Notes on Quantum Mechanics

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Contents

Chapter 1

Functional Analysis, Hilbert Spaces and Quantum Mechanics

1.1 Historical Notes and Overview

1.1.1 Introduction

The concept of a Hilbert space is seemingly technical and special. For example, the reader has probably heard of the space ℓ^2 (or, more precisely, $\ell^2(\mathbb{Z})$ of square-summable sequences of real or complex numbers.[In what follows, we mainly work over the reals in order to serve intuition, but many infinite-dimensional vector spaces, especially Hilbert spaces, are defined over the complex numbers].We also use standard math notation with occasionl Dirac examples. Hence we will write our formulae in a way that is correct also for $\mathbb{C}$ instead of $\mathbb{R}$. Of course, for $z \in \mathbb{R}$ the expression $|z|^2$ is just z^2. We will occasionally use the fancy letter $\mathbb{K}$, for *Korper*, which in these notes stands for either $\mathbb{K} = \mathbb{R}$ or $\mathbb{K} = \mathbb{C}$]. That is, ℓ^2 consists of all infinite sequences $\{..., c_{-2}, c_{-1}, c_0, c_1, c_2, ...\}$, $c_k \in \mathbb{K}$, for which

$$\sum_{-\infty}^{\infty} |c_k|^2 < \infty$$

Another example of a Hilbert space one might have seen is the space $L^2(\mathbb{R})$ of square-integrable complex-valued functions on $\mathbb{R}$, that is, of all functions[As we shall see, the elements of $L^2(\mathbb{R})$ are, strictly speaking, not simply functions but equivalence classes[In mathematics, given a set X and an equivalence relation $\sim$ on X, the equivalence class of an element a in X is the subset of all elements in X which are equivalent to a: $[a] = x \in X | x \sim a]$ of Borel functions] $f : \mathbb{R} \to \mathbb{K}$ for which

$$\int_{-\infty}^{\infty} dx |f(x)|^2 < \infty$$

In view of their special nature, it may therefore come as a surprise that Hilbert spaces play a central role in many areas of mathematics, notably in analysis,

but also including (differential) geometry, group theory, stochastics, and even number theory. In addition, the notion of a Hilbert space provides the mathematical foundation of quantum mechanics. Indeed, the definition of a Hilbert space was first given by von Neumann (rather than Hilbert!) in 1927 precisely for the latter purpose. However, despite his exceptional brilliance, even von Neumann would probably not have been able to do so without the preparatory work in pure mathematics by Hilbert and others, which produced numerous constructions (like the ones mentioned above) that are now regarded as examples of the abstract notion of a Hilbert space. It is quite remarkable how a particular development within pure mathematics crossed one in theoretical physics in this way; this crossing is reminiscent to the one leading to the calculus around 1670; see below. Today, the most spectacular new application of Hilbert space theory is given by Noncommutative Geometry, where the motivation from pure mathematics is merged with the physical input from quantum mechanics. Consequently, this is an important field of research in pure mathematics as well as in mathematical physics.

In what follows, we shall separately trace the origins of the concept of a Hilbert space in mathematics and physics. As we shall see, Hilbert space theory is part of functional analysis, an area of mathematics that emerged between approximately 1880-1930. Functional analysis is almost indistinguishable from what is sometimes called abstract analysis or modern analysis, which marked a break with classical analysis. The latter involves, roughly speaking, the study of properties of a single function, whereas the former deals with spaces of functions[The modern concept of a function as a map $f : [a, b] to \mathbb{R}$ was only arrived at by Dirichlet as late as 1837, following earlier work by notably Euler and Cauchy. But Newton already had an intuitive grasp of this concept, at least for one variable]. One may argue that classical analysis is tied to classical physics[Classical analysis grew out of the calculus of Newton, which in turn had its roots in both geometry and physics. (Some parts of the calculus were later rediscovered by Leibniz). In the 17th century, geometry was a practical matter involving the calculation of lengths, areas, and volumes. This was generalized by Newton into the calculus of integrals. Physics, or more precisely mechanics, on the other hand, had to do with velocities and accelerations and the like. This was abstracted by Newton into differential calculus. These two steps formed one of the most brilliant generalizations in the history of mathematics, crowned by Newtons insight that the operations of integration and differentiation are inverse to each other, so that one may speak of a unified differential and integral calculus, or briefly calculus. Attempts to extend the calculus to more than one variable and to make the ensuing machinery mathematically rigorous in the modern sense of the word led to classical analysis as we know it today. (Newton used theorems and proofs as well, but his arguments would be called heuristic or intuitive in modern mathematics)], whereas modern analysis is associated with quantum theory. Of course, both kinds of analysis were largely driven by intrinsic mathematical arguments as well[The jump from classical to modern analysis was as discontinuous as the one from classical to quantum mechanics.

The following anecdote may serve to illustrate this. G.H. Hardy was one of the masters of classical analysis and one of the most famous mathematicians altogether at the beginning of the 20th century. John von Neumann, one of the founders of modern analysis, once gave a talk on this subject at Cambridge in Hardys presence. Hardys comment was: *"Obviously a very intelligent man. But was that mathematics?"*]. The final establishment of functional analysis and Hilbert space theory around 1930 was made possible by combining a concern for rigorous foundations with an interest in physical applications.

1.1.2 Origins in Mathematics

The key idea behind functional analysis is to look at functions as points in some infinite-dimensional vector space. To appreciate the depth of this idea, it should be mentioned that the concept of a finite-dimensional vector space, today routinely taught to first-year students, only emerged in the work of Grassmann between 1844 and 1862 (to be picked up very slowly by other mathematicians because of the obscurity of Grassmanns writings), and that even the far less precise notion of a space (other than a subset of $\mathbb{R}^n$) was not really known before the work of Riemann around 1850. Indeed, Riemann not only conceived the idea of a manifold (albeit in embryonic form, to be made rigorous only in the 20th century), whose points have a status comparable to points in $\mathbb{R}^n$, but also explicitly talked about spaces of functions (initially analytic ones, later also more general ones). However, Riemanns spaces of functions were not equipped with the structure of a vector space. In 1885 Weierstrass considered the distance between two functions (in the context of the calculus of variations), and in 1897 Hadamard took the crucial step of connecting the set-theoretic ideas of Cantor with the notion of a space of functions. Finally, in his PhD thesis of 1906, which is often seen as a turning point in the development of functional analysis, Hadamards student Fréchet defined what is now called a metric space (i.e., a possibly infinite-dimensional vector space equipped with a metric, see below), and gave examples of such spaces whose points are functions. After 1914, the notion of a topological space due to Hausdorff led to further progress, eventually leading to the concept of a topological vector space, which contains all spaces mentioned below as special cases.

