defines the functional $\varphi_y(x) = \langle y|x\rangle$ on $\mathcal{H}$. It follows from the Cauchy–Schwarz inequality (Proposition 2.1.3) that for $x \in \mathcal{H}$ one has $|\varphi_y(x)| \leq \|y\|\,\|x\|$. On the other hand one has $\varphi_y(y/\|y\|) = \|y\|$ provided $y \neq 0$. This shows that $\varphi_y \in \mathcal{H}'$ with norm $\|y\|$ (the case $y = 0$ is obvious).

Remark 2.1.17. The space $\mathcal{H}'$ is called the *topological* dual space of $\mathcal{H}$ because one requires its elements to be continuous. Sometimes one also considers the so-called algebraic dual space which consists of *all* linear functionals $\mathcal{H} \to \mathbb{K}$. We will exclusively work with the topological dual space. Hence, no confusion can arise and we will often drop the term *topological*.

The Riesz representation theorem for Hilbert spaces says that indeed all elements of $\mathcal{H}'$ are of the form considered in Example 2.1.16.

Theorem 2.1.18 (Riesz representation theorem). *Let $\mathcal{H}$ be a Hilbert space and $\varphi \in \mathcal{H}'$. Then there exists a unique $y \in \mathcal{H}$ such that $\varphi = \varphi_y$. Moreover, the map*

$$\mathcal{H} \to \mathcal{H}' \qquad y \mapsto \varphi_y$$

is an anti-linear isometric isomorphism between $\mathcal{H}$ and $\mathcal{H}'$.

As an application of the Riesz representation theorem we now discuss the *bra–ket* formalism (often also called the *Dirac notation*) frequently used by physicists in quantum mechanics. In the following we will also work with the adjoints of operators although we have not yet introduced this concept. You can either ignore this part for the moment and return later or just work with the adjoints as known from linear algebra (the standpoint of most physicists). This makes no problems as long as all operators involved are bounded. We will later in the lecture introduce and discuss adjoints in a mathematical rigorous way.

Remark 2.1.19 (Bra–ket notation of quantum mechanics). Recall that by the postulates of quantum mechanics a physical (pure) state of a quantum mechanical system is described by an element in some Hilbert space $\mathcal{H}$. In physics notation such a state is often written as $|\psi\rangle \in \mathcal{H}$, a so-called *ket*. Further, elements in the dual space $\mathcal{H}'$ are called *bras*, and one writes $\langle\varphi| \in \mathcal{H}'$. One can now apply $|\psi\rangle$ to the functional $\langle\varphi|$. If the functional $\langle\varphi|$ is identified with a vector $|\varphi\rangle \in \mathcal{H}$ (which is possible in a unique way by the Riesz representation theorem) one has

$$\langle\varphi|(|\psi\rangle) = \varphi_{|\varphi\rangle}(|\psi\rangle) = \langle(|\varphi\rangle)|(|\psi\rangle)\rangle$$

To simplify notation, physicists usually use $\langle\varphi|\psi\rangle$ for the above expression. Note that by the last equality this evaluation indeed agrees with the scalar product of $|\psi\rangle$ with $\langle\varphi|$ after $\langle\varphi|$ is identified with the state $|\varphi\rangle$ via the isomorphism given by the Riesz representation theorem. Please note however that this argument only works if both sides can indeed by identified with elements of the Hilbert space $\mathcal{H}$. Note that nevertheless physicists often use the above notation when this condition is violated. For example, physicists usually call the system $(e^{ix\cdot})_{x\in\mathbb{R}}$ a generalized orthogonal basis and write

$$\langle e^{ix_1\cdot}|e^{ix_2\cdot}\rangle = \delta(x_1 - x_2).$$

We will later give more sense to expressions as above by introducing Gelfand triples and distributions.

The bra–ket notation can also be very convenient when working with linear operators. Given a linear operator A (bounded or unbounded) one

denotes by $A|\psi\rangle$ the value of $\psi\rangle$ under A in agreement with the notation used in mathematics. One extends the action of A to bras by defining

$$(\langle\varphi|A)(|\psi\rangle) = A(\langle\varphi|)(|\psi\rangle) := (\langle\varphi|)(A|\psi\rangle) = \langle(|\varphi\rangle)|(A|\psi\rangle)\rangle =: \langle\varphi|A|\psi\rangle.$$

In fact, if $A \in \mathcal{B}(\mathcal{H})$ one has $|A(\langle\varphi|)(|\psi\rangle)| \leq \|\langle\varphi|\| \, \|A\| \, \||\psi\rangle\|$ and therefore $A(\langle\varphi|) \in \mathcal{H}^*$ for all $\langle\varphi| \in \mathcal{H}^*$.

Now suppose one has given $A \in \mathcal{B}(\mathcal{H})$ and $|\psi\rangle \in \mathcal{H}$. Let us determine the bra $\langle\varphi|$ which corresponds to the ket $|\varphi\rangle = A|\psi\rangle$. One has

$$\langle\varphi|\eta\rangle = \langle(A|\psi\rangle)|(|\eta\rangle)\rangle = \langle(|\psi\rangle)|(A^*|\eta\rangle)\rangle = (\langle\psi|A^*)(|\eta\rangle).$$

One obtains $\langle\varphi| = \langle\psi|A^*$. Hence, the adjoint formally acts on kets. In particular, if A is self-adjoint, then A acts in the same way both on kets and bras.

Note that the definition of the action of A on bras is made in a way such that the value of the scalar product at the right hand side of the above equation agrees no matter whether A is applied to a ket or to a bra. This justifies the use of the notation $\langle\varphi|A|\psi\rangle$. Note that if $\mathcal{H}$ is finite dimensional and A is identified with a matrix everything can be computed using matrix multiplications.

One also often uses the so-called *outer product* of kets and bras. For a ket $|\varphi\rangle \in \mathcal{H}$ and a bra $\langle\psi| \in \mathcal{H}^*$ we define the bounded linear operator

$$(|\varphi\rangle\langle\psi|)(|\chi\rangle) := \langle\psi|\chi\rangle \cdot |\varphi\rangle \qquad \text{for } |\chi\rangle \in \mathcal{H}.$$

In the finite dimensional setting the operator $|\varphi\rangle\langle\psi|$ corresponds to the matrix obtained by multiplying the column vector $|\varphi\rangle$ with the row vector $\langle\psi|$. In particular, if $(e_n)_{n\in\mathbb{N}}$ is an orthonormal basis of a Hilbert space $\mathcal{H}$, then the finite rank operator

$$\sum_{n=1}^{N} |e_n\rangle\langle e_n|$$

for $N \in \mathbb{N}$ is an orthogonal projection onto $\operatorname{span}\{e_1, \ldots, e_N\}$ as considered in Example 2.1.14.

2.1.3 Sobolev Spaces

In this section we introduce an important class of Hilbert spaces, the so-called Sobolev spaces. These play a fundamental role in the mathematical treatment of differential operators and partial differential equations. We have seen that many important quantum mechanical observables can be realized by self-adjoint differential operators. The correct domain of these operators usually is some sort of Sobolev space as we will soon see. Hence, for the study of concrete quantum mechanical systems, we need some basic knowledge on those spaces.

Sobolev spaces generalize the notion of classical derivatives in a way that is very well adapted to the use of functional analytic methods such as Hilbert space theory. Indeed, the theory of Sobolev spaces is the correct framework for the study of partial differential equations.

Before introducing Sobolev spaces, we need some basic notation. For an open subset $\Omega \subset \mathbb{R}^n$ we denote by $C_c^\infty(\Omega)$ the set of all infinitely differentiable functions $\varphi\colon \Omega \to \mathbb{K}$ with compact support in Ω, i.e. the closure of $\{x \in \Omega : \varphi(x) \neq 0\}$ (in the metric space Ω) is a compact subset of Ω. Note that $C_c^\infty(\Omega)$ contains plenty of functions. For example, in the one-dimensional case consider the function

$$\psi(x) = \begin{cases} e^{-1/x^2} & \text{if } x > 0 \\ 0 & \text{if } x \leq 0. \end{cases}$$

Then one can verify that $\psi \in C^\infty(\mathbb{R})$. Now, the function $\varphi(x) = \psi(1+x)\psi(1-x)$ lies in $C^\infty(\mathbb{R})$ and vanishes outside $(-1,1)$. Hence, φ is a non-trivial element of $C_c^\infty(\mathbb{R})$. By taking suitable products of translations and dilations of the function φ just constructed one now easily obtains non-trivial elements of $C_c^\infty(\Omega)$.

In the following we use a short-hand notation for higher derivatives. Let $\Omega \subset \mathbb{R}^n$ be open and $\alpha = (\alpha_1, \dots, \alpha_n) \in \mathbb{N}_0^n$ be a multi-index. For a sufficiently differentiable function $f : \Omega \to \mathbb{R}$ we write $D^\alpha f = D^{\alpha_1} D^{\alpha_2} \cdots D^{\alpha_n} f = \frac{\partial^{|\alpha|} f}{\partial^{\alpha_1} x_1 \cdots \partial^{\alpha_n} x_n}$, where $|\alpha| = \alpha_1 + \cdots + \alpha_n$. Sometimes we will also write $D_x^\alpha f$ to make clear that we derivative with respect to the x-variables. Moreover, we use for $p \in [1, \infty]$

$$L^p_{\mathrm{loc}}(\Omega) := \Big\{ f : \Omega \to \mathbb{K} \text{ measurable} : \|f \mathbb{1}_K\|_p < \infty \text{ for all compact } K \subset \Omega \Big\}.$$

Note that by the L^p-inclusions for finite measure spaces (Proposition 1.3.8) we have $L^p_{\mathrm{loc}}(\Omega) \subset L^q_{\mathrm{loc}}(\Omega)$ for all $p \geq q$. In particular, we have the inclusion $L^p_{\mathrm{loc}}(\Omega) \subset L^1_{\mathrm{loc}}(\Omega)$ for all $p \geq 1$.

Definition 2.1.20. Let $\Omega \subset \mathbb{R}^n$ be open, $\alpha \in \mathbb{N}_0^n$ and $f \in L^1_{\mathrm{loc}}(\Omega)$. A function $g \in L^1_{\mathrm{loc}}(\Omega)$ is called a *weak α-th derivative* of f if for all (real) $\varphi \in C_c^\infty(\Omega)$

$$\int_\Omega f D^\alpha \varphi = (-1)^{|\alpha|} \int_\Omega g \varphi.$$

The space $C_c^\infty(\Omega)$ is a so-called space of *test functions*. Such spaces will later play an important role in the development of the mathematical theory of distributions.

In the following example we show that the terminology weak derivative makes sense.

Example 2.1.21. Let $f \in C^k(\Omega)$ be a k times continuously differentiable function on some open subset $\Omega \subset \mathbb{R}^n$ and $\alpha \in \mathbb{N}_0^n$ with $|\alpha| \leq k$. Successively using integrations by parts, we see that

$$\int_\Omega f D^\alpha \varphi = (-1)^{|\alpha|} \int_\Omega D^\alpha f \varphi \qquad \text{for all } \varphi \in C_c^\infty(\Omega).$$

This shows that $D^\alpha f$ is a weak α-th derivative of f. Notice that the continuity of all factors in the integrands and the compact support of φ guarantee the existence of both integrals.

Hence, we have generalized the concept of a classical derivative by making the validity of the integration by parts formula to our definition of a weak derivative. Moreover, there exist functions which have a weak derivative but are not classically differentiable.

Example 2.1.22. Consider the function $f \in L^1_{\mathrm{loc}}((-1,1))$ given by $f(x) = |x|$. It is well-known that f is not differentiable in the origin. However, $g(x) = \operatorname{sign} x$ is a weak derivative of f. Indeed, for $\varphi \in C_c^\infty((-1,1))$ one has

$$\begin{aligned}\int_{-1}^1 |x|\,\varphi'(x)\,dx &= \int_0^1 x\varphi'(x)\,dx - \int_{-1}^0 x\varphi'(x)\,dx \\ &= [x\varphi(x)]_0^1 - \int_0^1 \varphi(x)\,dx - [x\varphi(x)]_{-1}^0 + \int_{-1}^0 \varphi(x)\,dx \\ &= -\int_{-1}^1 \operatorname{sign} x\varphi(x)\,dx.\end{aligned}$$

We now substantially generalize the above example.

Example 2.1.23. Let $I = (a,b) \subset \mathbb{R}$ be an open (not necessarily bounded) interval and $g \in L^1(I)$. Now for some $x_0 \in \overline{I}$ consider the function $f(x) = \int_{x_0}^x g(y)\,dy$. Then f is weakly differentiable because for $\varphi \in C_c^\infty((a,b))$ we have by Fubini's theorem

$$\begin{aligned}\int_a^b f(x)\varphi'(x)\,dx &= \int_a^b \int_{x_0}^x g(y)\,dy\,\varphi'(x)\,dx = \int_a^b g(y) \int_y^b \varphi'(x)\,dx\,dy \\ &= -\int_a^b g(y)\varphi'(y)\,dy.\end{aligned}$$

This shows that the weak derivative of f is given by g, i.e. $f' = g$ in the weak sense. Observe that the same argument works if $f \in L^1_{\mathrm{loc}}(I)$ provided one makes the restriction $x_0 \in I$.

Before going any further, we need some approximation results for continuous and L^p functions.

Proposition 2.1.24. *Let $\Omega \subset \mathbb{R}^n$ be open, $p \in [1,\infty)$ and $f \in L^p(\Omega)$ such that $f = 0$ almost everywhere outside a subset $A \subset \Omega$ that has positive distance to $\partial\Omega$. Then there exists a sequence $(\varphi_k)_{k\in\mathbb{N}} \subset C_c^\infty(\Omega)$ with $\varphi_k \to f$ in $L^p(\Omega)$. Moreover, the sequence can be chosen to have the following properties.*

(a) *if $f \geq 0$ almost everywhere, then $\varphi_n(x) \geq 0$ for all $n \in \mathbb{N}$;*

(b) *if $f \in L^\infty(\Omega)$, then $\varphi_n \leq \|f\|_\infty \mathbb{1}$ for all $n \in \mathbb{N}$.*

Proof. Let $\psi \in C_c^\infty(\mathbb{R}^n)$ be a non-negative function with $\|\psi\|_1 = 1$ and support inside the unit ball. Now define $\psi_k(x) = k^n\psi(kx)$. Then $\psi_k \geq 0$ and $\|\psi_k\|_1 = 1$ for all $k \in \mathbb{N}$ and ψ_k vanishes outside the ball $B(0,1/k)$. Now consider the convolution

$$\varphi_k(x) = (f * \psi_k)(x) = \int_{\mathbb{R}^n} f(y)\psi_k(x-y)\,dy,$$

where we extend f by zero outside Ω. Notice that the convolution exists, for example as a consequence of Proposition 1.3.10 or by observing that for fixed $x \in \mathbb{R}^n$ both sides are integrable after passing to the compact support of the integrand. It follows from the dominated convergence theorem that $\varphi_k \in C^\infty(\mathbb{R}^n)$. More precisely, one can verify that for a multi-index $\alpha \in \mathbb{N}^n$ one has

$$(D^\alpha\varphi_k)(x) = \int_{\mathbb{R}^n} f(y)(D^\alpha\psi_k)(x-y)\,dy.$$

Moreover, it follows from the formula for the convolution that $\varphi_k(x)$ vanishes if $|x-y| \geq 1/k$ for all $y \in A$. Hence, φ_k vanishes outside $A + B(0,1/k)$. Since A has positive distance to $\partial\Omega$, we have $\varphi_k \in C_c^\infty(\Omega)$ for sufficiently large k.

We now show that $(\varphi_k)_{k\in\mathbb{N}}$ converges to f in L^p. We start with the case when f additionally is a compactly supported continuous function. Let $x \in \Omega$ and $\varepsilon > 0$. Since f is continuous in x, there exists $\delta > 0$ such that $|f(x)-f(y)| \leq \varepsilon$ for all $|x-y| \leq \delta$. Now if $k > 1/\delta$

$$\begin{aligned}
|f(x) - \varphi_k(x)| &= \left| \int_{\mathbb{R}^n} f(x)\psi_k(x-y)\,dy - \int_{\mathbb{R}^n} f(y)\psi_k(x-y)\,dy \right| \\
&\leq \int_{\mathbb{R}^n} |f(x)-f(y)|\psi_k(x-y)\,dy = \int_{\mathbb{R}^n} |f(x)-f(x-y)|\psi_k(y)\,dy \\
&= \int_{B(0,1/k)} |f(x)-f(x-y)|\psi_k(y)\,dy \leq \varepsilon \int_{B(0,1/k)} \psi_k(y)\,dy = \varepsilon.
\end{aligned}$$

Hence, $\varphi_k(x) \to f(x)$ for all $x \in \Omega$. As an immediate step we now show assertions (a) and (b). Note that (a) is obvious from our construction and that part (b) follows from the estimate

$$|\varphi_k(x)| \leq \int_{\mathbb{R}^n} \|f\|_\infty\, \psi_k(x-y)\,dy = \|f\|_\infty.$$

Since the functions φ_k are supported in $A + B(0,1)$ and are uniformly bounded by $\|f\|_\infty$ (which is finite because f is continuous and has compact support), it follows from the dominated convergence theorem that $\varphi_k \to f$ in L^p.

We now consider the case of arbitrary $f \in L^p(\Omega)$. Consider for $k \in \mathbb{N}$ the linear bounded operator

$$\begin{aligned} T_k \colon L^p(\Omega) &\to L^p(\mathbb{R}^n) \\ f &\mapsto f * \psi_k \end{aligned}$$

It follows from Minkowski's inequality for convolutions (Proposition 1.3.10) that $\|T_k\| \leq \|\psi_k\|_1 = 1$. Since $C_c(\Omega)$ is dense in $L^p(\Omega)$ by Proposition 1.3.6, Lemma 2.1.10 shows that $T_k f \to f \mathbb{1}_\Omega$ in $L^p(\mathbb{R}^n)$ for all $f \in L^p(\Omega)$. This finishes the proof. □

Notice that a priori a function f could have several different weak derivatives. We now show that this is not the case. The following lemma is often called the *du Bois-Reymond lemma*. In calculus of variations you have probably encountered variants of this lemma which are usually called *the fundamental lemma of calculus of variations*. There it is used to deduce the Euler–Lagrange equations from the variational principle. Although intuitively clear, a rigorous proof needs some effort because of measure theoretic difficulties.

Lemma 2.1.25 (du Bois-Reymond). *Let $\Omega \subset \mathbb{R}^n$ be open and $f \in L^1_{\mathrm{loc}}(\Omega)$ with*

$$\int_\Omega f\varphi = 0 \qquad \text{for all } \varphi \in C_c^\infty(\Omega).$$

Then $f = 0$ almost everywhere.

Proof. First observe that it is sufficient to consider the case when f is a real function. Indeed, the assumption implies

$$\int_\Omega f\varphi = \int_\Omega \operatorname{Re} f\varphi + i \int_\Omega \operatorname{Im} f\varphi = 0$$

for all real $\varphi \in C_c(\Omega)$. Since a complex number vanishes if and only if both the real and imaginary part vanish, both summands in the above formula must vanish. Hence, the complex case follows from the real case applied to both $\operatorname{Re} f$ and $\operatorname{Im} f$.

For $n \in \mathbb{N}$ let $\Omega_n = \{x \in \Omega \cap B(0,n) : \operatorname{dist}(x, \partial(\Omega \cap B(0,n)) > 1/n\}$. Then Ω_n is open and bounded. Suppose we can show that $f = 0$ almost everywhere on Ω_n. Then it follows that $f = 0$ almost everywhere on Ω because of $\cup_{n\in\mathbb{N}} \Omega_n = \Omega$ and the fact that the countable union of null sets is a null set.

Now assume that $f = 0$ does not hold almost everywhere on Ω_n. This means that $|\{x \in \Omega_n : |f(x)| > 0\}| > 0$. We may assume without loss of generality

that $|\{x \in \Omega_n : f(x) > 0\}| > 0$ (replace f by $-f$ if necessary). It now follows that there exists an $\varepsilon > 0$ and a measurable subset $A \subset \Omega_n$ of positive measure with $f(x) \geq \varepsilon$ for all $x \in A$.

Let B be an arbitary measurable subset of Ω_n. Since Ω_n has positive distance to the boundary of Ω, by Proposition 2.1.24 there exists a sequence $(\varphi_k)_{k\in\mathbb{N}} \subset C_c^\infty(\Omega_{n+1})$ with $0 \leq \varphi_k \leq \mathbb{1}$ and $\varphi_k \to \mathbb{1}_B$ in $L^1(\Omega)$. By Proposition 1.3.5 we can additionally assume after passing to a subsequence that $\varphi_k(x) \to \mathbb{1}_B(x)$ almost everywhere on Ω. Since Ω_n has finite measure, it follows from the dominated convergence theorem because of $|\varphi_k f| \leq |f|\mathbb{1}_{\Omega_{n+1}}$ that

$$\int_\Omega f\mathbb{1}_B = \lim_{k\to\infty} \int_\Omega f\varphi_k = 0.$$

Taking $B = A$, we however have by the considerations in the previous paragraph

$$\int_\Omega f\mathbb{1}_A \geq \varepsilon \int_\Omega \mathbb{1}_A = \varepsilon\,|A| > 0,$$

which is a contradiction. Hence, we must have $f = 0$ almost everywhere on Ω_n. □

The uniqueness of weak derivatives is now an immediate consequence of the Du Bois–Reymond lemma.

Corollary 2.1.26. *Let $\Omega \subset \mathbb{R}^n$ be open, $\alpha \in \mathbb{N}_0^n$ and $f : \Omega \to \mathbb{K}$. Suppose that f has two weak α-th derivatives g_1 and g_2 in $L^1_{\mathrm{loc}}(\Omega)$. Then $g_1 = g_2$ as elements in $L^1_{\mathrm{loc}}(\Omega)$, i.e. $g_1 = g_2$ almost everywhere.*

Proof. By definition, one has for all $\varphi \in C_c^\infty(\Omega)$

$$(-1)^{|\alpha|} \int_\Omega g_1\varphi = \int_\Omega f D^\alpha\varphi = (-1)^{|\alpha|} \int_\Omega g_2\varphi.$$

Hence, for all $\varphi \in C_c^\infty(\Omega)$ we obtain the identity

$$\int_\Omega (g_1 - g_2)\varphi = 0.$$

It now follows from the du Bois-Reymond Lemma 2.1.25 that $g_1 = g_2$ almost everywhere. □

Now suppose that $f \in L^1_{\mathrm{loc}}(\Omega)$ has a weak α-th derivative. By the above corollary a weak derivative is uniquely determined in $L^1_{\mathrm{loc}}(\Omega)$. It makes therefore sense to speak of *the* weak α-th derivative which we will denote by $D^\alpha f$. Recall that we have seen in Example 2.1.21 that if f is classically continuously differentiable, the weak derivative coincides with the classical derivative. Thus there is no conflict in notation.

We now can finally define Sobolev spaces.

Definition 2.1.27 (Sobelev spaces). Let $\Omega \subset \mathbb{R}^n$ be open, $k \in \mathbb{N}$ and $p \in [1, \infty]$. We define the *Sobolev spaces*

$$W^{k,p}(\Omega) \coloneqq \{f \in L^p(\Omega) : f \text{ is weakly } \alpha\text{-diff. and } D^\alpha f \in L^p(\Omega) \text{ for all } |\alpha| \leq n\}.$$

endowed with the norms

$$\|f\|_{W^{k,p}(\Omega)} \coloneqq \left(\sum_{|\alpha| \leq k} \|D^\alpha f\|^p_{L_p(\Omega)} \right)^{1/p}.$$

In the particular interesting case of $W^{k,2}$-spaces, one naturally obtains a Hilbert space structure.

Proposition 2.1.28. *Let $\Omega \subset \mathbb{R}^n$ be open and $k \in \mathbb{N}$. Then $W^{k,p}(\Omega)$ is a Banach space. In the case $p = 2$ the norm of $W^{k,2}(\Omega)$ is induced by the inner product*

$$\langle f | g \rangle_{W^{k,2}(\Omega)} \coloneqq \sum_{|\alpha| \leq k} \int_\Omega \langle D^\alpha f | D^\alpha g \rangle_{L^2(\Omega)},$$

which endows $W^{k,2}(\Omega)$ with the structure of a Hilbert space. We will also use the abbreviation $H^k(\Omega) = W^{k,2}(\Omega)$.

Proof. All assertions except for the completeness are obvious. For the completeness suppose that $(f_n)_{n \in \mathbb{N}}$ is a Cauchy sequence in $W^{k,p}(\Omega)$. In particular, $(D^\alpha f_n)_{n \in \mathbb{N}}$ is a Cauchy sequence in $L_p(\Omega)$ for all $|\alpha| \leq k$. Now, it follows from the completeness of $L^p(\Omega)$ that for all $|\alpha| \leq k$ there exists $f_\alpha \in L^p(\Omega)$ with $D^\alpha f_n \to f_\alpha$.

We now show that $f = f_{(0,\dots,0)}$ is weakly α-differentiable for all $|\alpha| \leq k$. For this observe that for all $\varphi \in C_c^\infty(\Omega)$ one has

$$\int_\Omega f D^\alpha \varphi = \lim_{n \to \infty} \int_\Omega f_n D^\alpha \varphi = \lim_{n \to \infty} (-1)^{|\alpha|} \int_\Omega D^\alpha f_n \varphi = (-1)^{|\alpha|} \int_\Omega f_\alpha \varphi.$$

Here we have used twice the fact that for $\psi \in C_c^\infty(\Omega)$ the functional $f \mapsto \int_\Omega f \psi$ is continuous by Hölder's inequality. Observe that the above calculation shows that $D^\alpha f = f_\alpha$. From this it is now clear that $f \in W^{k,p}(\Omega)$ and $f_n \to f$ in $W^{k,p}(\Omega)$. Hence, $W^{k,p}(\Omega)$ is complete. □

Note that we have seen in Example 2.1.22 that there exist Sobolev functions which are not classically differentiable. However, one has the following denseness result.

Theorem 2.1.29. *Let $n \in \mathbb{N}$, $p \in [1, \infty)$ and $k \in \mathbb{N}$. Then the space $C_c^\infty(\mathbb{R}^n)$ is dense in $W^{k,p}(\mathbb{R}^n)$.*

Proof. Let $f \in W^{k,p}(\mathbb{R}^n)$. By Proposition 2.1.24 the sequence in $C_c^\infty(\mathbb{R}^n)$ given by $\varphi_k = f * \psi_k$, where $\psi_k(x) = k^n \psi(kx)$ for some $C_c^\infty(\mathbb{R}^n)$ with $\|\psi\|_1 = 1$, converges to f in L^p. Moreover, we have seen that for $\alpha \in \mathbb{N}^n$

$$(D^\alpha \varphi_k)(x) = \int_{\mathbb{R}^n} f(y)(D_x^\alpha \psi_k)(x-y)\,dy.$$

Observe that $(D_x^\alpha \psi_k)(x-y) = (-1)^{|\alpha|}(D_y^\alpha \psi_k)(x-y)$ lies in $C_c^\infty(\mathbb{R}^n)$. Hence, for $|\alpha| \le k$ we have by the definition of the weak derivative

$$\begin{aligned}(D^\alpha \varphi_k)(x) &= (-1)^{-\alpha} \int_{\mathbb{R}^n} f(y)(D_y^\alpha \psi_k)(x-y)\,dy = \int_{\mathbb{R}^n} (D^\alpha f)(y)\psi_k(x-y)\,dy \\ &= D^\alpha f * \psi_k\end{aligned}$$

Hence, it follows again form Proposition 2.1.24 that $D^\alpha \varphi_k \to D^\alpha f$ in L^p. Altogether this shows that $\varphi_k \to f$ in $W^{k,p}(\mathbb{R}^n)$. Hence, $C_c(\mathbb{R}^n)$ is dense in $W^{k,p}(\mathbb{R}^n)$. □

Sobolev spaces are a fundamental tool in the modern treatment of partial differential equations. We only give one example to show the power of the functional analytic apparatus for the treatment of such equations.

Example 2.1.30 (Weak solutions for $-\Delta u + u = f$). On $\mathbb{R}^n$ consider the following elliptic problem for real functions closely related to Poisson's equation. We search a solution u to the inhomogeneous problem $-\Delta u + u = f$ on $\mathbb{R}^n$. For the moment assume that $u \in C^2(\mathbb{R}^n)$ is a classical solution of the problem. In particular, u and therefore f are continuous functions. Integrating both sides against a test function $w \in C_c^\infty(\mathbb{R}^n)$ we obtain by integration by parts

$$\int_{\mathbb{R}^n} (-\Delta u + u) w\,dx = \int_{\mathbb{R}^n} \nabla u \nabla w\,dx + \int_{\mathbb{R}^n} u w\,dx = \int_{\mathbb{R}^n} f w\,dx.$$

Conversely, suppose that $u \in C^2(\mathbb{R}^n)$ satisfies for some $f \in L^1_{\mathrm{loc}}(\mathbb{R}^n)$

$$\int_{\mathbb{R}^n} \nabla u \nabla w\,dx + \int_{\mathbb{R}^n} u w\,dx = \int_{\mathbb{R}^n} f w\,dx \tag{WS}$$

for all $w \in C_c(\mathbb{R}^n)$. Then we again see by integration by parts that

$$\int_{\mathbb{R}^n} (-\Delta u + u) w\,dx = \int_{\mathbb{R}^n} f w\,dx$$

for all $w \in C_c(\mathbb{R}^n)$. Hence, it follows from the Du Bois-Reymond lemma (Lemma 2.1.25) that $-\Delta u + u = f$, i.e. u is a classical solution of the equation. For $f \in L^2(\mathbb{R}^n)$ we say that $u \in H^1(\mathbb{R}^n)$ (we work over real Hilbert spaces in this example) is a *weak solution* of the equation if u satisfies (WS) for all

$w \in C_c^\infty(\mathbb{R}^n)$. Note that if u is a classical solution such that f as well as u and all of its partial derivatives of first order lie in $L^2(\mathbb{R}^n)$, then (WS) holds for all $w \in H^1(\mathbb{R}^n)$ by the density of $C_c(\Omega)$ in $H^1(\mathbb{R}^n)$. More generally, the validity of (WS) extends from all $w \in C_c^\infty(\mathbb{R}^n)$ to all $w \in H^1(\mathbb{R}^n)$ provided $u \in H^1(\mathbb{R}^n)$ and $f \in L^2(\mathbb{R}^n)$.

The advantage of the concept of weak solutions lies in the fact that one often can establish the existence and uniqueness of weak solutions with functional analytic methods. In our case consider the functional

$$\begin{aligned} \varphi\colon H^1(\mathbb{R}^n) &\to \mathbb{R} \\ w &\mapsto \int_{\mathbb{R}^n} f w \, dx. \end{aligned}$$

Notice that by the Cauchy–Schwarz inequality (CS) one has

$$|\varphi(w)| \leq \|f\|_2 \|w\|_2 \leq \|f\|_2 \|w\|_{H^1(\mathbb{R}^n)}$$

for all $w \in H^1(\mathbb{R}^n)$. This shows that $\varphi \in H^1(\mathbb{R}^n)^*$ and it now follows from the Riesz representation theorem (Theorem 2.1.18) that there exists a unique $u \in H^1(\mathbb{R}^n)$ such that

$$\langle u, w \rangle_{H^1(\mathbb{R}^n)} = \int_{\mathbb{R}^n} \nabla u \nabla w \, dx + \int_{\mathbb{R}^n} u w \, dx = \int_{\mathbb{R}^n} f w \, dx = \varphi(w)$$

for all $w \in H^1(\mathbb{R}^n)$. Hence, we have shown that there exists a unique weak solution u of the equation for all $f \in L^2(\mathbb{R}^n)$. We will later see that this solution already satisfies $u \in C^\infty(\mathbb{R}^n)$ if the inhomogeneity additionally has the regularity $f \in C^\infty(\mathbb{R}^n)$ and therefore is a classical solution of $-\Delta u + u = f$.

2.1.4 The Fourier Transform on $L^2(\mathbb{R}^n)$

The Fourier transform is an extremely important and powerful tool both in mathematics and physics. In physics the Fourier transform is often used to switch from the position space to the momentum space description of a quantum mechanical system and vice versa. In mathematics and concrete calculations the Fourier transform is extremely useful because it diagonalizes differential operators (with constant coefficients). We start with with the definition of the Fourier transform on L^1.

Definition 2.1.31 (The Fourier Transform on $L^1(\mathbb{R}^n)$). For $f \in L^1(\mathbb{R}^n)$ we define its *Fourier transform* as

$$(\mathcal{F} f)(x) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} f(y) e^{-ix\cdot y} \, dy,$$

where $x \cdot y = \sum_{k=1}^n x_k y_k$ stands for the Euclidean scalar product in $\mathbb{R}^n$.

For an open set $\Omega \subset \mathbb{R}^n$ we introduce the space of all continuous functions vanishing in infinity

$$C_0(\Omega) = \{u \colon \Omega \to \mathbb{K} \text{ continuous} : \forall \varepsilon > 0 \, \exists K \subset \Omega \text{ compact: } |f(x)| \leq \varepsilon \, \forall x \notin K\}.$$

Observe that $C_0(\Omega)$ becomes a Banach space when endowed with the norm $\|f\|_\infty := \sup_{x\in\Omega} |f(x)|$. This follows from the fact that the uniform limit of continuous functions is continuous and respects the vanishing condition. The Fourier transform has the following elementary but useful mapping property.

Lemma 2.1.32 (Riemann–Lebesgue). *The Fourier transform $\mathcal{F}$ maps $L^1(\mathbb{R}^n)$ into $C_0(\mathbb{R}^n)$.*

The above lemma can be explicitly verified for indicators of finite intervals and hence extends to simple functions by linearity. The general case then follows from a density argument and the fact that $C_0(\mathbb{R}^n)$ is a closed subspace of $L^\infty(\mathbb{R}^n)$. Note that for a function $f \in L^2(\mathbb{R}^n)$ the above Fourier integral may not converge. Nevertheless it is possible to extend the Fourier transform to $L^2(\mathbb{R}^n)$.

Definition 2.1.33. Let $\mathcal{H}$ be a Hilbert space. A bounded linear operator $U \in \mathcal{B}(\mathcal{H})$ is called a *unitary operator* if

(i) U is surjective and

(ii) $\langle Ux|Uy\rangle = \langle x|y\rangle$ for all $x, y \in \mathcal{H}$.

It follows from the *polarization identity*

$$\overline{\langle x|y\rangle} = \frac{1}{4} \sum_{k=1}^{4} i^k \|x + i^k y\|^2$$

that a bounded linear surjective operator U is unitary if and only if $\|Ux\| = \|x\|$ for all $x \in \mathcal{H}$, i.e. U is a surjective *isometry*. In fact, the next theorem shows that the Fourier transform can even be extended to a unitary operator on $L^2(\mathbb{R}^n)$.

Theorem 2.1.34. *The Fourier transform $\mathcal{F}$ has the following properties.*

(a) *Let $f \in L^1(\mathbb{R}^n)$ such that $\mathcal{F}f \in L^1(\mathbb{R}^n)$ as well. Then the Fourier inversion formula*

$$f(x) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} (\mathcal{F}f)(y) e^{ix\cdot y} \, dy$$

holds.

(b) *Let $f \in L^1(\mathbb{R}^n) \cap L^2(\mathbb{R}^n)$. Then $\mathcal{F}f \in L^2(\mathbb{R}^n)$ and*

$$\|\mathcal{F}f\|_2^2 = \int_{\mathbb{R}^n} |(\mathcal{F}f)(x)|^2 \, dx = \int_{\mathbb{R}^n} |f(x)|^2 \, dx = \|f\|_2^2.$$

Therefore the Fourier transform can be uniquely extended to a unitary operator $\mathcal{F}_2 \colon L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ which we will also denote by $\mathcal{F}$ (the density of $\mathcal{F}L^1(\mathbb{R}^n)$ in $L^2(\mathbb{R}^n)$ will be a consequence of Proposition 3.2.7).

Note that by the inversion formula we have $\mathcal{F}^2 = -\mathrm{Id}$ and therefore $\mathcal{F}^{-1} = -\mathcal{F}$. Hence, results such as the Riemann-Lebesgue lemma are also valid for the inverse Fourier transform. The importance of the Fourier transform lies in the fact that it diagonalizes differentiation operators. This is essentially the content of the next result.

Proposition 2.1.35. *Let $n \in \mathbb{N}$. The following criterion for a function $f \in L^2(\mathbb{R}^n)$ to be in $H^1(\mathbb{R}^n)$ holds:*

$$f \in H^1(\mathbb{R}^n) \qquad \Leftrightarrow \qquad x_j \mathcal{F}f \in L^2(\mathbb{R}^n) \quad \text{for all } j = 1, \dots, n.$$

More generally, one has $f \in H^k(\mathbb{R}^n)$ if and only if $x^\alpha \mathcal{F}f$ lies in $L^2(\mathbb{R}^n)$ for all $|\alpha| \leq k$. More precisely, for $\alpha \in \mathbb{N}^n$ the weak α-th partial derivative exists and lies in $L^2(\mathbb{R}^n)$ if and only if $x^\alpha \mathcal{F}f \in L^2(\mathbb{R}^n)$. In this case

$$\|D^\alpha f\|_{L^2(\mathbb{R}^n)} = \|x^\alpha \mathcal{F}f\|_{L^2(\mathbb{R}^n)}.$$

Proof. First let $f \in C_c^\infty(\mathbb{R}^n)$. Using integration by parts we obtain for $j = 1, \dots, n$ and $x \in \mathbb{R}^n$ the identity

$$\begin{aligned}\left(\mathcal{F}\left(\frac{\partial f}{\partial y_j}\right)\right)(x) &= \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} \frac{\partial f}{\partial y_j}(y) e^{-ixy} \, dy = ix_j \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} f(y) e^{-ixy} \, dy \\ &= ix_j (\mathcal{F}f)(x).\end{aligned}$$

Hence, $\mathcal{F}(\frac{\partial f}{\partial y_j}) = ix_j \mathcal{F}f$. Since the space of test functions $C_c^\infty(\mathbb{R}^n)$ is dense in $H^1(\mathbb{R}^n)$ by Proposition 2.1.29, it follows from a limiting argument that the above identity extends to all $f \in H^1(\mathbb{R}^n)$. Indeed, for $f \in H^1(\mathbb{R}^n)$ let $(f_n)_{n\in\mathbb{N}} \subset C_c^\infty(\mathbb{R}^n)$ be a sequence with $f_n \to f$ in $H^1(\mathbb{R}^n)$. Then it follows from the continuity of the Fourier transform on $L^2(\mathbb{R}^n)$ that

$$\mathcal{F}\left(D_j f\right) = \lim_{n\to\infty} \mathcal{F}\left(D_j f_n\right) = \lim_{n\to\infty} ix_j \mathcal{F}f_n$$

exists in $L^2(\mathbb{R}^n)$. It follows from Proposition 1.3.5 that $\lim_{n\to\infty} ix_j \mathcal{F}f_n$ agrees with $ix_j \mathcal{F}f$ almost everywhere. Hence, $ix_j \mathcal{F}f \in L^2(\mathbb{R}^n)$ with $\mathcal{F}(D_j f) = ix_j \mathcal{F}f$.

Conversely for $f \in L^2(\mathbb{R}^n)$, assume that $ix_j \mathcal{F}f$ is in $L^2(\mathbb{R}^n)$ for all $j = 1, \dots, n$. We show that $\mathcal{F}^{-1}(ix_j \mathcal{F}f)$ is the weak j-th partial derivative for $f \in L^2(\mathbb{R}^n)$. Observe that for all $\varphi \in C_c^\infty(\mathbb{R}^n)$ we have

$$\begin{aligned}\int_{\mathbb{R}^n} \mathcal{F}^{-1}(ix_j \mathcal{F}f)\varphi &= \int_{\mathbb{R}^n} \mathcal{F}^{-1}(ix_j \mathcal{F}f)\overline{\varphi} = \int_{\mathbb{R}^n} ix_j \mathcal{F}f \overline{\mathcal{F}\varphi} \\ &= -\int_{\mathbb{R}^n} \mathcal{F}f \overline{\mathcal{F}(D_j\varphi)} = -\int_{\mathbb{R}^n} f \overline{D_j\varphi} = -\int_{\mathbb{R}^n} f D_j \varphi.\end{aligned}$$

Hence, by definition $f \in H^1(\mathbb{R}^n)$. The general case and the norm identity follow on exactly the same lines of proof. □

A a direct consequence we obtain an embedding theorem for Sobolev spaces into classical function spaces.

Theorem 2.1.36 (Sobolev embedding). *Let $k, n \in \mathbb{N}$ with $k > \frac{n}{2}$. Then one has the inclusion $H^k(\mathbb{R}^n) \subset C_0(\mathbb{R}^n)$. Hence, $H^k(\mathbb{R}^n) \subset C^m(\mathbb{R}^n) \cap C_0(\mathbb{R}^n)$ if $k - m > \frac{n}{2}$. In particular $\cap_{k\in\mathbb{N}} H^k(\mathbb{R}^n) \subset C^\infty(\mathbb{R}^n)$.*

Proof. Let $k, n \in \mathbb{N}$ be such that $\frac{k}{2} > n$. It follows from Proposition 2.1.35 that $|x|^\alpha \mathcal{F}f \in L^2(\mathbb{R}^n)$ for all $|\alpha| \le k$. It then follows that for some constants c_α

$$\int_{\mathbb{R}^n} (1 + |x|^2)^k \, |(\mathcal{F}f)(x)|^2 \, dx = \sum_{|\alpha|\le k} c_\alpha \int_{\mathbb{R}^n} (x^\alpha)^2 \, |(\mathcal{F}f)(x)|^2 \, dx < \infty.$$

This shows $(1 + |x|^2)^{k/2} \mathcal{F}f \in L^2(\mathbb{R}^n)$. Now we obtain with the Cauchy–Schwarz inequality that

$$\|\mathcal{F}f\|_1 \le \|(1 + |x|^2)^{k/2} \mathcal{F}f\|_2 \|(1 + |x|^2)^{-k/2}\|_2.$$

By the above calculation the first factor factor is finite, whereas the second factor is finite because of the assumption $k > \frac{n}{2}$ (note that $(1 + |x|^2)^{-\alpha}$ is integrable if and only if $2\alpha > n$). Hence, $\mathcal{F}f \in L^1(\mathbb{R}^n)$. It now follows from the Riemann–Lebesuge lemma (Lemma 2.1.32) that $f = \mathcal{F}^{-1}\mathcal{F}f \in C_0(\mathbb{R}^n)$.

For the proof of the higher inclusions observe that if $k - 1 > \frac{n}{2}$ we have $D_j f \in H^{k-1}(\mathbb{R}^n)$ for all $j = 1, \dots, n$. Applying the just shown result to the partial derivatives, we obtain $D_j f \in C_0(\mathbb{R}^n)$. This shows $f \in C^1(\mathbb{R}^n)$. The general case now follows inductively. □

Remark 2.1.37 (More general Sobolev embeddings). More generally one can show that if $\Omega \subset \mathbb{R}^n$ is open and bounded and has C^1-boundary, then for $k, m \in \mathbb{N}$ and $p \in [1, \infty)$ with $k - m > \frac{n}{p}$ one has the inclusion $W^{k,p}(\Omega) \subset C^m(\overline{\Omega})$. In this case there exists a universal constant $C \ge 0$ such that

$$\|f\|_{C^m(\overline{\Omega}} \le \|f\|_{W^{k,p}(\Omega)}.$$

In fact, the existence of such a constant follows abstractly from the embedding result by the closed graph theorem (Theorem 2.2.9) that will be introduced later in the lecture. The Fourier transform has a lot of important applications as it gives a very easy description of very important operators in analysis. We illustrate this fact with an easy example.

Example 2.1.38 (Elliptic regularity of the Laplacian on L^2). Recall the inhomogeneous problem $-\Delta u + u = f$ on $\mathbb{R}^n$ considered in Example 2.1.30. We have seen that for each $f \in L^2(\mathbb{R}^n)$ this elliptic problem has a unique weak solution $u \in H^1(\mathbb{R}^n)$, i.e. u satisfies

$$\int_{\mathbb{R}^n} \nabla u \nabla \varphi + \int_{\mathbb{R}^n} u\varphi = \int_{\mathbb{R}^n} f\varphi$$

for all test functions $\varphi \in C_c^\infty(\mathbb{R}^n)$. In analogy to the notion of weak derivatives, we say a function $w \in L^1_{\mathrm{loc}}(\mathbb{R}^n)$ is the (unique) *weak Laplacian* of some function $u \in L^1_{\mathrm{loc}}(\mathbb{R}^n)$ provided the integration by parts formula

$$\int_{\mathbb{R}^n} u\Delta\varphi = \int_{\mathbb{R}^n} w\varphi$$

holds for all test functions $\varphi \in C_c^\infty(\mathbb{R}^n)$. Using this terminology for the weak solutions of $-\Delta u + u = f$, we see that because of

$$-\int_{\mathbb{R}^n} u\Delta\varphi = \int_{\mathbb{R}^n} \nabla u \nabla \varphi = \int_{\mathbb{R}^n} (f-u)\varphi$$

for all $\varphi \in C_c^\infty(\mathbb{R}^n)$ that the weak Laplacian of u lies in $L^2(\mathbb{R}^n)$ and satisfies $-\Delta u = f - u$. Since $\Delta u \in L^2(\mathbb{R}^n)$, it follows from Proposition 2.1.35 that $|x|^2 \mathcal{F}f$ and therefore also $(1+|x|^2)\mathcal{F}f$ is square integrable. We now want to show that all mixed second partial derivatives exist and are square integrable. By Proposition 2.1.35 this is equivalent to $x_i x_j \mathcal{F}f \in L^2(\mathbb{R}^n)$ for all $i, j = 1, \dots, n$. Fix such i, j. Then

$$\begin{aligned}\int_{\mathbb{R}^n} \left|x_i x_j (\mathcal{F}u)(x)\right|^2 dx &= \int_{\mathbb{R}^n} \left|\frac{x_i x_j}{1+|x|^2}\right|^2 \left|(1+|x|^2)(\mathcal{F}u)(x)\right|^2 dx \\ &\leq \sup_{x\in\mathbb{R}^n} \left|\frac{x_i x_j}{1+|x|^2}\right|^2 \int_{\mathbb{R}^n} (1+|x|^2)^2 |(\mathcal{F}u)(x)|^2 dx \leq \|\Delta u\|^2_{L^2(\mathbb{R}^n)}.\end{aligned}$$

A similar estimates holds for the first derivatives. Hence, $u \in H^2(\mathbb{R}^n)$ whenever $\Delta u \in L^2(\mathbb{R}^n)$. In particular, the weak solution $u \in H^1(\mathbb{R}^n)$ of $-\Delta u + u = f$ automatically has the higher regularity $u \in H^2(\mathbb{R}^n)$. Now suppose that the inhomogeneity even satisfies $f \in H^1(\mathbb{R}^n)$. Then $\Delta u = u - f \in H^1(\mathbb{R}^n)$. Using a variant of the above arguments we see that $u \in H^3(\mathbb{R}^n)$. Iterating this

argument we see that $f \in H^k(\mathbb{R}^n)$ implies the higher regularity $u \in H^{k+2}(\mathbb{R}^n)$. This is the so-called *elliptic regularity* of the Laplace operator. Note that this in particular implies by the Sobolev embedding Theorem 2.1.36 that $u \in C^\infty(\mathbb{R}^n)$ whenever $f \in C^\infty(\mathbb{R}^n)$ and additionally has suitable decay of all derivatives such that f lies in Sobolev spaces of arbitrary high order.

2.2 Symmetric and Self-Adjoint Operators

2.2.1 Unbounded Operators on Hilbert Spaces

Let us now consider for a moment the most prototypical operators in quantum mechanics, namely the position operator $\hat{x}$ and the momentum operator $\hat{p}$ for a single one-dimensional particle. Such a particle can be modeled in the Hilbert space $\mathcal{H} = L^2(\mathbb{R})$. Explicitly one then has (ignoring physical constants)

$$\hat{x}\colon f \mapsto [x \mapsto x \cdot f(x)] \qquad \hat{p}\colon f \mapsto [x \mapsto i\frac{d}{dx}f(x)].$$

Clearly, both $\hat{x}$ and $\hat{p}$ are linear. However, they do not define *bounded* operators on $L^2(\mathbb{R})$. There are two (closely related) obstructions:

1. $\hat{x}(f)$ does not lie in $L^2(\mathbb{R})$ for all $f \in L^2(\mathbb{R})$ (for example one can take $f(x) = \frac{1}{x}\mathbb{1}_{[1,\infty)}$). In the same spirit not every function in $L^2(\mathbb{R})$ has a (weak) derivative in $L^2(\mathbb{R}^n)$.

2. Both operators are not bounded when restricted to their maximal domains of definition. For example, one has

$$\sup_{\|f\|_2 \leq 1 : xf \in L^2(\mathbb{R})} \|\hat{x}(f)\| = \infty.$$

For applications in quantum mechanics one therefore has to study *unbounded linear operators* which are not defined on the whole Hilbert space.

Definition 2.2.1. An *unbounded (linear) operator* $(A, D(A))$ on a Hilbert space $\mathcal{H}$ is the datum of a linear subspace $D(A) \subset \mathcal{H}$ and a linear operator $A\colon D(A) \to \mathcal{H}$.

In particular, we say that two unbounded operators $(A, D(A))$ and $(B, D(B))$ agree and one writes $A = B$ if and only if $D(A) = D(B)$ and $Ax = Bx$ for all $x \in D(A) = D(B)$. If one has $D(A) \subset D(B)$ and $Bx = Ax$ for all $x \in D(A)$, we say that B is an *extension* of A. Moreover, we define the sum of two unbounded operators $(A, D(A))$ and $(B, D(B))$ on the same Hilbert space $\mathcal{H}$ in the natural way: $(D(A+B), A+B)$ is given by $D(A+B) = D(A) \cap D(B)$ and $(A+B)x := Ax + Bx$. In particular, the sum of an unbounded operator $(A, D(A))$

and a bounded operator $B \in \mathcal{B}(\mathcal{H})$ is defined on $D(A)$. In a similar fashion one defines the composition of A and B in the natural way with the domain $D(AB) = \{x \in D(B) : Bx \in D(A)\}$.

Remark 2.2.2. Be careful: by our definition an unbounded operator $(A, D(A))$ can be bounded in the sense of Definition 2.1.12. Our definition should be understood in the sense of a not necessarily bounded operator.

Recall that by the postulates of quantum mechanics the possible outcomes of a physical measurement of a quantum mechanical system are determined by the spectrum of the self-adjoint operator associated to this measurement. Hence, the physical treatment crucially relies on the spectral properties of those operators. It is now time to define in a precise way the spectrum of unbounded operator. We first define the inverse of an unbounded operator.

Definition 2.2.3. Let $(A, D(A))$ be an unbounded operator on some Hilbert space $\mathcal{H}$. If A is injective, we can define the operator $(A^{-1}, D(A^{-1}))$ with $D(A^{-1}) = \operatorname{Rg} A$ and $A^{-1}y = x$ if and only if $Ax = y$. The operator $(A, D(A))$ is called *invertible* if for each $y \in \mathcal{H}$ there exists a unique $x \in D(A)$ with $Ax = y$, i.e. $A\colon D(A) \to \mathcal{H}$ is bijective.

This now allows us to define the spectrum of an unbounded operator, generalizing the concept of an eigenvalue in the finite dimensional case.

Definition 2.2.4 (Spectrum and resolvent set of an operator). Let $(A, D(A))$ be an (unbounded) operator on some Hilbert space $\mathcal{H}$. We call the set

$$\rho(A) := \{\lambda \in \mathbb{K} : \lambda \operatorname{Id} - A \text{ is invertible}\}$$

the *resolvent set* of A. Its complement $\sigma(A) := \mathbb{K} \setminus \rho(A)$ is called the *(mathematical) spectrum* of A.

Clearly, every eigenvalue $\lambda \in \mathbb{C}$ of A lies in the spectrum $\sigma(A)$ because $\lambda \operatorname{Id} - A$ is not injective in this case. If $\mathcal{H}$ is finite dimensional and $A\colon \mathcal{H} \to \mathcal{H}$ is linear, then $\lambda \operatorname{Id} - A$ is injective if and only if $\lambda \operatorname{Id} - A$ is bijective. Hence, in the finite dimensional case, the spectrum of A consists exactly of the eigenvalues of A.

One can show that a bounded operator on a complex Hilbert space always has non-empty spectrum. Moreover, one can show that the spectrum of an operator is always a closed subset of the complex plane. If A is moreover bounded, then $\sigma(A)$ is bounded as well. This shows that a bounded operator can never model a physical system in which arbitrary high measure outcomes, e.g. arbitrary high energies, are possible. Further, it can happen that even a bounded operator on a complex Hilbert space has no eigenvalues in contrast to the finite dimensional case.

Example 2.2.5. On $\mathcal{H} = L^2([0,1])$ consider the spatially bounded analogue of the position operator given by

$$(Tf)(x) = xf(x).$$

Then $T \in \mathcal{B}(H)$ with $\|T\| = 1$. However, T has no complex eigenvalue. For if $\lambda \in \mathbb{C}$ is an eigenvalue of T, then $Tf = \lambda f$ for some $f \neq 0$. Hence, $xf(x) = \lambda f(x)$ almost everywhere on $[0,1]$. Equivalently, $(x-\lambda)f(x) = 0$ almost everywhere. But this implies $f = 0$ as element in $L^2([0,1])$, in contradiction to our assumption. Nevertheless $0 \in \sigma(A)$ since T is not surjective. For example, take $g(x) = x^{1/2} \in L^2([0,1])$. If $f \in L^2([0,1])$ such that $Tf = g$, i.e. $xf(x) = x^{1/2}$, then $f(x) = x^{-1/2}$. But we clearly have

$$\int_0^1 |f(x)|^2 \, dx = \int_0^1 \frac{1}{x} \, dx = \infty,$$

so $f \notin L^2([0,1])$. With similiar arguments one can further show that $[0,1] \subset \sigma(A)$. Note that on a (until now) formal level the Dirac measure δ_0 at zero is an eigenvalue of T because of

$$T\delta_0 = x\delta_0 = 0.$$

Here $x\delta_0$ is the Dirac measure with the density x, i.e. the Borel measure $A \mapsto \int_A x \, d\delta_0$. But please be aware that δ_0 is not an element of $L^2([0,1])$ as it is not even a function. At the end of the lecture we will give mathematical sense to such expressions by introducing the theory of distributions. Moreover, note that the same discussion applies to the unbounded position operator on $L^2(\mathbb{R})$, where one even obtains $\mathbb{R} \subset \sigma(A)$.

We will almost exclusively work with the class of *closed operators* on some Hilbert space.

Definition 2.2.6. An unbounded operator $(A, D(A))$ on a Hilbert space $\mathcal{H}$ is called *closed* if the graph

$$G(A) = \{(x,y) \in D(A) \times \mathcal{H} : Ax = y\}$$

of A is a closed subspace of $\mathcal{H} \times \mathcal{H}$. An unbounded operator $(A, D(A))$ is called *closable* if $\overline{G(A)}$ is the graph of a (necessarily closed) unbounded operator $(\overline{A}, D(\overline{A}))$ on $\mathcal{H}$. In this case $(\overline{A}, D(\overline{A}))$ is called the *closure* of A.

Observe that if $(A, D(A))$ is an injective closed operator, then the graph of A^{-1} is given by $G(A^{-1}) = \{(y,x) : (x,y) \in G(A)\}$. This shows that an injective operator A is closed if and only if A^{-1} is closed. In particular, if $\rho(A)$ is nonempty, then $\lambda - A$ is invertible for some $\lambda \in \mathbb{C}$. Hence, $(\lambda - A)^{-1}$ is bounded

and a fortiori closed. Now, it follows that $\lambda - A$ and therefore also A are closed. This shows that $\rho(A) \neq \emptyset$ implies that A is closed. Hence, a reasonable spectral theory is only possible for closed operators.

As a consequence we only encounter closed operators in our study of the mathematics behind quantum mechanics. Indeed, by the postulates of quantum mechanics a physical quantum mechanical system is modeled by a self-adjoint operator on some complex Hilbert space $\mathcal{H}$. The mathematical spectrum $\sigma(H)$ of H corresponds by the postulates of quantum mechanics to the possible outcomes of a physical measurement of the system. Naturally, one requires $\sigma(H) \subset \mathbb{R}$ (reality condition). A fortiori one has $\rho(A) \neq \emptyset$. In other words, there exists a $\lambda \in \mathbb{C}$ such that $(\lambda - A)^{-1} : \mathcal{H} \to \mathcal{H}$ is a bounded operator. By the above reasoning this implies that A must be closed.

Remark 2.2.7. One can easily verify that the definition of a closed operator is equivalent to the following condition: for $(x_n)_{n\in\mathbb{N}} \subset D(A)$ with $x_n \to x$ and $Ax_n \to y$ in $\mathcal{H}$ one has $x \in D(A)$ and $Ax = y$.

The following example shows that the domain of an operator plays a crucial role for its structural properties.

Example 2.2.8. Let $\mathcal{H} = L^2([-1,1])$ and $A = \frac{d}{dx}$ be the first derivative with domain

$$D(A) = \{f \in L^2([-1,1]) \cap C^1((-1,1)) : f' \in L^2([-1,1])\}.$$

Then $(A, D(A))$ is an unbounded operator which is not closed. For this consider the smooth functions given by $f_n(x) = \sqrt{x^2 + \frac{1}{n}}$ and for $n \in \mathbb{N}$ and the function $f(x) = |x|$. Then one has by the dominated convergence theorem or a direct calculation that

$$\lim_{n\to\infty} \int_{-1}^{1} |f_n(x) - f(x)|^2 \, dx = 0$$

and by the same reasoning

$$\lim_{n\to\infty} \int_{-1}^{1} |f_n'(x) - f'(x)| \, dx = \lim_{n\to\infty} \int_{-1}^{1} \left| \frac{x}{\sqrt{x^2 + \frac{1}{n}}} - \operatorname{sign} x \right|^2 dx = 0,$$

where the derivative of f is understood in the weak sense. From this one sees that $(f_n, Af_n) \in G(A)$ with $(f_n, Af_n) \to (f, f')$ in $\mathcal{H} \times \mathcal{H}$. Hence, $G(A)$ is not closed in $\mathcal{H} \times \mathcal{H}$ and $(A, D(A))$ does not define a closed operator.

However, if we choose $B = \frac{d}{dx}$ with $D(B) = H^1((0,1))$, one can immediately verify that B is a closed operator on $\mathcal{H}$. Moreover, it follows from the above calculations that $\overline{G(A)} \subset G(B)$. From this one sees that A is closable and that B is an extension of A.

In particular notice that in the above example one only obtains a closed operator if the domain consists of Sobolev and not classically differentiable functions. This is the prototypical behaviour for all differential operators. One has the following fundamental theorem on closed operators.

Theorem 2.2.9 (Closed Graph Theorem). *Let $(A, D(A))$ be a closed operator on some Hilbert space $\mathcal{H}$ with $D(A) = \mathcal{H}$. Then A is bounded, i.e. $A \in \mathcal{B}(H)$.*

Let us briefly discuss the consequences of the closed graph theorem for the mathematical description of quantum mechanics. A typical quantum mechanical system is described by a closed unbounded operator H (the Hamiltonian) on some Hilbert space $\mathcal{H}$. The closed graph theorem implies that one then automatically has $D(H) \subsetneq \mathcal{H}$, i.e. one has to restrict the domain of the operator.

2.2.2 The Difference Between Symmetry and Self-Adjointness

Recall that by the postulates of quantum mechanics a physical observable is described by a self-adjoint operator some Hilbert space. More precisely, one can only obtain elements of the spectrum as possible outcomes of the measurement of a pure quantum mechanical state. This fact is guaranteed by the postulated self-adjointness of the operator associated to the observable. In analogy to what we have learned in course in linear algebra, this is often defined as follows in the physics literature.

Definition 2.2.10. An operator $(A, D(A))$ on a Hilbert space $\mathcal{H}$ is called *symmetric* if

$$\langle x|Ay\rangle = \langle Ax|y\rangle \qquad \text{for all } x, y \in D(A).$$

Now let $0 \neq x \in D(A)$ be an eigenvalue of A, i.e. $Ax = \lambda x$ for some $\lambda \in \mathbb{C}$. Then

$$\overline{\lambda}\langle x|x\rangle = \langle \lambda x|x\rangle = \langle Ax|x\rangle = \langle x|Ax\rangle = \langle x|\lambda x\rangle = \lambda\langle x|x\rangle.$$

Hence, $(\overline{\lambda} - \lambda)\langle x|x\rangle = 0$. Since $x \neq 0$ we must have $\lambda = \overline{\lambda}$ which is equivalent to $\lambda \in \mathbb{R}$. This shows that the symmetry of $(A, D(A))$ implies that all eigenvalues of A are real. However, as we have already seen the spectrum $\sigma(A)$ may not contain one single eigenvalue. Hence, it is not clear that one has $\sigma(A) \subset \mathbb{R}$ for a symmetric operator A. In fact, this is not even true.

The next example shows that the symmetry of an operator A is not sufficient to guarantee that the spectrum of A is real.

Example 2.2.11. Let $\mathcal{H} := L^2([0, \infty))$ and consider $A = i\frac{d}{dx}$ with domain $D(A) = C_c^\infty((0, \infty))$. For $f, g \in C_c^\infty((0, \infty))$ we have by integration by parts

$$\langle f|Ag\rangle = \int_0^\infty \overline{f(x)} i g'(x)\, dx = i[\overline{f(x)}g(x)]_0^\infty - i\int_0^\infty \overline{f'(x)}g(x)\, dx$$

$$= \int_0^\infty \overline{if'(x)} g(x)\, dx = \langle Af|g\rangle.$$

This shows that A is symmetric. However, it follows along the same line of arguments as in Example 2.2.8 that A is not closed. Hence, by the comments after Definition 2.2.6 one has $\sigma(A) = \mathbb{C}$.

Before going further, we prove a very useful lemma for symmetric operators.

Lemma 2.2.12. *Let $(A, D(A))$ be a symmetric operator on some Hilbert space $\mathcal{H}$. Then for all $\lambda \in \mathbb{C}$ we have*

$$\|(\lambda - A)x\| \geq |\operatorname{Im}\lambda|\,\|x\| \qquad \text{for all } x \in D(A).$$

Proof. Let $x \in D(A)$. By symmetry, we have $\langle Ax|x\rangle = \overline{\langle x|Ax\rangle}$. Further, by the properties of a scalar product one also has $\langle Ax|x\rangle = \overline{\langle x|Ax\rangle}$. This shows that $\langle x|Ax\rangle$ must be a real number. Hence,

$$\operatorname{Im}(\langle x|(\lambda - A)x\rangle) = \operatorname{Im}\lambda \langle x|x\rangle.$$

Taking absolutes values and using the Cauchy–Schwarz inequality we obtain

$$|\operatorname{Im}\lambda|\,\|x\|^2 \leq |\langle x|(\lambda - A)x\rangle| \leq \|(\lambda - A)x\|\,\|x\|.$$

Now, if $x = 0$ the assertion trivially holds. In the case $x \neq 0$ the inequality follows by dividing both sides with $\|x\|$. □

The above lemma has the following very useful consequences which simplify the study of symmetric operators substantially.

Corollary 2.2.13. *Let $(A, (D(A))$ be a symmetric operator on some Hilbert space $\mathcal{H}$. Then the following are equivalent for $\lambda \in \mathbb{C} \setminus \mathbb{R}$.*

(i) $\lambda \in \rho(A)$;

(ii) $\lambda - A$ *is surjective.*

Proof. The first condition implies the first by definition. For the converse observe that $\lambda - A$ is injective by Lemma 2.2.12 or the fact that a symmetric operator does not have any eigenvalues. Hence, $\lambda - A$ is bijective. Now, it follows from the estimate in Lemma 2.2.12 that for $y \in \mathcal{H}$ with $(\lambda - A)x = y$ we have

$$\|(\lambda - A)^{-1}y\| = \|x\| \leq |\operatorname{Im}\lambda|^{-1}\,\|(\lambda - A)x\| = |\operatorname{Im}\lambda|^{-1}\,\|y\|.$$

This shows that $\|(\lambda - A)^{-1}\| \leq |\operatorname{Im}\lambda|^{-1}$. Hence, $\lambda \in \rho(A)$. □

Corollary 2.2.14. *Let $(A, D(A))$ be a symmetric operator on some Hilbert space $\mathcal{H}$. If $\lambda - A$ is surjective for some $\lambda \in \mathbb{C} \setminus \mathbb{R}$, then $D(A)$ is dense in $\mathcal{H}$.*

Proof. Assume that this is not the case. Then the closure $\overline{D(A)}$ of $\mathcal{H}$ is a proper subspace of $\mathcal{H}$. Hence, there exists $y \in \mathcal{H} \setminus \overline{D(A)}$. Let P be the orthogonal projection onto $\overline{D(A)}$. Replacing y by $y - Py$ if necessary, we may assume that y is orthogonal to all elements of $\overline{D(A)}$. By assumption, there exists $0 \neq x \in D(A)$ with $(\lambda - A)x = y$. Now, on the one hand

$$0 = \langle x|y\rangle = \langle x|(\lambda - A)x\rangle$$

On the other hand we have shown in Lemma 2.2.12 that

$$\mathrm{Im}\langle x|(\lambda - A)x\rangle = \mathrm{Im}\,\lambda\,\|x\|^2 > 0.$$

This is a contradiction. Hence, $D(A)$ must be dense in $\mathcal{H}$. □

Note that by Remark 2.1.37 one has the Sobolev embedding $H^1((0,1)) \subset C([0,1])$. More precisely, this means that every function $f \in H^1((0,1))$ has an (automatically unique) representative in $C([0,1])$. Note that in particular it then makes sense to talk about point evaluations of f, e.g. $f(0)$ or $f(1)$. Please remember that point evaluations are not well-defined for general functions in $L^2([0,1])$. The above inclusion into the continuous functions allows us to define the following subspace of $H^1((0,1))$.

Definition 2.2.15. Let $a < b \in \mathbb{R}$. Then we define the Sobolev space with vanishing boundary values as

$$H_0^1([a,b]) = \{f \in H^1((0,1)) : f(a) = f(b) = 0\}.$$

In the case of an one-sided unbounded interval we set in a similar manner

$$H_0^1([a,\infty)) = \{f \in H^1((0,1)) : f(1) = 0\}.$$

In an analogous way one also defines the spaces $H_0^1((-\infty, b])$.

Remark 2.2.16. Using the methods of the proof of Theorem 2.1.36 and a truncation argument one can show that $C_c((0,\infty))$ is a dense subset of $H_0^1([0,\infty))$. Analogously, $C_c((a,b))$ is a dense subset of $H_0^1((a,b))$.

In Example 2.2.11, one may argue that the essential obstruction is the fact that A is not closed. Indeed, this fact was used to show $\sigma(A) = \mathbb{C}$. However, there are even more obstructions.

Example 2.2.17 (Example 2.2.11 continued). Now consider the same mapping $A = i\frac{d}{dx}$, but with the different domain $D(A) = H_0^1([0,\infty))$. Now the derivative has to be understood in the weak sense. Then A is a closed operator. This can be checked as in the previous examples: for the additional problem of the boundary values please observe that $f_n \to f$ in $H^1((0,\infty))$ implies $f_n(x) \to f(x)$ for all $x \in [0,\infty)$ by the estimate for the Sobolev embedding theorem (see end of Remark 2.1.37). It is not clear that A is still symmetric on the bigger domain which we use now. Until now, we only know from Example 2.2.11 that

$$\langle f|Ag\rangle = \langle Af|g\rangle$$

for all $f,g \in C_c^\infty((0,\infty))$. Now let $f,g \in H_0^1([0,\infty))$. Since this space is dense by the remarks made before this example, there exists sequences $(f_n)_{n\in\mathbb{N}}$ and $(g_n)_{n\in\mathbb{N}}$ in $C_c^\infty([0,\infty))$ such that $f_n \to f$ and $g_n \to g$ in $H_0^1([0,\infty))$. A fortiori, we have $f_n \to f$ and $g_n \to g$ in $L^2([0,\infty))$. Moreover, for $h \in H_0^1([0,\infty))$ we have

$$\|Ah\|_2 = \|h'\|_2 \le \|h\|_2 + \|h'\|_2 = \|h\|_{H_0^1}.$$

This shows that A is continuous as a mapping from $D(A) = H_0^1([0,\infty))$ to $L^2([0,\infty))$. In particular $f_n \to f$ in $H_0^1([0,\infty))$ implies $Af_n \to Af$ in $L^2([0,\infty))$. Using the continuity of the scalar product we obtain

$$\langle f|Ag\rangle = \lim_{n\to\infty}\langle f_n|Ag_n\rangle = \lim_{n\to\infty}\langle Af_n|g_n\rangle = \langle Af|g\rangle.$$

Hence, $(A, D(A))$ is still symmetric. Note that loosely spoken the symmetry gets increasingly difficult to achieve for bigger domains. For example, if we would use $D(A) = H^1([0,\infty))$ instead, in the integration by parts argument the term $f(0)g(0)$ would not vanish in general. Hence, A is not symmetric with this even bigger domain.

We now deal with the spectrum of A. Let us first consider $\lambda \in \mathbb{C}$ with $\operatorname{Im}\lambda < 0$. Note that by Corollary 2.2.13 the essential question is whether $\lambda - A$ is surjective. For this let $g \in L^2([0,\infty))$. We have to find a (necessarily unique) $f \in H_0^1([0,\infty))$ with

$$\lambda f - Af = \lambda f - if' = g.$$

Using the well-known variation of parameters method we can write down the very reasonable candidate (ignoring problems such as weak differentiation for a moment)

$$f(t) = i\int_0^t g(s)e^{-i\lambda(t-s)}\,ds.$$

We now check that f is square integrable. For this observe that by the Cauchy–Schwarz inequality

$$|f(t)|^2 \le \left(\int_0^t |g(s)|\,e^{\operatorname{Im}\lambda(t-s)}\,ds\right)^2 \le \int_0^t |g(s)|^2\,e^{\operatorname{Im}\lambda(t-s)}\,ds\int_0^t e^{\operatorname{Im}\lambda(t-s)}\,ds$$

$$\leq \frac{1}{|\operatorname{Im}\lambda|}\int_0^t |g(s)|^2\, e^{\operatorname{Im}\lambda(t-s)}\,ds.$$

Integration of this inequality yields with Fubini's theorem

$$\begin{aligned}\int_0^\infty |f(t)|^2\,dt &\leq \frac{1}{|\operatorname{Im}\lambda|}\int_0^\infty\int_0^t |g(s)|^2\, e^{\operatorname{Im}\lambda(t-s)}\,ds\,dt\\ &= \frac{1}{|\operatorname{Im}\lambda|}\int_0^\infty |g(s)|^2\int_s^\infty e^{\operatorname{Im}\lambda(t-s)}\,dt\,ds = \frac{1}{|\operatorname{Im}\lambda|}\int_0^\infty |g(s)|^2\int_0^\infty e^{\operatorname{Im}\lambda t}\,dt\,ds\\ &= \frac{1}{|\operatorname{Im}\lambda|^2}\int_0^\infty |g(s)|^2\,ds < \infty.\end{aligned}$$

Hence, $f \in L^2([0,\infty))$ with $\|f\|_2 \leq |\operatorname{Im}\lambda|^{-1}\|g\|_2$. Now a calculation similar to that of Example 2.1.23 shows that f is weakly differentiable with $if' = \lambda f - g$. It follows that $f' \in L^2([0,\infty))$ and therefore $f \in H^1([0,\infty))$. In particular, f is continuous (this can also be easily verified directly by using the dominated convergence theorem) with $f(0) = 0$. Altogether this shows that $f \in H^1_0([0,\infty))$ with $(\lambda - A)f = g$. Corollary 2.2.13 shows that $\lambda \in \rho(A)$ whenever $\operatorname{Im}\lambda < 0$. Hence, the upper half-plane is contained in $\rho(A)$.

However, the situation is different for the upper half-plane. For example, take $\lambda = i$ and $g(t) = e^{-t} \in L^2([0,\infty))$. In this case the resolvent equation is the ordinary differential equation $-if(t) - if'(t) = e^{-t}$ with the initial condition $f(0) = 0$ whose unique solution (note that the right hand side lies in Sobolev spaces of arbitrary order, by bootstrapping this shows that a solution $f \in H^1([0,\infty))$ automatically satisfies $f \in C^\infty((0,\infty))$ and therefore is a classical solution of the ODE) is given by

$$f(t) = i\int_0^t e^{-s}e^{t-s}\,ds = ie^t\int_0^t e^{-2s}\,ds = \frac{i}{2}e^t(1-e^{-2t})$$

which satisfies $|f(t)| \to \infty$ as $t \to \infty$ and therefore cannot be square integrable. As a consequence we obtain $i \in \sigma(A)$. A similar argument applies for all $\lambda \in \mathbb{C}$ with positive imaginary part. Since the spectrum is always closed, this shows that $\sigma(A) = \{\lambda \in \mathbb{C} : \operatorname{Im}\lambda \geq 0\}$.

Note that if we would have worked with $B = -i\frac{d}{dx}$ and the same domain instead, then $\sigma(B) = \{\lambda \in \mathbb{C} : \operatorname{Im}\lambda \leq 0\}$. Concluding our discussion, we see that although A and B are closed symmetric operators, the spectrum may consist of non-real numbers. By using the operator $A \oplus B$ and the direct sum $L^2([0,\infty)) \oplus L^2([0,\infty))$ one moreover obtains an example of a closed symmetric operator for which the spectrum consists of the entire complex plane.

Remark 2.2.18 (Physical interpretation). Let us try to give a physical explanation of the above result from the naive standpoint of a mathematician. In fact, the above result may be surprising from a physical point of view. The

Hilbert space $L^2([0,\infty))$ should be associated to a quantum system which describes an one-sided well given by the potential

$$V(x) = \begin{cases} 0 & \text{if } x > 0 \\ \infty & \text{if } x \leq 0. \end{cases}$$

Indeed, we have shown that the momentum operator $\hat{p} = -i\frac{d}{dx}$ on the half-line $[0,\infty)$ with zero boundary condition is not self-adjoint and therefore is not a physical reasonable observable. Even worse, we will later show that the operator $-i\frac{d}{dx}$ defined on $C_c^\infty((0,\infty))$ has no self-adjoint extensions. Clearly, if ψ is a quantum mechanical wave function which is localized in a compact subset of $(0,\infty)$, the time evolution of the system should be given for sufficiently small times by the time evolution of a free particle, i.e. by translation as we have seen in the physics part of the lecture. Hence, on $C_c^\infty((0,\infty))$ the single choice we have is to set $\hat{p} = -i\frac{d}{dx}$. But since this operator does not have any self-adjoint extensions, by the postulates of quantum mechanics, there does not exist a well-defined momentum observable. Clearly, this odd behaviour should arise from the infinite high well at zero.

Since the well is infinitely high, we would expect that a wave function ψ is totally reflected at zero (or at least with some phase shift), i.e. the time evolution gets an immediate phase shift of π. You probably all know this kind of reasoning from classical mechanics where this argument works perfectly fine. But now for simplicity think of a wave function of the form $\psi(x) = \mathbb{1}_{[0,1]}$. Then one has $\|\psi\| = 1$. Let us for simplicity assume that the time evolution operators $U(t)$ of the momentum operator are given by translation of one per time unit. Assuming total reflection, the state has evolved after a time span of $1/2$ to the state $U(1/2)\psi$ which satisfies

$$\|U(1/2)\psi\|_2^2 = \|2\mathbb{1}_{[0,1/2]}\|_2^2 = 2 \neq 1.$$

Hence, $U(t)$ does not preserve the norm of the state and therefore violates a fundamental principle of quantum mechanics. Again physical and mathematical reasoning fits perfectly together!

The occurrence of half-planes as the spectrum of symmetric operators is no coincidence as the next result shows. Before we introduce the resolvent of an operator and need some technical tools.

Definition 2.2.19 (Resolvent). Let $(A, D(A))$ be an unbounded operator on some Hilbert space $\mathcal{H}$. Then the mapping

$$\begin{aligned} R(\cdot, A)\colon \rho(A) &\to \mathcal{B}(\mathcal{H}) \\ \lambda &\mapsto R(\lambda, A) := (\lambda - A)^{-1} \end{aligned}$$

is called the *resolvent* of A.

The next elementary result plays a fundamental role in the study of operators on Banach or Hilbert spaces.

Lemma 2.2.20 (Neumann series). *Let X be a Banach space and $T \in \mathcal{B}(X)$ a bounded operator. If $\|T\| < 1$, then $\mathrm{Id} - T$ is invertible. Moreover, one has*

$$(\mathrm{Id} - T)^{-1} = \sum_{n=0}^{\infty} T^n.$$

In particular, if $T \in \mathcal{B}(H)$ is invertible and $\|T - S\| < \|T^{-1}\|^{-1}$ for some $S \in \mathcal{B}(H)$, then S is invertible as well.

Proof. For the first assertion, simply calculate

$$(\mathrm{Id} - T)\sum_{n=0}^{N} T^n = (\mathrm{Id} - T)\sum_{n=0}^{N} T^n = \mathrm{Id} - T^{N+1}$$

which exists because of $\|T\| < 1$. The first assertion now follows by taking limits. For the second assertion write

$$S = T + S - T = T(\mathrm{Id} + T^{-1}(S - T)).$$

Note that T is invertible because of the assumptions and that $\mathrm{Id} + T^{-1}(S - T)$ is invertible because of the first part of this lemma and the estimate

$$\|T^{-1}(S - T)\| \leq \|T^{-1}\|\|T - S\| < 1.$$

Hence, S is invertible as the composition of two invertible operators. □

Note that it follows from the above lemma that the set of invertible operators is open in $\mathcal{B}(X)$ for every Banach space X. Moreover, one obtains directly the previously stated fact that the resolvent set $\rho(A)$ of an unbounded operator $(A, D(A))$ is open (and as a consequence that the spectrum $\sigma(A)$ is closed). We are now ready to describe the spectrum of a symmetric operator.

Proposition 2.2.21. *Let $(A, D(A))$ be a symmetric operator on some Hilbert space $\mathcal{H}$. If $\lambda \mathrm{Id} - A$ is surjective for some $\lambda \in \mathbb{C}$ with $\mathrm{Im}\,\lambda > 0$ (resp. $\mathrm{Im}\,\lambda < 0$), then the whole upper (resp. lower) half-plane is contained in the resolvent set $\rho(A)$ of A.*

Proof. We assume without loss of generality that $\lambda \mathrm{Id} - A$ is surjective for some $\lambda \in \mathbb{C}$ with $\mathrm{Im}\,\lambda > 0$. It follows from Corollary 2.2.13 that $\lambda \in \rho(A)$. Moreover, we have seen in Lemma 2.2.12 that $\|(\lambda - A)x\| \geq |\mathrm{Im}\,\lambda|\|x\|$ for all $x \in D(A)$. Taking inverses, we see that $\|R(\lambda, A)\| = \|(\lambda - A)^{-1}\| \leq 1/|\mathrm{Im}\,\lambda|$. Further note that for μ in the upper half plane

$$(\mu - A)R(\lambda, A) = (\lambda - A + \mu - \lambda)R(\lambda, A) = \mathrm{Id} + (\mu - \lambda)R(\lambda, A).$$

Hence, it follows from the Neumann series (Lemma 2.2.20) that the right hand side and therefore $\mu - A$ is surjective and consequently $\mu \in \rho(A)$ by Corollary 2.2.13 provided

$$|\mu - \lambda| \|R(\lambda, A)\| < 1 \qquad \Leftrightarrow \qquad \|R(\lambda, A)\| < \frac{1}{|\mu - \lambda|}.$$

This is satisfied if

$$\frac{1}{|\operatorname{Im} \lambda|} < \frac{1}{|\mu - \lambda|} \qquad \Leftrightarrow \qquad |\mu - \lambda| < |\operatorname{Im} \lambda|.$$

Hence, for every $\lambda \in \rho(A)$ the ball with center λ and radius $|\operatorname{Im} \lambda|$ is contained in $\rho(A)$ as well. By taking bigger and bigger disks we see that the whole upper half plane is contained in the resolvent set $\rho(A)$. □

As a direct corollary we obtain the following spectral properties of symmetric operators.