To understand the idea of a space of functions, we first reconsider $\mathbb{R}^n$ as the space of all functions $f : 1, 2, ..., n \to \mathbb{R}$, under the identification $x^1 = f(1), ..., x^n = f(n)$. Clearly, under this identification the vector space operations in $\mathbb{R}^n$ just correspond to pointwise operations on functions (e.g., $f + g$ is the function defined by $(f + g(k) := f(k) + g(k)$, etc). Hence $\mathbb{R}^n$ is a function space itself, consisting of functions defined on a finite set.

The given structure of $\mathbb{R}^n$ as a vector space may be enriched by defining the length of a vector f and the associated distance $d(f, g) = \|f - g\|$ between two vectors f and g. In addition, the angle θ between f and g in $\mathbb{R}^n$ is defined.

Lengths and angles can both be expressed through the usual inner product

$$(f,g) = \sum_{k=1}^{n} \overline{f(k)} g(k) \tag{1.1}$$

through the relations

$$\|f\| = \sqrt{(f,f)} \tag{1.2}$$

and

$$(f,g) = \|f\|\|g\| \cos\theta \tag{1.3}$$

In particular, one has a notion of orthogonality of vectors, stating that f and g are orthogonal whenever $(f,g) = 0$, and an associated notion of orthogonality of subspaces[A subspace of a vector space is by definition a linear subspace]: we say that $V \subset \mathbb{R}^n$ and $W \subset \mathbb{R}^n$ are orthogonal if $(f,g) = 0$ for all $f \in V$ and $g \in W$. This, in turn, enables one to define the (orthogonal) projection of a vector on a subspace of $\mathbb{R}^n$ [This is most easily done by picking a basis $\{e_i\}$ of the particular subspace V. The projection pf of f onto V is then given by $pf = \sum_i (e_i, f) e_i$]. Even the dimension n of $\mathbb{R}^n$ may be recovered from the inner product as the cardinality[In mathematics, the **cardinality** of a set is a measure of the *"number of elements of the set"*. For example, the set $A = \{2, 4, 6\}$ contains 3 elements, and therefore A has a cardinality of 3.] of an arbitrary orthogonal basis[This is the same as the cardinality of an arbitrary basis, as any basis can be replaced by an orthogonal one by the Gram-Schmidt procedure]. Now replace $\{1, 2, ..., n\}$ by an infinite set. In this case the corresponding space of functions will obviously be infinite-dimensional in a suitable sense[The dimension of a vector space is defined as the cardinality of some basis. The notion of a basis is complicated in general, because one has to distinguish between algebraic (or Hamel) and topological bases. Either way, the dimension of the spaces described below is infinite, though the cardinality of the infinity in question depends on the type of basis. The notion of an algebraic basis is very rarely used in the context of Hilbert spaces (and more generally Banach spaces), since the ensuing dimension is either finite or uncountable. The dimension of the spaces below with respect to a topological basis is countably infinite, and for a Hilbert space all possible cardinalities may occur as a possible dimension. In that case one may restrict oneself to an orthogonal basis]. The simplest example is $\mathbb{N} = \{1, 2, ..., n\}$, so that one may define $\mathbb{R}^\infty$ as the space of all functions $f : \mathbb{N} \to \mathbb{R}$, with the associated vector space structure given by pointwise operations. However, although $\mathbb{R}^\infty$ is well defined as a vector space, it turns out to be impossible to define an inner product on it, or even a length or distance. Indeed, defining

$$(f,g) = \sum_{k=1}^{\infty} \overline{f(k)} g(k) \tag{1.4}$$

it is clear that the associated length $\|f\|$ (still given by (4.2)) is infinite for most f. This is hardly surprising, since there are no growth conditions on f at infinity. The solution is to simply restrict $\mathbb{R}^\infty$ to those functions with $\|f\| < \infty$.

These functions by definition form the set $\ell^2(\mathbb{N})$, which is easily seen to be a vector space. Moreover, it follows from the Cauchy-Schwarz inequality

$$(f,g) \leq \|f\|\|g\| \tag{1.5}$$

that the inner product is finite on $\ell^2(\mathbb{N})$. Consequently, the entire geometric structure of $\mathbb{R}^n$ in so far as it relies on the notions of lengths and angles (including orthogonality and orthogonal projections) is available on $\ell^2(\mathbb{N})$. Running ahead of the precise definition, we say that $\mathbb{R}^n \cong \ell^2(\{1,2,....,n\})$ is a finite-dimensional Hilbert space, whereas $\ell^2(\mathbb{N})$ is an infinite-dimensional one. Similarly, one may define $\ell^2(\mathbb{Z})$ (or indeed $\ell^2(\mathcal{S})$ for any countable set $\mathcal{S}$) as a Hilbert space in the obvious way.

From a modern perspective, $\ell^2(\mathbb{N})$ or $\ell^2(\mathbb{Z})$ are the simplest examples of infinite-dimensional Hilbert spaces, but historically these were not the first to be found. The initial motivation for the concept of a Hilbert space came from the analysis of integral equations[Integral equations were initially seen as reformulations of differential equations. For example, the differential equation $Df = g$ or $f' = g(x)$ for unknown f is solved by $f = \int g$ or $f(x) = \int_0^x dyg(y) = \int_0^1 dyK(x,y)g(y)$ for $K(x,y) = \theta(x-y)$ (where $x \leq 1$), which is an integral equation for g] of the type

$$f(x) + \int_a^b dyK(x,y)f(y) = g(x) \tag{1.6}$$

where f, g, and K are continuous functions and f is unknown. Such equations were first studied from a somewhat modern perspective by Volterra and Fredholm around 1900, but the main breakthrough came from the work of Hilbert between 1904-1910. In particular, Hilbert succeeded in relating integral equations to an infinite-dimensional generalization of linear algebra by choosing an orthonormal basis $\{e_k\}$ of continuous functions on $[a,b]$ (such as $e_k(x) := \exp(2\pi kix)$ on the interval $[0,1]$), and defining the (generalized) Fourier coefficients of f by $f_k := (e_k, f)$ with respect to the inner product

$$(f,g) := \int_a^b dx\overline{f(x)}g(x) \tag{1.7}$$

The integral equation (4.6) is then transformed into an equation of the type

$$\hat{f}_k = \sum_l \hat{K}_{kl}\hat{f}_l = \hat{g}_l \tag{1.8}$$

Hilbert then noted from the Parseval relation (already well known at the time from Fourier analysis and more general expansions in eigenfunctions)

$$\sum_{k\in\mathbb{Z}} |\hat{f}_k|^2 = \int_a^b dx|f(x)|^2 \tag{1.9}$$

that the left-hand side is finite, so that $\hat{f} \in \ell^2(\mathbb{Z})$. This, then, led him and his students to study ℓ^2 also abstractly. E. Schmidt should be mentioned here

in particular. Unlike Hilbert, already in 1908 he looked at ℓ^2 as a space in the modern sense, thinking of sequences (c_k) as point in this space. Schmidt studied the geometry of ℓ^2 as a Hilbert space in the modern sense, that is, emphasizing the inner product, orthogonality, and projections, and decisively contributed to Hilberts work on spectral theory.

The space $L^2(a,b)$ appeared in 1907 in the work of F. Riesz and Fischer as the space of (Lebesgue) integrable functions14 on (u,b) for which

$$\int_a^b dx|f(x)|^2 < \infty$$

of course, this condition holds if f is continuous on $[a,b]$. Equipped with the inner product (4.7), this was another early example of what is now called a Hilbert space. The context of its appearance was what is now called the Riesz-Fischer theorem: *Given any sequence (c_k) of real (or complex) numbers and any orthonormal system (e_k) in $L^2(a,b)$, there exists a function $f \in L^2(a,b)$ for which $(e_k, f) = c_k$ if and only $c \in \ell^2$, i.e., if $\sum_k |c_k|2 < \infty$.*

At the time, the Riesz-Fischer theorem was completely unexpected, as it proved that two seemingly totally different spaces were the same from the right point of view. In modern terminology, the theorem establishes an isomorphism of ℓ^2 and Ł^2 as Hilbert spaces, but this point of view was only established twenty years later, i.e., in 1927, by von Neumann. Inspired by quantum mechanics (see below), in that year von Neumann gave the definition of a Hilbert space as an abstract mathematical structure, as follows. First, an inner product on a vector space V over a field $\mathbb{K}$ (where $\mathbb{K} = \mathbb{R}$ or $\mathbb{K} = \mathbb{C}$), is a map $V \times V \to \mathbb{K}$, written as $(f,g) \mapsto (f,g)$, satisfying, for all $f, g \in V$ and $t \in \mathbb{K}$,

1. $(f,f) \geq 0$;
2. $(g,f) = \overline{(f,g)}$;
3. $(f,tg) - t(f,g)$;
4. $(f,g+h) = (f,g) + (f,h)$;
5. $(f,f) = 0 \Rightarrow f = 0$

Given an inner product on V, one defines an associated length function or norm (see below) $\|\cdot\| : V \to \mathbb{R}^+$ by (4.2). A Hilbert space (over $\mathbb{K}$) is a vector space (over $\mathbb{K}$) with inner product, with the property that Cauchy sequences with respect to the given norm are convergent (in other words, V is complete in the given norm)[A sequence (f_n) is a Cauchy sequence in V when $\|f_n - f_m\| \to 0$ when $n, m \to \infty$; more precisely, for any $\epsilon > 0$ there is $N \in \mathbb{N}$ such that $\|f_n - f_m\| < \epsilon$ for all $n, m > N$. A sequence (f_n) converges if there is $f \in V$ such that $\lim_{n\to\infty} \|f_n - f_m\| = 0$]. Hilbert spaces are denoted by the letter H rather than V. Thus Hilbert spaces preserve as much as possible of the geometry

of $\mathbb{R}^n$.

It can be shown that the spaces mentioned above are Hilbert spaces. Defining an isomorphism of Hilbert spaces $U : H_1 \to H_2$ as an invertible linear map preserving the inner product (i.e., $(Uf, Ug)_2 = (f, g)_1$ for all $f, g \in H_1$), the Riesz-Fischer theorem shows that $\ell^2(\mathbb{Z})$ and $L^2(a, b)$ are indeed isomorphic.

In a Hilbert space the inner product is fundamental, the norm being derived from it. However, one may instead take the norm as a starting point (or, even more generally, the metric, as done by Fréchet in 1906). The abstract properties of a norm were first identified by Riesz in 1918 as being satisfied by the supremum[In mathematics, given a subset S of a partially ordered set T, the **supremum (sup)** of S, if it exists, is the least element of T that is greater than or equal to each element of S. Consequently, the supremum is also referred to as the *least upper bound (lub or LUB)*. If the supremum exists, it may or may not belong to S. If the supremum exists, it is unique] norm, and were axiomatized by Banach in his thesis in 1922. A norm on a vector space V over a field $\mathbb{K}$ as above is a function $\| \cdot \| : V \to \mathbb{R}^+$ with the properties:

1. $\|f + g\| \leq \|f\| + \|g\| \;\; for \;\; all \;\; f, g \in V$;
2. $\|tf\| = |t|\|f\|; \;\; for \;\; all \;\; f \in V \;\; and \;\; t \in \mathbb{K}$;
3. $\|f\| = 0 \Rightarrow f = 0$