Corollary 2.2.22. *Let $(A, D(A))$ be a symmetric operator on some Hilbert space $\mathcal{H}$. Then the spectrum $\sigma(A)$ of A is given by one of the following four possibilities: a closed subset of the real line, the upper or lower closed half-plane or the entire complex plane.*

Proof. By Lemma 2.2.21 the resolvent set $\rho(A)$ contains a whole open half-plane as soon as a single point of this half-plane is contained in $\rho(A)$. Passing to complements this means that either $\{\lambda \in \mathbb{C} : \operatorname{Re} \lambda > 0\}$ or no point of this half-plane are contained in the spectrum $\sigma(A)$. The same of course applies the lower half-plane. Since the spectrum $\sigma(A)$ is closed, only the above listed cases remain possible. □

In fact, one can construct for each of the above listed closed sets a closed (!) densely defined symmetric operator on some Hilbert space whose spectrum is exactly that set. Hence, the above statement is the best possible in the general case of a symmetric operator. In order to guarantee that the spectrum of an unbounded operator is real we therefore need a stronger condition than mere symmetry. It is now finally time to introduce the adjoint of a densely defined operator on some Hilbert space.

Definition 2.2.23. Let $(A, D(A))$ be a densely defined operator on some Hilbert space $\mathcal{H}$. The *adjoint* A^* of A is the operator defined by

$$\begin{aligned} D(A^*) &= \{x \in \mathcal{H} : \exists y \in \mathcal{H} \text{ with } \langle x|Az\rangle = \langle y|z\rangle \text{ for all } z \in D(A)\} \\ A^* x &= y. \end{aligned}$$

We now give some comments on the definition of the adjoint operator. Let $f \in D(A^*)$. Then it follows from the definition of $D(A^*)$ that the linear functional

$$\begin{aligned} \varphi \colon D(A) &\to \mathcal{H} \\ z &\mapsto \langle x | Ay \rangle \end{aligned}$$

is continuous, i.e. there exists a constant $C \geq 0$ such that $|\varphi(z)| \leq C \|z\|_{\mathcal{H}}$ for all $z \in D(A)$. Since $D(A)$ is dense in $\mathcal{H}$, there exists a unique extension $\tilde{\varphi} \in \mathcal{H}^*$ of φ to all of $\mathcal{H}$. In fact by the definition, one has $\tilde{\varphi}(z) = \langle g | z \rangle$ for all $z \in \mathcal{H}$. Note that by the Riesz representation theorem (Theorem 2.1.18) each continuous functional on $\mathcal{H}$ can be uniquely determined by such an element in $\mathcal{H}$, in our case by the element y. Hence, an equivalent definition of the domain is

$$D(A^*) = \{x \in \mathcal{H} : \langle x | A \cdot \rangle \text{ is continuous with respect to } \mathcal{H}\}.$$

Note that by the above definition the element y is uniquely determined. This shows that A^* is well-defined. Moreover, it follows from a direct computation that A^* is indeed linear. Further, the adjoint is always closed.

Lemma 2.2.24. *Let $(A, D(A))$ be a densely defined operator on some Hilbert space $\mathcal{H}$. Then the adjoint operator $(A^*, D(A^*))$ is closed.*

Proof. Let $(x_n)_{n \in \mathbb{N}} \subset D(A^*)$ with $x_n \to x$ and $A^* x_n \to y \in \mathcal{H}$. Then one has for all $z \in D(A)$

$$\langle x | Az \rangle = \lim_{n \to \infty} \langle x_n | Az \rangle = \lim_{n \to \infty} \langle A^* x_n | z \rangle = \langle y | z \rangle.$$

Hence, $x \in D(A^*)$ and $A^* x = y$. This shows that A^* is a closed operator. □

Let us as a first example calculate the adjoint operator of the variant of the momentum operator considered in Example 2.2.11.

Example 2.2.25. Recall that the operator from Example 2.2.11 was given by $A = i\frac{d}{dx}$ with domain $D(A) = H_0^1([0, \infty))$. Assume that $f \in D(A^*)$. Then we have for all $g \in D(A)$

$$\int_0^\infty \overline{A^* f} g = \langle A^* f | g \rangle = \langle f | Ag \rangle = \int_0^\infty \overline{f(x)} i g'(x) \, dx$$

In particular, if we only consider real $\varphi = g \in C_c^\infty([0, \infty))$ and use the anti-symmetry of the scalar product, we obtain

$$-\int_0^\infty i A^* f \varphi = -\int_0^\infty f(x) \varphi'(x) \, dx.$$

Hence, f is weakly differentiable with $f' = -iA^* f$. This shows that $f \in H^1([0, \infty))$ and $A^* f = if'$. Altogether these arguments shows that $D(A^*) \subset$

$H^1([0,\infty))$ and that A^* is a restriction of the differential operator $i\frac{d}{dx}$ with domain $H^1([0,\infty))$. We now show that $D(A^*) = H^1([0,\infty))$. For this let $f \in H^1([0,\infty))$. Then one has for all $g \in D(A) = H_0^1([0,\infty))$ using integration by parts that

$$\begin{aligned}\langle f|Ag\rangle &= \int_0^\infty \overline{f(x)} i g'(x)\,dx = \left[i\overline{f(x)}g(x)\right]_0^\infty - \int_0^\infty \overline{f'(x)} i g(x)\,dx \\ &= \int_0^\infty \overline{if'(x)} g(x)\,dx = \langle if'|g\rangle.\end{aligned}$$

Note that equality relying upon integration by parts holds for all test functions $g \in C_c^\infty((0,\infty))$ and extends to all $g \in H_0^1[0,\infty)$ by continuity because the test functions $C_c^\infty([0,\infty))$ are dense in $H_0^1([0,\infty))$ as stated in Remark 2.2.16. The above identity implies that $H^1([0,\infty)) \subset D(A^*)$ and $A^*f = if'$ for all $f \in H^1([0,\infty))$. Altogether, we have shown that $A^* = i\frac{d}{dx}$ with domain $D(A^*) = H^1((0,\infty))$. Hence, we do not have $A = A^*$. However, A^* is an extension of A.

Note that $(A^*, D(A^*))$ is not symmetric although $(A, D(A))$ is symmetric. Indeed, let $f(x) = g(x) = e^{-x/2} \in H^1([0,\infty))$. Then by integration by parts we see that the symmetry is violated as

$$\langle f|A^*g\rangle = \langle f|ig'\rangle = -i\int_0^\infty e^{-x}\,dx = i + i\int_0^\infty e^{-x}\,dx = i + \langle if'|g\rangle = i + \langle A^*f|g\rangle.$$

It is no coincidence that the adjoint operator A^* in the last example is an extension of A as the next lemma shows.

Lemma 2.2.26. *Let $(A, D(A))$ be a densely defined symmetric operator on some Hilbert space. Then $(A^*, D(A^*))$ is a closed extension of A. In particular, $(A, D(A))$ is closable.*

Proof. We have seen in Lemma 2.2.24 that the adjoint is a closed operator. It remains to show that A^* extends A. Let $x \in D(A)$. Then one has for all $y \in D(A)$ by the symmetry of A

$$\langle x|Ay\rangle = \langle Ax|y\rangle.$$

Hence, $x \in D(A^*)$ with $A^*x = Ax$ as desired. □

It is now finally time to introduce self-adjoint operators. We will soon see that for this definition the behavior is exactly as desired.

Definition 2.2.27. A densely defined operator $(A, D(A))$ on a Hilbert space $\mathcal{H}$ is *self-adjoint* if $A = A^*$. Moreover, a densely defined symmetric operator $(A, D(A))$ is called *essentially self-adjoint* if its closure is self-adjoint.

Using this definition, we have shown in Example 2.2.25 that the operator $A = i\frac{d}{dx}$ with domain $D(A) = H^1([0,\infty))$ is not self-adjoint as the adjoint is a true extension of A.

We now give some basic positive examples of self-adjoint operators.

Example 2.2.28 (Multiplication Operators). Let (Ω, Σ, μ) be a measure space and $m\colon \Omega \to \mathbb{R}$ a measurable function. One defines the multiplication operator M_m on $L^2(\Omega) = L^2(\Omega, \Sigma, \mu)$ as

$$\begin{aligned} D(M_m) &= \{f \in L^2(\Omega) : m \cdot f \in L^2(\Omega)\} \\ M_m f &= m \cdot f. \end{aligned}$$

First observe that M_m is densely defined. For this consider the set $A_n = \{x \in \Omega : |m(x)| \leq n\}$ for $n \in \mathbb{N}$. Since m is bounded on A_n, one has $f\,\mathbb{1}_{A_n} \in D(M_m)$ for all $f \in L^2(\Omega)$ and all $n \in \mathbb{N}$. Moreover, it follows from the dominated convergence theorem that $f\,\mathbb{1}_{A_n} \to f$ in $L^2(\Omega)$ for all $f \in L^2(\Omega)$. Hence, $\overline{D(M_m)} = L^2(\Omega)$. Note that since $D(M_m)$ is dense, we can now speak of the adjoint.

Now let us compute the adjoint of M_m. First assume that $f, g \in D(M_m)$. Then one has

$$\langle f | M_m g \rangle = \int_\Omega \overline{f} m g \, d\mu = \int_\Omega \overline{mf} g \, d\mu = \langle M_m f | g \rangle.$$

This shows that M_m is symmetric and (therefore automatically) M_m is a restriction of $(M_m)^*$. It remains to show that the converse inclusion $M_m^* = (M_m)^* \subseteq M_m$ holds as well. Suppose that $f \in D(M_m^*)$. Then one has for all $g \in D(M_m)$ by definition of the adjoint

$$\int_\Omega \overline{M_m^* f} g \, d\mu = \langle M_m^* f | g \rangle = \langle f | M_m g \rangle = \int_\Omega \overline{f} m g \, d\mu \Leftrightarrow \int_\Omega \overline{M_m^* f - mf} g \, d\mu = 0.$$

Since $D(M_m)$ is dense in $L^2(\Omega)$, the above identity extends to all $g \in L^2(\Omega)$ by continuity of the scalar product. In particular, we may choose $g = M_m^* f - mf$ and obtain

$$\int_\Omega |M_m^* f - mf|^2 \, d\mu = 0.$$

This shows that $M_m^* f = mf$. In particular, $mf \in L^2(\Omega)$ and therefore $f \in D(M_m)$ with $M_m f = mf = M_m^* f$. This shows $M_m^* \subset M_m$. Altogether, we have $M_m = M_m^*$ and M_m is self-adjoint.

Note that if we choose $(\mathbb{R}, \mathcal{B}(\mathbb{R}), \lambda)$ as measure space and $m(x) = x$ as multiplier, we obtain the (one-dimensional) position operator from quantum mechanics. Similarly, for $(\mathbb{R}^3, \mathcal{B}(\mathbb{R}^3), \lambda)$ and $m_j(x) = x_j$ for $j = 1, 2, 3$ we obtain the self-adjointness of the momentum operators $\hat{x}, \hat{y}$ and $\hat{z}$ in three-dimensional space. It is now time to treat some more basic operators / observables from quantum mechanics which are given by differential operators. We start with momentum operators.

Example 2.2.29 (Momentum operators). On $\mathbb{R}^n$ we consider the momentum operator $A = -i\frac{\partial}{\partial x_j}$ with domain

$$D(A) = \left\{ f \in L^2(\mathbb{R}^n) : D_j f \text{ exists in the weak sense and is in } L^2(\mathbb{R}^n) \right\}.$$

It follows from the mapping properties of the Fourier transform on $L^2(\mathbb{R}^n)$ stated in Proposition 2.1.35 that for $f \in D(A)$ one has

$$-i\frac{\partial f}{\partial x_j} = i\mathcal{F}^{-1} M_{ix_j} \mathcal{F} f = \mathcal{F}^{-1} M_{x_j} \mathcal{F}.$$

Moreover, it follows that the unitary operator $\mathcal{F}$ maps the domain of $-i\frac{\partial}{\partial x_j}$ bijectively onto the domain of the multiplication operator M_{x_j}. This shows that $A = \mathcal{F}^{-1} M_{x_j} \mathcal{F}$ with the appropriate domain mapping condition $D(M_{x_j}) = \mathcal{F}(D(A))$. Since the Fourier transform $\mathcal{F}$ on $L^2(\mathbb{R}^n)$ is a unitary operator by Theorem 2.1.34, we have shown that $-i\frac{\partial}{\partial x_j}$ is unitarily equivalent to the multiplication operator M_{x_j}. Hence, the self-adjointness of the momentum operators directly follows from the self-adjointness of the multiplication operators shown in Example 2.2.28.

Notice that in the above example we have in particular considered the operator $-i\frac{d}{dx}$ on $L^2(\mathbb{R})$ with domain $H^1(\mathbb{R}) = H_0^1(\mathbb{R})$ which is a self-adjoint operator, whereas for the analogous situation on $L^2([0,\infty))$ with domain $H_0^1([0,\infty))$ one does not obtain a self-adjoint operator a shown in Example 2.2.25.

Using the same methods one can treat the Hamiltonian of a free particle in $\mathbb{R}^n$.

Example 2.2.30 (Hamiltonian of a free particle). On $\mathbb{R}^n$ consider the Hamiltonian of a free particle. In classical mechanics the Hamiltonian (the energy) is given by $H = \frac{1}{2m}\sum_{k=1}^n p_k^2$, where m denotes the mass of the particle and the $\hat{p}_k$ are the momenta in the respective directions. Hence, using the formal quantization rules we obtain that the Hamiltonian is given by

$$\hat{H} = \frac{1}{2m}\sum_{k=1}^n \hat{p}_k^2.$$

As usual in mathematics ignoring physical constants or setting them equal to one has

$$\hat{H} = \sum_{k=1}^n \left(i\frac{\partial}{\partial x_k} \right)^2 = -\sum_{k=1}^n \frac{\partial^2}{\partial^2 x_k} = -\Delta,$$

where Δ denotes the Laplace operator. Of course, we are not done with this formal calculation because we must also deal with the domain of $\hat{H}$. Let us

start with the domain of $\frac{\partial^2}{\partial^2 x_k}$. For a function $f \in L^2(\mathbb{R}^n)$ to be in its domain we require that the k-th partial derivative of f exists and again lies in $L^2(\mathbb{R}^n)$. Moreover, also the weak k-th partial derivative of $\frac{\partial f}{\partial x_k}$ must exist and lie in $L^2(\mathbb{R}^n)$. Taking the Fourier description obtained in Proposition 2.1.35 we see that $x_k^2 \mathcal{F} f \in L^2(\mathbb{R}^n)$ for all $k = 1, \dots, n$. Equivalently, $(1 + |x|^2)\mathcal{F} f \in L^2(\mathbb{R}^n)$. As already used in the proof of the Sobolev embedding theorem (Theorem 2.1.36) this is equivalent to $f \in H^2(\mathbb{R}^n)$. Hence, $\hat{H} = -\Delta$ with domain $H^2(\mathbb{R}^n)$. Arguing as in the previous example, we see that $-\Delta$ is unitarily equivalent to the multiplication operator $M_{|x|^2}$ via the Fourier transform. Hence, $-\Delta$ with domain $H^2(\mathbb{R}^n)$ is a self-adjoint operator.

We now shortly comment on the easier case of adjoints of bounded operators.

Remark 2.2.31 (Adjoints of bounded operators). Let $A \in \mathcal{B}(\mathcal{H})$ be a bounded operator on some Hilbert space $\mathcal{H}$. In particular, we have $D(A) = \mathcal{H}$. Then it follows from the Cauchy–Schwarz inequality and the boundedness of the operator that

$$|\langle f | Ag \rangle| \leq \|f\| \|A\| \|g\|.$$

This shows that $D(A^*) = \mathcal{H}$. Moreover, one has

$$\begin{aligned} \|A^*\| &= \sup_{\|f\| \leq 1} \|A^* f\| = \sup_{\|f\| \leq 1} \sup_{\|g\| \leq 1} \langle g | A^* f \rangle = \sup_{\|f\| \leq 1} \sup_{\|g\| \leq 1} \langle Ag | f \rangle = \sup_{\|g\| \leq 1} \sup_{\|f\| \leq 1} \langle Ag | f \rangle \\ &= \sup_{\|g\| \leq 1} \|Ag\| = \|A\|. \end{aligned}$$

In particular, A^* is bounded if A is bounded. In particular, this shows that every bounded symmetric operator is already self-adjoint. Hence, the difficulties vanish in the bounded case.

Let us also determine the adjoint of a bounded operator.

Example 2.2.32 (Adjoint of orthogonal projections). Let $\mathcal{H}$ be a Hilbert space and $M \subset \mathcal{H}$ a closed subspace. We denote by P the orthogonal projection onto M as introduced in Example 2.1.14. Then for every $x \in \mathcal{H}$ we have the decomposition $x = Px + (x - Px)$ into the orthogornal subspaces $\operatorname{Ker} P$ and $\operatorname{Im} P$. Now, for $x, y \in \mathcal{H}$ we have

$$\langle y | Px \rangle = \langle Py + (y - Py) | Px \rangle = \langle Py | Px \rangle = \langle Py | Px + (x - Px) \rangle = \langle Py | x \rangle.$$

Hence, we have $P = P^*$, i.e. P is self-adjoint. In fact, the self-adjointness characterizes orthogonal projections among all bounded projections. This is left as an exercise to the reader.

2.2.3 Basic Criteria for Self-Adjointness

Until now we have checked the self-adjointness of concrete symmetric operators by direct calculations. As this can be a quite difficult endeavour, we now give some characterizations and criteria for self-adjoint operators which will simplify our life.

We will use the following lemma which is proved by an argument analogous to the one used in the proof of Corollary 2.2.14.

Lemma 2.2.33. *Let $(A, D(A))$ be a densely defined operator on some Hilbert space $\mathcal{H}$. Then the following are equivalent.*

(i) *A^* is injective;*

(ii) *A has dense range.*

Proof. (ii) $\Rightarrow$ (i): Let $x \in D(A^*)$ with $A^*x = 0$. Then one has for all $y \in D(A)$

$$0 = \langle A^*x|y\rangle = \langle x|Ay\rangle.$$

Since A has dense range, we conclude that $0 = \langle x|z\rangle$ for all $z \in \mathcal{H}$. Choosing $z = x$, this shows $x = 0$. Hence, A^* is injective.

(i) $\Rightarrow$ (ii): Assume that A has not dense range. Then the closure $\overline{\mathrm{Rg}\,A}$ is a proper closed subspace of $\mathcal{H}$. Then there exists some $x \in \mathcal{H} \setminus \overline{\mathrm{Rg}\,A}$. By replacing x by $x - Px$ where P is the orthogonal projection onto $\overline{RgA}$, we may assume that $x \neq 0$ and x is orthogonal to $\overline{RgA}$. Then we have for all $y \in D(A)$ the identity $0 = \langle x|Ay\rangle$. This shows that $x \in D(A^*)$ and $A^*x = 0$. Since $x \neq 0$ by construction, A^* cannot be injective which contradicts the assumption. □

The following theorem gives a very convenient characterization of self-adjoint operators.

Theorem 2.2.34. *Let $(A, D(A))$ be a symmetric operator on some Hilbert space $\mathcal{H}$. Then the following are equivalent.*

(i) *A is densely defined and self-adjoint;*

(ii) *A is closed, densely defined and* $\mathrm{Ker}(A^* \pm i) = 0$*;*

(iii) $\mathrm{Rg}(A \pm i) = \mathcal{H}$.

Proof. (i) $\Rightarrow$ (ii): If A is self-adjoint, one has $A = A^*$. Since the latter is closed by Proposition 2.2.24, A is a closed operator. Moreover, one has $\mathrm{Ker}(A^* \pm i) = \mathrm{Ker}(A \pm i) = 0$, since the latter is injective by Lemma 2.2.12.

(ii) $\Rightarrow$ (iii): By Lemma 2.2.33 the operators $A \pm i$ have dense range. We now show that this already implies that $A \pm i$ are surjective. We only treat the case of $A + i$ as the other case works completely analogously. Recall that one has

the estimate $\|(A+i)x\| \geq \|x\|$ for all $x \in D(A)$ by Lemma 2.2.12. Now let $y \in \mathcal{H}$. Since $\mathrm{Rg}(A+i)$ is dense, there exist $y_n \in \mathcal{H}$ and $x_n \in D(A)$ with $(A+i)x_n = y_n$ and $y_n \to y$ in $\mathcal{H}$. One has

$$\|x_n - x_m\| \leq \|(A+i)(x_n - x_m)\| = \|y_n - y_m\|$$

Since the right hand side converges it is Cauchy sequence. By the above estimate $(x_n)_{n\in\mathbb{N}}$ is a Cauchy sequence as well. Hence, there exists $x \in \mathcal{H}$ with $x_n \to x$. To summarize we have $x_n \to x$ and $(A+i)x_n \to y$. Since A is closed, this implies $x \in D(A)$ and $(A+i)x = y$. This shows that $A+i$ is surjective.

(iii) $\Rightarrow$ (i): Note first that by Lemma 2.2.14 the domain $D(A)$ is dense. It therefore makes sense to consider the adjoint. By Lemma 2.2.26, the adjoint A^* is an extension of A. It therefore remains to show that A extends A^*. For this let $y \in D(A^*)$. By assumption, there exists $x \in D(A)$ with $(A+i)x = (A^*+i)y$. Since A^* extends A, we have $(A^*+i)x = (A^*+i)y$. It follows from Lemma 2.2.33 that $(A-i)^* = A^*+i$ is injective. Hence, $y = x \in D(A)$ and A extends A^*. □

We now show using the example of real multiplication operators that this result simplifies verifying self-adjointness.

Example 2.2.35. Let (Ω, Σ, μ) be a measure space and M_m the multiplication operator on $L^2(\Omega, \Sigma, \mu)$ for some measurable $m\colon \Omega \to \mathbb{R}$ as in Example 2.2.28. The symmetry (the easy part) can be checked by a direct calculation. We now check the range condition of Theorem 2.2.34. For this we have to find for a given $g \in L^2$ a function $f \in L^2$ with $mf \in L^2$ such that

$$(M_m \pm i)f = (m \pm i)f = g \qquad \Leftrightarrow \qquad f = \frac{1}{m \pm i} g.$$

Note that $|m \pm i| \geq 1$ because m is a real function and therefore

$$\|f\|_2 \leq \|1/(m \pm i)\|_\infty \|g\|_2 \leq \|g\|_2 .$$

This shows $f \in L^2$. Moreover, one has $\|m/(m \pm i)\|_\infty \leq 1$ which implies $f \in D(M_m)$. Hence, M_m is a symmetric operator with $\mathrm{Rg}(M_m \pm i) = L^2(\Omega)$. Theorem 2.2.34 now implies that M_m is self-adjoint.

Note the above argument works without checking the denseness of the domain or determining the adjoint. With a similar condition one can also check whether a symmetric operator is essentially self-adjoint or not.

Theorem 2.2.36. *Let $(A, D(A))$ by a densely defined symmetric operator on some Hilbert space $\mathcal{H}$. Then the following are equivalent.*

(i) *A is essentially self-adjoint;*

(ii) $\mathrm{Ker}(A^* \pm i) = 0$;

(iii) $\mathrm{Rg}(A \pm i)$ *is dense in* $\mathcal{H}$.

We will only give a sketch of the proof of the theorem here and leave the details as an exercise to the reader. One can show that for a symmetric operator A^{**} is again symmetric and the closure of A. Moreover, one always has $A^* = A^{***}$. Hence, the above result follows from Theorem 2.2.34 applied to A^{**} and Lemma 2.2.33.

Remark 2.2.37. Recall that in Example 2.2.25 we have seen a closed densely defined symmetric operator A whose adjoint A^* is not symmetric. In fact, this is no coincidence. Suppose that A is a closed densely defined symmetric operator whose adjoint A^* is also symmetric. If follows from the symmetry of A that $A \subset A^*$. Analogously, it follows from the symmetry of A^* that $A^* \subset A^{**}$. Since, A is closed, it follows from the comments before this remark that $A = A^{**}$. Hence, $A^* \subset A$ and therefore A is self-adjoint.

2.2.4 Self-Adjoint Extensions

It may be difficult to explicitly write down the domain of a self-adjoint operator. For example, this situation arises in the study of Hamiltonians if the potential is non-trivial. Therefore one often as a first step defines a symmetric operator with some dense domain, e.g. some class of smooth functions. After that one asks whether this symmetric operator can be extended to a self-adjoint operator. In this direction we have given a characterization of essentially self-adjoint operators in the last section. However, it may happen that a symmetric operator has several different self-adjoint extensions. In this section we give a characterization of all self-adjoint extensions of a symmetric operator and give some physical examples.

We extend the notion of an isometry in a natural way to unbounded operators.

Definition 2.2.38 (Isometry). An unbounded operator $(U, D(U))$ on some Hilbert space $\mathcal{H}$ is called an *isometry* if

$$\langle Ux|Uy\rangle = \langle x|y\rangle \qquad \text{for all } x, y \in D(U).$$

Note that as after Definition 2.1.33 it follows from the polarization identity that $(U, D(U))$ is an isometry if and only if $\|Ux\| = \|x\|$ for all $x \in D(U)$. As a motivation for the following argument we take a quick look at the Möbius transform

$$z \mapsto \frac{z-i}{z+i}.$$

It is a well-known fact from complex analysis that this defines a bijection between the real line and the unit circle in the complex plane without the

point 1 (considered in the extended complex plan the point ∞ is mapped to 1). Indeed, for $z \in \mathbb{R}$ the absolute value of the nominator and the denominator agree and the inverse can be easily calculated as

$$w \mapsto i\frac{1+w}{1-w}.$$

We now apply the above transformation to a symmetric operator. This transformation is called the *Cayley transformation*. In the next proposition we study its basic properties.

Proposition 2.2.39 (Properties of the Cayley transform). *Let $(A, D(A))$ be a symmetric operator on some Hilbert space $\mathcal{H}$. Then the Cayley transform of A*

$$V := (A-i)(A+i)^{-1}$$

is a well-defined isometry from $\mathrm{Rg}(A+i)$ onto $\mathrm{Rg}(A-i) \subset \mathcal{H}$.

Proof. Note that for $x \in D(A)$ one has by the symmetry of A

$$\begin{aligned}\|(A \pm i)x\|^2 &= \langle (A \pm i)x | (A \pm i)x\rangle = \langle Ax|Ax\rangle + \langle x|x\rangle \pm i\langle Ax|x\rangle \mp i\langle x|Ax\rangle \\ &= \|Ax\|^2 + \|x\|^2 \pm \langle Ax|x\rangle \mp i\langle Ax|x\rangle = \|Ax\|^2 + \|x\|^2.\end{aligned}$$

This again shows that $A \pm i$ is injective and therefore that the inverse $(A+i)^{-1}$ is well-defined as an unbounded operator with domain $\mathrm{Rg}(A+i)$. Moreover, for $x \in D(A)$ we have

$$\|(A+i)x\|^2 = \|(A-i)x\|^2.$$

Now, it follows for $x \in \mathrm{Rg}(A+i)$ and $y = (A+i)^{-1}x$ that

$$\|Vx\|^2 = \|(A-i)y\|^2 = \|(A+i)y\|^2 = \|x\|^2.$$

This shows that V is an isometry. Moreover, if $y \in \mathrm{Rg}(A-i)$, then $x = (A+i)(A-i)^{-1}y$ satisfies $Vx = y$. This finishes the proof. □

Lemma 2.2.40. *Let $(A, D(A))$ be a symmetric operator on some Hilbert space $\mathcal{H}$. Then the Cayley transform of A is unitary on $\mathcal{H}$ if and only if A is densely defined and self-adjoint.*

Proof. First assume that A is self-adjoint. Then it follows from Theorem 2.2.34 that $\mathrm{Rg}(A \pm i) = \mathcal{H}$. By Proposition 2.2.39 the Cayley transform V is an isometric operator from $\mathcal{H} = \mathrm{Rg}(A+i)$ onto $\mathcal{H} = \mathrm{Rg}(A-i)$. This yields that V is a surjective isometric operator $\mathcal{H} \to \mathcal{H}$. It now follows from the polarization identity that V is unitary on $\mathcal{H}$.

Conversely, if $V\colon \mathcal{H} \to \mathcal{H}$ is unitary, then $\mathrm{Rg}(A \pm i) = \mathcal{H}$ by Proposition 2.2.39. The self-adjointness now follows from Theorem 2.2.34. □

Suppose that V is the Cayley transform of some symmetric operator A. Then one would expect that one can recover A from V by the natural formula $A = i(\mathrm{Id}+V)(\mathrm{Id}-V)^{-1}$. Indeed, one can show by direct calculations that if A is an unbounded operator such that $A+i$ is injective, then $\mathrm{Id}-V$ is injective, $\mathrm{Rg}(\mathrm{Id}-V) = D(A)$ and $A = i(\mathrm{Id}+V)(\mathrm{Id}-V)^{-1}$ as unbounded operators. Moreover, if some given $V\colon \mathcal{H} \to \mathcal{H}$ is unitary such that $\mathrm{Id}-V$ is injective, one can always write V as the Cayley transform of some self-adjoint operator.

Lemma 2.2.41. *Let $\mathcal{H}$ be a Hilbert space and $V \in \mathcal{B}(H)$ a unitary operator such that $\mathrm{Id}-V$ is injective. Then there exists a self-adjoint operator $(A, D(A))$ on $\mathcal{H}$ such that V is the Cayley transform of A.*

Proof. It is sufficient to find a symmetric operator on $\mathcal{H}$ whose Cayley transform is V: the self-adjointness of A then follows directly from Lemma 2.2.40. Since $\mathrm{Id}-V$ is injective, the operator

$$A = i(\mathrm{Id}+V)(\mathrm{Id}-V)^{-1}$$

is well-defined with $D(A) = \mathrm{Rg}(\mathrm{Id}-V)$. We show that A is symmetric. For this let $x, y \in \mathrm{Rg}(\mathrm{Id}-V)$. There exist $w, z \in \mathcal{H}$ with $x = (\mathrm{Id}-V)w$ and $y = (\mathrm{Id}-V)z$. We have

$$\begin{aligned}
\langle Ax|y\rangle &= \langle i(\mathrm{Id}+V)(\mathrm{Id}-V)^{-1}x|y\rangle = \langle i(\mathrm{Id}+V)w|(\mathrm{Id}-V)z\rangle \\
&= -i\langle w|z\rangle + i\langle Vw|Vz\rangle - i\langle Vw|z\rangle + i\langle w|Vz\rangle = i\langle w|Vz\rangle - i\langle Vw|z\rangle \\
&= i\langle w|z\rangle - i\langle Vw|Vz\rangle - i\langle Vw|z\rangle + i\langle w|Vz\rangle = \langle (\mathrm{Id}-V)w|i(\mathrm{Id}+V)z\rangle \\
&= \langle x|Ay\rangle.
\end{aligned}$$

Now, one can verify with a direct computation that the Cayley transform of A is indeed V, a task which is left to the reader. □

Note that the last step of the above proof only used the fact that V is isometric. Hence, the proof shows that for every isometry U there exists a symmetric operator A whose Cayley transform is U.

By the above arguments the problem of finding self-adjoint extensions of a symmetric operator A is reduced to the problem of finding unitary extensions of the Cayley transform $V\colon \mathrm{Rg}(A+i) \to \mathrm{Rg}(A-i)$. Now working with orthogonal complements becomes quite handy, a notion which we already have used implicitly several times.

Definition 2.2.42 (Orthogonal complement). Let $M \subset \mathcal{H}$ be a subset of some Hilbert space. Then its *orthogonal complement* is defined as the closed subspace

$$M^{\perp} := \{x \in \mathcal{H} : \langle x|y\rangle = 0 \text{ for all } y \in M\}.$$

The orthogonal complement $M^\perp$ has a straightforward geometrical interpretation. It consists of all vectors which are perpendicular to all elements of M. Note that for a closed subspace $M \subset \mathcal{H}$ one always has the orthogonal direct decomposition $\mathcal{H} = M \oplus M^\perp$. For $x \in \mathcal{H}$ this decomposition is given by $x = Px + (\mathrm{Id} - P)x$, where P is the orthogonal projection onto M defined in Example 2.1.14. We will use the following relation for unbounded operators.

Lemma 2.2.43. *Let $(A, D(A))$ be a densely defined unbounded operator on some Hilbert space $\mathcal{H}$. Then*

$$\operatorname{Ker} A^* = \operatorname{Rg}(A)^\perp.$$

Proof. Suppose $x \in \operatorname{Ker} A^*$. Then we have for all $Az = y \in \operatorname{Rg}(A)$

$$\langle x|y\rangle = \langle x|Az\rangle = \langle A^*x|z\rangle = 0.$$

Hence, $x \in \operatorname{Rg}(A)^\perp$. Conversely, let $x \in \operatorname{Rg}(A)^\perp$. Then we have for all $y \in D(A)$ the identity $\langle x|Ay\rangle = 0$. This implies that $x \in D(A^*)$ and $A^*x = 0$. Therefore $x \in \operatorname{Ker} A^*$. □

We now return to the above extension problem. Note that if such a unitary extension $U : \mathcal{H} \to \mathcal{H}$ exists, then U splits as a componentwise isomorphism

$$\overline{\operatorname{Rg}(A+i)} \oplus \operatorname{Rg}(A+i)^\perp \to \overline{\operatorname{Rg}(A-i)} \oplus \operatorname{Rg}(A-i)^\perp.$$

Hence, $\operatorname{Rg}(A+i)^\perp$ and $\operatorname{Rg}(A+i)^\perp$ are isomorphic as Hilbert spaces. Conversely, one sees directly that an isometry $\operatorname{Rg}(A+i) \to \operatorname{Rg}(A-i)$ extends uniquely to an isometry between the closures. Hence, a unitary isomorphism between $\operatorname{Rg}(A+i)^\perp$ and $\operatorname{Rg}(A-i)^\perp$ yields a unitary operator $U : \mathcal{H} \to \mathcal{H}$ extending the Cayley transform of A. One can check that for such an extension U the operator $\mathrm{Id} - U$ is injective and therefore is the Cayley transform of some self-adjoint operator B by Lemma 2.2.41. In fact, this gives an one-to-correspondence between unitary extensions of the Cayley transform and self-adjoint extensions of A. A crucial role is played by the dimensions of the orthogonal complements just used.

Definition 2.2.44 (Deficiency indices). The *deficiency indices* $d_+(A)$ and $d_-(A)$ of a densely defined symmetric operator $(A, D(A))$ are defined as

$$d_+(A) = \dim \operatorname{Ker}(A^* + i) \qquad \text{and} \qquad d_-(A) = \dim \operatorname{Ker}(A^* - i).$$

Note that by Lemma 2.2.43 one has $d_+(A) = \dim \operatorname{Rg}(A-i)^\perp$ and $d_-(A) = \dim \operatorname{Rg}(A+i)^\perp$. We have just sketched a proof of the following theorem (we omit a detailed proof).

Theorem 2.2.45. *Let $(A, D(A))$ be a densely defined symmetric operator on some Hilbert space $\mathcal{H}$. Then*

(a) *A has self-adjoint extensions if and only if $d_+(A) = d_-(A)$.*

(b) *There is a one-to-one correspondence between self-adjoint extensions of A and unitary extensions $\mathcal{H} \to \mathcal{H}$ of its Cayley transform, i.e. unitary operators between* $\operatorname{Ker}(A^* - i)$ *and* $\operatorname{Ker}(A^* + i)$.

In particular, A admits a unique self-adjoint extension if and only if $d_+(A) = d_-(A) = 0$, i.e. if and only if A is essentially self-adjoint by Theorem 2.2.36. Moreover, if $U\colon \operatorname{Ker}(A^* - i) \to \operatorname{Ker}(A^* + i)$ is unitary, the corresponding self-adjoint extension A_U is given by

$$\begin{aligned} D(A_U) &= \{f + g - Ug : f \in D(\overline{A}), g \in \operatorname{Ker}(A^* - i)\} \\ A_U(f + g - Ug) &= \overline{A}f + i(g + Ug). \end{aligned}$$

In fact, more generally one can show that there is an one-to-one correspondence between isometries $(U, D(U))$ into $\operatorname{Ker}(A^* + i)$ with $D(U) \subset \operatorname{Ker}(A^* - i)$ and closed symmetric extensions of A. Let us illustrate the theorem with some examples.

Example 2.2.46 (Self-adjoint extensions of the momentum operator on the half-line). Let us again consider the momentum operator $A = -i\frac{d}{dx}$ with domain $D(A) = C_c^\infty((0,\infty))$ on $L^2([0,\infty))$. The calculations in Example 2.2.25 show that its adjoint is $A^* = -i\frac{d}{dx}$ with $D(A^*) = H^1((0,\infty))$. Let us determine the deficiency indices of A. First we consider the equation

$$(A^* + i)f = -if' + if = 0 \qquad \Leftrightarrow \qquad f' - f = 0.$$

Every solution of this equation is a solution in the classical sense: we have $f \in H^1((0,\infty))$ and the above equation implies that $f' \in H^1((0,1))$ as well. Therefore $f \in H^2((0,\infty))$. Iterating this argument shows that $f \in H^k((0,\infty))$ for all $k \in \mathbb{N}$. The Sobolev embedding theorems (Remark 2.1.37) show that $f \in C^\infty((0,\infty))$ and therefore a classical solution. This shows that all solutions of the above ordinary differential equation are scalar multiples of $f(t) = e^t$. However, these solutions are not-square integrable. This shows $d_+(A) = 0$. For $d_-(A)$ we have to solve

$$(A^* - i)f = -if' - if = 0 \qquad \Leftrightarrow \qquad f' + f = 0.$$

As above all solutions of the above equation are scalar multiples of $f(t) = e^{-t}$ which are square-integrable. Hence, $d_-(A) = 1$. Altogether we have $d_+(A) \neq d_-(A)$ and we see from Theorem 2.2.45 that A has no self-adjoint extensions.

Please recall that we have already discussed the non-existence of self-adjoint extensions of the momentum operator on the half-line from a physical perspective in Remark 2.2.18.