The usual norm on $\mathbb{R}^n$ satisfies these axioms, but there are many other possibilities, such as

$$\|f\|_p := \left(\sum_{k=1}^{n} |f(k)|^p \right)^{1/p} \tag{1.10}$$

for any $p \in \mathbb{R}$ with $1 \leq p < \infty$, or

$$\|f\|_\infty := sup\{|f(k)|, k = 1, ..., n\}$$

In the finite-dimensional case, these norms (and indeed all other norms) are all equivalent in the sense that they lead to the same criterion of convergence (technically, they generate the same topology): if we say that $f_n \to f$ when $\|f_n - f\| \to 0$ for some norm on $\mathbb{R}^n$, then this implies convergence with respect to any other norm. This is no longer the case in infinite dimension. For example, one may define $\ell^p(\mathbb{N})$ as the subspace of $\mathbb{R}^\infty$ that consists of all vectors $f \in \mathbb{R}^\infty$ for which

$$\|f\|_p := \left(\sum_{k=1}^{n} |f(k)|^p \right)^{1/p} \tag{1.11}$$

is finite. It can be shown that $\| \cdot \|_p$, is indeed a norm on $\ell^p(\mathbb{N})$, and that this space is complete in this norm. As with Hilbert spaces, the examples that originally motivated Riesz to give his definition were not ℓ^p spaces but the far

more general L^p spaces, which he began to study in 1910. For example, $L^P(a,b)$ consists of all (equivalence classes of Lebesgue) integrable functions f on (a,b) for which

$$\|f\|_p := \left(\sum_{k=1}^{n} |f(k)|^p \right)^{1/p} \tag{1.12}$$

is finite, still for $1 \leq p < \infty$, and also $\|f\|_\infty := sup\{|f(x)|, x \in (a,b)$. Eventually, in 1922 Banach defined what is now called a **Banach space** as a vector space (over $\mathbb{K}$ as before) that is complete in some given norm.

Long before the abstract definitions of a Hilbert space and a Banach space were given, people began to study the infinite-dimensional generalization of functions on $\mathbb{R}^n$. In the hands of Volterra, the calculus of variations originally inspired the study of functions $\varphi : V \to \mathbb{K}$, later called functionals, and led to early ideas about possible continuity of such functions. However, although the calculus of variations involved nonlinear functionals as well, only linear functionals turned out to be tractable at the time (until the emergence of nonlinear functional analysis much later). Indeed, even today (continuous) linear functionals still form the main scalar-valued functions that are studied on infinite-dimensional (topological) vector spaces. For this reason, throughout this text a **functional** will denote a **continuous linear functional**. For $H = L^2(a,b)$, it was independently proved by Riesz and Fréchet in 1907 that any functional on H is of the form $g \mapsto (f,g)$ for some $f \in H$. The same result for arbitrary Hilbert spaces H was written down only in 1934-35, again by Riesz, although it is not very difficult.

The second class of functions on Hilbert spaces and Banach spaces that could be analyzed in detail were the generalizations of matrices on $\mathbb{R}^n$, that is, linear maps from the given space to itself. Such functions are now called operators[Or linear operators, but for us linearity is part of the definition of an operator]. For example, the integral equation (4.6) is then simply of the form $(1+K)f = g$, where $1 : L^2(a,b) \to L^2(a,b)$ is the identity operator $1f = f$, and $K : L^2(a,b) \to L^2(a,b)$ is the operator given by $(Kf)(x) = \int_a^b dy K(x,y)f(y)$.

This is easy for us to write down, but in fact it took some time before integral of differential equations were interpreted in terms of operators acting on functions. They managed to generalize practically all results of linear algebra to operators, notably the existence of a complete set of eigenvectors for operators of the stated type with symmetric kernel, that is, $K(x,y) = K(y,x)$. The abstract concept of a (bounded) operator (between what we now call Banach spaces) is due to Riesz in 1913. It turned out that Hilbert and Schmidt had studied a special class of operators we now call compact, whereas an even more famous student of Hilberts, Weyl, had investigated a singular class of operators now called unbounded in the context of ordinary differential equations. Spectral theory and eigenfunctions expansions were studied by Riesz himself for general bounded operators on Hilbert spaces (seen by him as a special case of general normed

spaces), and later, more specifically in the Hilbert space case, by Hellinger and Toeplitz (culminating in their pre-von Neumann review article of 1927).

In the Hilbert space case, the results of all these authors were generalized almost beyond recognition by von Neumann in his book from 1932, to whose origins we now turn.

1.1.3 Origins in Physics

From 1900 onwards, physicists had begun to recognize that the classical physics of Newton, Maxwell and Lorentz (i.e., classical mechanics, Newtonian gravity, and electrodynamics) could not describe all of Nature. The fascinating era that was thus initiated by Planck, to be continued mainly by Einstein, Bohr, and De Broglie, ended in 1925-1927 with the discovery of quantum mechanics. This theory replaced classical mechanics, and was initially discovered in two guises.

First, Heisenberg discovered a form of quantum mechanics that at the time was called matrix mechanics. Heisenbergs basic idea was that in atomic physics physical observables (that is, measurable quantities) should not depend on continuous variables like position and momentum (as he did not believe the concept of an electronic orbit in an atom made sense), but on discrete quantities, like the natural numbers $n = 1, 2, 3, ...$ labeling the orbits in Bohrs model of the atom. Specifically, Heisenberg thought that in analogy to a quantum jump from one orbit to the other, everything should be expressed in terms of two such numbers. Thus he replaced the functions $f(x, p)$ of position and momentum in terms of which classical physics is formulated by quantities $f(m, n)$. In order to secure the law of conservation of energy in his new mechanics, he was forced to postulate the multiplication rule $f * g(m, n) = \sum_l f(m, l)g(l, n)$, replacing the rule $fg(x, p) = f(x, p)g(x, p)$ of classical mechanics. He noted that $f * g \neq g * f$, unlike in classical mechanics, and saw in this non-commutativity of physical observables the key revolutionary character of quantum mechanics. When he showed his work to his boss Born, a physicist who as a former assistant to Hilbert was well versed in mathematics, Born saw, after a sleepless night, that Heisenbergs multiplication rule was the same as the one known for matrices, but now of infinite size[At the time, matrices and linear algebra were unknown to practically all physicists]. Thus Heisenbergs embryonic formulation of quantum theory, written down in 1925 in a paper generally seen as the birth of quantum mechanics, came to be known as matrix mechanics.

Second, Schrodinger was led to a formulation of quantum theory called wave mechanics, in which the famous symbol Ψ, denoting a wave function, played an important role. To summarize a long story, Schrodinger based his work on de Broglies idea that in quantum theory a wave should be associated to each particle; this turned Einsteinss concept of a photon from 1905 on its head[Einsteins revolutionary proposal, which marked the true conceptual beginning of quantum theory, had been that light, universally seen as a wave phenomenon at the

time, had a particle nature as well. The idea that light consists of particles had earlier been proposed by none other than Newton, but had been discredited after the discovery of Young around 1800 (and its further elaboration by Fresnel) that light displays interference phenomena and therefore should have a wave nature. This was subsequently confirmed by Maxwells theory, in which light is an oscillation of the electromagnetic field. In his PhD thesis from 1924, de Broglie generalized and inverted Einsteins reasoning: where the latter had proposed that light waves are particles, the former postulated that particles are waves]. De Broglies waves should, of course, satisfy some equation, similar to the fundamental wave equation or Maxwells equations. It is this equation that Schrodinger proposed in 1926 and which is now named after him. Schrodinger found his equation by studying the transition from wave optics to geometric optics, and by (wrongly) believing that there should be a similar transition from wave mechanics to classical mechanics.