Example 2.2.47 (Self-adjoint extensions of the momentum operator on a bounded interval). We now study a slight variation of the previous example. In fact, we consider the momentum operator $A = -i\frac{d}{dx}$ on $L^2([0,1])$ with domain $D(A) = C_c^\infty((0,1))$. Similar as in the previous example one calculates its adjoint to be $A^* = -i\frac{d}{dx}$ with $D(A^*) = H^1((0,1))$. For $d_+(A)$ we solve

$$(A^* + i)f = 0 \qquad \Leftrightarrow \qquad f' - f = 0.$$

Every solution of the above equation is a scalar multiple of $f(t) = e^t$. Hence, $d_+(A) = 1$. An analogous calculation shows that $d_-(A) = 1$. By Theorem 2.2.45, A has self-adjoint extensions. Moreover, the self-adjoint extensions are in one-to-one correspondence to unitaries between $\mathbb{C} \simeq \mathrm{Ker}(A^* - i)$ and $\mathbb{C} \simeq \mathrm{Ker}(A^* + i)$. Every unitary map between in $\mathbb{C}$ is uniquely determined by a real number $\alpha \in [0, 2\pi)$, i.e. $z \mapsto e^{i\alpha}z$. Now let us determine the self-adjoint extensions of A concretely. For this we first need to determine the closure of A. Notice that the norm $\|\cdot\| + \|A\cdot\|$ agrees with the norm of $H^1((0,1))$. It follows from the denseness of $C_c((0,1))$ in $H_0^1((0,1))$ (see Remark 2.2.16) that $\overline{A} = -i\frac{d}{dx}$ with $D(\overline{A}) = H_0^1((0,1))$. To write down the unitary mappings between $\mathrm{Ker}(A^* - i)$ and $\mathrm{Ker}(A^* + i)$ we need normalized elements in the kernels. For this we calculate

$$\int_0^1 e^{-2t}\,dt = \frac{1}{2}(1 - e^{-2}) = \frac{1}{2}e^{-2}(e^2 - 1) \qquad \text{and} \qquad \int_0^1 e^{2t}\,dt = \frac{1}{2}(e^2 - 1).$$

The normalized elements are therefore given by

$$f_-(t) = \frac{\sqrt{2}e}{\sqrt{e^2 - 1}}e^{-t} \qquad \text{and} \qquad f_+(t) = \frac{\sqrt{2}}{\sqrt{e^2 - 1}}e^{t}.$$

Hence, the unitary $U_\alpha \colon \mathrm{Ker}(A^* - i) \to \mathrm{Ker}(A^* + i)$ is determined by $f_- \mapsto e^{i\alpha}f_+$. Every element of $D(A_{U_\alpha})$ can be written as the sum $g + \lambda(f_- - U_\alpha f_-)$ for some $g \in H_0^1((0,1))$. Evaluating at the boundaries gives

$$\begin{aligned} f_-(0) - e^{i\alpha}f_+(0) &= \frac{\sqrt{2}e}{\sqrt{e^2 - 1}} - e^{i\alpha}\frac{\sqrt{2}}{\sqrt{e^2 - 1}} \\ f_-(1) - e^{i\alpha}f_+(1) &= \frac{\sqrt{2}}{\sqrt{e^2 - 1}} - e^{i\alpha}\frac{\sqrt{2}e}{\sqrt{e^2 - 1}}. \end{aligned}$$

The quotient of both is

$$\left|\frac{e - e^{i\alpha}}{1 - e^{i\alpha}e}\right| = \left|\frac{e - e^{i\alpha}}{e^{-i\alpha} - e}\right| = 1.$$

Moreover, one can directly verify or use the theory of Möbius transformations that $z \mapsto (e - z)/(1 - ez)$ restricts to a bijection on the unit circle. Hence, there

exists a $\beta \in [0, 2\pi)$ (uniquely determined by α) such that for every $f \in D(U_\alpha)$ we have $f(0) = e^{i\beta} f(1)$. Conversely, one sees that every $f \in H^1((0,1))$ with $f(0) = e^{i\beta} f(1)$ can be written as $g + \lambda(f_- U_\alpha f_-)$ for some $g \in H_0^1((0,1))$ and some $\lambda \in \mathbb{C}$. Hence, the self-adjoint operators $(A_\beta, D(A_\beta))$ defined by

$$\begin{aligned} D(A_\beta) &= \{f \in H^1((0,1)) : f(0) = e^{i\beta} f(1)\} \\ A_\beta f &= -if'. \end{aligned}$$

for some $\beta \in [0, 2\pi)$ are exactly the self-adjoint extensions of A.

It is again time to discuss the physical relevance of the above calculations. This time we describe a particle which is located in a finite spatial region due to the potential

$$V(x) = \begin{cases} 0 & \text{if } 0 \le x \le 1 \\ \infty & \text{else} \end{cases}.$$

Given a compactly supported wave function $\psi \in C_c^\infty((0,1))$ the time evolution described by the momentum operator should be given by translation of ψ. But this of course does not completely describe the time evolution for all times because after some time the wave function will meet the boundary. Since the time evolution must be described by some unitary operator, we cannot loose probability mass of the function. Hence, what goes out at one side of the well should come in at the other side. However, we have the freedom to choose a phase shift for the outcoming wave. By the superposition principle, this phase shift is independent of the wave function. In this way one exactly obtains the just calculated self-adjoint extensions, where $e^{i\beta}$ is the global phase shift of the outcoming waves.

What can we learn from this example? Different self-adjoint extensions really correspond to different *physics*! Hence, the concrete choice of a self-adjoint extension of a given symmetric operator is not just some mathematical freedom which is irrelevant for the description of the physical world, but has real physical consequences.

Example 2.2.48 (The Hamiltonian in the half-line). We now consider the free Hamiltonian associated to the momentum operator of the last example, i.e. $A = -\frac{d^2}{d^2x}$ with $D(A) = C_c^\infty((0,\infty))$. Let us calculate its adjoint. For this let $f \in D(A^*)$. Then one has for all $g \in C_c^\infty((0,\infty))$ that

$$\int_0^\infty \overline{(A^* f)(x)} g(x)\, dx = \langle A^* f | g \rangle = \langle f | Ag \rangle = -\int_0^\infty \overline{f(x)} g''(x)\, dx.$$

Taking complex conjugates, we obtain for real $g \in C_c^\infty((0,\infty))$

$$\int_0^\infty (A^* f)(x) g(x)\, dx = -\int_0^\infty f(x) g''(x)\, dx.$$

This shows that the second derivative of f exists in the weak sense and is given by $-A^*f$. Conversely, if the second derivative of f exists in the weak sense and lies in $L^2((0,\infty))$, the same calculations read backwards show that $f \in D(A^*)$ and $A^*f = -f''$. Now let us determine the deficiency indices of A. For $d_+(A)$ we solve

$$(A^* + i)f = -f'' + if = 0.$$

It follows from the elliptic regularity theory presented in Example 2.1.38 (the half-line case follows from the real line case via a reduction argument, simply extend all solutions to the real line by reflecting the solution along at the origin; in fact this argument also shows $D(A^*) = H^2((0,\infty))$ that a solution of the equation in the weak sense already satisfies $f \in C^\infty((0,\infty))$ and therefore is a classical solution. Every classical solution of this second ordinary differential equation is of the form

$$\lambda_1 \exp((1-i)x/\sqrt{2}) + \lambda_2 \exp(-(1+i)x/\sqrt{2})$$

for some $\lambda_1, \lambda_2 \in \mathbb{C}$. This solution is in $L^2((0,\infty))$ if and only if $\lambda_1 = 0$. Hence, $d_+(A) = 1$. An analogous calculation shows $d_-(A) = 1$. Hence, it follows from Theorem 2.2.45 that A has self-adjoint extensions. In fact, along the reasoning of Example 2.2.47 the self-adjoint extensions of A are precisely the operators $-\frac{d^2}{d^2x}$ with domains

$$D(A_a) = \{f \in H^2((0,\infty)) : f'(0) + af(0) = 0\}$$

for $a \in \mathbb{R}$ and in the formal limit case $a = \infty$

$$D(A_\infty) = \{f \in H^2((0,\infty)) : f(0) = 0\}.$$

This result is very interesting from a physical perspective. Although one cannot define a reasonable momentum observable in the half-line case as shown in Example 2.2.46, the situation changes when one considers the Hamiltonian as its formal square. In fact, the previous example shows that there are infinitely many self-adjoint realizations of the Hamiltonian with different boundary conditions. Let us show that these realizations again correspond to different physics. Let us for the following moment ignore the behaviour of the wave function at infinity, i.e. all integrability issues. Then the plane waves $e^{\pm ikx}$ for $k \in \mathbb{R}$ do not lie in $D(A_a)$ since they do not satisfy the boundary conditions. However, if we consider a supposition of both incoming and outcoming waves $\psi(x) = e^{-ikx} + \lambda e^{ikx}$ we have

$$\psi'(0) + a\psi(0) = -ik + ik\lambda + a + \lambda a = 0 \qquad \Leftrightarrow \qquad \lambda = \frac{ik - a}{ik + a}.$$

Note that $|\lambda| = 1$. Hence, A_a generates a dynamic in which a plane wave is reflected at the origin with a phase change depending on the value of a and the momentum k. The limit case $a = \infty$ corresponds to the case of total reflection on a hard wall where the phase change is -1 independent of the momentum.

We now come back to an old example from the other part of the lecture. Sadly, this example is more difficult than the previous ones and is best treated within the theory of distributions which we will introduce in the next chapter. We will state all necessary facts explicitly. The reader may skip the example and return later or simply believe the used results.

Example 2.2.49. On $L^2(\mathbb{R})$ consider the operator $A = -ix^3\frac{d}{dx} - i\frac{d}{dx}x^3$. We have already studied this operator in the physics part of the lecture. Using naive reasoning, it seems that

$$f(x) = \frac{1}{|x|^{3/2}} e^{-1/4x^2} \in L^2(\mathbb{R})$$

satisfies $Af = -if$, i.e. f is an imaginary eigenvalue of A. The problem is that, once precisely written down, f does not lie in the domain $D(A)$. We now give a mathematical precise study of the operator with the aim to get another perspective on the operator with the help of the theory just developed. For this we use the domain $D(A) = C_c^\infty(\mathbb{R})$. Let us first show that the operator $(A, D(A))$ is symmetric. Using integration by parts, for $f, g \in D(A)$ we obtain the desired identity

$$\begin{aligned}\langle f|Ag\rangle &= \int_{-\infty}^{\infty} \overline{f(x)}(Ag)(x)\,dx = -i\int_{-\infty}^{\infty} \overline{f(x)}(x^3 g'(x) + (x^3 g(x))')\,dx \\ &= i\int_{-\infty}^{\infty} \overline{(f(x)x^3)'}g(x) + \overline{f'(x)}x^3 g(x)\,dx \\ &= \int_{-\infty}^{\infty} \overline{-i(x^3 f'(x) + (f(x)x^3)')}g(x)\,dx = \langle Af|g\rangle.\end{aligned}$$

It is somewhat difficult to describe the domain of the adjoint more explicitly without using the theory of distributions that we will cover in the next chapter. For the moment we assume that we can give sense to the derivative of an arbitrary L^1_{loc}-function and that these derivatives can be multiplied with smooth functions of polynomial growth. The domain $D(A^*)$ is then given by those functions $f \in L^2(\mathbb{R})$ for which the distribution $x^3 f'(x) + (x^3 f(x))' = 2x^3 f'(x) + 3x^2 f(x)$ lies in $L^2(\mathbb{R})$ (assuming the usual rules of calculus). Let us now calculate the deficiency indices. For $d_+(A)$ we obtain the equation

$$(A^* + i)f = 0 \quad \Leftrightarrow \quad f(x) - 2x^3 f'(x) - 3x^2 f(x) = (1 - 3x^2)f(x) - 2x^3 f'(x) = 0.$$

We can restrict the above equation to the open right and left half-plane (this is also valid for distributions). For $x > 0$ respectively $x < 0$ we obtain the

equation

$$f'(x) = \frac{1-3x^2}{2x^3} f(x).$$

We now treat the case $x > 0$. If $f \in L^2(\mathbb{R})$ solves the equation on $[\varepsilon, \infty)$ for some $\varepsilon > 0$, then it follows from the fact the factor on the right hand side is bounded that $f' \in L^2([\varepsilon, \infty))$. Hence, $f \in H^1([\varepsilon, \infty))$ because we will see from the definition of distributions that if the distributional derivative exists as a locally integrable function, then the weak derivative exists and agrees with the function representing the distributional derivative. Iterating this argument and using the Sobolev embeddings we see that $f \in C^\infty((\varepsilon, \infty))$. Hence, f is smooth away from zero. Hence, away from zero it is sufficient to work with classical solution of the differential equation. Using separation of variables, we see that all solutions are scalar multiples of

$$f_+(x) = \exp\left(\int \frac{1-3y^2}{2y^3}\, dy \right) = \exp\left(-\frac{1}{4} y^{-2} - \frac{3}{2} \log y \right) = \frac{\exp(-1/4y^2)}{y^{3/2}}.$$

Analogously, one obtains for the case $x < 0$ that the solution is a multiple of

$$f_-(x) = \exp\left(\int \frac{1-3y^2}{2y^3}\, dy \right) = \exp\left(-\frac{1}{4} y^{-2} - \frac{3}{2} \log|y| \right) = \frac{\exp(-1/4y^2)}{|y|^{3/2}}.$$

One now sees directly that both are square-integrable in the respective half-planes. Hence, $\lambda_1 f_+ \mathbb{1}_{[0,\infty)} + \lambda_2 f_- \mathbb{1}_{(-\infty,0]} \in \operatorname{Ker}(A^* + i)$ for $\lambda_1, \lambda_2 \in \mathbb{C}$. This shows $d_+(A) = 2$.

Let us continue with $d_-(A)$. For this we have to find all solutions of

$$(A^* - i)f = 0 \quad \Leftrightarrow \quad f(x) + 2x^3 f'(x) + 3x^2 f(x) = (1 + 3x^2) f(x) + 2x^3 f(x) = 0.$$

For $x \neq 0$ we therefore have by the same reasoning

$$f'(x) = -\frac{1+3x^2}{2x^3} f(x).$$

Integrating this equation we obtain that on both open half-lines one must have scalar multiples of the functions

$$f(x) = \exp\left(-\int \frac{1+3y^2}{2y^3}\, dy \right) = \exp\left(\frac{1}{4} y^{-2} - \frac{3}{2} \log|y| \right) = \frac{\exp(1/4y^2)}{|y|^{3/2}}.$$

However, these functions have non-square integrable singularities at zero and therefore cannot be combined to a non-zero $L^2(\mathbb{R})$-function. This shows that $d_-(A) = 0$.

Altogether we see from Theorem 2.2.45 that A does not have any self-adjoint extensions. Moreover, observe that the potential eigenvector for i does not lie in the domain of A. However, it does lie in the domain of A^* as we just shown. However, the domain $D(A^*)$ is too big in order for A^* to be self-adjoint.

2.2.5 The Spectrum of Self-Adjoint Operators

Recall that our actual interest for self-adjoint operators stems from the fact that self-adjoint operators describe quantum mechanical observables by the postulates of quantum mechanics. In particular, a key issue here is the fact that the spectrum of a self-adjoint operator should be real because the spectrum of an observable corresponds to its possible measurement outcomes. Recall that for symmetric operators the spectrum can contain complex numbers. We now show that the reality condition on the spectrum characterizes self-adjoint operators among the symmetric operators. Hence, self-adjointness as introduced before is exactly the right concept for the mathematical treatment of quantum mechanics.

Theorem 2.2.50. *Let $(A, D(A))$ be a densely defined symmetric operator on some Hilbert space. Then*

$$\sigma(A) \subset \mathbb{R} \qquad \Leftrightarrow \qquad A \text{ is self-adjoint.}$$

Proof. Suppose first that A is self-adjoint. Then it follows from the characterization of self-adjoint operators given in Theorem 2.2.34 (iii) and Lemma 2.2.13 that $\pm i \in \rho(A)$. By the structural properties of the spectrum of a symmetric operator proved in Corollary 2.2.22, the spectrum of A must be contained in the real axis.

Conversely, if $\sigma(A) \subset \mathbb{R}$, then we have $\pm i \rho(A)$. The self-adjointness of A then follows directly from Proposition 2.2.21. □

Nevertheless it can take some work to determine the spectrum of self-adjoint operators explicitly. We now do this for the important case of real multiplication operators.

Example 2.2.51 (Spectrum of multiplication operators). Consider again the multiplication operator $M_m f = mf$ on the Hilbert space $L^2(\Omega, \Sigma, \mu)$ for some σ-finite measure space (Ω, Σ, μ) and a measurable function $m\colon \Omega \to \mathbb{R}$ with domain $D(M_m) = \{f \in L^2 : mf \in L^2\}$. We now want to determine the spectrum $\sigma(M_m)$ of M_m. For this we introduce the *essential range* of m as

$$\operatorname{essim}(m) := \{z \in \Omega : \text{for all } \varepsilon > 0 \text{ one has } \mu(\{\omega : |m(\omega) - z|) < \varepsilon\} > 0\}.$$

We claim that $\sigma(M_m) = \operatorname{essim}(m)$. For this let us first assume that $z \notin \operatorname{essim}(m)$. Then there exists $\varepsilon > 0$ such that $\mu(\{\omega : |m(\omega) - z| < \varepsilon\}) = 0$. Hence, $|m(\omega) - z| \geq \varepsilon$ almost everywhere. We show that $z \in \rho(A)$. For this we have to solve $(z - m)f = g$ for $g \in L^2(\Omega)$. In fact, the unique solution of this equation is given by $f(\omega) = g(\omega)/(z - m(\omega))$ almost everywhere. This solution is indeed square integrable because of

$$\int_\Omega |f(\omega)|^2 \, d\omega = \int_\Omega \frac{|g(\omega)|^2}{|z - m(\omega)|^2} \, d\omega \leq \varepsilon^{-2} \int_\Omega |g(\omega)|^2 \, d\omega.$$

This shows $\sigma(A) \subseteq \operatorname{essim}(A)$. It remains to show the converse inclusion $\operatorname{essim}(A) \subset \sigma(A)$. For this let $z \in \operatorname{essim}(A)$. Then for all $n \in \mathbb{N}$ there exist $c_n > 0$ with $\mu(A_n) = c_n$, where $A_n = \{\omega : |m(\omega) - z| < 4^{-n}\}$. Now consider the function $g = \sum_{n=1}^{\infty} c_n^{-1/2} 2^{-n} \mathbb{1}_{A_n}$. Then

$$\|g\|_2 \leq \sum_{n=1}^{\infty} c_n^{-1/2} 2^{-n} \|1_{A_n}\|_2 = \sum_{n=1}^{\infty} c_n^{-1/2} 2^{-n} c_n^{1/2} = 1.$$

Let $f(\omega) = g(\omega)/(z - m(\omega))$ be the unique solution of the resolvent equation. Then for all $n \in \mathbb{N}$ we have

$$\|f\|_2^2 \geq \int_{A_n} \frac{|g(\omega)|^2}{|z - m(\omega)|^2} \, d\omega \geq \int_{A_n} \frac{c_n^{-1} 4^{-n}}{|z - m(\omega)|^2} \, d\omega \geq 4^n \int_{A_n} c_n^{-1} \, d\omega = 4^n.$$

This shows that f is not square integrable and that $z - M_m$ is not surjective. A fortiori, $z \in \sigma(A)$ and the converse inclusion $\operatorname{essim}(A) \subset \sigma(A)$ is shown.

As particular examples we can determine the spectrum of the position and momentum operators and the Laplace operator on $\mathbb{R}^n$.

Example 2.2.52. For $j = 1, \ldots, n$ let $\hat{x_j}$ and $\hat{p_j}$ be the position and momentum operators on $\mathbb{R}^n$ as introduced before and in Example 2.2.29. These operators are self-adjoint and satisfy

$$\sigma(\hat{p}_j) = \sigma(\hat{x}_j) = \mathbb{R} \qquad \text{for all } j = 1, \ldots, n.$$

Proof. The case of the momentum operators is a particular instance of Example 2.2.51. For the momentum operators recall that these are unitarily equivalent via the Fourier transform to the multiplication operators with $m(x) = x_j$. Since the spectrum is invariant under similarity transforms, the result again follows from Example 2.2.51. □

Note that the full spectrum of the position and momentum operators is exactly the result we would expect from physics: if one measures the momentum (or the position) of a particle, one can obtain arbitrary real values as measurement outcomes.

An analogous approach yields the spectrum of the negative Laplacian $-\Delta$ with domain $H^2(\mathbb{R}^n)$.

Example 2.2.53 (Spectrum of $-\Delta$). For $n \in \mathbb{N}$ consider the negative Laplacian $-\Delta$ with domain $H^2(\mathbb{R}^n)$. We have seen that this operator is unitarily equivalent via the Fourier transform to the multiplication operator with $m(x) = |x|^2$. Hence, $\sigma(-\Delta) = [0, \infty)$ by Example 2.2.51.

Note that the result $\sigma(-\Delta) = [0, \infty)$ perfectly corresponds to the physical intuition. In fact, recall that $-\Delta = \sum_{j=1}^{n} \hat{p}_j^2$ is the Hamiltonian for the free particle on $\mathbb{R}^n$ if we ignore all physical constants. As the spectrum of $\hat{H}$ corresponds to the possible measurable energy values of the particle, we expect that the spectrum is non-negative because there should not be a particle with negative energy (using the natural gauge). Moreover, since the particle is free and therefore no constraints whatsoever apply, in principle all energy values should be possible. Hence, by physical reasoning one has $\sigma(-\Delta) = [0, \infty)$ which is exactly our mathematical result.

Note that for more difficult Hamiltonians it can be extremely difficult to exactly determine their spectrum. Therefore it is desirable to at least have some information on the structure of the spectrum, for example whether there exists an orthonormal basis of eigenvectors. We will deal to some extend with such problems in the next section. However, we will not have the time to give a systematic study of the spectral properties of typical Hamiltonians of the form $-\Delta + V$.

2.3 The Spectral Theorem for Self-Adjoint Operators

Let us shortly recall the spectral theorem in the finite dimensional setting. Suppose that A is a symmetric operator on some finite dimensional complex inner product space V. Then the spectral theorem guarantees the existence of an orthonormal basis of V consisting of eigenvectors of A. With respect to this orthonormal basis, A is represented as a diagonal matrix. This is in general not possible for self-adjoint operators in the infinite dimensional setting. In fact, we have seen that there exist bounded operators on some infinite dimensional Hilbert space which not have a single eigenvalue. However, in some important physical examples, for example the Hamiltonians for an infinite high well or the harmonic oscillator, there exists an orthonormal basis of eigenvectors.

2.3.1 The Spectral Theorem for Compact Self-Adjoint Operators

In fact, with an additional assumption one obtains such an orthonormal basis. We deal with this case first before we proceed with general self-adjoint operators.

Definition 2.3.1 (Compact subsets). A subset $K \subset \mathcal{H}$ of some Hilbert space (or more generally of some metric space) is called *compact* if one of the following equivalent conditions holds.

(i) For every sequence $(x_n)_{n\in\mathbb{N}} \subset K$ there exists a subsequence $(x_{n_k})_{k\in\mathbb{N}}$ and $x \in K$ with $x_{n_k} \to x$ for $k \to \infty$.

(ii) Let $K \subset \cup_{i\in I} U_i$ be a covering of K with open subsets $U_i \subset \mathcal{H}$. Then there exist finitely many $i_1, \dots, i_n \in I$ with $K \subset \cup_{k=1}^{n} U_{i_k}$, i.e. every open covering of K has a finite sub-covering.

The second point is the definition of compact subsets for general topological spaces, whereas the (in the case of metric spaces equivalent) second point is called *sequentially compactness*. You have learned in calculus that a subset K of some finite dimensional normed vector space V is compact if and only if K is closed and bounded. This changes fundamentally in the infinite dimensional setting.

Example 2.3.2 (Non-compact unit ball). Let B be the closed unit ball of some infinite dimensional separable Hilbert space $\mathcal{H}$. Then B clearly is bounded and closed by definition. However, we now show that B is not compact. Choose an orthonormal basis $(e_n)_{n\in\mathbb{N}}$ of $\mathcal{H}$ which exists by Theorem 2.1.7. By orthogonality we have for $n \neq m$

$$\|e_n - e_m\|^2 = \|e_n\|^2 + \|e_m\|^2 = 2.$$

Since the mutual distance of two different arbitrary elements is equal to $\sqrt{2}$, the sequence $(e_n)_{n\in\mathbb{N}}$ cannot have a convergent subsequence. Hence, B is not compact.

It is an instructive exercise for the reader to explicitly construct an infinite disjoint open covering of the closed unit ball of some infinite-dimensional Hilbert space. We now introduce the important class of bounded operators.

Definition 2.3.3 (Compact operator). A linear operator $T\colon \mathcal{H}_1 \to \mathcal{H}_2$ between two Hilbert spaces (or more generally between two Banach spaces) $\mathcal{H}_1$ and $\mathcal{H}_2$ is *compact* if $\overline{T(B)}$ is a compact subset of $\mathcal{H}_2$, where B denotes the closed unit ball in $\mathcal{H}_1$. We denote the space of all compact operators between $\mathcal{H}_1$ and $\mathcal{H}_2$ by $\mathcal{K}(\mathcal{H}_1, \mathcal{H}_2)$.

The reader should verify the following elementary facts: a compact linear operator $T\colon \mathcal{H}_1 \to \mathcal{H}_2$ is automatically bounded and $\overline{T(B)}$ is compact for arbitrary bounded subsets B of $\mathcal{H}_1$. Moreover, the compact operators form a subspace of $\mathcal{B}(\mathcal{H}_1, \mathcal{H}_2)$ and the composition of a bounded and a compact operator is again a compact operator (hence, in algebraic terms, $\mathcal{K}(\mathcal{H})$ is an ideal in $\mathcal{B}(\mathcal{H})$).

We start our journey through the spectral theorems with the easiest (infinite dimensional) case, namely the spectral theorem for compact self-adjoint or more generally normal operators.

Definition 2.3.4 (Normal operator). An operator $N \in \mathcal{B}(H)$ is called *normal* if $NN^* = N^*N$.

Theorem 2.3.5 (The spectral theorem for compact normal operators). *Let $T\colon \mathcal{H} \to \mathcal{H}$ be a compact normal operator on some Hilbert space $\mathcal{H}$. Then there exists a countable orthonormal system $(e_n)_{n\in\mathbb{N}}$ and $(\lambda_n)_{n\in\mathbb{N}} \subset \mathbb{C}\setminus\{0\}$ such that*

$$\mathcal{H} = \operatorname{Ker} T \oplus \overline{\operatorname{span}\{e_n : n \in \mathbb{N}\}}$$

and

$$Tx = \sum_{n\in\mathbb{N}} \lambda_n \langle e_n|x\rangle e_n \qquad \text{for all } x \in \mathcal{H}.$$

Moreover, the only possible accumulation point of $(\lambda_n)_{n\in\mathbb{N}}$ is 0 and every non-zero eigenvalue of T has finite multiplicity, i.e. $\dim\operatorname{Ker}(T-\lambda) < \infty$ for all $\lambda \neq 0$ and all eigenvalues λ_n are real if T is self-adjoint.

In particular, after choosing an orthonormal basis of $\operatorname{Ker} T$, we have an orthonormal basis of $\mathcal{H}$ consisting of eigenvectors of T. The above formulation has the advantage that it is valid arbitrary Hilbert spaces. Ultimately, we are mostly interested in the spectral theory of unbounded self-adjoint operators which will not be bounded. Nevertheless the spectral theorem for compact self-adjoint operators has direct consequences for the study of unbounded operators, such as some Hamiltonians, as the next corollary shows.

Corollary 2.3.6. *Let $(A, D(A))$ be a self-adjoint operator on some separable infinite-dimensional Hilbert space $\mathcal{H}$ with compact resolvent, i.e. $R(\lambda, A)$ is a compact operator for some λ in the resolvent set $\rho(A)$. Then there exists an orthonormal basis $(e_n)_{n\in\mathbb{N}}$ of $\mathcal{H}$ and a sequence $(\lambda_n)_{n\in\mathbb{N}} \subset \mathbb{R}$ with $\lim_{n\to\infty}|\lambda_n| = \infty$ such that*

$$D(A) = \left\{ x \in \mathcal{H} : \sum_{n=1}^{\infty} |\lambda_n|^2 \, |\langle e_n|x\rangle|^2 < \infty \right\}$$
$$Ax = \sum_{n=1}^{\infty} \lambda_n \langle e_n|x\rangle e_n.$$

Proof. Consider the bounded operator $R(\lambda, A) = (\lambda - A)^{-1}$. One can verify that its adjoint is given by $R(\overline{\lambda}, A^*) = R(\overline{\lambda}, A)$. It is easy to see that the resolvents at different values commute, in particular we have $R(\lambda, A)R(\overline{\lambda}, A) = R(\overline{\lambda}, A)R(\lambda, A)$. Hence, $R(\lambda, A)$ is a compact normal operator. By the spectral theorem for such operators (Theorem 2.3.5) there exists an orthonormal system $(e_n)_{n\in\mathbb{N}}$ of $\mathcal{H}$ and sequence $(\mu_n)_{n\in\mathbb{N}}$ with $\lim_{n\to\infty}\mu_n = 0$ such that

$$R(\lambda, A) = \sum_{n=1}^{\infty} \mu_n \langle e_n|x\rangle e_n.$$

Since $R(\lambda, A)$ is invertible, its kernel is trivial and therefore $(e_n)_{n\in\mathbb{N}}$ must be an orthonormal basis of $\mathcal{H}$. For $\lambda_n = \lambda - \mu_n^{-1}$ define the operator B as in the

assertion of the theorem, i.e.

$$D(B) = \left\{ x \in \mathcal{H} : \sum_{n=1}^{\infty} |\lambda_n|^2 \, |\langle e_n | x \rangle|^2 < \infty \right\}$$
$$Bx = \sum_{n=1}^{\infty} \lambda_n \langle e_n | x \rangle e_n.$$

Note that by definition of B we have $\lambda \in \rho(B)$ and $R(\lambda, A) = R(\lambda, B)$. In other words, $(\lambda - A)^{-1} = (\lambda - B)^{-1}$. Hence, $\lambda - A = \lambda - B$ as unbounded operators and therefore $A = B$. Further observe that since $A = B$ is self-adjoint, all eigenvalues λ_n of A must be real. Further $\lim_{n\to\infty} |\mu_n| = 0$ implies $\lim_{n\to\infty} |\lambda_n| = \infty$. □

We now give a physical example that illustrate the above methods. However, before we present a powerful characterization of compact subsets of L^p-spaces. Its proof uses a smooth approximation of the members of $\mathcal{F}$ for which the Arzelà–Ascoli theorem is applied.

Theorem 2.3.7 (Fréchet–Kolmogorov). *Let $n \in \mathbb{N}$, $p \in [1, \infty)$ and $\mathcal{F} \subset L^p(\mathbb{R}^n)$ be a bounded subset. Suppose that $\mathcal{F}$ satisfies*

$$\lim_{h\to 0} \int_{\mathbb{R}^n} |f(x+h) - f(x)|^p \, dx = 0 \qquad \text{uniformly on } \mathcal{F}.$$

Then the closure of $\mathcal{F}_{|\Omega}$ is compact in $L^p(\Omega)$ for any measurable subset $\Omega \subset \mathbb{R}^n$ of finite measure. Moreover $\overline{\mathcal{F}}$ is compact in $L^p(\mathbb{R}^n)$ if one additionally has

$$\lim_{r\to\infty} \int_{|x|\geq r} |f(x)|^p \, dx = 0 \qquad \text{uniformly on } \mathcal{F}.$$

Note that $\mathcal{F}_{|\Omega} = \{g \colon \Omega \to \mathbb{K} : g = f_{|\Omega} \text{ for some } f \in \mathcal{F}\}$. Further the first assumption can be rephrased as: for all $\varepsilon > 0$ there exists $\delta > 0$ such that $\int_{\mathbb{R}^n} |f(x+h) - f(x)|^p \, dx \leq \varepsilon$ for all $|h| \leq \delta$ and all $f \in \mathcal{F}$. An analogous version with quantifiers can be of course formulated for the second condition.

We now apply the Fréchet–Kolmogorov theorem to some basic examples and show its consequences for concrete quantum mechanical systems. We start with compact embeddings of Sobolev spaces.

Example 2.3.8 (Compact embedding of $H^1((a,b))$). Consider $\mathcal{F} = \overline{B}_R$, the closed ball of radius $R > 0$ in $H^1((a,b))$ for some $-\infty < a < b < \infty$. For $f \in \mathcal{F}$ define

$$\tilde{f}(x) = \begin{cases} (1 - (a-x))^2 f(a) & x \in [a-1, a] \\ f(x) & x \in (a,b) \\ (1-(x-b))^2 f(b) & x \in [b, b+1] \\ 0 & \text{else} \end{cases}.$$

We have $\tilde{f} \in H^1(\mathbb{R})$ for all $f \in \mathcal{F}$. Moreover, verify with the help of Remark 2.1.37 that there exists a universal constant $C > 0$ such that $\|\tilde{f}\|_{H^1(\mathbb{R})} \leq C\|f\|_{H^1((a,b))}$. We set $\tilde{\mathcal{F}} = \{\tilde{f} : f \in \mathcal{F}\}$. Note that $\tilde{\mathcal{F}}_{|(a,b)} = \mathcal{F}$. We now check that $\tilde{\mathcal{F}}$ satisfies the condition of the Fréchet–Kolmogorov theorem (Theorem 2.3.7). First assume that $f \in C^1(\mathbb{R}) \cap \tilde{\mathcal{F}}$. Then the Cauchy–Schwarz inequality implies

$$\begin{aligned} |f(x+h) - f(x)| &\leq \int_x^{x+h} |f'(y)|\,dy \leq |h|^{1/2} \left(\int_x^{x+h} |f'(y)|^2\,dy \right)^{1/2} \leq |h|^{1/2} \|f'\|_2^2 \\ &\leq |h|^{1/2} \|f\|_{H^1(\mathbb{R})}. \end{aligned}$$

Hence, for $|h| < 1$ we have

$$\int_{\mathbb{R}} |f(x+h) - f(x)|^2\,dx \leq \|f\|_{H^1(\mathbb{R})}^2 |h| \int_{a-2}^{b+2} dx \leq |h| \|f\|_{H^1(\mathbb{R})}^2 (b-a+4).$$

Now let $\tilde{f} \in \tilde{\mathcal{F}}$ be arbitrary. Then there exists a sequence $(f_n)_{n\in\mathbb{N}} \subset C^1(\mathbb{R}) \cap \tilde{\mathcal{F}}$ with $f_n \to \tilde{f} \in H^1(\mathbb{R})$. In particular we have

$$\begin{aligned} \|f_n(\cdot + h) - f_n - (\tilde{f}(\cdot + h) - \tilde{f})\|_2 &\leq \|(f_n - \tilde{f})(\cdot + h)\|_2 + \|f_n - \tilde{f}\|_2 \\ &= 2\|f_n - \tilde{f}\|_2 \xrightarrow[n\to\infty]{} 0. \end{aligned}$$

It then follows that

$$\begin{aligned} \int_{\mathbb{R}} |\tilde{f}(x+h) - \tilde{f}(x)|^2\,dx &= \lim_{n\to\infty} \int_{\mathbb{R}} |f_n(x+h) - f_n(x)|^2\,dx \\ &\leq |h|(b-a+4) \lim_{n\to\infty} \|f_n\|_{H^1(\mathbb{R})}^2 = |h|(b-a+4)\|f\|_{H^1(\mathbb{R})}^2 \\ &\leq C|h|(b-a+4)\|\tilde{f}\|_{H^1(a,b)}. \end{aligned}$$

From this inequality we immediately get that the left hand side converges uniformly to zero as $h \to 0$. This shows that the closure of bounded sets in $H^1((a,b))$ are compact subsets of $L^2((a,b))$. This result can also be rephrased in the following way: the natural inclusion

$$\iota\colon H^1((a,b)) \hookrightarrow L^2((a,b))$$

is a compact operator. Further note that similar arguments to Sobolev spaces of recantangles or higher dimensional bounded subsets of $\mathbb{R}^n$. The only difficulty that arises for more complicated sets is the fact that it is difficult to extend Sobolev functions to all of $\mathbb{R}^n$. In fact, this may not be possible if not the boundary of the set has some bad regularity.

Moreover, one can alternatively directly apply the Arzelà–Ascoli theorem to show the compactness if the embedding $\iota\colon H^1((a,b)) \hookrightarrow L^2((a,b))$. In fact,

the Arzelà–Ascoli theorem gives the stronger fact that the Sobolev embedding $H^1((a,b)) \hookrightarrow C([a,b])$ is compact.

We now apply the above embedding to a particle in an infinitely high square well.

Example 2.3.9 (Hamiltonian for an infinitely high square well). Consider an one-dimensional particle in an infinitely high square well, i.e. a particle subject to the potential

$$V(x) = \begin{cases} 0, & x \in [a,b] \\ \infty, & x \notin [a,b] \end{cases}$$

for some $-\infty < a < b < \infty$. Ignoring physical constants, the Hamiltonian of this system is a self-adjoint extension of $A = -\frac{d^2}{d^2x}$ with $D(A) = C_c^\infty((a,b))$ and the underlying Hilbert space $\mathcal{H} = L^2((a,b))$. The most common choice here is

$$\{f \in H^2((a,b)) : f(a) = f(b) = 0\},$$

for which we have already solved the eigenvalue problem in the physics parts of the lecture. We leave it to the reader the verify the self-adjointness of the operator with this domain. However, there are also other possbile self-adjoint extensions corresponding to different physics. Let $(B, D(B))$ be an arbitrary self-adjoint extension of A. Then we have $D(B) \subset H^2((a,b))$. In particular, we have

$$R(i,B)L^2((a,b)) \subset D(B) \subset H^2((a,b)) \subset H^1((a,b)).$$

and therefore $R(i,B)$ is compact as the composition of the bounded operator $R(i,B)\colon L^2((a,b)) \to H^1((a,b))$ and the compact operator $\iota\colon H^1((a,b)) \to L^2((a,b))$. Hence, it follows from Corollary 2.3.6 that $L^2((a,b))$ has an orthonormal basis consisting of eigenvectors of B.

It is interesting to compare this with the situation of a particle in a finitely high square well.

Remark 2.3.10 (Hamiltonian for a finitely high square well). In physics one usually considers the easiest case, i.e. the potential is constant outside the box and one therefore has

$$V(x) = \begin{cases} 0, & x \in [a,b] \\ V_0, & x \notin [a,b] \end{cases}$$

for some $V_0 > 0$. The Hamiltonian is then given as $\hat{H} = -\Delta + V$ with domain $H^2(\mathbb{R})$. Note that $H^2(\mathbb{R})$ is the natural domain of $-\Delta$, where $V(x)$ is a multiplication operator with a bounded function and therefore a bounded operator on $L^2(\mathbb{R})$. We will later see that the sum of a self-adjoint operator with a bounded

symmetric (and therefore self-adjoint) operator is always a self-adjoint operator with the domain of the unbounded self-adjoint operator. In contrast to the case of a subset of finite measure, $H^2(\mathbb{R})$ is not compactly embedded in $L^2(\mathbb{R})$. We therefore cannot deduce that $\hat{H}$ has an orthonormal basis of eigenvalues. In fact, it is well-known from physics that although there may exist some eigenvectors of $\hat{H}$ representing bounded states of the system whose energy is smaller than V_0, the other part of the spectrum corresponding to states whose energy is bigger than V_0 is continuous. Hence, as long as the energy is smaller than the potential barrier, the part of the spectrum looks like the spectrum for a constrained particle, whereas when the energy is bigger than the barrier, the part of the spectrum looks like the spectrum of a free particle. This situation is prototypical for systems with a potential.

Moreover, notice the following fun fact: when one ususally solves the above eigenvalue problem explicitly, one obtains three differential equations in the spatial regions $(-\infty, a)$, $[a, b]$ and (b, ∞) with solutions ψ_1, ψ_2 and ψ_3. One then usually argues with some (maybe mysterious) hand-waving that $\psi_1(a) = \psi_2(a)$ and $\psi_2(b) = \psi_3(b)$ and the same holds for the first derivatives. From a mathematical perspective this is very clear: The solution ψ must lie in $D(\hat{H}) = H^2(\mathbb{R}^n)$. By Sobolev embeddings a solution ψ of the eigenvalue problem must lie in $H^2(\mathbb{R}) \subset C^1(\mathbb{R})$. But ψ and its first derivative are continuous at a and b if and only if the above conditions are satisfied! However, the second derivative of an $H^2(\mathbb{R})$-function must not be continuous and therefore we do not require combability conditions such as $\psi_1''(a) = \psi_2''(a)$.

2.3.2 Trace Class Operators

The spectral theorem for compact self-adjoint operators also allows us to give sense to the definition of trace-class operators. Recall that there are two different types of states of a quantum mechanical systems: pure states which are often modeled as elements in the underlying Hilbert space and the more general mixed states which are thought of as (infinite) convex combinations of pure states. Mixed states are modeled as trace class operators with trace equal to one. With this motivation in our minds we now define trace class operators. We only deal with the infinite dimensional case. The obvious modifications for the finite dimensional case are left to the reader. Note that if A is a compact linear operator, the compact operator A^*A has an orthonormal basis of eigenvectors $(e_n)_{n\in\mathbb{N}}$ by the spectral theorem (Theorem 2.3.5). Moreover, each eigenvalue λ_n is non-negative. This allows us to define the bounded operator

$$(A^*A)^{1/2}x = \sum_{n=1}^{\infty} \sqrt{\lambda_n}\langle e_n|x\rangle e_n.$$

This is a particular easy instance of the so-called functional calculus for (unbounded) self-adjoint operators studied in the next section.

Definition 2.3.11 (Trace class operator). Let $\mathcal{H}$ be a separable Hilbert space of infinite dimension. An operator $A \in \mathcal{K}(\mathcal{H})$ is called *trace class* if for one (equiv. all) orthonormal bases $(e_n)_{n\in\mathbb{N}}$ of $\mathcal{H}$

$$\|A\|_1 := \sum_{n=1}^{\infty} \left\langle (A^*A)^{1/2} e_n \,\middle|\, e_n \right\rangle < \infty.$$

In this case the sum

$$\operatorname{Tr} A := \sum_{n=1}^{\infty} \langle Ae_n | e_n \rangle$$

is independent of the orthonormal basis and called the *trace* of A.

One can show that the space of trace class operators endowed with the norm $\|\cdot\|_1$ is a Banach space in which the finite rank operators are dense.

Note that every linear operator on a finite dimensional Hilbert space is trace class and its trace coincides with the usual trace for matrices. Using the general functional calculus for self-adjoint operators, we will soon see that we can give sense to the square of A^*A for arbitrary bounded operators. One can then define trace class operators without assuming the compactness of A. Nevertheless one obtains the same class of operators as one can show that trace class implies compactness. Moreover, observe that if a trace-class operator A has a basis of eigenvectors $(e_n)_{n\in\mathbb{N}}$ with corresponding eigenvalues $(\lambda_n)_{n\in\mathbb{N}}$, we obtain

$$\operatorname{Tr} A = \sum_{n=1}^{\infty} \langle Ae_n | e_n \rangle = \sum_{n=1}^{\infty} \lambda_n.$$

Note that it makes no sense to consider unbounded operators in connection with the trace. Even if an unbounded operator A has an orthonormal basis of eigenvectors, the associated eigenvalues are not summable unless they are bounded (they must even form a zero sequence) and therefore define a bounded (even compact) operator.

One now can precisely define a *mixed state* as a positive trace class operator $\rho \in \mathcal{K}(\mathcal{H})$ with $\operatorname{Tr}\rho = 1$. Here positive means that ρ is self-adjoint and all eigenvalues of ρ are non-negative. It follows from the spectral theorem for compact self-adjoint operators (Theorem 2.3.5) that there exists an orthonormal basis $(\psi_n)_{n\in\mathbb{N}}$ of eigenvectors with eigenvalues $p_n \geq 0$ such that $\rho(\varphi) = \sum_{n=1}^{\infty} p_n \langle \psi_n | \varphi \rangle \psi_n$ for all $\varphi \in \mathcal{H}$. Hence,

$$\operatorname{Tr}\rho = \sum_{n=1}^{\infty} p_n = 1.$$

The state ρ can be interpreted as a discrete probability distribution: the system is in the state ψ_n with probability p_n. Such a situation arises naturally when one considers an entangled state ψ on a composite system described by a tensor product $\mathcal{H}_1 \otimes \mathcal{H}_2$ for which only the information on H_1 is accessbile to the observer due to some limitations. Alternatively, one works with mixed states if the system under consideration has an uncertain probabilistic preparation history, for example if you measure the unpolarized light emitted by a light bulb. In physics ρ is also often called a *density matrix* or *density operator*.

Recall that a pure state $|\psi\rangle \in \mathcal{H}$ can be represented as the density matrix

$$\rho = |\psi\rangle\langle\psi|,$$

i.e. as the one-dimensional projection onto the span of $|\psi\rangle$ (provided $|\psi\rangle$ is normalized).

Remark 2.3.12. Please be careful: there are two different notions in quantum mechanics related with probabilistic measurements. Let us illustrate the two concepts in a two-dimensional Hilbert space $\mathbb{C}^2$ with *pure* states $\psi_1 = (1,0)^T$ and $\psi_2 = (0,1)^T$ which are both eigenvalues for the observable $\hat{H} = \mathrm{diag}(1,2)$. Both states are eigenstates for $\mathcal{H}$ and therefore have a certain measurement outcome, namely 1 for ψ_1 and 2 for ψ_2. Now consider the superposition

$$\psi = \frac{1}{\sqrt{2}}(\psi_1 + \psi_2).$$

This is again a *pure* state. Measuring the observable $\hat{H}$, we will obtain both outcomes 1 and 2 with probability equal to 1. Nevertheless we will know for sure that the system is in the state ψ. Now consider the density matrix

$$\rho = \frac{1}{2}(\psi_1\psi_1^T + \psi_2\psi_2^T) = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}.$$

Now measuring $\hat{H}$ gives

$$\mathrm{Tr}(\rho\hat{H}) = \frac{1}{2}(1+2) = \frac{3}{2}.$$

This time ρ models a mixed state which is in state ψ_1 and in state ψ_2 with chances equal to 1/2 each, i.e. a *statistical* mixture of both states. In contrast, the state ψ zero probability to be in one of the states ψ_1 and ψ_2, it is definitely in the state ψ. The measurement of $\rho\hat{H}$ gives the expectation value of the measurement outcome of $\hat{H}$ of such an ensemble.

The difference of $|\psi\rangle\langle\psi|$ and ρ may be seen experimentally if one takes the measurement of some non-commuting observable. In fact, consider the observable

$$\hat{I} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

The operator $\hat{I}$ has the eigenvalues 1 and -1 with normalized eigenvectors

$$\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} = \psi = \frac{1}{\sqrt{2}}(\psi_1 + \psi_2) \qquad \text{and} \qquad \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} = \frac{1}{\sqrt{2}}(\psi_1 - \psi_2).$$

If one considers the pure state $|\psi\rangle\langle\psi|$ the measurement outcome for $\hat{I}$ is equal to 1 with probability 1. If one however considers the mixed state ρ, one has a 50% chance to be in the states ψ_1 or ψ_2. For both states one has a 50% chance to obtain the measurement outcome 1 for $\hat{I}$, e.g. for ψ_1 one calculates the square of the norm of

$$(|\psi\rangle\langle\psi|)(\psi_1) = \frac{1}{2}\begin{pmatrix}1 & 1\\1 & 1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1\\1\end{pmatrix}.$$

as being equal to 1/2. Altogether for the mixed state ρ we have a 50% chance to measure 1 for $\hat{I}$ in contrast to the pure state $|\psi\rangle\langle\psi|$.

Remark 2.3.13. If you still feel unsure about pure and mixed states, the following analogy to classical mechanics may help: in classical mechanics the state of a system (say particle) is determined by its coordinate in the phase space, e.g. by its position and momentum, whereas in analogy a quantum mechanical systems is determined by its state $\psi \in \mathcal{H}$. The time evolution of these states is then governed by the Hamiltonian respectively Schrödinger equations. In practice, one however often has to work with huge ensembles of individual particles. In classical mechanics this is usually seen as a collection of individual systems in different states and modelled via a probability distribution over the phase space. The quantum mechanical analogue for such ensembles are mixed states which are represented by densities operators.

Remark 2.3.14. It may seem unsatisfactory to only allow discrete probability distributions for density matrices. This is what is usually done in most introductory texts for quantum mechanics and allows the description of most physical phenomena. Ultimately one can generalize the algebras of observables from Hilbert space operators to abstract operator algebras such as C^*- and von Neumann algebras. In this context one also obtains a general concept of pure and mixed states. This is the so called *algebraic* formulation of quantum mechanics. The introduction of abstract algebras is motivated by the by now mostly accepted fact that not all self-adjoint operators can indeed be realized as physical observables. Moreover, the algebraic approach has become a very useful tool in the study of quantum systems with infinite degree of freedoms, for example in quantum statistical mechanics and quantum field theory.

We now state some basic properties of trace class operators which are commonly used in practice.

Proposition 2.3.15 (Properties of trace class operators). *Let $\mathcal{H}$ be a (separable) Hilbert space. The trace class operators have the following properties.*

(a) *They form a subspace of $\mathcal{B}(H)$ and the composition of a bounded and a trace class operator is again trace class.*

(b) *The trace mapping from the trace class operators is linear and satisfies*

$$\mathrm{Tr}(ST) = \mathrm{Tr}(TS)$$

for all $S \in \mathcal{B}(\mathcal{H})$ and all trace class operators T.

2.3.3 The Spectral Theorem for Unbounded Self-Adjoint Operators

We now come to one of the central results of this lecture, the spectral theorem for unbounded self-adjoint operators. We will motivate and give two different equivalent formulations of the spectral theorem. For the first version observe that the spectral theorem for a compact self-adjoint operator T on an infinite-dimensional separable Hilbert space (Theorem 2.3.5) can be reformulated as follows. Let $(\lambda_n)_{n\in\mathbb{N}}$ be the sequence of eigenvalues with respect to the orthonormal basis of eigenvectors $(e_n)_{n\in\mathbb{N}}$ given by the spectral theorem. Define the multiplication operator

$$\begin{aligned} M\colon \ell^2(\mathbb{N}) &\to \ell^2(\mathbb{N}) \\ (x_n)_{n\in\mathbb{N}} &\mapsto (\lambda_n x_n)_{n\in\mathbb{N}} \end{aligned}$$

Then the spectral theorem says that T is unitarily equivalent to M, i.e. $T = U^{-1}MU$ for $U\colon x \mapsto (\langle e_n|x\rangle)_{n\in\mathbb{N}}$. For general self-adjoint operators this cannot remain true as stated above, however it holds true if one allows different L^2-spaces than $\ell^2(\mathbb{N})$. This is the following multiplicative version of the spectral theorem.

Theorem 2.3.16 (Spectral theorem for self-adjoint operators – multiplicative version). *Let $(A, D(A))$ be a self-adjoint operator on some Hilbert space $\mathcal{H}$. Then there exists a measure space (Ω, Σ, μ) (σ-finite if $\mathcal{H}$ is separable), a measurable function $m\colon \Omega \to \mathbb{C}$ and a unitary operator $U\colon \mathcal{H} \to L^2(\Omega, \Sigma, \mu)$ such that*

(a) *$x \in D(T)$ if and only if $m \cdot Ux \in L^2(\Omega, \Sigma, \mu)$*

(b) *$UTU^{-1}f = m \cdot f$ for all $f \in D(M_m) = \{f \in L^2(\Omega, \Sigma, \mu) : mf \in L^2(\Omega, \Sigma, \mu)\}$.*

Recall that we have seen in Example 2.2.28 that M_m with the above domain is a self-adjoint operator. The spectral theorem shows that up to unitary equivalence every self-adjoint operator is of this form. The spectral theorem is

usually first proved for bounded normal operators. The case of an unbounded self-adjoint operator A is then reduced to the bounded normal case via the Cayley transform of A. However, we do not want to delve into the details and refer to the literature instead. Instead, we present an example.

Example 2.3.17 (The spectral theorem for $-\Delta$). We have seen that $-\Delta$ with domain $H^2(\mathbb{R}^n)$ is a self-adjoint operator in Example 2.2.30. As exploited in the argument for its self-adjointness, $-\Delta$ is equivalent to the multiplication operator M_m on $L^2(\mathbb{R}^n)$ with $m(x) = |x|^2$ via the unitary operator given by the Fourier transform $\mathcal{F}\colon L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$.

Note that the spectral theorem allows one to define a functional calculus for self-adjoint operators. In fact, if A is a self-adjoint operator and $f\colon \sigma(A) \to \mathbb{C}$ is a measurable function, we may define the closed operator

$$f(A)x = U^{-1}(f(m)\cdot Ux) \qquad \text{with } D(A) = \{x \in \mathcal{H} : f(m)\cdot Ux \in L^2(\Omega, \Sigma, \mu)\}.$$

We will discuss this functional calculus in more detail soon when considering the other variant of the spectral theorem via spectral measures.

Before given the exact definition of such measures, let us again motivative this version of the spectral theorem. Let A be a self-adjoint operator on $\mathbb{C}^n$. Let $P_1, \dots, P_k$ denote the orthogonal projections onto the pairwise orthogonal eigenspaces of A for the eigenvalues $\lambda_1, \dots, \lambda_k$. Since by the spectral theorem these eigenspaces span the complete space $\mathbb{C}^n$, we obtain

$$A = A\cdot I = A\left(\sum_{l=1}^{k} \lambda_l P_l\right) = \sum_{l=1}^{k} \lambda_l P_l.$$

Hence, A can be decomposed as the sum of the orthogonal projections onto its eigenspaces. The natural generalization of the family $(P_1, \dots, P_k)$ is the concept of a projection-valued measure.

Definition 2.3.18 (Projection-valued measure). Let $\mathcal{H}$ be a Hilbert space. A *projection-valued measure* on $\mathbb{R}$ is a mapping $P\colon \mathcal{B}(\mathbb{R}) \to \mathcal{B}(\mathcal{H})$ satisfying the following properties.

(i) For every $\Omega \in \mathcal{B}(\mathbb{R})$ the operator $P(\Omega)$ is an orthogonal projection;

(ii) $P(\emptyset) = 0$ and $P(\mathbb{R}) = \mathrm{Id}$;

(iii) For $(\Omega_n)_{n\in\mathbb{N}} \subset \mathcal{B}(\mathbb{R})$ pairwise disjoint one has

$$P\left(\bigcup_{n\in\mathbb{N}} \Omega_n\right)x = \lim_{N\to\infty} \sum_{n=1}^{N} P(\Omega_n)x \qquad \text{for all } x \in \mathcal{H}.$$

The last property in the definition is called the *strong continuity* of P. Of course, analogously one can define a projection-valued measure on $\mathbb{R}^n$. One can deduce from the above properties the non-trivial fact that

$$P(\Omega_1)P(\Omega_2) = P(\Omega_1 \cap \Omega_2) \qquad \text{for all } \Omega_1, \Omega_2 \in \mathcal{B}(\mathbb{R}).$$

First observe that for $\Omega_1, \Omega_2 \in \mathcal{B}(\mathbb{R})$ we have

$$\begin{aligned} P(\Omega_1 \cap \Omega_2) + P(\Omega_1 \cup \Omega_2) &= P(\Omega_1 \cap \Omega_2) + P(\Omega_1 \cup (\Omega_2 \setminus (\Omega_1 \cap \Omega_2)) \\ &= P(\Omega_1 \cap \Omega_2) + P(\Omega_1) + P(\Omega_2 \setminus (\Omega_1 \cap \Omega_2)) \\ &= P(\Omega_1 \cap \Omega_2) + P(\Omega_1) + P(\Omega_2) - P(\Omega_1 \cap \Omega_2) \\ &= P(\Omega_1) + P(\Omega_2). \end{aligned}$$

Now, if Ω_1 and Ω_2 are disjoint, we obtain by taking squares in the last equation

$$\begin{aligned} P(\Omega_1 \cup \Omega_2) = P^2(\Omega_1 \cup \Omega_2) &= (P(\Omega_1) + P(\Omega_2))^2 \\ &= P(\Omega_1) + P(\Omega_2) + P(\Omega_1)P(\Omega_2) + P(\Omega_2)P(\Omega_1) \\ &= P(\Omega_1 \cap \Omega_2) + P(\Omega_1)P(\Omega_2) + P(\Omega_2)P(\Omega_1). \end{aligned}$$

This shows that

$$P(\Omega_1)P(\Omega_2) + P(\Omega_2)P(\Omega_1) = 0.$$

Multiplying both sides of the equation with $P(\Omega_2)$ from the right we see that $P(\Omega_1)P(\Omega_2) = -P(\Omega_2)P(\Omega_1)P(\Omega_2)$, which is self-adjoint (an orthogonal projection satisfies $P = P^*$). This shows that

$$P(\Omega_1)P(\Omega_2) = (P(\Omega_1)P(\Omega_2))^* = P(\Omega_2)P(\Omega_1) = 0.$$

Now, for the general case we obtain as desired

$$\begin{aligned} P(\Omega_1)P(\Omega_2) &= (P(\Omega_1 \setminus \Omega_2) + P(\Omega_1 \cap \Omega_2))(P(\Omega_2 \setminus \Omega_1) + P(\Omega_1 \cap \Omega_2)) \\ &= P^2(\Omega_1 \cap \Omega_2) = P(\Omega_1 \cap \Omega_2). \end{aligned}$$

Further we leave it as an exercise to the reader that a projection-valued measure is monotone in the sense that $\Omega_1 \subset \Omega_2$ for two Borel sets implies $\langle P(\Omega_1)x|x\rangle \leq \langle P(\Omega_2)x|x\rangle$ for all $x \in \mathcal{H}$. In particular $P(\Omega_2) = 0$ implies $P(\Omega_1) = 0$ for $\Omega_1 \subset \Omega_2$.

To a projection-valued measure P on $\mathbb{R}$ there corresponds a projection-valued function $\lambda \mapsto P_\lambda = P((-\infty, \lambda))$, a so called *projection-valued resolution of the identity*. This function is characterized by the following properties.

(a) $P_\lambda P_\mu = P_{\min\{\lambda,\mu\}}$ for all $\lambda, \mu \in \mathbb{R}$;

(b) $\lim_{\lambda\to-\infty} P_\lambda x = 0$ and $\lim_{\lambda\to\infty} P_\lambda x = x$ for all $x \in \mathcal{H}$;

(c) $\lim_{\mu\uparrow\lambda} P_\mu x = P_\lambda x$ for all $x \in \mathcal{H}$.

Note that the above properties imply that for all $x \in \mathcal{H}$ the resolution of the function $\lambda \mapsto \langle x|P_\lambda x\rangle$ is a distribution function of the bounded measure $\Omega \mapsto \langle x|P(\Omega)x\rangle$. If $\|x\| = 1$, this is a distribution function of a probability measure. Conversely, a standard result from measure and probability theory says that for every bounded distribution function there exist a unique bounded measure with the given distribution function. This allows one to recover the spectral measure P from its set of distribution functions $\lambda \mapsto \langle x|P_\lambda x\rangle$ for $x \in \mathcal{H}$. For general $x, y \in \mathcal{H}$ we moreover obtain (complex-valued!) measures related to the just considered distribution functions via the polarization identity by

$$\langle y|P(\Omega)x\rangle = \frac{1}{4}\sum_{k=1}^{4} i^k \langle x + i^k y|P(\Omega)(x + i^k y)\rangle$$

for $\Omega \in \mathcal{B}(\mathbb{R})$.

Note that for $x \in \mathcal{H}$ the map $\Omega \mapsto \langle x|P(\Omega)x\rangle$ defines a Borel measure in the usual sense of measure theory because of

$$\langle x|P(\Omega)x\rangle = \langle x|P^2(\Omega)x\rangle = \langle P(\Omega)x|P(\Omega)x\rangle \geq 0 \qquad \text{for all } x \in \mathcal{H}.$$

Hence, we can apply the usual theory of Lebesuge integration to these measures. In particular, a measurable function $f\colon \mathbb{R} \to \mathbb{K}$ is said to be finite almost everywhere with respect to P if it is finite almost everywhere with respect to all measures $\langle x|Px\rangle$ for $x \in \mathcal{H}$.

We now can state the spectral theorem in its version for projection-valued measures and its various consequences. To motivate the domains involved below, consider a step function $f = \sum_{k=1}^{n} a_k \mathbb{1}_{\Omega_k}$ for some pairwise disjoint $\Omega_k \in \mathcal{B}(\mathbb{R})$ and $a_k \in \mathbb{C}$. Then as for the usual Lebesgue integral we can directly define the bounded operator

$$\int_{\mathbb{R}} f(\lambda)\, dP(\lambda) := \sum_{k=1}^{n} a_k P(\Omega_k).$$

Note that for the value of the norm of this operator evaluated at some $x \in \mathcal{H}$ we obtain

$$\begin{aligned}
\left\| \int_{\mathbb{R}} f(\lambda)\, dP(\lambda) x \right\|^2 &= \left\langle \sum_{k=1}^{n} a_k P(\Omega_k)x \middle| \sum_{l=1}^{n} a_l P(\Omega_l)x \right\rangle \\
&= \sum_{k=1}^{n}\sum_{l=1}^{n} \overline{a_k} a_l \langle P(\Omega_k)x|P(\Omega_l)x\rangle = \sum_{k=1}^{n}\sum_{l=1}^{n} \overline{a_k} a_k \langle x|P(\Omega_k)P(\Omega_l)x\rangle \\
&= \sum_{k=1}^{n}\sum_{l=1}^{n} \overline{a_k} a_k \langle x|P(\Omega_k \cap \Omega_l)x\rangle = \sum_{k=1}^{n} |a_k|^2 \langle x|P(\Omega_k)x\rangle
\end{aligned}$$

$$= \int_{\mathbb{R}} |f(\lambda)|^2 \, d\langle x|P(\lambda)x\rangle.$$

The above isometry allows one to extend the integral on the left hand side pointwise for a given $x \in \mathcal{H}$ for all measurable functions $f : \mathbb{R} \to \mathbb{C}$ which are square-integrable with respect to the measure $\Omega \mapsto \langle x|P(\Omega)x\rangle = \|P(\Omega)x\|^2$ via a limiting argument. Moreover, this calculation together with the Cauchy Schwarz inequality also shows the less exact inequality

$$\left| \int_{\mathbb{R}} f(\lambda) \, d\langle y|P(\lambda)x\rangle \right| \leq \|f\|_\infty \|x\| \|y\|$$

for all $x, y \in \mathcal{H}$ which is fundamental for the bounded functional calculus of A. However, in order to avoid dealing with such operator-valued integrals we will work with the measures $\Omega \mapsto \langle y|P(\Omega)x\rangle$ instead.

Theorem 2.3.19 (Spectral theorem for self-adjoint operators – version with projection-valued measures). *For every self-adjoint operator $(A, D(A))$ on some Hilbert space $\mathcal{H}$ there exists a unique projection-valued measure P with the following properties.*

(a) *We have*

$$D(A) = \left\{ x \in \mathcal{H} : \int_{\mathbb{R}} \lambda^2 \, d\langle x|P(\lambda)x\rangle < \infty \right\}$$

and for every $x \in D(A)$ and $y \in \mathcal{H}$ we have

$$\langle y|Ax\rangle = \int_{\mathbb{R}} \lambda \, d\langle y|P(\lambda)x\rangle.$$

Further, for the spectrum we have

$$\lambda \in \sigma(A) \qquad \Leftrightarrow \qquad P((\lambda - \varepsilon, \lambda + \varepsilon)) \neq 0 \quad \text{for all } \varepsilon > 0.$$

(b) *Let $f : \mathbb{R} \to \mathbb{C}$ be measurable and finite almost everywhere with repsect to P. Then one obtains a densely defined linear operator $f(A)$ with*

$$D(f(A)) = \left\{ x \in \mathcal{H} : \int_{\mathbb{R}} |f(\lambda)|^2 \, d\langle x|P(\lambda)x\rangle < \infty \right\}$$

which is defined for $x \in D(f(A))$ and $y \in \mathcal{H}$ by

$$\langle y|f(A)x\rangle = \int_{\mathbb{R}} f(\lambda) \, d\langle y|P(\lambda)x\rangle.$$

Moreover, the correspondence $f \mapsto f(A)$ has the following properties: one has $f(A)^* = \overline{f}(A)$ and $f(A)$ is bounded if and only if f is bounded on $\sigma(A)$. Further, $f \mapsto f(A)$ is an algebra homomorphism from the space of bounded measurable functions on $\mathbb{R}$ to $\mathcal{B}(\mathcal{H})$.

Let us now give some examples of projection-valued measures and the associated functional calculus.

Example 2.3.20 (The PVM for the position operator). Let $\mathcal{H} = L^2(\mathbb{R})$ and for $\Omega \in \mathcal{B}(\mathbb{R})$ let $P(\Omega)u = \mathbb{1}_\Omega u$ for all $u \in L^2(\mathbb{R})$. We leave it to the reader to verify that P is a projection-valued measure (for the third property use the dominated convergence theorem). We have for all $u, w \in L^2(\mathbb{R})$ and $\Omega \in \mathcal{B}(\mathbb{R})$

$$\langle u|P(\Omega)w\rangle = \int_{\mathbb{R}} \overline{u(x)}\mathbb{1}_\Omega(x)w(x)\,dx = \int_\Omega \overline{u(x)}w(x)\,dx.$$

Hence, the measure is given by the density $\overline{u}w$. For the integral over the projection-valued measure we obtain for a bounded measurable function $f\colon \mathbb{R} \to \mathbb{C}$ that (if you do not know this identity check its validity first for simple functions and then write a general function as the monotone limit of step functions and use the monotone convergence theorem; you can take the more general arguments in the next example as a guidline)

$$\int_{\mathbb{R}} f(\lambda)\,d\langle u|P(\lambda)w\rangle = \int_{\mathbb{R}} f(x)\overline{u(x)}w(x)\,dx.$$

This is exactly $\langle u|T_f w\rangle$, where $T_f w = f \cdot w$, i.e. T_f acts as multiplication with f. It now follows, for example by comparing resolvents or carefully repeating the above argument for unbounded functions, that P is the resolution of the identity for the position operator on $\mathbb{R}$.

Example 2.3.21 (PVMs for multipliers). Let (X, Σ, μ) be a measure space and $m\colon X \to \mathbb{R}$ a measurable function. We have already seen that we have a functional calculus for the self-adjoint multiplication operator M_m: to a bounded measurable function $f\colon \mathbb{R} \to \mathbb{R}$ it associates the bounded operator $f(M_m)u = f \circ m \cdot u$. In particular, if $\Omega \in \mathcal{B}(\mathbb{R})$, we obtain the orthogornal projection $\mathbb{1}_\Omega u = \mathbb{1}_\Omega \circ m \cdot u = \mathbb{1}_{m^{-1}(\Omega)}u$. We therefore expect that the family of these projections is the projection-valued measure for M_m. Let us verify this explicitly.

Hence, generalizing the previous example, for $\Omega \in \mathcal{B}(\mathbb{R})$ we let $P(\Omega)u = \mathbb{1}_{m^{-1}(\Omega)}u$ for $u \in L^2(X, \Sigma, \mu)$. With the same arguments as in the previous example one can directly verify that P is a projection-valued measure on $L^2(X, \Sigma, \mu)$. Now, let $u = \mathbb{1}_A$ and $w = \mathbb{1}_B$ for some $A, B \in \Sigma$ and $\Omega \in \mathcal{B}(\mathbb{R})$. Then

$$\langle u|P(\Omega)w\rangle = \int_X \mathbb{1}_A(x)\mathbb{1}_B(x)\mathbb{1}_{m^{-1}(\Omega)}(x)\,d\mu(x) = \mu(A \cap B \cap m^{-1}(\Omega)).$$

Now, if $f = \sum_{k=1}^n a_k \mathbb{1}_{\Omega_k}$ for some $a_k \geq$ and disjoint $\Omega_k \in \mathcal{B}(\mathbb{R})$ is a step function, we obtain

$$\int_{\mathbb{R}} f(\lambda)\,d\langle u|P(\lambda)w\rangle = \sum_{k=1}^n a_k \langle u|P(\Omega_k)u\rangle = \sum_{k=1}^n a_k \mu(A \cap B \cap m^{-1}(\Omega_k))$$

$$= \int_{A\cap B} \sum_{k=1}^{n} a_k \mathbb{1}_{m^{-1}(\Omega_k)}\, d\mu = \int_{A\cap B} \sum_{k=1}^{n} a_k \mathbb{1}_{\Omega_k} \circ m\, d\mu = \int_{A\cap B} f\circ m\, d\mu$$
$$= \int_X \mathbb{1}_{A\cap B} f\circ m\, d\mu = \int_X \overline{\mathbb{1}_A}\mathbb{1}_B f\circ m\, d\mu.$$

Using the monotone convergence theorem we see that the above identity extends to all positive functions $f\colon \mathbb{R}\to\mathbb{R}$. By linearity one then can pass to all functions which are integrable with respect to the measure $\Omega\mapsto\langle u|P(\Omega)w\rangle$. In particular, the identity holds for all bounded functions if A and B have finite measure. Since both sides of the equality are sesquilinear, the identity therefore holds for all integrable step functions u and w and all bounded f. Since the step functions are dense in $L^2(X,\Sigma,\mu)$, the identity extends to all square integrable functions u and w. Written this out, we have for all $u,w\in L^2(X,\Sigma,\mu)$ and all measurable bounded $f\colon\mathbb{R}\to\mathbb{R}$ that

$$\int_{\mathbb{R}} f(\lambda)\, d\langle u|P(\lambda)w\rangle = \int_X \overline{u}wf\circ m\, d\mu = \langle u|M_{f\circ m}w\rangle_{L^2(X,\Sigma,\mu)}.$$

Again, by comparing resolvents, we see that P is the projection valued measure associated to the multiplication operator M_m on $L^2(X,\Sigma,\mu)$.

In fact, notice that this example actually gives a proof of the spectral theorem in the version with projection-valued measures based on the multiplicative version of the spectral theorem. In fact, one can verify that one version of the spectral theorem implies the other. The arguments for the converse implication can be found in [Tes12, Lemma 3.3 and following results].

Example 2.3.22 (PVM for orthonormal bases of eigenvectors). Let $(A,D(A))$ be a self-adjoint operator on a separable infinite-dimensional Hilbert space and $(e_n)_{n\in\mathbb{N}}$ an orthonormal basis of eigenvectors for A for the real eigenvalues $(\lambda_n)_{n\in\mathbb{N}}$. For $\Omega\in\mathcal{B}(\mathbb{R})$ we define

$$P(\Omega) = \sum_{n:\lambda_n\in\Omega} |e_n\rangle\langle e_n|.$$

Then $P(\Omega)$ is the orthogonal projection onto the span of the eigenspaces for the eigenvalues which lie in Ω. Moreover, P is a projection-valued measure. In fact, after an unitary transformation this example is again a special case of the previous one. Nevertheless let us verify directly the required properties. In fact, everything is clear except for the σ-additivity. For this note that one a direct decomposition

$$\mathcal{H} = \bigoplus_k \mathcal{H}_k,$$

where $\mathcal{H}_k$ are the pairwise orthogonal eigenspaces for the different eigenvalues λ_k of A. Let P_k be the orthogonal projection onto $\mathcal{H}_k$. Then $P_k = \sum_{n:\lambda_n=\lambda_k} |e_n\rangle\langle e_n|$. It follows from orthogonality that

$$\|x\|^2 = \sum_k \|P_k x\|^2 \qquad \text{for all } x \in \mathcal{H}. \tag{2.2}$$

Now, let $(\Omega_n)_{n\in\mathbb{N}} \subset \mathcal{B}(\mathbb{R})$ be pairwise disjoint. Then we have for $x \in \mathcal{H}$

$$\begin{aligned}\left\|\sum_{n=1}^{N} P(\Omega_n)x - P(\cup_{n\in\mathbb{N}}\Omega_n)x\right\|^2 &= \left\|\sum_{k:\lambda_k\in\cup_{n=1}^{N}\Omega_n} P_k x - \sum_{k:\lambda_k\in\cup_{n=1}^{\infty}\Omega_n} P_k x\right\|^2 \\ &= \left\|\sum_{k:\lambda_k\in\cup_{n=N+1}^{\infty}} P_k x\right\|^2 = \sum_{k:\lambda_k\in\cup_{n=N+1}^{\infty}} \|P_k x\|^2 \xrightarrow[N\to\infty]{} 0.\end{aligned}$$

because of the absolute square-summability of (2.2). We leave it to the reader to work out the concrete representation of the functional calculus for P. For example by comparing resolvents, one then can see that P is the projection-valued measure for A.

2.3.4 Measurement in Quantum Mechanics

The spectral theorem allows us to model quantum mechanical measurements in a mathematically exact way. From an abstract point of view a physical theory (for example classical mechanics or quantum mechanics) is described by a set of observables $\mathcal{A}$ and a set of states $\mathcal{S}$ in which the physical system can be. A process of measurement is then the assignment $\mathcal{A}\times\mathcal{S} \ni (A,\rho) \mapsto \mu_A$, where μ_A is a probability measure on $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$. For every Borel set $\Omega \subset \mathbb{R}$ the value $\mu_A(\Omega)$ is then the probability that for a system in the state ρ the result of a measurement of the observable A belongs to Ω.

The Born–von Neumann formula We have seen that for *quantum mechanics* $\mathcal{S}$ is the set of all trace class operators on some fixed (separable) Hilbert space $\mathcal{H}$ and $\mathcal{A}$ is the set of all self-adjoint operators on $\mathcal{H}$. Let P_A be the projection-valued measure of A. Then μ_A is given by the *Born–von Neumann formula*

$$\mu_A(\Omega) = \operatorname{Tr} P_A(\Omega)\rho \qquad \text{for } \Omega \in \mathcal{B}(\mathbb{R}).$$

Note that the trace is well-defined because $P_A(E)\rho$ is trace class as the composition of a bounded and a trace class operator. However, one still has to check that μ_A is a probability measure. The only non-trivial fact is the σ-additivity of μ_A. For this let $(\Omega_k)_{k\in\mathbb{N}}$ be pairwise disjoint. Then for an orthonormal basis

$(e_n)_{n\in\mathbb{N}}$

$$\sum_{k=1}^{N} \mu_A(\Omega_k) = \mathrm{Tr}(P_A(\cup_{k=1}^{N}\Omega_k)\rho) = \sum_{n=1}^{\infty} \langle e_n | P_A(\cup_{k=1}^{n}\Omega_k)\rho e_n\rangle.$$

Note that for all $n \in \mathbb{N}$ the sequence $P_A(\cup_{k=1}^{N}\Omega_k)e_n$ converges to $P_A(\cup_{k\in\mathbb{N}}\Omega_k)e_n$ by the properties of a projection-valued measure. Since moreover the n-th summand is dominated by $\langle e_n|\rho e_n\rangle$ which is summable because ρ is trace class, the series converges to $\mathrm{Tr}(P_A(\cup_{k\in\mathbb{N}}\Omega_k)\rho)$ by the dominated convergence theorem.

Further, the expectation value of the observable A in the state ρ is (provided it exists)

$$\langle A\rangle_\rho = \int_{\mathbb{R}} \lambda \, d\mu_A(\lambda).$$

Some useful results We now state some useful related results without proofs which are often used in physics. The first result can be verified by simply checking the definitions and shows that under mild assumptions the expectation value of a state can be calculated as shown in the physics part of the lecture.

Proposition 2.3.23. *Let A be an observable and ρ a state such that $\langle A\rangle_\rho$ exists (as finite value) and $\mathrm{Im}\,\rho \subset D(A)$. Then $A\rho$ is trace class and*

$$\langle A\rangle_\rho = \mathrm{Tr}(A\rho).$$

In particular, if $\rho = |\psi\rangle\langle\psi|$ is a pure state and $\psi \in D(A)$, then

$$\langle A\rangle_\rho = \langle A\psi|\psi\rangle \qquad \text{and} \qquad \langle A^2\rangle_\rho = \|A\psi\|^2.$$

We now come to the simultaneous measurement of severable observables. We already know from physics that this is only possible if the observables commute. Note that it is not clear what we mean with commuting observables in the unbounded case. The spectral theorem helps us here again.

Definition 2.3.24. We say that two self-adjoint operators A and B commute if the corresponding projection-valued measures P_A and P_B commute, i.e.

$$P_A(\Omega_1)P_B(\Omega_2) = P_B(\Omega_2)P_A(\Omega_1) \qquad \text{for all } \Omega_1, \Omega_2 \in \mathcal{B}(\mathbb{R}).$$

One can show that the above definition is equivalent to the fact that the resolvents of A and B commute, i.e. one has $R(\lambda, A)R(\mu, B) = R(\mu, B)R(\lambda, A)$ for all $\lambda, \mu \in \mathbb{C}\setminus\mathbb{R}$. For commuting observables one has the following generalization of the spectral theorem.

Proposition 2.3.25. *Let $A_1,\dots,A_n$ be finitely many pairwise commuting self-adjoint operators on some Hilbert space $\mathcal{H}$. Then there exists a unique projection-valued measure P on $\mathcal{B}(\mathbb{R}^n)$ with the following properties.*

(a) *For every $\Omega = \Omega_1 \times \cdots \times \Omega_n \in \mathcal{B}(\mathbb{R}^n)$ we have*

$$P(\Omega) = P_{A_1}(\Omega_1)\cdots P_{A_n}(\Omega_n).$$

(b) *If λ_k is the k-th coordinate functional in $\mathbb{R}^n$, i.e. $\lambda_k(x_1,\dots,x_n) = x_k$, we have for all $k = 1,\dots,n$*

$$D(A_k) = \left\{ x \in \mathcal{H} : \int_{\mathbb{R}} |\lambda_k|^2 \, d\langle x|Px\rangle < \infty \right\}$$

and for every $x \in D(A)$ and $y \in \mathcal{H}$ we have

$$\langle y|Ax\rangle = \int_{\mathbb{R}^n} \lambda_k \langle x|Px\rangle.$$

Moreover, as in the case of a single operator one obtains a joint functional calculus by integrating measurable functions on $\mathbb{R}^n$ against the spectral measure.

Note that as in the case of one observable the simultaneous measurement of observables $\mathbb{A} = \{A_1,\dots,A_n\}$ of a quantum mechanical system in a state ρ should be described by the probability measure μ_A on $\mathbb{R}^n$ given by the following natural generalization of the Born-von Neumann formula:

$$\mu_{\mathbb{A}}(\Omega) = \mathrm{Tr}(P_{A_1}(\Omega_1)\cdots P_{A_n}(\Omega_n)\rho) \qquad \text{for all } \Omega = \Omega_1 \times \cdots \times \Omega_n \in \mathcal{B}(\mathbb{R}^n).$$

However, for the above formula to define a probability measure for all states ρ and all Ω as above we need that $\Omega_1 \times \cdots \times \Omega_n \mapsto P_{A_1}(\Omega_1)\cdots P_{A_n}(\Omega_n)$ extends to a projection-valued measure on $\mathbb{R}^n$. Since the product of two orthogonal projections is an orthogonal projection if and only if the projections commute, we see that the observables must commute pairwise. From a physical perspective this agrees with the requirement that the simultaneous measurement of several observables should be independent of the order of the measurements of the individual observables.

2.3.5 The Schrödinger Equation and Stone's Theorem on One-Parameter Unitary Groups

We now come to the time evolution of quantum mechanical systems. Recall from the postulates of quantum mechanics that although measurements of states are of a probabilistic nature, the time evolution of a state is deterministic. In fact, given a system described by the Hilbert space $\mathcal{H}$, the time evolution of

its states is completely determined by a special observable, i.e. a self-adjoint operator, H on $\mathcal{H}$. This operator is called the *Hamiltonian* of the system. This time evolution is governed for a pure state $\psi \in \mathcal{H}$ by the *Schrödinger equation*

$$i\hbar \frac{\partial}{\partial t}\psi(t) = H\psi(t).$$

From a mathematical perspective there are several problems with the above equation. First of all the equation does not make sense in the usual meaning if the initial value ψ_0 or the solution $\psi(t)$ does not lie in the domain of H. So how one has to interpret the above equation? And even if $\psi_0 \in D(H)$, why does the above equation have a unique solution? In fact, if H is unbounded, the usual theorems for existence and uniqueness of solutions involving a Lipschitz condition do not apply.