Thus in 1926 one had two alternative formulations of quantum mechanics, which looked completely different, but each of which could explain certain atomic phenomena. The relationship and possible equivalence between these formulations was, of course, much discussed at the time. The most obvious difficulty in relating Heisenbergs work to Schrodingers was that the former was a theory of observables lacking the concept of a state, whereas the latter had precisely the opposite feature: Schrodingers wave functions were states, but where were the observables? To answer this question, Schrodinger introduced his famous expressions $Q = x$ (more precisely, $Q\Psi(x) = x\Psi(x)$ and $P = -i\hbar\partial/\partial x$, defining what we now call unbounded operators on the Hilbert space $L^2(\mathbb{R}^3)$. Subsequently, Dirac, Pauli, and Schrodinger himself recognized that wave mechanics was related to matrix mechanics in the following way: Heisenbergs matrix $x(m, n)$ was nothing but the matrix element (e_n, Qe_m) of the position operator Q with respect to the orthonormal basis of $L^2(\mathbb{R}^3)$ given by the eigenfunctions of the Hamiltonian $H = P^2/2m + V(Q)$. Conversely, the vectors in ℓ^2 on which Heisenbergs matrices acted could be interpreted as states. However, these observations fell far short of an equivalence proof of wave mechanics and matrix mechanics (as is sometimes claimed), let alone of a mathematical understanding of quantum mechanics.

Heisenbergs paper was followed by the Dreimännerarbeit of Born, Heisenberg, and Jordan (1926); all three were in Gottingen at the time. Born turned to his former teacher Hilbert for mathematical advice. Hilbert had been interested in the mathematical structure of physical theories for a long time; his Sixth Problem (1900) called for the mathematical axiomatization of physics. Aided by his assistants Nordheim and von Neumann, Hilbert ran a seminar on the mathematical structure of quantum mechanics, and the three wrote a joint paper on the subject (now obsolete).

It was von Neumann alone who, at the age of 23, recognized the mathematical structure of quantum mechanics. In this process, he defined the abstract

concept of a Hilbert space discussed above; as we have said, previously only some examples of Hilbert spaces had been known. Von Neumann saw that Schrodingers wave functions were unit vectors in the Hilbert space $L^2(\mathbb{R}^3)$, and that Heisenbergs observables were linear operators on the Hilbert space ℓ^2. The Riesz-Fischer theorem then implied the mathematical equivalence between wave mechanics and matrix mechanics. In a series of papers that appeared between 1927-1929, von Neumann defined Hilbert space, formulated quantum mechanics in this language, and developed the spectral theory of bounded as well as unbounded normal operators on a Hilbert space. This work culminated in his book, which to this day remains the definitive account of the mathematical structure of elementary quantum mechanics[Von Neumanns book was preceded by Diracs The Principles of Quantum Mechanics (1930), which contains another brilliant, but this time mathematically questionable account of quantum mechanics in terms of linear spaces and operators].

Von Neumann proposed the following mathematical formulation of quantum mechanics. The observables of a given physical system are the self-adjoint (possibly unbounded) linear operators a on a Hilbert space H. The pure states of the system are the unit vectors in H. The expectation value of an observable a in a state ψ is given by $(\psi, a\psi)$. The transition probability between two states ψ and φ is $|(\psi, \varphi)|^2$. As we see from (4.3), this number is just $(\cos\theta)^2$, where θ is the angle between the unit vectors ψ and φ. Thus the geometry of Hilbert space has a direct physical interpretation in quantum mechanics, surely one of von Neumanns most brilliant insights. Later on, he would go beyond his Hilbert space approach to quantum theory by developing such topics and quantum logic and operator algebras.

See end of this chapter for a discussion of Lebesgue integration and associated concepts.

1.2 Metric Spaces, Normed Spaces, and Hilbert Spaces

1.2.1 Basic Definitions

We repeat two basic definitions from the Introduction, and add a third:

Definition 4.2.1 *Let V be a vector space over a field $\mathbb{K}$ (where $\mathbb{K} = \mathbb{R}$ or $\mathbb{K} = \mathbb{C}$).*

*An **inner product** on V is a map $V \times V \to \mathbb{K}$, written as $\langle f, g\rangle \mapsto (f, g)$, satisfying, for all $f, g, h \in V$ and $t \in \mathbb{K}$:*

1. $(f, f) \in \mathbb{R}^+ := [0, \infty)$ (positivity);

2. $(g, f) = \overline{(f, g)}$ (symmetry);

3. $(f, tg) = t(f, g)$ (linearity 1);

4. $(f, g + h) = (f, g) + (f, h)$ (linearity 2);

5. $(f, f) = 0 \Rightarrow f = 0$ (positive definiteness)

*A **norm** on V is a function $\|\cdot\| : V \to \mathbb{R}^+$ satisfying, for all $f, g, h \in V$ and $t \in \mathbb{K}$:*

1. $\|f + g\| \leq \|f\| + \|g\|$ (triangle inequality);

2. $\|tf\| = |t|\|f\|$ (homogeneity);

3. $\|f\| = 0 \Rightarrow f = 0$ (positive definiteness)

*A **metric** on V is a function $d : V \times V \to \mathbb{R}^+$ satisfying, for all $f, g, h \in V$:*

1. $d(f, g) \leq d(f, h) + d(h, g)$ (triangle inequality);

2. $d(f, g) = d(g, f)$ for all $f, g \in V$ (symmetry);

3. $d(f, g) = 0 \Leftrightarrow f = g$ (definiteness)