The case of bounded Hamiltonians Nevertheless let us first take a look at the case of a bounded Hamiltonian, i.e. $H \in \mathcal{B}(\mathcal{H})$, to get a feeling for the problem. From now on we again ignore all physical constants. As for linear systems of ordinary differential equations, we can explicitly write down the solution of the Schrödinger equation. For arbitrary $\psi_0 \in \mathcal{H}$ a solution is given by

$$\psi(t) = e^{-iHt}\psi_0, \quad \text{where} \quad e^{-iHt} = \sum_{k=0}^{\infty} \frac{(-iHt)^k}{k!}.$$

Note that the series is absolute convergent in $\mathcal{B}(\mathcal{H})$. In fact, we have for $t \in \mathbb{R}$ because of the boundedness of H

$$\sum_{k=0}^{\infty} \frac{\|(iHt)^k\|}{k!} \leq \sum_{k=0}^{\infty} \frac{\|H\|^k\,|t|^k}{k!} = e^{|t|\|H\|}.$$

Moreover, the solution is unique by the Picard–Lindelöf theorem which also holds on Banach spaces with the same proof or by a direct argument as in the case systems of linear ordinary differential equations. Note that the above argument does not work in the case of unbounded operators.

The case of unbounded Hamiltonians Note that in the case of a bounded Hamiltonian the family $U(t) = e^{-Hit}$ of solution operators are unitary and satisfy the exponential law $U(t+s) = U(t)U(s)$ for all $t, s \in \mathbb{R}$. Moreover, one has $U(0) = \mathrm{Id}$. This leads to the following abstract definition.

Definition 2.3.26 (Unitary Group). A family of unitary operators $(U(t))_{t\in\mathbb{R}}$ on a Hilbert space $\mathcal{H}$ is called a *unitary group* if

(a) $U(0) = \mathrm{Id}$;

(b) $U(t+s) = U(t)U(s)$ for all $t, s \in \mathbb{R}$.

Further, $(U(t))_{t\in\mathbb{R}}$ is called *strongly continuous* if $t \mapsto U(t)x$ is continuous for all $x \in \mathcal{H}$.

From a physical perspective it is very reasonable to describe the time evolution of a quantum mechanical system by a unitary group. In fact, the existence of family of mappings statisfying the exponential law follows from the fact the the time evolution of a system is uniquely determined. Morever, by the superposition principle these mappings should be linear. Further, by the probabilistic interpretation of states each member of this family should preserve the norm of pure states, i.e. should be given by isometries. The surjectivity of these isometries comes from the requirement that the history of each state can be traced back and the assumption that each pure state (or at least a dense set) is physically realizable.

Moreover, it is natural to require some regularity on the map $t \mapsto U(t)$. A result of J. von Neumann says that a unitary group $(U(t))_{t\in\mathbb{R}}$ is already strongly continuous if the orbits are weakly measurable, i.e. $t \mapsto \langle y|U(t)x\rangle$ is measurable for all $x, y \in \mathcal{H}$. Hence, we would expect that for each Hamiltonian there is an associated unitary group. This is indeed true.

Proposition 2.3.27. *Let $(A, D(A))$ be a self-adjoint operator on a Hilbert space. Then $(U(t))_{t\in\mathbb{R}}$ defined by*

$$U(t) = e^{itA} \qquad \text{for } t \in \mathbb{R}$$

by the functional calculus of A is a strongly continuous unitary group.

Proof. For $t \in \mathbb{R}$ define $f_t(\lambda) = e^{it\lambda}$. Then f is a bounded function on $\mathbb{R}$. By the functional calculus for self-adjoint operators $U(t) = f_t(A)$ defines a bounded operator on $\mathcal{H}$. Since the bounded functional calculus is compatible with multiplication of functions, we have $U(t)U(s) = f_t(A)f_s(A) = f_{t+s}(A) = U(t+s)$ and we have verified the exponential law. Further, we have clearly $U(0) = \mathrm{Id}$. Moreover, we have for all $x \in \mathcal{H}$ and $t \in \mathbb{R}$

$$\begin{aligned}\langle y|U^*(t)U(t)x\rangle = \langle y|\overline{f_t}(A)f_t(A)x\rangle &= \int_{\mathbb{R}} f_t(\lambda)\overline{f_t}(\lambda)\langle y|P(\lambda)x\rangle \\ &= \int_{\mathbb{R}} \langle y|P(\lambda)x\rangle = \langle x|y\rangle.\end{aligned}$$

Hence, $U(t)$ is unitary. Finally, for the strong continuity observe that for $x \in \mathcal{H}$ we have

$$\|U(t)x - U(s)x\|^2 = \int_{\mathbb{R}} \left|e^{i\lambda t} - e^{i\lambda s}\right|^2 d\langle x|P(\lambda)x\rangle = \int_{\mathbb{R}} \left|e^{i\lambda(t-s)} - 1\right|^2 d\langle x|P(\lambda)x\rangle.$$

The right hand side goes to zero as $t \to s$ because of the dominated convergence theorem. Altogether $(U(t))_{t\in\mathbb{R}}$ is a unitary group. □

Conversely, we want to recover the self-adjoint operator out of the group $U(t) = e^{itA}$. In the bounded case this is again easy: the group mapping $\mathbb{R} \to \mathcal{B}(\mathcal{H})$ is differentiable and one has $A = -i\frac{d}{dt}U(t)_{|t=0}$. This cannot work in the unbounded case because A is simply not bounded. However, the approach works pointwise.

Definition 2.3.28 (Infinitesimal generator). Let $\mathcal{H}$ be a Hilbert space. The *infinitesimal generator* of the strongly continuous unitary group $(U(t))_{t\in\mathbb{R}}$ on $\mathcal{H}$ is the unbounded operator $(A, D(A))$ defined as

$$D(A) = \left\{ x \in \mathcal{H} : \lim_{t\to 0} \frac{U(h)x - x}{h} \text{ exists} \right\}$$
$$Ax = -i \lim_{t\to 0} \frac{U(h)x - x}{h}.$$

Moreover, one would expect a relation between solutions of the differential equation $\dot{x}(t) = -iAx(t)$, i.e. the Schrödinger equation, and the unitary group. This is studied in the next result.

Proposition 2.3.29. *Let $(U(t))_{t\in\mathbb{R}}$ be a strongly continuous unitary group a Hilbert space $\mathcal{H}$ with infinitesimal generator A. Then for every $x_0 \in D(A)$ the function $x(t) = U(t)x_0$ satisfies $x(t) \in D(A)$ for all $t > 0$. Moreover, $x(t)$ is the unique (classical) solution of the problem*

$$\begin{cases} \dot{x}(t) = -iA(x(t)) & (t \geq 0) \\ x(0) = x_0. \end{cases}$$

Proof. Let $x_0 \in D(A)$. Then we have for all $t > 0$

$$\lim_{h\to 0} \frac{U(t+h)x_0 - U(t)x_0}{h} = \lim_{h\to 0} \frac{U(h)U(t)x_0 - U(t)x_0}{h} = U(t)\left(\lim_{h\to 0} \frac{U(h)x_0 - x_0}{h}\right).$$

Hence, $U(t)x_0 \in D(A)$ and $x(t)$ is differentiable with $\dot{x}(t) = -iAU(t)x_0 = -iU(t)Ax_0$. Now, let y be a second solution of the problem. For $t > 0$ consider the function $z(s) = U(t-s)y(s)$. Then it follows from a variant of the product rule that

$$\dot{z}(s) = iAU(t-s)y(s) + U(t-s)\dot{y}(s) = iU(t-s)Ay(s) - iU(t-s)Ay(s) = 0.$$

This shows that $\dot{z}(s) = 0$ for all $s \in \mathbb{R}$. By reducing to the case of the functions $s \mapsto \langle w|z(s)\rangle$ for $w \in \mathcal{H}$, we see from the scalar case that the function z is constant. In particular, we have $U(t)x_0 = z(0) = z(t) = y(t)$. This establishes the uniqueness of the solutions. □

Hence, for elements in the domain of the generator we obtain classical solutions of the Schrödinger equation. In the general case $x_0 \in \mathcal{H}$ we may therefore interpret $U(t)x_0$ as a generalized solution of the Schrödinger equation.

As one would hope the infinitesimal generator of every strongly continuous unitary group is self-adjoint. As a preliminary results in this direction we show the following lemma.

Lemma 2.3.30. *Let $(U(t))_{t\in\mathbb{R}}$ be a strongly continuous unitary group on some Hilbert space $\mathcal{H}$. Then its infinitesimal generator A is essentially self-adjoint.*

Proof. For $x, y \in D(A)$ we have because of $U^*(t) = U(-t)$ for all $t \in \mathbb{R}$

$$\langle y|Ax\rangle = \left\langle y\middle| -i\lim_{h\to 0}\frac{U(h)x-x}{h}\right\rangle = \left\langle \lim_{h\to 0} i\frac{U(-h)y-y}{h}\middle| x\right\rangle = \langle Ay|x\rangle.$$

This shows that A is symmetric. Hence, A is closable by Lemma 2.2.26. Now let $x \in \mathcal{H}$. Note that as in the scalar case we can define the Riemann integral of continuous functions as the limit of approximating sums. We have for $R > 0$ and $x_R = \int_0^R e^{-t}U(t)x\,dt$

$$\begin{aligned} e^{-h}\frac{U(h)-x_R}{h} + \frac{e^{-h}x_R - x_R}{h} &= \frac{e^{-h}U(h)x_R - x_R}{h} \\ &= \frac{1}{h}\int_0^R e^{-(t+h)}U(t+h)x - e^{-t}U(t)x\,dt \\ &= \frac{1}{h}\int_R^{R+h} e^{-t}U(t)x\,dt - \frac{1}{h}\int_0^h e^{-t}U(t)x\,dt \xrightarrow[h\to 0]{} e^{-R}U(R)x - x. \end{aligned}$$

Hence, $x_R \in D(A)$ and $(iA-1)x_R = e^{-R}U(R)x - x$. Note that both x_R and $(iA-1)x_R$ converge as $R \to \infty$. Since $\overline{A}$ is closed this implies that the improper Riemann integral $\int_0^\infty e^{-t}U(t)x\,dt$ lies in the domain of $\overline{A}$ and

$$(i\overline{A}-1)\int_0^\infty e^{-t}U(t)x\,dt = \lim_{R\to\infty} e^{-R}U(R)x - x = -x.$$

Hence, $i\overline{A}-1$ and therefore $\overline{A}+i$ are surjective. For the self-adjointness of $\overline{A}$ it remains to show that $\overline{A}-i$ is surjective as well.

Now consider the adjoint group $(U^*(t))_{t\in\mathbb{R}}$. Clearly, one has $U^*(0) = \mathrm{Id}^* = \mathrm{Id}$ and for all $x, y \in \mathcal{H}$ and $t, s \in \mathbb{R}$

$$\langle y|U^*(t+s)x\rangle = \langle U(t+s)y|x\rangle = \langle U(s)U(t)y|x\rangle = \langle y|U^*(t)U^*(s)x\rangle.$$

This shows that $(U^*(t))_{t\in\mathbb{R}}$ is a unitary group. We now show that the group is strongly continuous. For this observe that for all $x, y \in \mathcal{H}$

$$\langle y|U^*(s)x\rangle = \langle U(s)y|x\rangle \xrightarrow[s\to t]{} \langle U(t)y|x\rangle = \langle y|U^*(t)x\rangle$$

by the strong continuity of $(U(t))_{t\in\mathbb{R}}$. We obtain that for all $x \in \mathcal{H}$

$$\begin{aligned}\|U^*(t)x - U^*(s)x\|^2 &= \|U^*(t)x\|^2 + \|U^*(s)x\|^2 - 2\,\mathrm{Re}\langle U^*(t)x|U^*(s)x\rangle \\ &= 2\|x\|^2 - 2\,\mathrm{Re}\langle x|U^*(s-t)x\rangle \xrightarrow[s\to t]{} 0.\end{aligned}$$

Since $(U^*(t))_{t\in\mathbb{R}}$ is strongly continuous, we may calculate its infinitesimal generator B. Note that because of

$$-i\frac{U^*(h)x - x}{h} = -i\frac{U(-h)x - x}{h}$$

one has $B = -A$. By the first part of the proof we know that $-\overline{A} + i$ and therefore also $\overline{A} - i$ are surjective. The self-adjointness of $\overline{A}$ now follows from Theorem 2.2.34. But this is by definition equivalent to A being essentially self-adjoint. □

We now determine the infinitesimal generator of the unitary groups defined by the functional calculus for self-adjoint operators.

Lemma 2.3.31. *Let $(A, D(A))$ be a self-adjoint operator on a Hilbert space $\mathcal{H}$. Then A is the infinitesimal generator of the strongly continuous unitary group $U(t) = e^{itA}$.*

Proof. Let B denote the infinitesimal generator of $(U(t))_{t\in\mathbb{R}}$. By Lemma 2.3.30 the operator B is essentially self-adjoint. For $x \in D(A)$ we have by the spectral theorem for self-adjoint operators (Theorem 2.3.19) that

$$\begin{aligned}\left\|-i\frac{U(h)x - x}{h} - Ax\right\|^2 &= \int_{\mathbb{R}}\left|-i\frac{e^{ih\lambda} - 1}{h} - \lambda\right|^2 d\langle x|P(\lambda)x\rangle \\ &= \int_{\mathbb{R}}\left|\frac{e^{ih\lambda} - 1}{h} - i\lambda\right|^2 d\langle x|P(\lambda)x\rangle \xrightarrow[h\to\infty]{} 0\end{aligned}$$

by the dominated convergence theorem. Hence, $x \in D(B)$ and $A \subset B$. This shows that B is a symmetric extension of the self-adjoint operator A. But if A satisfies the range condition for self-adjoint operators (Theorem 2.2.34 (iii)), then so does B. This shows $(i + A)^{-1} = (i + B)^{-1}$, which implies $A = B$. □

We now come to the fundamental theorem of this section which shows that the description of the evolution via the Schrödinger equation is equivalent to the description via unitary groups.

Theorem 2.3.32 (Stone's theorem). *Let $\mathcal{H}$ be a Hilbert space. There is a one-to-one correspondence between self-adjoint operators on $\mathcal{H}$ and strongly continuous unitary groups on $\mathcal{H}$ given by*

$$A \mapsto (e^{itA})_{t\in\mathbb{R}}.$$

Proof. Let $(U(t))_{t\in\mathbb{R}}$ be a strongly continuous unitary group. Then its infinitesimal generator A is essentially self-adjoint by Lemma 2.3.30. Therefore the self-adjoint operator $\overline{A}$ generates the strongly continuous unitary group $(e^{it\overline{A}})_{t\in\mathbb{R}}$. Since $\overline{A}$ is self-adjoint, we see that $D(\overline{A})$ and therefore also $D(A)$ are dense in $\mathcal{H}$. Note that for $x \in D(A)$ both unitary groups yield classical solutions for the problem $\dot{x}(t) = Ax(t)$ with initial value x_0. By the uniqueness of the solutions shown in Proposition 2.3.29, the operators $e^{it\overline{A}}$ and $U(t)$ therefore agree on the dense subset $D(A)$ for all $t \in \mathbb{R}$. Since these operators are bounded, we indeed have $e^{it\overline{A}} = U(t)$ for all $t \in \mathbb{R}$. This shows $(e^{it\overline{A}})_{t\in\mathbb{R}} = (U(t))_{t\in\mathbb{R}}$. In particular, as the groups agree, so do the generators and we have $A = \overline{A}$. Altogether we have shown that the map $A \mapsto (e^{itA})_{t\in\mathbb{R}}$ is onto. For the injectivity simply note again that if $(e^{itA})_{t\in\mathbb{R}}$ and $(e^{itB})_{t\in\mathbb{R}}$ define the same unitary groups, then one clearly has $A = B$. □

We now study the unitary groups generated by the position and momentum operators. Since both are particular instances of multiplication operators, we study this class first.

Example 2.3.33 (Multiplication semigroup). Let (Ω, Σ, μ) be an arbitary measure space and $m\colon \Omega \to \mathbb{R}$ a measurable function. We have seen in Example 2.2.28 that the multiplication operator M_m is self-adjoint. By Stone's theorem (Theorem 2.3.32) $U(t) = e^{itM_m}$ for $t \in \mathbb{R}$ is the associated unitary group. We have seen in Example 2.3.21 that

$$(e^{itM_m} f)(x) = e^{itm(x)} f(x) \qquad \text{for all } f \in L^2(\Omega, \Sigma, \mu).$$

In particular, we obtain for the position operators the following.

Corollary 2.3.34. *Let $n \in \mathbb{N}$ and for $j = 1, \dots, n$ let $\hat{x}_j$ denote the position operator on $L^2(\mathbb{R}^n)$ in direction j. Then $\hat{x}_j$ generates the unitary group*

$$(U(t)f)(x) = e^{itx_j} f(x) \qquad \textit{for all } f \in L^2(\mathbb{R}^n).$$

Hence, these groups simply act on pure states by a uniform phase rotation. After a Fourier transform an analogous argument applies to the momentum operators.

Corollary 2.3.35. *Let $n \in \mathbb{N}$ and for $j = 1, \dots, n$ let $\hat{p}_j = -i\frac{\partial}{\partial x_j}$ be the momentum operator on $L^2(\mathbb{R}^n)$ in direction j. Then $\hat{p}_j$ generates the unitary group*

$$(U(t)f)(x) = f(x + te_j) \qquad \textit{for all } f \in L^2(\mathbb{R}^n),$$

where e_j denotes the j-th unit vector.

Proof. Recall that we have seen in Example 2.2.29 that under the unitary Fourier transform $\hat{p}_j$ becomes the multiplication operator with x_j. Hence, it follows that for all $f \in L^2(\mathbb{R}^n)$ one has almost everywhere

$$(U(t)f)(x) = \mathcal{F}^{-1}(e^{itx_j}\mathcal{F}f)(x) = f(x + te_j). \qquad \square$$

We now come back to the abstract description of the time evolution of a quantum mechanical system. Let A be a self-adjoint operator and $(U(t))_{t\in\mathbb{R}}$ the unitary group generated by A. Then a quantum mechanical state initially given by ψ evolves into the state $U(t)\psi$ after time t. Written as a density matrix, we obtain

$$|U(t)\psi\rangle\langle U(t)\psi| = U(t)|\psi\rangle\langle\psi|U^*(t).$$

Requiring linearity of the time evolution for mixed states, the same formula holds for (non-normalized) mixed states made of finitely many pure states. Assuming again continuity of the time evolution, it follows from the density of the finite rank operators in the space of trace class operators that the identity indeed holds for all trace class operators. In particular, it holds for all density operators. Hence, we obtain the following mathematical description of the time evolution in quantum mechanics.

Time evolution in Schrödinger's picture. The dynamics of a quantum system under a self-adjoint operator H is described by the strongly continuous unitary group $(U(t))_{t\in\mathbb{R}}$ associated to H via Stone's theorem. Quantum observables do not depend on time and the evolution of states is given by

$$\rho \mapsto U(t)\rho U(t)^{-1}.$$

2.4 Further Criteria for Self-Adjointness

Recall that until now we introduced self-adjoint operators and checked self-adjointness for several elementary examples, such as the position and momentum operators or the Hamiltonian of a free particle on $\mathbb{R}^n$ provided one works with the right domains. However, most Hamiltonians such as for the harmonic oscillator or the hydrogen atom are more complicated as they additionally involve potentials, i.e. are of the form

$$-\Delta + V.$$

In this general case we cannot rely on simple Fourier transform techniques and more advanced criteria for self-adjointness are needed. In particular, it can be very difficult to determine the domains explicitly. We will now present several criteria for self-adjointness – partially with proofs – and apply them to concrete quantum mechanical operators of physical importance.

2.4.1 von Neumann's criterion

A sometimes very handy criterion is von Neumann's criterion. In concrete situations it is sometimes trivial to verify this criterion. However, it has the disadvantage that it only shows the existence of self-adjoint extensions and not the essentially self-adjointness of symmetric operators. Von Neumann's criterion is formulated in terms of conjugations.

Definition 2.4.1 (Conjugation). A surjective map $V\colon \mathcal{H} \to \mathcal{H}$ on a Hilbert space $\mathcal{H}$ is called *anti-unitary* if

(i) V is anti-linear, i.e. $V(\lambda x+\mu y) = \overline{\lambda} Vx+\overline{\mu} V(y)$ for all $\lambda, \mu \in \mathbb{C}$ and $x, y \in \mathcal{H}$.

(ii) V is anti-isometric, i.e. $\langle Vx|Vy\rangle = \overline{\langle x|y\rangle}$ for all $x, y \in \mathcal{H}$.

Moreover, an anti-unitary operator $C\colon \mathcal{H} \to \mathcal{H}$ is called a *conjugation* if $C^2 = C$.

Now, von Neumann's criterion reads as follows.

Theorem 2.4.2 (von Neumann's criterion). *Let $(A, D(A))$ be a densely defined symmetric operator on a Hilbert space $\mathcal{H}$. If there is a conjugation $C\colon \mathcal{H} \to \mathcal{H}$ such that $C(D(A)) \subset D(A)$ and*

$$AC = CA \qquad \text{on } D(A),$$

then A has self-adjoint extensions.

Proof. We first show that $C(D(A^*)) \subset D(A^*)$ and that $A^*C = CA^*$. For this let $x \in D(A)$ and $y \in D(A^*)$. Then by assumption

$$\langle Cy|Ax\rangle = \overline{\langle y|CAx\rangle} = \overline{\langle y|ACx\rangle} = \overline{\langle A^*y|Cx\rangle} = \langle CA^*y|x\rangle.$$

This shows thats $Cy \in D(A^*)$ and $A^*Cy = CA^*y$. Hence, $A^*C = CA^*$ on $D(A^*)$. Now let $x \in \mathrm{Ker}(A^* + i)$. Hence,

$$(A^* + i)x = 0 \quad \Rightarrow \quad C(A^* + i)x = A^*Cx - iCx = (A^* - i)Cx = 0.$$

Since C is an isometry, C induces an injective map $\mathrm{Ker}(A^* + i) \to \mathrm{Ker}(A^* - i)$. We now show that this map is onto. In fact, as above for $y \in \mathrm{Ker}(A^* - i)$ we have for $x = Cy$ that $x \in D(A^*)$, $Cx = C^2y = y$ and

$$(A^* + i)Cy = C(A^*y - iy) = C((A^* - i)y) = 0.$$

Since C preserves angles, it maps orthonormal bases to orthonormal bases. Hence, $\mathrm{Ker}(A^* + i)$ and $\mathrm{Ker}(A^* - i)$ are isomorphic as Hilbert spaces. This shows that the deficiency indices $d_+(A)$ and $d_-(A)$ agree. It follows from Theorem 2.2.45 that A has self-adjoint extensions. □

Von Neumann's criterion immediately gives the following results on Hamiltonians with potential terms.

Example 2.4.3 (Hamiltonians with potential terms). Let us consider the Hamiltonian $-\Delta + V$ for a real-valued function $V \in L^1_{\mathrm{loc}}(\mathbb{R}^n)$ on the Hilbert space $L^2(\mathbb{R}^n)$. Using the test functions $C_c^\infty(\mathbb{R}^n)$ as domain, we that for $f, g \in C_c^\infty(\mathbb{R}^n)$

$$\begin{aligned}\langle g|(-\Delta + V)f\rangle &= -\int_{\mathbb{R}^n} \overline{g(x)}\Delta f(x)\,dx + \int_{\mathbb{R}^n} g(x)\overline{V(x)f(x)}\,dx \\ &= -\int_{\mathbb{R}^n} \overline{\Delta g(x)} f(x)\,dx + \int_{\mathbb{R}^n} V(x)g(x)\overline{f(x)}\,dx = \langle(-\Delta + V)g|f\rangle.\end{aligned}$$

Here we have used integration by parts twice for the first summand. Hence, $-\Delta + V$ is a densely defined symmetric operator on $L^2(\mathbb{R}^n)$. Now observe that the complex conjugation $C\colon f \mapsto \overline{f}$ clearly is a conjugation that leaves $C_c^\infty(\mathbb{R}^n)$ invariant and statisfies $AC = CA$ on $C_c^\infty(\mathbb{R}^n)$. Hence, by von Neumann's criterion (Theorem 2.4.2) the operator A has self-adjoint extensions.

Note that although a conjugation as required by von Neumann's criterion for a given symmetric operator may exist, it can be somewhat difficult to find it. For example, you might want to try to find conjugations for the momentum operators both on a bounded interval and on $\mathbb{R}$ with domains equal to the space of test functions.

2.4.2 Kato–Rellich Theory

Note that it is however more difficult to establish essentially self-adjointness for Hamiltonians with potential terms. This will be our goal now and is the content of the so-called Kato–Rellich theory. The central idea is to see the potential term as a perturbation of the self-adjoint operator $-\Delta$. In fact, as one would expect, perturbations preserve self-adjointness if they are small in a certain sense. This is shown in the next abstract result.

Theorem 2.4.4 (Kato–Rellich). *Let $(A, D(A))$ and $(B, D(B))$ be two self-adjoint operators on a Hilbert space $\mathcal{H}$. Suppose that $D(A) \subset D(B)$ and that there exist constants $0 < a < 1$ and $0 < b$ such that*

$$\|Bx\| \le a\|Ax\| + b\|x\| \qquad \text{for all } x \in D(A).$$

Then $(A + B, D(A))$ is a self-adjoint operator on $\mathcal{H}$.

Proof. Use a positive sufficiently large number $\mu \in \mathbb{R}$ such that $a + b/\mu < 1$. This is possible because of $a < 1$. Now for all $x \in D(A)$ we have

$$(A + B + i\mu)x = (B(A + i\mu)^{-1} + \mathrm{Id})(A + i\mu)x.$$

The second factor on the right hand side is invertible because A is self-adjoint. Now let us deal with the first factor. Observe that because of $D(A) \subset D(B)$ this factor is a closed operator which is defined on the whole Hilbert space. For all $x \in \mathcal{H}$ we have by the assumption and the estimate of Lemma 2.2.12 that

$$\begin{aligned}\|B(A+i\mu)^{-1}x\| &\leq a\|A(A+i\mu)^{-1}x\| + b\|(A+i\mu)^{-1}x\| \\ &\leq a\|A(A+i\mu)^{-1}x\| + \frac{b}{\mu}\|x\|.\end{aligned}$$

Further note that because of the self-adjointness of A one has $\langle Az|z\rangle \in \mathbb{R}$ for all $z \in D(A)$ and therefore

$$\begin{aligned}\|x\|^2 = \|(A(A+i\mu)^{-1}x + i\mu(A+i\mu)^{-1}x\|^2 = \|(A(A+i\mu)^{-1}x\|^2 + \|\mu(A+i\mu)^{-1}x\|^2 \\ + 2\,\mathrm{Re}\langle A(A+i\mu)^{-1}x|i\mu(A+i\mu)^{-1}x\rangle = \|(A(A+i\mu)^{-1}x\|^2 + \|\mu(A+i\mu)^{-1}x\|^2.\end{aligned}$$

Forgetting the second summand at the right hand side, we therefore obtain

$$\|B(A+i\mu)^{-1}x\| \leq (a + b/y)\,\|x\|.$$

Since the factor on the right is smaller than 1 by the choice of μ, using the Neumann series (Lemma 2.2.20) we see that $B(A+i\mu)^{-1} + \mathrm{Id}$ and therefore $A + B + i\mu = \mu(\mu^{-1}A + \mu^{-1}B + i)$ are invertible. Of course, the same argument applies to $(A + B - i\mu)$. It now follows from Theorem 2.2.34 that $A + B$ is self-adjoint with domain $D(A)$. □

Furthermore, one can show with similar arguments that $(A + B, D)$ is essentially self-adjoint whenever (A, D) is essentially self-adjoint. We now apply the Kato–Rellich theorem to Hamiltonians with potentials.

Theorem 2.4.5. *Let $n \leq 3$ and $V\colon \mathbb{R}^n \to \mathbb{R}$ be measurable such that $V = V_1 + V_2$ with $V_1 \in L^2(\mathbb{R}^n)$ and $V_2 \in L^\infty(\mathbb{R}^n)$. Then $-\Delta + V$ is self-adjoint on $H^2(\mathbb{R}^n)$.*

Proof. We want to apply the Kato–Rellich theorem (Theorem 2.4.4) with $A = -\Delta$ and domain $D(A) = H^2(\mathbb{R}^n)$ and B the multiplication operator with the potential V. Note that in particular we have to check that $D(B) \subset D(A)$. Let $f \in H^2(\mathbb{R}^n)$ and $\varepsilon > 0$. One now argues almost analogously to the proof of the Sobolev embedding theorem (Theorem 2.1.34): we have by the Cauchy–Schwarz inequality

$$\begin{aligned}\|\mathcal{F}f\|_1 &\leq \|(1+\varepsilon|x|^2)\mathcal{F}f\|_2\|(1+\varepsilon|x|^2)^{-1}\|_2 = C_\varepsilon\|f + \varepsilon\Delta f\|_2 \\ &\leq C_\varepsilon(\varepsilon\|\Delta f\|_2 + \|f\|_2).\end{aligned}$$

Here we have used the fact that the integral $\int_{\mathbb{R}^n} 1/(1+\varepsilon|x|^2)^2\,dx$ is finite for $n \leq 3$. Since $\mathcal{F}f \in L^1(\mathbb{R}^n)$, it follows that

$$\|f\|_\infty \leq \|\mathcal{F}f\|_1 \leq C_\varepsilon(\varepsilon\|\Delta f\|_2 + \|f\|_2).$$

Hence, for all $\varepsilon > 0$ there exists a constant $c_\varepsilon > 0$ such that

$$\|f\|_\infty \leq \varepsilon \|\Delta f\|_2 + c_\varepsilon \|f\|_2 .$$

Using this estimate, we obtain for all $f \in H^2(\mathbb{R}^n)$ that

$$\begin{aligned} \|Vf\|_2 &\leq \|V_1 f\|_2 + \|V_2 f\|_2 \leq \|V_1\|_2 \|f\|_\infty + \|V_2\|_\infty \|f\|_2 \\ &\leq \varepsilon \|V_1\|_2 \|\Delta f\|_2 + (c_\varepsilon \|V_1\|_2 + \|V_2\|_\infty) \|f\|_2 \\ &= \varepsilon \|V_1\|_2 \|Af\|_2 + (c_\varepsilon \|V_1\|_2 + \|V_2\|_\infty) \|f\|_2 < \infty. \end{aligned}$$

This shows that $f \in D(B)$. Moreover, if we choose $\varepsilon < \|V_1\|_2^{-1}$, then the assumptions of the Kato–Rellich theorem are fulfilled and therefore $-\Delta + V$ with domain $H^2(\mathbb{R}^n)$ is self-adjoint. □

One can show that the theorem still holds for $n \geq 4$ if one replaces the assumption $V_1 \in L^2(\mathbb{R}^n)$ by $V_1 \in L^p(\mathbb{R}^n)$ for some $p > n/2$. For a proof see [RS75, Theorem X.20]. As a particular instance of the above theorem we obtain the self-adjointness of the hydrogen atom.

Example 2.4.6 (Hydrogen atom). Let $n = 3$ and consider the Hamiltonian of the hydrogen atom given by $-\Delta + 1/|x|$, once again ignoring physical constants. This means that the potential is given by $1/|x|$. We now use the decomposition

$$V(x) = V_1(x) + V_2(x) = \frac{1}{|x|} \mathbb{1}_{|x| \leq 1} + \frac{1}{|x|} \mathbb{1}_{|x|>1}.$$

Then clearly $V_2 \in L^\infty(\mathbb{R}^3)$. Moreover, for V_1 we have using polar coordinates

$$\int_{\mathbb{R}^2} |V_2(x)|^2 \, dx = \int_{|x|\leq 1} \frac{1}{|x|^2} \, dx = \int_0^1 \int_{\mathbb{S}^2} d\theta \frac{1}{r^2} r^2 \, dr = 4\pi < \infty.$$

Hence, it follows from Theorem 2.4.5 that $-\Delta + \frac{1}{|x|}$ is self-adjoint with domain $H^2(\mathbb{R}^3)$.

With more effort one can prove a variant of Theorem 2.4.5 due to T. Kato which allows a wider range of potentials. However, in this case one only obtains essentially self-adjointness on the space of test functions and one has no exact information on the domain of the closure. We omit the proof because of its complexity and refer to [RS75, Theorem X.29].

Theorem 2.4.7 (Kato). *Let $n \leq 3$ and $V \colon \mathbb{R}^n \to \mathbb{R}$ be measurable such that $V = V_1 + V_2 + V_3$ with $V_1 \in L^2(\mathbb{R}^n)$, $V_2 \in L^\infty(\mathbb{R}^n)$ and $0 \leq V_3 \in L^2_{\mathrm{loc}}(\mathbb{R}^n)$. Then $-\Delta + V$ is essentially self-adjoint on $C_c^\infty(\mathbb{R}^n)$.*

The theorem again holds for $n \geq 4$ if one replaces the condition $V_1 \in L^2(\mathbb{R}^n)$ with $V_1 \in L^p(\mathbb{R}^n)$ for some $p > n/2$. Note that the above theorem in particular applies for non-negative continuous potentials. For example, $-\Delta + x^4$ is essentially self-adjoint on $C_c^\infty(\mathbb{R}^n)$. The sign of the potential here plays a crucial role as the next example makes clear. We do not discuss it here and refer the reader to [Hal13, Section 9.10] where a detailed exposition is given.

Example 2.4.8. The operator $-\Delta - x^4$ with domain $C_c^\infty(\mathbb{R}^n)$ is not essentially self-adjoint.

In contrast to this negative result recall that we have seen in Example 2.4.3 that $-\Delta - x^4$ has self-adjoint extensions. In fact, since $-\Delta - x^4$ on $C_c^\infty(\mathbb{R}^n)$ is not essentially self-adjoint, the above example even yields that there must exist several self-adjoint extensions.

2.4.3 Nelson's criterion

We now come to our last criterion, namely Nelson's criterion. This result is particularly useful in connection with the algebraic method of raising and lowering operators. In fact, it sometimes allows to verify self-adjointness with the usual arguments used by physicists. For the criterion we need the notion of analytic vectors.

Definition 2.4.9. Let $(A, D(A))$ be an unbounded operator on a Hilbert space $\mathcal{H}$.

(i) An element $x \in D(A)$ is called a C^∞-vector for A if $A^n x \in D(A)$ for all $n \in \mathbb{N}$.

(ii) A C^∞-vector $x \in D(A)$ is called an *analytic vector* for A if

$$\sum_{n=0}^{\infty} \frac{\|A^n x\|}{n!} t^n < \infty \qquad \text{for some } t > 0.$$

Observe that the defining condition for an analytic vector implies that the map $z \mapsto \sum_{n=0}^\infty \frac{\|A^n x\|}{n!} z^n$ is well-defined and analytic. In particular, it follows form the fact that derivatives are analytic and the triangle inequality that $\operatorname{span}\{A^n x : n \in \mathbb{N}\}$ entirely consists of analytic vectors if x is analytic.

Let us consider a self-adjoint operator $(A, D(A))$ on $\mathcal{H}$ with the projection-valued measure P. Then for $M > 0$ the operator A leaves $P([-M, M])\mathcal{H}$ invariant and therefore restricts to a bounded operator on $P([-M, M])\mathcal{H}$. Therefore the exponential series $\sum_{n=0}^\infty \frac{A^n}{n!} t^n$ converges in absolutely operator norm for

all $t \in \mathbb{R}$. This implies that for x in the dense set $\cup_{M\in\mathbb{N}} P([-M,M])\mathcal{H}$ we have a C^∞-vector

$$\sum_{n=0}^{\infty} \frac{\|A^n x\|}{n!} t^n < \infty \qquad \text{for all } t > 0.$$

Hence, for a self-adjoint operators its set of analytic vector is dense. In fact, this property characterizes self-adjoint operators. This is Nelson's criterion for self-adjointness which we will not prove here due to time constraints. A proof can be found in [Mor13, Theorem 5.47] and [RS75, Theorem X.39].

Theorem 2.4.10 (Nelson's criterion). *Let $(A, D(A))$ be a symmetric operator on a Hilbert space $\mathcal{H}$. Suppose that $D(A)$ contains a set of analytic vectors for A whose span is dense in $\mathcal{H}$. Then A is essentially self-adjoint.*

Let us give a fundamental example of Nelson's criterion, the quantum mechanical one-dimensional harmonic oscillator.

Example 2.4.11 (Harmonic oscillator). Recall from the physics part that the quantum mechanical harmonic oscillator is given by $-\frac{d^2}{dx^2} + x^2$ ignoring physical constants. This time the space of test functions $C_c^\infty(\mathbb{R})$ is not the optimal choice as we have already seen in the physics part that the operator has Hermite functions as eigenvectors. Therefore we work with the space of Schwartz function $\mathcal{S}(\mathbb{R})$ instead. This is is the space of all C^∞-functions with rapid decay at infinity. This space plays a fundamental role in the theory of distributions where you can also find an exact definition (Definition 3.2.1).

A direct calculation now shows that $-\frac{d^2}{dx^2} + x^2$ with domain $\mathcal{S}(\mathbb{R})$ is a densely defined symmetric operator on $L^2(\mathbb{R})$. Using the ladder operators

$$a = x - \frac{d}{dx} \qquad \text{and} \qquad a^\dagger = x + \frac{d}{dx}$$

with domains $\mathcal{S}(\mathbb{R})$, we obtain the factorization $H = a^\dagger a + 1$ on $\mathcal{S}(\mathbb{R}^n)$. Now, repeating the calculations done in the physics part we obtain for all $n \in \mathbb{N}$ the vectors $\psi_n(x) = p_n(x)e^{-x^2/2}$ for some polynomial of degree n which appropriately normalized form an orthonormal system of eigenvectors for $-\frac{d^2}{dx^2} + x^2$. In fact, the polynomials p_n are – ignoring possbile scaling issues – the Hermite polynomials. Note that we have used the notation $a^\dagger$ instead of a^* because $a^\dagger$ *is not* the adjoint of a. Moreover, there are no domain problems because for arbitrary polynomial expressions in a and $\hat{a}^\dagger$ their domain is again $\mathcal{S}(\mathbb{R})$ if a and $a^\dagger$ are chosen with domain $\mathcal{S}(\mathbb{R})$ because $\mathcal{S}(\mathbb{R})$ is left invariant by those operators.

We now sketch how one can show that $(\psi_n)_{n\in\mathbb{N}}$ in fact forms an orthonormal basis of $L^2(\mathbb{R})$. Therefore we must show that $V = \operatorname{span}\{\psi_n : n \in \mathbb{N}\}$ is dense in $L^2(\mathbb{R})$. Note that it follows from the fact that the polynomials p_n

have degree n that $V = \{p(x)e^{-x^2/2} : p \text{ polynomial}\}$. One now shows that for all $\alpha \in \mathbb{C}$

$$\sum_{n=0}^{N} \frac{\alpha^n x^n}{n!} e^{-x^2/2} \xrightarrow[n\to\infty]{} e^{\alpha x} e^{-x^2/2} \qquad \text{in } L^2(\mathbb{R}).$$

Hence, if ψ is orthogornal to every element in the closure of V, we have

$$\int_{\mathbb{R}} e^{-ikx} e^{-x^2/2} \psi(x)\, dx = 0 \qquad \text{for all } k \in \mathbb{R}.$$

This means that the Fourier transform of $e^{-x^2/2}\psi(x)$ is identically zero. By Plancherel's theorem (Theorem 2.1.34) this implies that $e^{-x^2/2}\psi(x)$ and therefore also $\psi(x)$ are the zero function. Hence, $\overline{V}^{\perp} = V^{\perp} = 0$ which is equivalent to the denseness of V in $L^2(\mathbb{R}^n)$.

Now observe that eigenvalues of an operator A are clearly analytic vectors for A. Hence, $(\psi_n)_{n\in\mathbb{N}}$ is a set of analytic vectors for $-\frac{d^2}{dx^2} + x^2$ whose span is dense in $L^2(\mathbb{R}^n)$. Nelson's criterion (Theorem 2.4.10) now shows that $-\frac{d^2}{dx^2} + x^2$ with domain $\mathcal{S}(\mathbb{R})$ is essentially self-adjoint.