The notion of a metric applies to any set, not necessarily to a vector space, like an inner product and a norm. These structures are related in the following way[Apart from a norm, an inner product defines another structure called a transition probability, which is of great importance to quantum mechanics; (see the Introduction). Abstractly, a transition probability on a set $\mathcal{S}$ is a function $p : S \times S \to [0, 1]$ satisfying $p(x, y) = 1 \Leftrightarrow x = y$ (see Property 3 of a metric) and $p(x, y) = p(y, x)$. Now take the set $\mathcal{S}$ of all vectors in a complex inner product space that have norm 1, and define an equivalence relation on $\mathcal{S}$ by $f \sim g$ iff $f = zg$ for some $z \in \mathbb{C}$ with $|z| = 1$. (Without taking equivalence classes the first axiom would not be satisfied). The set $\mathcal{S} = S/\sim$ is then equipped with a transition probability defined by $p([f], [g]) := |(f, g)|^2$. Here $[f]$ is the equivalence class of f with $\|f\| = 1$, etc. In quantum mechanics vectors of norm 1 are (pure) states, so that the transition probability between two states is determined by their angle θ. (Recall the elementary formula from Euclidean geometry $(x, y) = \|x\|\|y\| \cos\theta$, where θ is the angle between x and y in $\mathbb{R}^n$)]:

Proposition 4.2.2

1. *An inner product on V defines a norm on V by means of $\|f\| = \sqrt{(f, f)}$.*

2. *A norm on V defines a metric on V through $d(f, g) := \|f - g\|$.*

The proof is based on the **Cauchy-Schwarz inequality**

$$|(f, g)| \leq \|f\|\|g\| \tag{1.13}$$

The three axioms on a norm immediately imply the corresponding properties of the metric. The question arises when a norm comes from an inner product

in the stated way: this question is answered by the **Jordan - von Neumann theorem**:

Theorem 4.2.3 *A norm $\|\cdot\|$ on a vector space comes from an inner product through $\|f\| = \sqrt{(f,f)}$ if and only if*

$$\|f+g\|^2 + \|f-g\|^2 = 2(\|f\|^2 + \|g\|^2) \tag{1.14}$$

In that case, one has

$$4(f,g) = \|f+g\|^2 + \|f-g\|^2 \;\; for \;\; \mathbb{K} = \mathbb{R}$$

and

$$4(f,g) = \|f+g\|^2 - \|f-g\|^2 + i\|f-ig\|^2 - i\|f+ig\|^2 \;\; for \;\; \mathbb{K} = \mathbb{C}$$

Applied to the ℓ^p and L^p spaces mentioned in the introduction, this yields the result that the norm in these spaces comes from an inner product if and only if $p = 2$; see below for a precise definition of $L^p(\Omega)$ for $\Omega \subseteq \mathbb{R}^n$. There is no (known) counterpart of this result for the transition from a norm to a metric. It is very easy to find examples of metrics that do not come from a norm: on any vector space (or indeed any set) V the formula $d(f,g) = \delta_{fg}$ defines a metric not derived from a norm. Also, if d is any metric on V , then $d' = d/(1+d)$ is a metric, too: since clearly $d'(f,g) \leq 1$ for all f, g, this metric can never come from a norm.

1.2.2 Convergence and completeness

The reason we look at metrics in a Hilbert space course is, apart from general education, that many concepts of importance for Hilbert spaces are associated with the metric rather than with the underlying inner product or norm. The main such concept is convergence:

Definition 4.2.4 *Let $(x_n) := \{x_n\}, n \in \mathbb{N}$ be a sequence in a metric space (V,d). We say that $x_n \to x$ (i.e., (x_n) converges to $x \in V$) when $\lim_{n\to\infty} d(x_n, x) = 0$, or, more precisely: for any $\epsilon > 0$ there is $N \in \mathbb{N}$ such that $d(x_n, x) < \epsilon$ for all $n > N$*

In a normed space, hence in particular in a space with inner product, this therefore means that $\lim_{n\to\infty} \|x_n - x\| = 0$[Such convergence is sometimes called **strong convergence**, in contrast to **weak convergence**, which for an inner product space means that $\lim_n |(y, x_n - x)| = 0$ for each $y \in V$].

A sequence (x_n) in (V,d) is called a Cauchy sequence when $d(x_n, x_m) \to 0$ when $n, m \to \infty$; more precisely: for any $\epsilon > 0$ there is $N \in \mathbb{N}$ such that $d(x_n, x_m) < \epsilon$ for all n, m ¿ N. Clearly, a convergent sequence is Cauchy: from the triangle inequality and symmetry one has

$$d(x_n, x_m) \leq d(x_n, x) + d(x_n, x)$$

So for given $\epsilon > 0$ there is $N \in \mathbb{N}$ such that $d(x_n, x) < \epsilon/2$, etcetera. However, the converse statement does not hold in general, as is clear from the example of the metric space $(0, 1)$ with metric $d(x, y) = |x - y|$: the sequence $x_n = 1/n$ does not converge in $(0, 1)$ (for an example involving a vector space see the exercises). In this case one can simply extend the given space to $[0, 1]$, in which every Cauchy sequence does converge.

Definition 4.2.5

A metric space (V, d) is called complete when every Cauchy sequence converges.

- *A vector space with norm that is complete in the associated metric is called a* **Banach space**.
- *A vector space with inner product that is complete in the associated metric is called a* **Hilbert space**.

The last part may be summarized as follows: *a vector space H with inner product $(\ ,\ )$ is a Hilbert space when every sequence (x_n) such that $\lim_{n,m\to\infty} \|x_n - x_m\| = 0$ has a limit $x \in H$ in the sense that $\lim_{n\to\infty} \|x_n - x\| = 0$ (where $\|x\| = \sqrt{(x, x)}$). It is easy to see that such a limit is unique.*

Like any good definition, this one too comes with a theorem:

Theorem 4.2.6 *For any metric space (V, d) there is a complete metric space $(\tilde{V}, \tilde{d})$, (unique up to isomorphism) containing (V, d) as a dense subspace[This means that any point in $\tilde{V}$ is the limit of some convergent sequence in V with respect to the metric $\tilde{d}$] on which $\tilde{d} = d$. If V is a vector space, then so is $\tilde{V}$. If the metric d comes from a norm, then $\tilde{V}$ carries a norm inducing $\tilde{d}$ (so that $\tilde{V}$, being complete, is a Banach space). If the norm on V comes from an inner product, then $\tilde{V}$ carries an inner product, which induces the norm just mentioned (so that $\tilde{V}$ is a Hilbert space), and whose restriction to V is the given inner product.*

This theorem is well known and basic in analysis so we will not give a complete proof, but will just sketch the main idea. In these notes one only needs the case where the metric comes from a norm, so that $d(x_n, y_n) = \|x_n - y_n\|$ etc. in what follows.