Of course, the fact that $-\frac{d^2}{dx^2} + x^2$ with domain $\mathcal{S}(\mathbb{R})$ is essentially self-adjoint also follows directly from Theorem 2.4.7.

3 Distributions

We have already seen that the domains of self-adjoint realizations of differential operators contain functions which are not classically differentiable, i.e. non-differentiable Sobolev functions. However, there are still many locally integrable functions which do not have a derivative even in the weak sense. This disadvantage has already made some arguments very difficult or impossible, for example in Example 2.1.38 or Example 2.2.49. In this section we give an introduction to the theory of distributions which also can be differentiated and have the huge advantage that they are closed with respect to differentiation. Moreover, we have formally seen (see Example 2.2.5) that such generalized functions can naturally arise as some kind of generalized eigenfunctions for self-adjoint operators which may not have eigenvalues in the usual sense. In fact, the spectral theorem can be generalized to this situation and we will see that typical quantum mechanical operators have an orthonormal basis if one allows for eigenvectors in this generalized sense. This is the statement of the main results of this chapter, the so-called nuclear spectral theorem.

3.1 The Space of Distributions

We now introduce distributions. Later on we will mainly work with a special class of distributions, the so-called tempered distributions for which some technical issues are more easily to handle. Nevertheless, for the sake of completeness we first shortly introduce general distributions. The general idea of the theory of distributions is to replace functions by functionals which act in some continuous way on a given class of particularly nice functions which are often called test functions. The exact mathematical objects one obtains depend on the concrete choice of the space of test functions. A first natural choice is here the class of all smooth functions with compact support.

Definition 3.1.1 (Space of Test Functions). Let $\Omega \subset \mathbb{R}^n$ be open. We say that a sequence $(f_n)_{n\in\mathbb{N}} \subset C_c^\infty(\Omega)$ converges to $f \in C_c^\infty(\Omega)$ if

(i) there exists a compact subset $K \subset \Omega$ such that $\operatorname{supp} f_n \subset K$ for all $n \in \mathbb{N}$ and

(ii) for all $\alpha \in \mathbb{N}_0^n$ the α-th derivative $\partial^\alpha f_n$ converges uniformly in K to $\partial^\alpha f$, i.e. $\sup_{x\in K} |\partial^\alpha (f_n - f)| \to 0$.

We call $C_c(\Omega)$ with this notation of convergence the *space of all test functions* on Ω und write $\mathcal{D}(\Omega)$.

More precisely, there exists a locally convex topology on the vector space $C_c(\Omega)$ for which the convergence of a sequence $(f_n)_{n\in\mathbb{N}}$ is equivalent to (i) and (ii). However, we will ignore such topological concepts to a great extent and instead work directly with the notion of convergence induced by the topology.

Distributions are then defined as continuous linear functionals on $\mathcal{D}(\Omega)$.

Definition 3.1.2 (Distribution). A *distribution* is a continuous linear functional on $\mathcal{D}(\Omega)$, i.e. a linear function $u\colon \mathcal{D}(\Omega) \to \mathbb{C}$ for which

$$f_n \to f \text{ in } \mathcal{D}(\Omega) \qquad \text{implies} \qquad \langle u, f_n\rangle \to \langle u, f\rangle.$$

Let us start with the most prominent example of all, the infamous Dirac distribution.

Example 3.1.3 (Dirac distribution). Let $\Omega \subset \mathbb{R}^n$ open and $a \in \Omega$. We define

$$\begin{aligned} \delta_a\colon \mathcal{D}(\Omega) &\to \mathbb{C} \\ \varphi &\mapsto \varphi(a). \end{aligned}$$

Then δ_a is a distribution, the *Dirac distribution* in a. Indeed, let $f_n \to f$ in $\mathcal{D}(\Omega)$. A fortiori, one has $f_n(a) \to f(a)$ which shows $\langle \delta_a, f_n\rangle \to \langle \delta_a, f\rangle$.

One has the following useful criterion for a linear functional $u\colon \mathcal{D}(\Omega) \to \mathbb{C}$ to be a distribution.

Proposition 3.1.4. *Let $u\colon \mathcal{D}(\Omega) \to \mathbb{C}$ be linear. Then u is a distribution if and only if for every compact subset $K \subset \Omega$ there exists a constant $C_K \geq 0$ and $n \in \mathbb{N}$ such that*

$$|\langle u, \varphi\rangle| \leq C_K \sum_{|\alpha|\leq n} \|\partial^\alpha \varphi\|_\infty \qquad \text{for all } \varphi \in \mathcal{D}(\Omega) \text{ with } \operatorname{supp}\varphi \subset K.$$

Let us apply the criterion to some concrete and important examples of distributions.

Example 3.1.5 (Principal value). Let $\Omega = \mathbb{R}$. We define

$$\begin{aligned} \operatorname{PV}\left(\frac{1}{x}\right)\colon \mathcal{D}(\mathbb{R}) &\to \mathbb{C} \\ \varphi &\mapsto \lim_{\varepsilon\downarrow 0} \int_{|x|\geq\varepsilon} \frac{\varphi(x)}{x}\, dx. \end{aligned}$$

Note that for $\varphi \in \mathcal{D}(\Omega)$ one has

$$\lim_{\varepsilon\downarrow 0} \int_{|x|\geq\varepsilon} \frac{\varphi(x)}{x}\, dx = \lim_{\varepsilon\to 0} \int_\varepsilon^\infty \frac{\varphi(x) - \varphi(-x)}{x}\, dx.$$

Note that the integrand can be extended to a continuous function on $\mathbb{R}$ by setting its value at zero to $2\varphi'(0)$. Together with the compactness of the support of φ it follows that the improper integral exists. Let $K \subset \mathbb{R}$ be compact. Applying the mean value theorem, we obtain for $\varphi \in \mathcal{D}(\Omega)$ with $\operatorname{supp}\varphi \subset K$

$$\left| \int_0^\infty \frac{\varphi(x) - \varphi(-x)}{x}\, dx \right| \leq 2 \int_0^\infty \sup_{x\in\mathbb{R}} \left|\varphi'(x)\right| dx \leq 2\lambda(K) \sup_{x\in\mathbb{R}} \left|\varphi'(x)\right|.$$

Hence, Proposition 3.1.4 shows that $\mathrm{PV}(1/x)$ is a distribution.

The space of locally integrable functions can be naturally identified with a subspace of the space of distributions.

Example 3.1.6 (Locally integrable functions). Let $\Omega \subset \mathbb{R}^n$ be open. For $f \in L^1_{\mathrm{loc}}(\Omega)$ consider the linear functional $u_f \colon \mathcal{D}(\Omega) \to \mathbb{C}$ defined via

$$\langle u_f, \varphi \rangle \coloneqq \int_\Omega f(x)\varphi(x)\, dx.$$

This is well-defined because f is integrable over compact subsets of Ω. Moreover, one has for $\varphi \in \mathcal{D}(\Omega)$ with $\operatorname{supp}\varphi \subset K$ for some $K \subset \Omega$ compact

$$|\langle u, \varphi \rangle| \leq \sup_{x\in\Omega} |\varphi(x)| \int_K |f(x)|\, dx.$$

This shows that u_f is a distribution. Moreover, it follows from the Du Bois-Reymond lemma (Lemma 2.1.25) that the mapping $f \mapsto u_f$ from $L^1_{\mathrm{loc}}(\Omega)$ into the space of distributions is injective.

Along the same line one can identify finite Borel measures with distributions.

Example 3.1.7 (Borel measures). Let $\Omega \subset \mathbb{R}^n$ be open and $\mu \colon \mathcal{B}(\Omega) \to \mathbb{C}$ be a locally finite Borel measure, i.e. $\mu(K) < \infty$ for all compact subsets $K \subset \Omega$. Consider the functional $u_\mu \colon \mathcal{D}(\Omega) \to \mathbb{C}$ defined via

$$\langle u_\mu, \varphi \rangle \coloneqq \int_\Omega \varphi\, d\mu.$$

Then u_μ is a distribution because for $\varphi \in \mathcal{D}(\Omega)$ with $\operatorname{supp}\varphi \subset K$ one has

$$|\langle u_\mu, \varphi \rangle| \leq \sup_{x\in K} |\varphi(x)| \int_K d\mu = \sup_{x\in\Omega} |\varphi(x)|\, \mu(K).$$

One can show that the embedding $\mu \mapsto u_\mu$ from the locally finite Borel measures into the space of distributions is injective. This can be seen as a stronger

variant of the Du Bois-Reymond lemma (Lemma 2.1.25) as every locally integrable function defines a locally finite Borel measure. The injectivity essentially is a generalized version of the Riesz–Markov representation theorem: there is a one-to one correspondence between positive linear functionals on $\mathcal{D}(\Omega)$ and locally finite Borel measures on Ω.

Now, that we have got a basic feeling for distributions, we introduce a notion of convergence on the space of all distributions.

Definition 3.1.8. Let $\Omega \subset \mathbb{R}^n$ be open. We denote by $\mathcal{D}'(\Omega)$ the *space of all distributions*. We say that a sequence of distributions $(u_n)_{n\in\mathbb{N}}$ converges to $u \in \mathcal{D}'(\Omega)$ in $\mathcal{D}'(\Omega)$ if

$$\lim_{n\to\infty} \langle u_n, \varphi\rangle = \langle u, \varphi\rangle \qquad \text{for all } \varphi \in \mathcal{D}(\Omega).$$

Again, we do not define a topology on the space of distributions. However, if you are more interested in these issues, read the next remarks. Otherwise simply ignore it.

Remark 3.1.9 (For experts). The notation $\mathcal{D}'(\Omega)$ for the space of distributions actually has a deeper mathematical meaning. It stands for the topological dual of the space $\mathcal{D}(\Omega)$, i.e. the space of all continuous linear functionals on $\mathcal{D}(\Omega)$. The above definition says that a sequence of distributions converges in $\mathcal{D}'(\Omega)$ if and only it converges with respect to the weak*-topology. However, for deeper results on distributions it may be more suitable to not endow $\mathcal{D}'(\Omega)$ with the weak*-topology. Indeed, often $\mathcal{D}'(\Omega)$ is defined with a different topology (the so-called strong topology) which however agrees on bounded sets (note that we have and will not define the notion of boundedness on topological vector spaces) with the weak*-topology. Hence, the notion of convergence of sequences is independent of the choice between these topologies.

In physics (and also in mathematics) one often works with approximating δ-functions. In our newly introduced language this simply means that the δ-distribution can be written as the limit of ordinary functions in the space of distributions.

Example 3.1.10 (Approximations of the δ-distribution). Let f be a positive and normalized function in $L^1(\mathbb{R})$. We define $f_n(x) = nf(nx)$. Then one has

$$\int_{-\infty}^{\infty} f_n(x)\,dx = \int_{-\infty}^{\infty} f(x)\,dx = 1$$

for all $n \in \mathbb{N}$. Suppose further that for all $\varepsilon > 0$ one has

$$\lim_{n\to\infty} \int_{|x|\geq\varepsilon} f_n(x)\,dx = 0.$$

This means that the masses of the functions f_n concentrate on arbitrary small intervals as n goes to infinity. Under these assumptions one has $f_n \to \delta_0$ in $\mathcal{D}'(\Omega)$. Indeed, for $\varphi \in \mathcal{D}(\Omega)$ one has

$$\begin{aligned}|\langle \delta_0, \varphi\rangle - \langle f_n, \varphi\rangle| &= \left|\varphi(0) - \int_{-\infty}^{\infty} f_n(x)\varphi(x)\,dx\right| = \left|\int_{\infty}^{\infty} f_n(x)(\varphi(0)-\varphi(x))\,dx\right| \\ &\leq \int_{-\infty}^{\infty} f_n(x)\,|\varphi(0)-\varphi(x)|\,dx\end{aligned}$$

and therefore one obtains for all $\varepsilon > 0$

$$\begin{aligned}\limsup_{n\to\infty} |\langle \delta_0, \varphi\rangle - \langle f_n, \varphi\rangle| &\leq \limsup_{n\to\infty} \sup_{x\in[-\varepsilon,\varepsilon]} |\varphi(0)-\varphi(x)| \int_{|x|\leq\varepsilon} f_n(x)\,dx \\ &\leq \sup_{x\in[-\varepsilon,\varepsilon]} |\varphi(0)-\varphi(x)|.\end{aligned}$$

Since φ is continuous, the right hand side tends to zero as $\varepsilon \to 0$. Hence, we have shown that f_n converges to the delta distribution in the sense of distributions. As concrete examples of approximations one for example has for $f(x) = (\pi)^{-1/2}e^{-x^2}$ and $g(x) = \pi^{-1}(1+x^2)^{-1}$

$$f_n(x) = \frac{n}{\sqrt{\pi}}\exp(-(nx)^2) \quad \text{and} \quad g_n(x) = \frac{1}{\pi}\frac{n}{1+(nx)^2}$$

or using the substitution $\varepsilon(n) = n^{-1/2}$ one obtains the approximations for $\varepsilon = \varepsilon(n) \to 0$

$$f_\varepsilon(x) = \frac{1}{\sqrt{\pi\varepsilon}}\exp\left(-\frac{x^2}{\varepsilon}\right) \quad \text{and} \quad g_\varepsilon(x) = \frac{1}{\pi}\frac{\varepsilon}{\varepsilon^2+x^2}.$$

The main advantage of distributions is that classical analytical operations like taking derivatives have very well-behaved extensions to distributions. Indeed, these operations are bounded with respect to the topology of distributions and therefore by density can be extended from $\mathcal{D}(\Omega)$ to $\mathcal{D}'(\Omega)$. However, it is more practical to define the extensions directly by using duality.

Definition 3.1.11. Let $\Omega \subset \mathbb{R}^n$ be open and $u \in \mathcal{D}'(\Omega)$. For $\alpha \in \mathbb{N}_0^n$ we define the *α-th derivative of u* as

$$\langle D^\alpha u, \varphi\rangle = (-1)^{|\alpha|}\langle u, \partial^\alpha \varphi\rangle \qquad \text{for } \varphi \in \mathcal{D}(\Omega).$$

Clearly, this is well-defined, i.e. $D^\alpha u$ is a distribution. Note that the above definition extends the concept of weak derivatives in the context of Sobolev spaces given in Definition 2.1.20. We now give some elementary examples of derivatives of distributions which are often used in physics.

Example 3.1.12 (Derivative of the delta function). Consider the Dirac distribution $\delta_0 \in \mathcal{D}'(\mathbb{R})$. For $\varphi \in \mathcal{D}(\Omega)$ and $n \in \mathbb{N}$ one has

$$\langle D^n \delta_0, \varphi \rangle = (-1)^n \langle \delta_0, D^n \varphi \rangle = (-1)^n \frac{\partial^n \varphi}{\partial^n x}(0).$$

Hence, the distributional derivative of the Dirac distribution is given by $(-1)^n$ times the evaluation of the n-th derivative at zero.

Example 3.1.13 (Derivative of the signum function). We come back to the signum function considered in Example 2.1.22. As we have seen this function does not have a derivative in the sense of Sobolev spaces. However, considered as a distribution we have for $\varphi \in \mathcal{D}(\mathbb{R})$

$$\begin{aligned}\langle D \operatorname{sign}, \varphi \rangle &= -\langle \operatorname{sign}, \varphi' \rangle = -\int_{-\infty}^{\infty} \operatorname{sign}(x) \varphi'(x)\, dx = \int_{-\infty}^{0} \varphi'(x)\, dx - \int_{0}^{\infty} \varphi'(x)\, dx \\ &= \varphi(0) - (-\varphi(0)) = 2\langle \delta_0, \varphi \rangle\end{aligned}$$

Hence, the distributional derivative of sign is given by two times the Dirac distribution.

Remark 3.1.14 (Non-commuting derivatives). It is a well-known fact from real analysis that there exist continuous functions $f : \mathbb{R}^2 \to \mathbb{R}$ which are twice differentiable and satisfy $D_x D_y f \neq D_y D_x f$, i.e. the mixed partial derivatives do not commute. For example, take $f : \mathbb{R}^2 \to \mathbb{R}$ defined as

$$f(x,y) = \begin{cases} \frac{xy(x^2-y^2)}{x^2+y^2} & \text{if } (x,y) \neq (0,0) \\ 0 & \text{if } (x,y) = (0,0). \end{cases}$$

However, the situation changes when one considers f as a distribution. Now it follows from the mere definition of the derivative and the fact that the order of differentiation can be changed for smooth functions that for all $\varphi \in \mathcal{D}(\mathbb{R})$

$$\langle D_x D_y f, \varphi \rangle = \langle f, D_x D_y \varphi \rangle = \langle f, D_y D_x \varphi \rangle = \langle D_y D_x f, \varphi \rangle.$$

Hence, $D_x D_y f = D_y D_x f$ as elements in $\mathcal{D}'(\mathbb{R})$. In particular this means that if $D_x D_y f$ and $D_y D_x f$ exist in the classical sense and define $L^1_{\mathrm{loc}}(\mathbb{R}^n)$ functions, then one has a consequence of the Du Bois-Reymond lemma (Lemma 2.1.25) that $D_x D_y f = D_y D_x f$ almost everywhere.

We now want to define the multiplication of distributions with smooth functions. For this note that for $m \in C^\infty(\Omega)$, a function $f \in L^1_{\mathrm{loc}}(\Omega)$ and a test function $\varphi \in \mathcal{D}(\Omega)$ we have

$$\langle u_{mf}, \varphi \rangle = \int_\Omega m(x) f(x) \varphi(x)\, dx = \int_\Omega f(x) m(x) \varphi(x) = \langle u_f, m \cdot \varphi \rangle.$$

Note that if $\varphi \in \mathcal{D}(\Omega)$ and m is smooth, then the product $m \cdot \varphi$ is again a test function. This allows us to extend the above identity as a definition to general distributions.

Definition 3.1.15 (Multiplication of distributions with smooth functions). Let $u \in \mathcal{D}'(\Omega)$ be a distribution and $m \in C^\infty(\Omega)$. Then their product is the distribution defined via

$$\langle m \cdot u, \varphi \rangle = \langle u, m \cdot \varphi \rangle \qquad \text{for } \varphi \in \mathcal{D}(\Omega).$$

Note that one sees directly that $m \cdot u$ is linear and continuous and therefore a well-defined distribution. Let us give a very elementary example to see how one works with such multiplications.

Example 3.1.16. Let $\delta_0 \in \mathcal{D}'(\mathbb{R})$ be the Dirac distribution and let $m \colon \mathbb{R} \to \mathbb{R}$ be an arbitrary smooth function. Then we have for $\varphi \in \mathcal{D}(\mathbb{R})$

$$\langle m\delta_0, \varphi \rangle = \langle \delta_0, m\varphi \rangle = m(0)\varphi(0) = \langle m(0)\delta_0, \varphi \rangle.$$

Hence, we have $m\delta_0 = m(0)\delta_0$ as one would intuitively expect. However, things can also be slightly more complicated. For example, one has

$$\begin{aligned} \langle m\delta_0', \varphi \rangle &= \langle \delta_0', m\varphi \rangle = -\langle \delta_0, (m\varphi)' \rangle = -m'(0)\varphi(0) - m(0)\varphi'(0) \\ &= \langle -m'(0)\delta_0, \varphi \rangle + \langle m(0)\delta_0', \rangle. \end{aligned}$$

Hence, $m \cdot \delta_0' = -m'(0)\delta_0 + m(0)\delta_0'$.

3.2 Tempered Distributions

We now come to a special class of distributions, the so-called tempered distributions. These are the right space for extending the theory of Fourier transform to distributions and are moreover even easier to handle from a technical perspective. For the tempered distributions we work with a different class of test functions than $\mathcal{D}(\Omega)$, namely the Schwartz functions.

Definition 3.2.1 (Schwartz functions). Let $n \in \mathbb{N}$. For $\alpha, \beta \in \mathbb{N}_0^n$ and a smooth function $f \in C^\infty(\mathbb{R}^n)$ we define

$$\|f\|_{\alpha,\beta} \coloneqq \sup_{x \in \mathbb{R}^n} |x^\alpha D^\beta f(x)|.$$

We then define the *Schwartz space* or the *space of all rapidly decreasing functions* as

$$\mathcal{S}(\mathbb{R}^n) \coloneqq \{f \in C^\infty(\mathbb{R}^n) : \|f\|_{\alpha,\beta} < \infty \text{ for all } \alpha, \beta \in \mathbb{N}_0^n\}.$$

More intuitively, the above definition means that f and all of its derivatives exist and decay faster than any inverse power of x. As for the test functions $\mathcal{D}(\Omega)$ we need a notion of convergence for Schwartz functions.

Definition 3.2.2 (Convergence of Schwartz functions). We say that a sequence of Schwartz functions $(f_m)_{m\in\mathbb{N}} \subset \mathcal{S}(\mathbb{R}^n)$ converges to $f \in \mathcal{S}(\mathbb{R}^n)$ if $\|f_m - f\|_{\alpha,\beta} \to 0$ for all $\alpha, \beta \in \mathbb{N}_0^n$.

It is a good exercise to check that $(f_m)_{m\in\mathbb{N}} \subset \mathcal{S}(\mathbb{R}^n)$ tends to $f \in \mathcal{S}(\mathbb{R}^n)$ as $m \to \infty$ if and only if $(f_m)_{m\in\mathbb{N}}$ converges to f with respect to the metric

$$d(f,g) := \sum_{\alpha,\beta\in\mathbb{N}_0^n} 2^{-(|\alpha|+|\beta|)} \frac{\|f-g\|_{\alpha,\beta}}{1+\|f-g\|_{\alpha,\beta}} \qquad (f,g \in \mathcal{S}(\mathbb{R}^n)).$$

Moreover, one can show that $(\mathcal{S}(\mathbb{R}^n), d)$ is a complete metric space. These properties show in mathematical terms that $\mathcal{S}(\mathbb{R}^n)$ is a so-called *Fréchet space*. Let us give the exact definition for later use. First we need the concept of a semi-norm which we have already met in our study of $\mathcal{L}^p$-spaces.

Definition 3.2.3 (Semi-norm). Let V be a $\mathbb{K}$-vector space. A map $p\colon V \to [0,\infty)$ is called a *semi-norm* on V if

(i) p is homogeneous, i.e. $p(\lambda x) = \lambda p(x)$ for all $x \in V$ and $\lambda \in \mathbb{K}$;

(ii) p satisfies the triangle inequality, i.e. $p(x+y) \le p(x)+p(y)$ for all $x, y \in V$.

Hence, the only difference between a norm and a semi-norm is the fact that a semi-norm p may not satisfy the definiteness condition $p(x) = 0 \Leftrightarrow x = 0$. Fréchet spaces are defined in terms of a countable family of semi-norms.

Definition 3.2.4 (Fréchet space). Let $\mathcal{G}$ be a vector space and $(p_k)_{k\in\mathbb{N}}$ a countable family of semi-norms on $\mathcal{G}$ with the following properties:

(i) If $x \in \mathcal{G}$ satisfies $p_k(x) = 0$ for all $k \in \mathbb{N}$, then $x = 0$.

(ii) If $(x_n)_{n\in\mathbb{N}} \subset \mathcal{G}$ is Cauchy with respect to each semi-norm p_k, i.e. for all $k \in \mathbb{N}$ and for all $\varepsilon > 0$ there exists $N \in \mathbb{N}$ such that

$$p_k(x_n - x_m) < \varepsilon \qquad \text{for all } n, m \ge N,$$

then there exists $x \in \mathcal{G}$ such that $(x_n)_{n\in\mathbb{N}}$ converges to x with respect to each semi-norm, i.e. $p_k(x_n - x) \to 0$ as $n \to \infty$ for all $k \in \mathbb{N}$.

Then $\mathcal{G}$ together with the datum of these semi-norms is called a *Fréchet space*. In this case $(\mathcal{G}, d)$ is a complete metric space for the metric

$$d(f,g) := \sum_{k=1}^{\infty} 2^{-k} \frac{\|f-g\|_k}{1+\|f-g\|_k} \qquad (f,g \in \mathcal{G}).$$

If $\mathcal{G}$ is a Fréchet space, we agree that all topological notions such a convergence, closedness or compactness or understood with respect to the metric induced by the family of semi-norms.

Remark 3.2.5. One can always replace the family $(p_k)_{k\in\mathbb{N}}$ by a family of increasing semi-norms $(q_k)_{k\in\mathbb{N}}$ by setting $q_k = \sup_{n\leq k} q_n$. In fact, the family $(q_k)_{k\in\mathbb{N}}$ induces an equivalent metric on $\mathcal{G}$ and we are only interested in the topological properties and not on the concrete values of the metric itself. Hence, we may assume that the semi-norms satisfy

$$q_1(x) \leq q_2 \leq q_3(x) \leq \cdots \qquad \text{for all } x \in \mathcal{G}.$$

Note that in contrast to this situation for $\mathcal{S}(\mathbb{R}^n)$ one can show that the convergence in $\mathcal{D}(\Omega)$ for $\emptyset \neq \Omega \subset \mathbb{R}^n$ is not induced by a translation-invariant metric.

As for distributions we define the tempered distributions as the space of all continuous functionals on $\mathcal{S}(\mathbb{R}^n)$.

Definition 3.2.6 (Tempered distribution). A *tempered distribution* is a continuous linear functional $u\colon \mathcal{S}(\mathbb{R}^n) \to \mathbb{C}$. The space of all tempered distributions is denoted by $\mathcal{S}'(\mathbb{R}^n)$. We say that a sequence of tempered distributions $(u_m)_{m\in\mathbb{N}} \subset \mathcal{S}'(\mathbb{R}^n)$ converges to $u \in \mathcal{S}'(\mathbb{R}^n)$ if

$$\langle u_m, \varphi\rangle \to \langle u, \varphi\rangle \qquad \text{for all } \varphi \in \mathcal{S}(\mathbb{R}^n).$$

All comments made for distributions also apply to tempered distributions: the definition of convergence of tempered distributions means in mathematical terms that we endow the space of tempered distributions with the weak*-topology. Notice further that with almost the identical proofs one can see that locally integrable functions define tempered distributions as long as they have polynomial growth. A similar statement also holds for measures. Moreover, distributional derivatives of tempered distributions are tempered distributions and the product of a function with polynomial growth and a tempered distribution is a tempered distribution as well.

For an example of a distribution in $\mathcal{D}'(\mathbb{R})$ which is not tempered one can take u_f for $f(x) = e^{|x|}$.

3.2.1 The Fourier Transform of Tempered Distributions

Now let us come to the Fourier transform of tempered distributions which will ultimately allow us to take for example the Fourier transform of Delta-functions. For this we first need to understand the Fourier transform on Schwartz functions.

Proposition 3.2.7 (Fourier transform on Schwartz functions). *For all $n \in \mathbb{N}$ the Fourier transform restricts to a bijection of $\mathcal{S}(\mathbb{R}^n)$. Moreover, one has $\mathcal{F} f_m \to \mathcal{F} f$ in $\mathcal{S}(\mathbb{R}^n)$ if $f_m \to f$ in $\mathcal{S}(\mathbb{R}^n)$.*

This follows from the fact that under the Fourier transform differentiation becomes multiplication. The details should be verified by the reader. Note that moreover for Schwartz functions $f, \varphi \in \mathcal{S}(\mathbb{R}^n)$ we have by Plancherel's formula (Theorem 2.1.34)

$$\begin{aligned}\langle u_{\mathcal{F}f}, \varphi\rangle &= \int_{\mathbb{R}^n} (\mathcal{F}f)(x)\varphi(x)\,dx = \int_{\mathbb{R}^n} f(x)\overline{(\mathcal{F}^{-1}\overline{\varphi})}(x)\,dx = \int_{\mathbb{R}^n} f(x)(\mathcal{F}\varphi)(x)\,dx \\ &= \langle u_f, \mathcal{F}\varphi\rangle.\end{aligned}$$

This equality can now be used to extend the Fourier transform to tempered distributions.

Definition 3.2.8 (The Fourier transform of tempered distributions). Let $u \in \mathcal{S}'(\mathbb{R}^n)$ be a tempered distribution. Its Fourier transform is defined as

$$\langle \mathcal{F}u, \varphi\rangle = \langle u, \mathcal{F}\varphi\rangle \qquad \text{for } \varphi \in \mathcal{S}(\mathbb{R}^n).$$

Note that since the Fourier transform is continuous on $\mathcal{S}(\mathbb{R}^n)$ by Proposition 3.2.7, $\mathcal{F}u$ is a well-defined tempered distribution. Further, the Fourier transform on the tempered distribution is a bijection.

Proposition 3.2.9. *The Fourier transform $\mathcal{F}\colon \mathcal{S}'(\mathbb{R}^n) \to \mathcal{S}'(\mathbb{R}^n)$ is one-to-one. Its inverse is given by the extension of the inverse Fourier transform via*

$$\langle \mathcal{F}^{-1}u, \varphi\rangle := \langle u, \mathcal{F}^{-1}\varphi\rangle \qquad \textit{for } \varphi \in \mathcal{S}(\mathbb{R}^n).$$

Proof. As in the case of the Fourier transform, one has a well-defined mapping $\mathcal{F}^{-1}\colon \mathcal{S}'(\mathbb{R}^n) \to \mathcal{S}'(\mathbb{R}^n)$. We now show that as the notation already indicates that $\mathcal{F}^{-1}$ is the inverse of $\mathcal{F}$. In fact, we have for $u \in \mathcal{S}'(\mathbb{R}^n)$ and $\varphi \in \mathcal{S}(\mathbb{R}^n)$ using the mere definitions

$$\langle \mathcal{F}^{-1}\mathcal{F}u, \varphi\rangle = \langle \mathcal{F}u, \mathcal{F}^{-1}\varphi\rangle = \langle u, \mathcal{F}\mathcal{F}^{-1}\varphi\rangle = \langle u, \varphi\rangle.$$

This shows that $\mathcal{F}^{-1}\mathcal{F} = \mathrm{Id}_{\mathcal{S}'(\mathbb{R}^n)}$. An analogous calculation also shows that $\mathcal{F}\mathcal{F}^{-1} = \mathrm{Id}_{\mathcal{S}'(\mathbb{R}^n)}$. □

Let us now give some examples which are particularly relevant for physics.

Example 3.2.10 (Fourier transform of Delta function). Let us calculate the Fourier transform of the Delta distribution δ_0. For this observe that for all $\varphi \in \mathcal{S}(\mathbb{R}^n)$ we have

$$\langle \mathcal{F}\delta_0, \varphi\rangle = \langle \delta_0, \mathcal{F}\varphi\rangle = (\mathcal{F}\varphi)(0) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} \varphi(x)\,dx = (2\pi)^{-n/2}\langle \mathbb{1}, \varphi\rangle.$$

Hence, we have shown that $\mathcal{F}\delta_0 = (2\pi)^{-n/2}\mathbb{1}$. Physically this means that one obtains the delta function if one takes all frequencies with equal (normalized) strength.

Essentially in the converse direction, let us take a look at the Fourier transform of planes waves.

Example 3.2.11 (Fourier transform of plane wave). For $k \in \mathbb{R}$ consider the plain wave $f(x) = e^{ikx} \in L^1_{\mathrm{loc}}(\mathbb{R}^n)$. By the Fourier inversion formula we obtain for all $\varphi \in \mathcal{S}(\mathbb{R}^n)$

$$\begin{aligned}\langle \mathcal{F}f, \varphi\rangle = \langle f, \mathcal{F}\varphi\rangle &= \int_{\mathbb{R}^n} f(x)(\mathcal{F}\varphi)(x)\,dx = \int_{\mathbb{R}^n} e^{ikx}(\mathcal{F}\varphi)(x)\,dx \\ &= (2\pi)^{n/2}(\mathcal{F}^{-1}\mathcal{F}\varphi)(k) = (2\pi)^{n/2}\varphi(k) = \langle (2\pi)^{n/2}\delta_k, \varphi\rangle.\end{aligned}$$

Hence, we have shown that $\mathcal{F}(e^{ik\cdot}) = (2\pi)^{n/2}\delta_k$. Physically this gives the obvious fact that one obtains a plain wave if one picks a single frequency (via a delta-distribution).

We now shortly sketch an application of tempered distributions to differential operators, a topic which is often used in physics courses. As a starting point we define linear differential operators with constant coefficients, the class of differential operators to be considered from now on.

Definition 3.2.12 (Linear differential operator with constant coefficients). Let $n \in \mathbb{N}$. A linear operator $L\colon C^\infty(\mathbb{R}^n) \to C^\infty(\mathbb{R}^n)$ is called a *linear differential operator with constant coefficients* if there exists a polynomial P in n variables such that

$$Lf = P\left(\frac{\partial}{\partial x_1}, \ldots, \frac{\partial}{\partial x_n}\right) f \qquad \text{for all } f \in C^\infty(\mathbb{R}^n).$$

Of course, the Laplace operator is an example of a differential operator with constant coefficients. Such differential operators can be treated very well with the help of distributions. An important concept here is that of a fundamental solution.

Definition 3.2.13 (Fundamental solution). Let L be a linear differential operator with constant coefficients. A distribution $u \in \mathcal{D}'(\mathbb{R}^n)$ is called a *fundamental solution* for L if u satisfies

$$Lu = \delta_0.$$

One may wonder if fundamental solutions do exist at all. This is indeed not the case for general differential operators. However, the Malgrange–Ehrenpreis theorem states that every non-zero linear differential operator with constant coefficients has a fundamental solution.

In order to apply fundamental solutions to the study of differential equations, we need to define convolutions of tempered distributions with Schwartz functions. For this consider first three Schwartz functions $f, g, \varphi \in \mathcal{S}(\mathbb{R}^n)$. Let us set $\tilde{g}(x) = g(-x)$. Then we have

$$\begin{aligned}\langle u_{f*g}, \varphi\rangle &= \int_{\mathbb{R}^n} (f*g)(x)\varphi(x)\,dx = \int_{\mathbb{R}^n}\int_{\mathbb{R}^n} f(y)g(x-y)\,dy\varphi(x)\,dx \\ &= \int_{\mathbb{R}^n}\int_{\mathbb{R}^n} g(x-y)\varphi(x)\,dx f(y)\,dy = \int_{\mathbb{R}^n}\int_{\mathbb{R}^n} \tilde{g}(y-x)\varphi(x)\,dx f(y)\,dy \\ &= \langle u_f, \tilde{g}*\varphi\rangle.\end{aligned}$$

Again, the right hand side makes sense if u_f is replaced by an arbitrary tempered distribution $u \in \mathcal{S}'(\mathbb{R}^n)$ because one can verify that the convolution of two Schwartz functions is again a Schwartz function. Therefore it can be used to extend the definition of convolutions of tempered distributions with Schwartz functions.

Definition 3.2.14 (Convolution of tempered distributions with Schwartz functions). Let $u \in \mathcal{S}'(\mathbb{R}^n)$ and $g \in \mathcal{S}(\mathbb{R}^n)$. Then $u*g$ is the distribution which for $\varphi \in \mathcal{S}(\mathbb{R}^n)$ is defined as

$$\langle u*g, \varphi\rangle = \langle u, \tilde{g}*\varphi\rangle.$$

Note that for $u*g$ to be a well-defined distribution, we need that $u*g$ is a continuous functional, a fact which should be checked by the reader. The usefulness of fundamental solutions lies in the following observation.

Proposition 3.2.15. *Let $n \in \mathbb{N}$ be fixed and $L\colon C^\infty(\mathbb{R}^n) \to C^\infty(\mathbb{R}^n)$ be linear differential operator with constant coefficients. Further, let $u \in \mathcal{S}'(\mathbb{R}^n)$ be a fundamental solution for L. Then for $f \in \mathcal{S}(\mathbb{R}^n)$ a distributional solution of the inhomogeneous problem*

$$Lw = f$$

is given by the convolution $w = u*f$.

Proof. The statement follows by a direct calculation. Let $L = P(\partial_1, \dots, \partial_n)$ and L^* the adjoint obtained by replacing ∂_i by $-\partial_i$ for all $i = 1, \dots, n$. Then for $\varphi \in \mathcal{S}(\mathbb{R}^n)$ we have

$$\begin{aligned}\langle Lw, \varphi\rangle &= \langle L(u*f), \varphi\rangle = \langle u*f, L^*\varphi\rangle = \langle u, \tilde{f}*L^*\varphi\rangle = \langle u, L^*(\tilde{f}*\varphi)\rangle = \langle Lu, \tilde{f}*\varphi\rangle \\ &= \langle \delta_0, \tilde{f}*\varphi\rangle = (\tilde{f}*\varphi)(0) = \int_{\mathbb{R}^n} f(y)\varphi(y)\,dy = \langle f, \varphi\rangle.\end{aligned}$$

This shows that $Lw = f$ and finishes the proof. □

We now show for the example of the three dimensional Laplace operator how a fundamental solution for a linear differential operator with constant coefficients can in principle be obtained.

Example 3.2.16 (Laplace operator in three dimensions). Let $L = \Delta$ be the Laplace operator in $\mathbb{R}^3$. Suppose that $u \in \mathcal{S}'(\mathbb{R}^3)$ is a fundamental solution for Δ, i.e. $\Delta u = \delta_0$. Taking Fourier transforms on both sides we obtain for $\varphi \in \mathcal{S}(\mathbb{R}^3)$

$$\begin{aligned}\langle (2\pi)^{-3/2}\mathbb{1}, \varphi\rangle &= \langle \mathcal{F}(\delta_0), \varphi\rangle = \langle \mathcal{F}(\Delta u), \varphi\rangle = \langle \Delta u, \mathcal{F}\varphi\rangle = \langle u, \Delta\mathcal{F}\varphi\rangle \\ &= \langle u, \mathcal{F}(-|\cdot|^2\,\varphi(\cdot))\rangle = \langle \mathcal{F}u, -|\cdot|^2\,\varphi(\cdot)\rangle = \langle -|x|^2\,\mathcal{F}u, \varphi\rangle.\end{aligned}$$

Hence, $(2\pi)^{-3/2}\mathbb{1} = -|x|^2\,\mathcal{F}u$ almost everywhere. Therefore we can try the choice $(\mathcal{F}u)(x) = -(2\pi)^{-3/2}\,|x|^{-2}$. Since the Fourier transform is a bijection on the space of tempered distributions, this equation is equivalent to $u = -(2\pi)^{-3/2}\mathcal{F}^{-1}(|x|^{-2})$. Note that

$$\int_{|x|\le R} \frac{1}{|x|^2}\,dx = \int_0^R \int_{\mathbb{S}^2} r^{-2} r^2\,d\theta\,dr = 4\pi R < \infty.$$

This shows that $x \mapsto |x|^{-2} \in L^1_{\mathrm{loc}}(\mathbb{R}^3)$. Therefore its Fourier transform exists in the sense of tempered distributions. Moreover, one has $|x|^{-2}\,\mathbb{1}_{B(0,R)} \to |x|^{-2}$ in $\mathcal{S}'(\mathbb{R}^3)$ as $R \to \infty$. This is a direct consequence of the dominated convergence theorem. By the continuity of the Fourier transform, we therefore obtain $\mathcal{F}^{-1}\,|x|^{-2}\,\mathbb{1}_{B(0,R)} \to \mathcal{F}^{-1}\,|x|^{-2}$ as $R \to \infty$. Hence for $\varphi \in \mathcal{S}(\mathbb{R}^n)$, we can determine the action of u on φ via the calculation

$$\begin{aligned}\langle u, \varphi\rangle &= \langle (2\pi)^{-3/2}\mathcal{F}^{-1}(-|\cdot|^{-2}), \varphi\rangle = -\lim_{R\to\infty} \langle (2\pi)^{-3/2}\mathcal{F}^{-1}(|\cdot|^{-2}\,\mathbb{1}_{B(0,R)}), \varphi\rangle \\ &= -\lim_{R\to\infty} (2\pi)^{-3/2}\langle |\cdot|^{-2}\,\mathbb{1}_{B(0,R)}, \mathcal{F}^{-1}\varphi\rangle \\ &= -\lim_{R\to\infty} (2\pi)^{-3/2} \int_{\mathbb{R}^3} |x|^{-2}\,\mathbb{1}_{B(0,R)}(x)(\mathcal{F}^{-1}\varphi)(x)\,dx \\ &= -\frac{1}{(2\pi)^3}\lim_{R\to\infty} \int_{|x|\le R} |x|^{-2} \int_{\mathbb{R}^3} \varphi(y) e^{ixy}\,dy\,dx \\ &= -\frac{1}{(2\pi)^3}\lim_{R\to\infty} \int_{\mathbb{R}^3}\int_{|x|\le R} |x|^{-2}\,e^{ixy}\,dx\varphi(y)\,dy.\end{aligned}$$

We now deal with the inner integral. For $R > 0$ we have by change of coordinates

$$\int_{|x|\le R}\int_{\mathbb{S}^2} |x|^{-2}\,e^{ixy}\,dx = \int_0^R \int_{\mathbb{S}^2} r^{-2} e^{ir\theta y}\,d\theta r^2\,dr = \int_0^R \int_{\mathbb{S}^2} \cos(r\theta y)\,d\theta\,dr.$$

Let us again first take a look at the inner integral. The following argument holds for all $r > 0$ and $|y| \neq 0$: Choose an orthogonal matrix O such that $Oe_z =$

$y/|y|$. Then using the substitution $s = \theta_z = \cos\varphi$ (in spherical coordinates with $\varphi \in [0,\pi)$) and consequently $\frac{d\varphi}{ds} = (\arccos s)' = -1/\sqrt{1-s^2}$, we obtain

$$\begin{aligned}\int_{\mathbb{S}^2} \cos(r\theta y)\,d\theta &= \int_{\mathbb{S}^2} \cos(r|y|\theta\cdot Oe_z)\,d\theta = \int_{\mathbb{S}^2} \cos(r|y|O^{-1}\theta\cdot e_z)\,d\theta \\ &= \int_{\mathbb{S}^2} \cos(r|y|\theta\cdot e_z)\,d\theta = \int_{\mathbb{S}^2} \cos(r|y|\theta_z)\,d\theta \\ &= -\int_{-1}^{1}\int_{\sqrt{1-s^2}\mathbb{S}^1} d\alpha\cos(r|y|s)\frac{ds}{\sqrt{1-s^2}} = -2\pi\int_{-1}^{1}\cos(r|y|s)\,ds \\ &= -2\pi\left[\frac{\sin(r|y|s)}{r|y|}\right]_{s=-1}^{s=1} = -4\pi\frac{\sin(r|y|)}{r|y|}\end{aligned}$$

Recall the identity $\int_0^\infty \frac{\sin x}{x}\,dx = \pi/2$ for the sinc-function. By the substitution formula we therefore obtain for $|y| \neq 0$

$$\int_0^\infty \frac{\sin(r|y|)}{r|y|}\,dr = \frac{\pi}{2|y|}.$$

Putting all calculations together, we obtain

$$\begin{aligned}\langle u,\varphi\rangle &= \frac{1}{(2\pi)^3}\lim_{R\to\infty}\int_{\mathbb{R}^3}\int_0^R 4\pi\frac{\sin(r|y|)}{r|y|}\,dr\varphi(y)\,dy \\ &= \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3} 2\pi^2\frac{1}{|y|}\varphi(y)\,dy = \frac{1}{4\pi}\int_{\mathbb{R}^3}\frac{1}{|y|}\varphi(y)\,dy\end{aligned}$$

Here we can exchange the limit and the integral with the help of the dominated convergence theorem, where we use the fact that there exists a universal constant $M > 0$ such that

$$\left|\int_0^R \frac{\sin x}{x}\,dx\right| \leq M \text{ for all } R>0 \quad\Rightarrow\quad \left|\int_0^R \frac{\sin ax}{ax}\,dx\right| \leq \frac{M}{a} \text{ for all } a,R>0.$$

Hence, altogether we have shown that $u(y) = (1/4\pi)|y|^{-1}$ is a fundamental solution for the Laplace operator on $\mathbb{R}^3$.

By a similar calculation one can see that an analogue formula holds for the case $n \geq 3$, whereas for $n = 2$ one obtains a logarithmic term.

3.3 The Nuclear Spectral Theorem

We now come back to the considerations related to the spectral theorem. For this let us again consider the momentum operator $A = -i\frac{d}{dx}$ with $D(A) = H^1(\mathbb{R})$. We have seen that the spectrum is given by $\sigma(A) = \mathbb{R}$ and that A has

no eigenvectors in $L^2(\mathbb{R})$. Nevertheless one can find non-square integrable eigenfunctions. In fact, for each $\xi \in \mathbb{R}$ the function $f_\xi(x) = e^{ix\xi} \notin L^2(\mathbb{R})$ satisfies

$$(Af_\xi)(x) = -i \cdot i\xi e^{ix\xi} = \xi e^{ix\xi} = \xi f_\xi(x).$$

Hence, in a generalized sense A has a complete system of generalized eigenfunctions.

A similar argument can also be applied for the position operator M_x. In fact, for $x_0 \in \mathbb{R}$ the delta-distribution $\delta_{x_0} \in \mathcal{S}'(\mathbb{R})$ satisfies in the sense of distributions

$$M_x(\delta_{x_0}) = x \cdot \delta_{x_0} = x_0 \delta_{x_0}.$$

Intuitively, this again means that there exist a complete system of generalized eigenfunctions in a certain sense. One sees however that in order to obtain these eigenfunctions one needs to extend the operator to a larger class of functions or distributions.

3.3.1 Gelfand Triples

This can be formalized with the help of Gelfand triples. For this we must again consider Fréchet spaces (actually, it is more natural to formulate the most concepts in the context of general locally convex topological vector spaces, however we do not want to delve too deeply into this theory). Recall that a *Fréchet space* can be described by a complete metric which is invariant with respect to translations, i.e. one has $d(x+z, y+z) = d(x,y)$ for all $x, y, z \in \mathcal{G}$. All topological notions such as convergence or closedness are understood with respect to this metric. As for Hilbert spaces we now define dual spaces of Fréchet spaces.

Definition 3.3.1 (Dual of Fréchet spaces). Let $\mathcal{G}$ be a Fréchet space. Its *dual space* $\mathcal{G}'$ is defined as

$$\mathcal{G}' := \{\varphi \colon \mathcal{G} \to \mathbb{C} \text{ linear and continuous }\}.$$

We endow $\mathcal{G}'$ with the weak*-topology, i.e. a sequence $(\varphi_n)_{n\in\mathbb{N}} \subset \mathcal{G}'$ satisfies $\varphi_n \to \varphi \in \mathcal{G}'$ if and only if $\varphi_n(g) \to \varphi(g)$ for all $g \in \mathcal{G}$.

Further, consider additionally a Hilbert space $\mathcal{H}$ together with a continuous linear embedding $i \colon \mathcal{G} \to \mathcal{H}$ with dense range. Here continuous as usual means that $x_n \to x$ in $\mathcal{G}$ implies $i(x_n) \to x$ in $\mathcal{H}$. Observe that i induces a continuous *anti-linear* embedding $i^\dagger \colon \mathcal{H} \to \mathcal{G}'$ given by

$$i^\dagger \colon x \mapsto [g \mapsto \langle x | i(g) \rangle].$$

In fact, $g_n \to g$ in $\mathcal{G}$ implies $i(g_n) \to i(g)$ in $\mathcal{H}$ and therefore $i^\dagger(x)(g_n) \to i^\dagger(x)(g)$ by the continuity of the scalar product. With the same argument one sees

that $x_n \to x$ in $\mathcal{H}$ implies $i^\dagger(x_n)(g) \to i^\dagger(x)(g)$ for all $g \in \mathcal{G}$. This shows the continuity of the map $i^\dagger \colon \mathcal{H} \to \mathcal{G}'$. Furthermore, the injectivity of $i^\dagger$ follows from the density of $\mathcal{G}$ in $\mathcal{H}$ because an element in the dual space $\mathcal{H}^*$ is uniquely by its values on a dense subset.

Definition 3.3.2 (Gelfand triple). Let $\mathcal{G}$ be a Fréchet space and $\mathcal{H}$ a Hilbert space together with a continuous linear embedding $i \colon \mathcal{G} \to \mathcal{H}$ with dense range. The induced structure

$$\mathcal{G} \overset{i}{\hookrightarrow} \mathcal{H} \overset{i^\dagger}{\hookrightarrow} \mathcal{G}'$$

is called the *Gelfand triple* associated to $(\mathcal{G}, \mathcal{H}, \iota)$.

In the following we will often ignore the embedding i and directly identify elements of $\mathcal{G}$ with elements in $\mathcal{H}$. However, one has to be careful when one identifies elements of $\mathcal{H}$ with elements of $\mathcal{G}'$ because the embedding $i^\dagger$ is *anti-linear*. The next example is probably the most important Gelfand triple.

Example 3.3.3. Consider $\mathcal{S}(\mathbb{R}^n) \overset{i}{\hookrightarrow} L^2(\mathbb{R}^n) \overset{i^\dagger}{\hookrightarrow} \mathcal{S}'(\mathbb{R}^n)$, where the embedding $i \colon \mathcal{S}(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ is the natural inclusion and $i^\dagger \colon \mathcal{H} \to \mathcal{S}'(\mathbb{R}^n)$ is given by

$$i^\dagger \colon f \mapsto \left[\mathcal{S}(\mathbb{R}^n) \ni \varphi \mapsto \int_{\mathbb{R}^n} \overline{f(x)} \varphi(x)\, dx \right].$$

Hence, except for a change with the complex conjugate $i^\dagger$ is the restriction of the inclusion of L^1_{loc}-functions into the space of distributions.

From now on let $\mathcal{G} \hookrightarrow \mathcal{H} \hookrightarrow \mathcal{G}'$ be a fixed Gelfand triple. Before we can talk in a mathematical rigorous way about generalized eigenvectors, we must extend the action of a self-adjoint operator $(A, D(A))$ on $\mathcal{H}$ to the Gelfand triple. For this we make the additional assumption that $\mathcal{G} \subseteq D(A)$ and $A\mathcal{G} \subseteq \mathcal{G}$, i.e. A leaves $\mathcal{G}$ invariant. This means that A restricts to a linear bounded operator on $\mathcal{G}$ (which is automatically continuous by the variant of the closed graph theorem for Fréchet spaces). One then obtains the dual map

$$\begin{aligned} A' \colon \mathcal{G}' &\to \mathcal{G}' \\ \varphi &\mapsto [g \mapsto \varphi(Ag) =: \langle \varphi, Ag \rangle_{\mathcal{G}', \mathcal{G}}]. \end{aligned}$$

We leave it to the reader to verify that this map is well-defined.

Definition 3.3.4 (Generalized eigenvector). Let $(A, D(A))$ be a self-adjoint operator on some Hilbert space $\mathcal{H}$ and $\mathcal{G} \hookrightarrow \mathcal{H} \hookrightarrow \mathcal{G}'$ a Gelfand tripel with $G \subseteq D(A)$ and $A\mathcal{G} \subseteq \mathcal{G}$. Then the eigenvectors of $A' \colon \mathcal{G}' \to \mathcal{G}'$ are called the *generalized eigenvectors* of A.

Suppose that $y \in D(A)$ is a eigenvalue of A, i.e. $Ay = \lambda y$ for some $\lambda \in \mathbb{R}$. Then we have for all $x \in \mathcal{G}$

$$\langle A' i^\dagger y, x\rangle_{\mathcal{G}',\mathcal{G}} = \langle i^\dagger y, Ax\rangle_{\mathcal{G}',\mathcal{G}} = \langle y|Ax\rangle = \lambda\langle y|x\rangle = \langle \lambda i^\dagger y, x\rangle_{\mathcal{G}',\mathcal{G}}.$$

Hence, $A' i^\dagger y = \lambda i^\dagger y$. This shows that every eigenvalue of A in the classical sense is also a generalized eigenvalue of A. More structurally spoken, by adapting the above reasoning we see that for $y \in D(A)$ and $x \in \mathcal{G}$

$$\langle A' i^\dagger y, x\rangle_{\mathcal{G}',\mathcal{G}} = \langle i^\dagger y, Ax\rangle_{\mathcal{G}',\mathcal{G}} = \langle y|Ax\rangle = \langle Ay|x\rangle = \langle i^\dagger Ay, x\rangle_{\mathcal{G}',\mathcal{G}},$$

which shows that (in a certain sense) A' is an extension of A to $\mathcal{G}'$.

Observe that until now we have only defined generalized eigenvalues but we do not know yet when a system of generalized eigenvalues is complete. For $\lambda \in \mathbb{R}$ let $E(\lambda) := \operatorname{Ker}(\lambda \operatorname{Id} - A') \subseteq \mathcal{G}'$ be the eigenspace of A'. We now define a generalized variant of the Fourier transform for elements in $\mathcal{G}$.

Definition 3.3.5 (Generalized Fourier transform). Let $\mathcal{G} \hookrightarrow \mathcal{H} \hookrightarrow \mathcal{G}'$ be a Gelfand triple and $(A, D(A))$ a self-adjoint operator on $\mathcal{H}$ with $D(A) \subseteq \mathcal{H}$ and $A\mathcal{G} \subseteq \mathcal{G}$. Then one defines the *generalized Fourier transform*

$$\begin{aligned} \hat{\cdot}\colon \mathcal{G} &\to \prod_{\lambda\in\mathbb{R}} E(\lambda)' \\ g &\mapsto (\varphi \ni E(\lambda) \mapsto \langle \varphi, g\rangle_{\mathcal{G}',\mathcal{G}})_{\lambda\in\mathbb{R}} \end{aligned}$$

We say that A has a *complete system of generalized eigenvectors* (with respect to A) in $\mathcal{G}'$ if the generalized Fourier transform is injective, i.e. $\hat{g} = 0$ implies $g = 0$.

Of course, $E(\lambda)'$ may be trivial for certain values of $\lambda \in \mathbb{R}$. One can show that A has a complete system of generalized eigenvectors if and only if the span of all $E(\lambda)$ is dense in $\mathcal{G}'$ for the weak*-topology. As before we will ignore this topological issues and will instead consider some examples. First we consider the momentum operator in one dimension.

Example 3.3.6 (Generalized eigenvectors for the momentum operator). We consider the momentum operator $A = -i\frac{d}{dx}$ with $D(A) = H^1(\mathbb{R})$. We choose $\mathcal{G} = \mathcal{S}(\mathbb{R})$. Then $\mathcal{G}' = \mathcal{S}'(\mathbb{R})$ is the space of all tempered distributions. We choose $i\colon \mathcal{S}(\mathbb{R}) \hookrightarrow L^2(\mathbb{R})$ as the canonical inclusion. Then we obtain the Gelfand triple $\mathcal{S}(\mathbb{R}) \hookrightarrow L^2(\mathbb{R}) \hookrightarrow \mathcal{S}'(\mathbb{R})$ considered in Example 3.3.3. Observe that $\mathcal{S}(\mathbb{R}) \subset H^1(\mathbb{R})$ and $A\mathcal{S}(\mathbb{R}) \subset \mathcal{S}(\mathbb{R})$. Hence, there exists the extension $A'\colon \mathcal{S}'(\mathbb{R}) \to \mathcal{S}'(\mathbb{R})$ of A. Explicitly, one has for $u \in \mathcal{S}'(\mathbb{R})$ and $\varphi \in \mathcal{S}(\mathbb{R})$

$$\begin{aligned} \langle A'u, \varphi\rangle_{\mathcal{S}'(\mathbb{R}),\mathcal{S}(\mathbb{R})} &= \langle u, A\varphi\rangle_{\mathcal{S}'(\mathbb{R}),\mathcal{S}(\mathbb{R})} = \langle u, -i\varphi'\rangle_{\mathcal{S}'(\mathbb{R}),\mathcal{S}(\mathbb{R})} = \langle u', i\varphi\rangle_{\mathcal{S}'(\mathbb{R}),\mathcal{S}(\mathbb{R})} \\ &= \langle iu', \varphi\rangle_{\mathcal{S}'(\mathbb{R}),\mathcal{S}(\mathbb{R})}. \end{aligned}$$

This shows that $A'u = iu'$ in the sense of distributions. Note that for $\varphi \in \mathcal{S}(\mathbb{R})$ one has $A'i^\dagger\varphi = i\varphi' = i^\dagger(-i\varphi') = i^\dagger A\varphi$ as it should hold in general. Now let us determine the generalized real eigenvalues of A, i.e. the eigenvalues of A'. For this we must find for given $\lambda \in \mathbb{R}$ all distributional solutions $u \in \mathcal{S}'(\mathbb{R})$ of

$$A'u = iu' = \lambda u.$$

One can show that all distributional solutions of the above equation already are smooth functions (we have already used and proved an easier variant of this result where we additionally assumed that $u' \in L^1_{\mathrm{loc}}(\mathbb{R})$). Hence, every solution of the above equation is of the form $u(x) = ce^{-i\lambda x}$ for some $c \in \mathbb{C}$. In other words, this shows that $E(\lambda) = \{ce^{-i\lambda x} : c \in \mathbb{C}\}$ for all $\lambda \in \mathbb{R}$. We now determine the generalized Fourier transform with respect to A. For $\varphi \in \mathcal{S}(\mathbb{R})$ we have

$$ce^{-i\lambda x} \mapsto \langle ce^{-i\lambda x}, \varphi\rangle_{\mathcal{S}'(\mathbb{R}),\mathcal{S}(\mathbb{R})} = c\int_{\mathbb{R}} \varphi(x)e^{-i\lambda x}\,dx.$$

Hence, if we identify linear mappings $\mathbb{C} \to \mathbb{C}$ with a complex number, we obtain $\prod_{\lambda\in\mathbb{R}} E(\lambda)' \simeq \prod_{\lambda\in\mathbb{R}} \mathbb{C}$, which is the space of all functions $f\colon \mathbb{R} \to \mathbb{C}$. Using this identification, for $\varphi \in \mathcal{S}(\mathbb{R})$ the generalized Fourier transform $\hat{\varphi}$ agrees with the function $\lambda \mapsto \int_{\mathbb{R}} \varphi(x)e^{-i\lambda x}\,dx$, i.e. up to a normalization constant with the usual Fourier transform. Since a Schwartz function is uniquely determined by its Fourier transform, we see that A has a complete system of generalized eigenvectors.

As a second example we consider the position operator in one dimension.

Example 3.3.7 (Generalized eigenvectors for the position operator). We consider the position operator M_x on $L^2(\mathbb{R})$. We again work with the Gelfand triple $\mathcal{S}(\mathbb{R}) \hookrightarrow L^2(\mathbb{R}) \hookrightarrow \mathcal{S}'(\mathbb{R})$ as in the last example. Note that one has $\mathcal{S}(\mathbb{R}) \subset D(M_x)$ and $M_x\mathcal{S}(\mathbb{R}) \subset \mathcal{S}(\mathbb{R})$. The extension $A'\colon \mathcal{S}'(\mathbb{R}) \to \mathcal{S}'(\mathbb{R})$ is explicitly given for $u \in \mathcal{S}'(\mathbb{R})$ and $\varphi \in \mathcal{S}(\mathbb{R})$ as

$$\langle M_x'u, \varphi\rangle_{\mathcal{S}'(\mathbb{R}),\mathcal{S}(\mathbb{R})} = \langle u, M_x\varphi\rangle_{\mathcal{S}'(\mathbb{R}),\mathcal{S}(\mathbb{R})} = \langle u, x\cdot\varphi\rangle_{\mathcal{S}'(\mathbb{R}),\mathcal{S}(\mathbb{R})} = \langle x\cdot u, \varphi\rangle_{\mathcal{S}'(\mathbb{R}),\mathcal{S}(\mathbb{R})}$$

Hence, $M_x'\colon u \mapsto x\cdot u$ is the multiplication of the function $x \mapsto x$ with the given distribution. Now, $M_x'\delta_{x_0} = x\delta_{x_0} = x_0\delta_{x_0}$ holds in a mathematical rigorous way. Moreover, one can show that all solutions of the eigenvalue equation

$$M_x'u = x\cdot u = x_0u \qquad \Leftrightarrow \qquad (x - x_0)\cdot u = 0$$

are constant multiples of δ_{x_0}. In fact, passing to the Fourier transform (for tempered distributions) the problem reduces to the eigenvalue problem of the previous example. Put differently, we have $E(\lambda) = \{c\delta_\lambda : c \in \mathbb{C}\}$ for all $\lambda \in \mathbb{R}$.

Let us now calculate the generalized Fourier transform with respect to A. For $\varphi = c\delta_\lambda \in E(\lambda)$ and $\varphi \in \mathcal{S}(\mathbb{R})$ we have

$$c\delta_\lambda \mapsto \langle c\delta_\lambda, \varphi\rangle_{\mathcal{S}'(\mathbb{R}),\mathcal{S}(\mathbb{R})} = c\varphi(\lambda).$$

Hence, if we again identify linear mappings $\mathbb{C} \to \mathbb{C}$ with a complex number, we obtain $\prod_{\lambda\in\mathbb{R}} E(\lambda)' \simeq \prod_{\lambda\in\mathbb{R}} \mathbb{C}$, the space of all functions $f : \mathbb{R} \to \mathbb{C}$. Using this identification, for $\varphi \in \mathcal{S}(\mathbb{R})$ the Fourier transform $\hat{\varphi}$ agrees with the function $\lambda \mapsto \varphi(\lambda)$, that is $\hat{\varphi} = \varphi$ and the Fourier transform is the identity mapping. Of course, from this it follows immediately that A has a complete system of generalized eigenvectors.

The nuclear spectral theorem says that one can always find a complete system of generalized eigenvalues for a self-adjoint operator A which is compatible with a Gelfand triple $(\mathcal{G}, \mathcal{H}, \iota)$ provided the Fréchet space $\mathcal{G}$ is nice enough. This niceness condition is in mathematical terms that $\mathcal{G}$ is a so-called *nuclear* space. This is a rather abstract mathematical concept from the theory of locally convex topological vector spaces and needs some work to be properly presented. Physics students may ignore the following definitions and simply work with the fact that the space of Schwartz functions $\mathcal{S}(\mathbb{R}^n)$ is nuclear if they feel overwhelmed by the amount of definitions and may therefore directly jump to the statement of the nuclear theorem.

From now on let $\mathcal{G}$ be a Fréchet space given by a countable family of increasing semi-norms $(p_n)_{n\in\mathbb{N}}$. For such a semi-norm we can define its *local Banach space*.

Definition 3.3.8 (Local Banach space). Let $\mathcal{G}$ be a Fréchet space and p one its defining semi-norms. Then for the null space $N_p = \{x \in \mathcal{G} : p(x) = 0\}$ define the quotient vector space

$$\mathcal{G}_p := \mathcal{G}/N_p = \{x + N_p : x \in \mathcal{G}\}.$$

Then $(\mathcal{G}_p, p)$ is a normed vector space and its completion $\hat{\mathcal{G}}_p$ is called the *local Banach space* for p.

Note that for $p \le q$ one has $p(x) = 0$ whenever $q(x) = 0$. Hence, $N_q \subseteq N_p$ and one obtains a natural contractive linear map $\mathcal{G}_q \to \mathcal{G}_p$ sending $x + N_q$ to $x + N_p$. Passing to the completions, we obtain a contractive operator $\hat{\mathcal{G}}_q \to \hat{\mathcal{G}}_p$ between the two local Banach spaces. In particular in our situation, using the shorthand notation $\mathcal{G}_k = \mathcal{G}_{p_k}$ and so on, we obtain natural maps $\hat{\mathcal{G}}_l \to \hat{\mathcal{G}}_k$ for $l \ge k$.

We now generalize the concept of trace class operator to mappings between general Banach spaces. This concept goes back to the work of A. Grothendieck.

Definition 3.3.9. A linear map $T\colon X \to Y$ between two Banach spaces is called *nuclear* if there exists an absolutely summable sequence $(\lambda_n)_{n\in\mathbb{N}}$ and $(x_n')_{n\in\mathbb{N}} \subset X'$ and $(y_n)_{n\in\mathbb{N}} \subset Y$ with $\|x_n\|, \|y_n\| \leq 1$ for all $n \in \mathbb{N}$ such that

$$Tx = \sum_{n=1}^{\infty} \lambda_n \langle x_n', x\rangle_{X',X} y_n \qquad \text{for all } x \in X.$$

We now can define nuclear spaces.

Definition 3.3.10. A Fréchet space $\mathcal{G}$ given by an increasing family $(p_k)_{k\in\mathbb{N}}$ of semi-norms is called *nuclear* if for all $k \in \mathbb{N}$ there is some $l > k$ such that the natural map $\hat{\mathcal{G}}_l \to \hat{\mathcal{G}}_k$ is nuclear.

Intuitively, a nuclear map has a very small image. Hence, in a nuclear space the unit balls with respect to the semi-norms decrease rapidly. As a rule of thumb one can say that all natural important function spaces which are Fréchet spaces are either Banach spaces or nuclear spaces. Nuclear Fréchet spaces – in contrast to infinite dimensional Banach spaces – behave in many regards very similar to finite dimensional spaces. For example, the Heine–Borel characterization of compact subsets holds for nuclear Fréchet spaces.

Let us illustrate all this with a concrete example.

Example 3.3.11 (The space of smooth functions). Let us consider the space $\mathcal{G} = C^\infty([0,1])$. We naturally want that a sequence in $(f_n)_{n\in\mathbb{N}} \in C^\infty([0,1])$ converges to some $f \in C^\infty([0,1])$ if and only if $D^k f_n \to D^k f$ uniformly on $[0,1]$ for all $k \in \mathbb{N}$. This is achieved if we require that $(f_n)_{n\in\mathbb{N}}$ converges with respect to all semi-norms $p_k(f) \coloneqq \sup_{x\in[0,1]} |f(x)|$ for $k \in \mathbb{N}$. One sees that the family $(p_k)_{k\in\mathbb{N}}$ satisfies all requirements in the definition of a Fréchet spaces. Hence, $(p_k)_{k\in\mathbb{N}}$ gives $C^\infty([0,1])$ the structure of a Fréchet space. Alternatively, one can also work with the norms $q_k(f) = \|f\|_{H^k(0,1)}$ for $k \in \mathbb{N}$. Note that $p_k(f_n - f) \to 0$ for all $n \in \mathbb{N}$ if and only if $q_k(f_n - f) \to 0$ for all $n \in \mathbb{N}$. This is a consequence of the fact that by the Sobolev embedding theorems (Theorem 2.1.36) convergence in $H^m((0,1))$ implies convergence in $C^k(\mathbb{R}^n)$ provided m is large enough. Observe that the family $(q_k)_{k\in\mathbb{N}}$ is monotone, i.e $q_k \leq q_{k+1}$ for all $k \in \mathbb{N}$.

We now show that $C^\infty([0,1])$ is a nuclear space. Since q_k is already a norm, the local Banach spaces are given by $\mathcal{G}_k = H^k((0,1))$. For $l > k$ the natural map $\hat{\mathcal{G}}_l \to \hat{\mathcal{G}}_k$ is the natural inclusion $H^l((0,1)) \hookrightarrow H^k((0,1))$ of Sobolev spaces. We must show that for l large enough these inclusions are nuclear mappings. For this let us consider the discrete Fourier transform $\mathcal{F}\colon L^2([0,1]) \to \ell^2(\mathbb{Z})$ which is an isomorphism because the trigonometric system $(e^{2\pi i m \cdot})_{m\in\mathbb{Z}}$ is an orthonormal basis of $L^2([0,1])$. Analogous to the continuous case, the image of $H^k((0,1))$ under $\mathcal{F}$ is the space of all sequences $(x_n)_{n\in\mathbb{N}}$ for which $(n^k x_n)_{n\in\mathbb{N}}$ lies in $\ell^2(\mathbb{Z})$ or equivalently $(x_n)_{n\in\mathbb{N}}$ lies in $\ell^2(\mathbb{Z}, (n^{2k}))$. Hence, under the

Fourier transform the inclusion $H^l((0,1)) \hookrightarrow H^k((0,1))$ becomes the identity mapping

$$\ell^2(\mathbb{Z},(n^{2l})) \hookrightarrow \ell^2(\mathbb{Z},(n^{2k})).$$

Choose $y_n = n^{-2k}e_n$, where e_n is the n-th unit vector, and $x_n = n^{-2l}e_n$. Then $\|x_n\|_{\ell^2(\mathbb{Z},(n^{2l}))} = \|y_n\|_{\ell^2(\mathbb{Z},(n^{2k}))} = 1$ and (x_n) and (y_n) form orthonormal bases in the respective spaces. Hence, for all $z \in \ell^2(\mathbb{Z},(n^{2l}))$ we have

$$z = \sum_{n=1}^{\infty} \langle x_n | z \rangle_{\ell^2(\mathbb{Z},(n^{2l}))} x_n = \sum_{n=1}^{\infty} \langle x_n | z \rangle_{\ell^2(\mathbb{Z},(n^{2l}))} n^{2(k-l)} y_n.$$

This shows that for $l > k$ the identity mapping between the weighted spaces is nuclear because in this case the sequence $(n^{2(k-l)})_{n\in\mathbb{N}}$ is absolutely summable. Hence, $C^\infty((0,1))$ is a nuclear Fréchet space.

With the above result one can further easily deduce that the Fréchet space $C^\infty(\mathbb{R})$ is nuclear. The ambitious reader may try to prove that the space of Schwartz functions $\mathcal{S}(\mathbb{R}^n)$ is a nuclear Fréchet space as well, a fact which we will use soon. The less ambitious readers can find a proof of this fact in [Kab14, p. 279].

We now come to the final result of our lecture, the nuclear spectral theorem.

Theorem 3.3.12 (Nuclear spectral theorem). *Let $\mathcal{G}$ be a nuclear Fréchet space, $\mathcal{G} \hookrightarrow \mathcal{H} \hookrightarrow \mathcal{H}'$ a Gelfand triple and $(A, D(A))$ a self-adjoint operator on $\mathcal{H}$ with $\mathcal{G} \subseteq D(A)$ and $A\mathcal{G} \subseteq \mathcal{G}$. Then for some set K the operator A has a complete system $\{\eta_{\lambda,k} : \lambda \in \mathbb{R}, k \in K\}$ of generalized eigenvectors in $\mathcal{G}'$. Further, there exist finite Borel measures $(\mu_k)_{k\in K}$ such that for $x \in \mathcal{G}$ one has the expansions*

$$x = \sum_{k\in K} \int_{\mathbb{R}} \langle \eta_{\lambda,k}, x \rangle \eta_{\lambda,k} \, d\mu_k(\lambda)$$

and

$$Ax = \sum_{k\in K} \int_{\mathbb{R}} \lambda \langle \eta_{\lambda,k}, x \rangle \eta_{\lambda,k} \, d\mu_k(\lambda)$$

Further for $x \in \mathcal{G}$ one has Plancherel's formula

$$\|x\|_{\mathcal{H}}^2 = \sum_{k\in K} \int_{\mathbb{R}} |\langle \eta_{\lambda,k}, x \rangle|^2 \, d\mu_k(\lambda).$$

We now sketch some main steps of the proof. For a complete proof see [Kab14, Satz 16.41]. One first establishes the following refined variant of the spectral theorem for unbounded self-adjoint operators: for a self-adjoint operator $(A, D(A))$ on $\mathcal{H}$ there exists a family of finite Borel measures $(\mu_k)_{k\in K}$

and a unitary operator $U : H \to \bigoplus_{k\in K} L^2(\sigma(A), \mathcal{B}(\sigma(A)), \mu_k)$ such that UAU^{-1} is the multiplication operator

$$\bigoplus_{k\in K} L^2(\sigma(A), \mathcal{B}(\sigma(A)), \mu_k) \to \bigoplus_{k\in K} L^2(\sigma(A), \mathcal{B}(\sigma(A)), \mu_k)$$
$$(f_k)_{k\in K} \mapsto (\lambda \mapsto \lambda f_k(\lambda))_{k\in K}.$$

This version of the spectral theorem can first be proven for bounded normal operators and thereafter the self-adjoint case can be deduced with the help of the Cayley transform. An elegant way to prove the spectral theorem for a normal operator $T \in \mathcal{B}(\mathcal{H})$ is to establish a continuous functional calculus $C(\sigma(T)) \to \mathcal{B}(\mathcal{H})$ for T. One then decomposes the above representation into the direct sum of cyclic representations which can be shown to be unitary equivalent to multiplication operators. For proofs of these facts we refer to the literature on functional analysis given in the bibliography.

With the above unitary transform one can essentially reduce the problem to the case of multiplication operators. One now tries to define delta-distributions $\delta_{k,\lambda}$ for $k \in K$ and $\lambda \in \mathbb{R}$. These distributions would be generalized eigenfunctions for A provided they are well-defined elements in $\mathcal{G}'$. In order to prove that these delta-distributions are indeed well-defined one uses the fact that $\mathcal{G}$ is nuclear. In fact, one can show that if $\mathcal{K}$ is a nuclear Fréchet space and one has a Gelfand triple of the form $\mathcal{K} \hookrightarrow L^2(\Omega, \Sigma, \mu) \hookrightarrow \mathcal{K}'$ for some measure space (Ω, Σ, μ), then for almost all $\omega \in \Omega$ the delta-distributions δ_ω are well-defined elements of $\mathcal{K}'$.

As a particular instance of the nuclear spectral theorem we obtain the following corollary for differential operators which includes some quantum mechanical operators.

Corollary 3.3.13 (Generalized eigenfunctions for differential operators). *Let $m, n \in \mathbb{N}$ and $a_\alpha \in C^\infty(\mathbb{R}^n)$ smooth real functions of polynomial growth for $|\alpha| \leq m$. Then the symmetric differential operator $D = \sum_{|\alpha|\leq m} a_\alpha D^\alpha$ on $L^2(\mathbb{R}^n)$ with $D(A) = \mathcal{S}(\mathbb{R}^n)$ can be extended to a self-adjoint operator A on $L^2(\mathbb{R}^n)$. Further, A has a complete system of generalized eigenfunctions in $\mathcal{S}'(\mathbb{R}^n)$.*

Recall that the existence of self-adjoint extensions in the above situation is guaranteed by von Neumann's criterion (Theorem 2.4.2). Hence, the corollary is a direct consequence of the nuclear spectral theorem. The above Corollary applies to some quantum mechanical operators, however it does not apply to Hamiltonians of the form $-\Delta + V$ for singular potentials V. A prominent example for this situation is the Hamiltonian of the hydrogen atom.

However, the definition of nuclear spaces extends to general locally convex topological vector spaces (you know how to do this if you know the theory of locally convex spaces). Further, the nuclear spectral theorem in fact holds

for such general nuclear locally convex spaces which may not be Fréchet spaces. We have avoided general locally convex spaces in this lecture to reduce topological difficulties. In fact, the topology of general locally convex space is not induced by a (translation-invariant) metric in contrast to the case of Fréchet spaces and concepts such as continuity are more difficult to formulate correctly. A prominent and important example of a nuclear space which is not a Fréchet space is the space of test functions $\mathcal{D}(\Omega)$ for some open $\Omega \neq \emptyset$. Taking the nuclear spectral theorem for granted in the case of $\mathcal{D}(\Omega)$, we obtain the following strengthening of the previous corollary.

Corollary 3.3.14. *Let $m, n \in \mathbb{N}$, $\Omega \subset \mathbb{R}^n$ open and $a_\alpha \in C^\infty(\Omega)$ smooth real functions for $|\alpha| \leq m$. Then the symmetric differential operator $D = \sum_{|\alpha| \leq m} a_\alpha D^\alpha$ on $L^2(\Omega)$ with $D(A) = \mathcal{D}(\Omega)$ can be extended to a self-adjoint operator A on $L^2(\Omega)$. Further, A has a complete system of generalized eigenfunctions in $\mathcal{D}'(\Omega)$.*

Note that the above corollary can in fact be applied to the Hamiltonian $\hat{H} = -\Delta + |x|^{-1}$ of the hydrogen atom. In fact, we can choose $\Omega = \mathbb{R}^3 \setminus \{0\}$ as the potential is smooth outside the singularity at zero. The above corollary then shows that there exists a complete system of generalized eigenfunctions in $\mathcal{D}'(\mathbb{R}^3 \setminus \{0\})$.

A

The postulates of quantum mechanics

In this short appendix we present all postulates of quantum mechanics used in our lectures in a condensed and mathematical manner. Our formulation of the postulates closely follows the presentation in [Tak08].

Postulate 1. A *quantum system* is described by a complex Hilbert space $\mathcal{H}$. The Hilbert space of a composite system is the tensor product of Hilbert spaces of the single component systems.

Postulate 2. The set of *observables* $\mathcal{A}$ of a quantum mechanical system with Hilbert space $\mathcal{H}$ consists of all self-adjoint operators on $\mathcal{H}$.

Postulate 3. The set of *states* $\mathcal{S}$ of a quantum system with a Hilbert space $\mathcal{H}$ consists of all positive trace class operators ρ with $\operatorname{Tr}\rho = 1$. *Pure states* are projection operators onto one-dimensional subspaces of $\mathcal{H}$. All other states are called *mixed states*.

Postulate 4. The process of measurement in quantum mechanics is described by the assignment

$$\mathcal{A} \times \mathcal{S} \ni (A, M) \mapsto \mu_A,$$

where μ_A is the probability measure on $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$ given by the *Born–von Neumann formula*

$$\mu_A(\Omega) = \operatorname{Tr} P_A(\Omega)\rho \qquad \text{for } \Omega \in \mathcal{B}(\mathbb{R}),$$

where P_A is the projection-valued measure associated to the self-adjoint operator A. For every Borel set $\Omega \subseteq \mathbb{R}$, the quantity $0 \leq \mu_A(\Omega) \leq 1$ is the probability that for a quantum system in the state ρ the result of a measurement of the observable A belongs to Ω.

Postulate 5. A finite set of observables $\mathbb{A} = \{A_1, \ldots, A_n\}$ can be measure simultaneously (*simultaneously measured observables*) if and only if they form a commutative family. The simultaneous measurement of the commutative family $\mathbb{A}$ in the state $\rho \in \mathcal{S}$ is described by the probability measure $\mu_{\mathbb{A}}$ on $\mathbb{R}^n$ given by

$$\mu_{\mathbb{A}}(\Omega) = \operatorname{Tr} P_{\mathbb{A}}(\Omega)\rho \qquad \text{for } \Omega \in \mathcal{B}(\mathbb{R}^n),$$

where $P_{\mathbb{A}}$ is the projection-valued measure associated to the family $\mathbb{A}$. For every Borel set $\Omega \subseteq \mathbb{R}^n$ the quantity $0 \leq \mu_{\mathbb{A}}(\Omega) \leq 1$ is the probability that for a quantum system in the state ρ the result of the simultaneous measurement of the observables $A_1, \ldots, A_n$ belongs to Ω.

Postulate 6 (Schrödinger's picture of time evolution). The dynamics of a quantum system is described by a strongly continuous unitary group $(U(t))_{t\in\mathbb{R}}$ on the Hilbert space $\mathcal{H}$ of the system. Quantum observables do not depend on time and the evolution of states is given by

$$\mathcal{S} \ni \rho \mapsto \rho(t) = U(t)\rho U(t)^{-1}.$$

Recall that by Stone's theorem (Theorem 2.3.32) there is a one-to-one correspondence between self-adjoint operators and strongly continuous unitary groups on $\mathcal{H}$. This gives the connection to the usually used well-known Schrödinger equation.

One may add additional postulates if one considers particles with spin or systems of identical particles with spins (bosons and fermions), physical phenomena which we have not discussed thoroughly in our lectures. Further, for concrete physics one would like to have a mapping which assigns a quantum observable to its classical counterpart. Such mappings are called *quantization rules* and were discussed in Kedar's part of the lecture.

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