One defines the completion $\tilde{V}$ as the set of all Cauchy sequences (x_n) in V, modulo the equivalence relation $(x_n) \sim (y_n)$ when $\lim_n d(x_n, y_n) = 0$. (When x_n and y_n converge in V, this means that they are equivalent when they have the same limit). The metric $\tilde{d}$ on the set of such equivalence classes $[x_n] := [(x_n)]$ is defined by $\tilde{d}([x_n], [y_n]) := \lim_n d(x_n, y_n)$. The embedding $\iota : V \hookrightarrow \tilde{V}$ is given by identifying $x \in V$ with the Cauchy sequence $(x_n = x \forall n)$, i.e., $\iota(x) = [x_n = x]$. It follows that a Cauchy sequence (x_n) in $V \subseteq \tilde{V}$ converges to$[x_n]$, for

$$\lim_m \tilde{d}(\iota(x_m), [x_n]) = \lim_m \tilde{d}([x_n = x_m], [x_n]) = \lim_m \lim_n d(x_m, x_n) = 0$$

by definition of a Cauchy sequence. Furthermore, one can show that any Cauchy sequence in $\tilde{V}$ converges by approximating its elements by elements of V.

If V is a vector space, the corresponding linear structure on $\tilde{V}$ is given by $[x_n] + [y_n] := [x_n + y_n]$ and $t[x_n] := [tx_n]$. If V has a norm, the corresponding norm on $\tilde{V}$ is given by $\|[x_n]\| := \lim_n \|x_n\|$.

If V has an inner product, the corresponding inner product on $\tilde{V}$ is given by $([x_n], [y_n]) := \lim_n (x_n, y_n)$.

A finite-dimensional vector space is complete in any possible norm. In infinite dimension, completeness generally depends on the norm (which often can be chosen in many different ways, even apart from trivial operations like rescaling by a positive constant). For example, take $V = \ell_c$, the space of functions $f : \mathbb{N}- \to (C)$ (or, equivalently, of infinite sequence $(f(1), f(2), ..., f(k), ...)$) with only finitely many $f(k) \neq 0$. Two interesting norms on this space are:

$$\|f\|_\infty := sup_k\{|f(k)|\} \tag{1.15}$$

$$\|f\|_2 := \left(\sum_{k=1}^{\infty} |f(k)|^2\right)^{1/2} \tag{1.16}$$

ℓ_c is not complete in either norm. However, the space

$$\ell^\infty := \{f : \mathbb{N} \to \mathbb{C} | \|f\|_\infty < \infty \tag{1.17}$$

is complete in the norm $\|\cdot\|_\infty$, and the space

$$\ell^2 := \{f : \mathbb{N} \to \mathbb{C} | \|f\|_2 < \infty \tag{1.18}$$

is complete in the norm $\|\cdot\|_2$. In fact, ℓ^2 is a Hilbert space in the inner product

$$(f, g) := \sum_{k=1}^{\infty} \overline{f(k)} g(k) \tag{1.19}$$

Now we seem to face a dilemma. On the one hand, there is the rather abstract completion procedure for metric spaces just sketched: it looks terrible to use in practice. On the other hand, we would like to regard ℓ^∞ as the completion of ℓ_c in the norm $\|f\|_\infty$ and similarly we would like to see ℓ^2 as the completion of ℓ_c in the norm $\|f\|_2$.

This can indeed be done through the following steps, which we just outline for the Hilbert space case ℓ^2 (similar comments hold for ℓ^∞):

1. Embed $V = \ell_c$ is some larger space W: in this case, W is the space of all sequences (or of all functions $f : \mathbb{N} \to \mathbb{C}$).

2. Guess a maximal subspace H of W in which the given norm $\|\cdot\|_2$ is finite: in this case this is $H = \ell^2$.

3. Prove that H is complete.

4. Prove that V is dense in H, in the sense that each element $f \in H$ is the limit of a Cauchy sequence in V.

The last step is usually quite easy. For example, any element $f \in \ell^2$ is the limit (with respect to the norm $\|\cdot\|_2$, of course), of the sequence (f_n) where $f_n(k) = f(k)$ if $k \leq n$ and $f_n(k) = 0$ if $k > n$. Clearly, $f_n \in \ell_c$ for all n.

The third step may in itself be split up in the following way:

- Take a generic Cauchy sequence (f_n) in H and guess its limit f in W.
- Prove that $f \in H$.
- Prove that $\lim_n \|f_n - f\| = 0$

Here also the last step is often easy, given the previous ones.

In our example this procedure is implemented as follows.

- If (f_n) is any sequence in ℓ^2, the the definition of the norm implies that for each k one has

  $$|f_n(k) - f_m(k)| \leq \|f_n - f_m\|_2$$

  So if (f_n) is a Cauchy sequence in ℓ^2, then for each k, $(f_n(k)$ is a Cauchy sequence in $\mathbb{C}$. Since $\mathbb{C}$ is complete, the latter has a limit called $f(k)$. This defines $f \in W$ as the candidate limit of (f_n), simply by $f : k \mapsto f(k) := \lim_n f_n(k)$.

- For each n one has:

  $$\|fn - f\|_2^2 = \sum_{k=1}^{\infty} |f_n(k) - f|^2 = \lim_{N\to\infty} \lim_{m\to\infty} \sum_{k=1}^{N} |f_N(k) - f_m(k)|^2$$

  By the definition of *lim sup* and using the positivity of all terms one has

  $$\lim_{m\to\infty} \sum_{k=1}^{N} |f_N(k) - f_m(k)|^2 \leq \lim \sup_{m\to\infty} \sum_{k=1}^{\infty} |f_N(k) - f_m(k)|^2 = \lim \sup_{m\to\infty} \|f_n - f_m\|_2^2$$

  Hence

  $$\|f_n - f\|_2^2 = \lim \sum_{m\to\infty} \|f_n - f_m\|_2^2$$

  Since (f_n) is Cauchy, this can be made $< \epsilon^2$ for $n > N$. Hence $\|f_n - f\|_2 \leq \epsilon$, so $f_n - f \in \ell^2$ and since $f_n \in \ell^2$ and ℓ^2 is a vector space, it follows that $f \in \ell^2 = H$, as desired.

- The claim $\lim_n \|f_n - f\| = 0$ follows from the same argument.

Returning to our dilemma, we wish to establish a link between the practical completion ℓ^2 of ℓ_c and the formal completion $\tilde{\ell}_c$. Such a link is given by the concept of **isomorphism** of two Hilbert spaces H_1 and H_2. As in the Introduction, we define an **isomorphism** of Hilbert spaces $U : H_1 \to H_2$ as an invertible linear map preserving the inner product (i.e., $(Uf, Ug)_2 = (f, g)_1$ for all $f, g \in H_1$). Such a map U is called a **unitary transformation** and we write $H_1 \cong H_2$.

So, in order to identify ℓ^2 with $\tilde{\ell}_c$ we have to find such a $U : \tilde{\ell}_c \to \ell^2$. This is easy: if (f_n) is Cauchy in ℓ_c we put

$$U(|f_n|) := f = \lim_n f_n \tag{1.20}$$

where f is the limit as defined above. It is easy to check that:

1. This map is well-defined, in the sense that if $f_n \sim g_n$ then $\lim_n f_n = \lim_n g_n$
2. This map is indeed invertible and preserves the inner product

We now apply the same strategy to a more complicated situation. Let $\Omega \subseteq \mathbb{R}^n$ be an open or closed subset of $\mathbb{R}^n$, just think of $\mathbb{R}^n$ itself for the quantum theory of a particle, of $[-\pi, \pi] \subset \mathbb{R}$ for Fourier analysis. The role of ℓ_c in the previous analysis is now played by $C_c(\Omega)$, the vector space of complex-valued continuous functions on Ω with compact support[The support of a function is defined as the smallest closed set outside which it vanishes]. Again, one has two natural norms on $C_c(\Omega)$:

$$\|f\|_\infty := \sup_{x \in \Omega} \{|f(x)|\} \tag{1.21}$$

$$\|f\|_2 := \left(\int_\Omega d^n x |f(x)|^2 \right)^{1/2} \tag{1.22}$$

The first norm is called the **supremum-norm** or **sup-norm**. The second norm is called the $\mathbf{L^2-norm}$ (see below). It is, of course, derived from the inner product

$$(f, g) := \left(\int_\Omega d^n x \overline{f(x)} g(x) \right)^{1/2} \tag{1.23}$$

But even the first norm will turn out to play an important role in Hilbert space theory.

Interestingly, if Ω is compact, then $C_c(\Omega) = C(\Omega)$ is complete in the norm $\|\cdot\|_\infty$. This claim follows from the theory of uniform convergence.

However, $C_c(\Omega)$ fails to be complete in the norm $\|\cdot\|_2$. Consider $\Omega = [0, 1]$. The sequence of functions

$$f_n(x) = \begin{cases} 0 & (x \leq 1/2) \\ n(x - 1/2) & (1/2 \leq x \leq 1/2 + 1/n) \\ 1 & (x \geq 1/2 + 1/n) \end{cases}$$

is a Cauchy sequence with respect to $\|\cdot\|_2$ that converges to a discontinuous function $f(x) = 0$ for $x \in [0, 1/2)$ and $f(x) = 1$ for $x \in (1/2, 1]$ (the value at $x = 1/2$ is not settled; see below, but in any case it cannot be chosen in such a way that f is continuous).

Clearly, $C_c(\Omega)$ lies in the space W of all functions $f : \Omega \to \mathbb{C}$, and according to the above scenario our task is to find a subspace $H \subseteq W$ that plays the role of the completion of $C_c(\Omega)$ in the norm $\|\cdot\|_2$. There is a complication, however, which does not occur in the case of ℓ^2. Let us ignore this complication first. A detailed study shows that the analogue of ℓ^2 is now given by the space $\mathcal{L}^2(\Omega)$, defined as follows.

Definition 4.2.7 The space $\mathcal{L}^2(\Omega)$ consists of all functions $f : \Omega \to \mathbb{C}$ for which there exists a Cauchy sequence (f_n) in $C_c(\Omega)$ with respect to $\|\cdot\|_2$ such that $f_n(x) \to f(x)$ for all $x \in \Omega \backslash N$, where $N \subset \Omega$ is a set of (Lebesgue) measure zero.

Now a subset $N \subset \mathbb{R}^n$ has measure zero if for any $\epsilon > 0$ there exists a covering of N by an at most countable set (I_n) of intervals for which $\sum_n |I_n| < \epsilon$, where $\sum_n |I_n|$ is the sum of the volumes of the I_n. (Here an interval in $\mathbb{R}^n$ is a set of the form $\Pi_{k=1}^n [a_k, b_k]$). For example, any countable subset of $\mathbb{R}^n$ has measure zero, but there are others.

The space $\mathcal{L}^2(\Omega)$ contains all functions f for which $|f|^2$ is Riemann-integrable over Ω (so in particular all of$C_c(\Omega)$, as was already clear from the definition), but many other, much wilder functions. We can extend the inner product on $C_c(\Omega)$ to $\mathcal{L}^2(\Omega)$ by means of

$$(f, g) = \lim_{n\to\infty} (f_n, g_n) \tag{1.24}$$

where (f_n) and (g_n) are Cauchy sequences as specified in the definition of $\mathcal{L}^2(\Omega)$.

Consequently, taking $g_n = f_n$, the following limit exists:

$$\|f\|_2 := \lim_{n\to\infty} \|f_n\|_2 \tag{1.25}$$

The problem is that (4.24) does not define an inner product on $\mathcal{L}^2(\Omega)$ and that (4.25) does not define a norm on it because these expressions fail to be positive definite. For example, take a function f on $\Omega = [0, 1]$ that is nonzero in finitely (or even countably) many points. The Cauchy sequence with only zeros defines f as an element of $\mathcal{L}^2(\Omega)$, so $\|f\|_2 = 0$ by (4.25), yet $f \neq 0$ as a function. This is related to the following point: the sequence (f_n) does not define f except outside a set of measure zero.

Everything is solved by introducing the space

$$\mathcal{L}^2(\Omega) := \mathcal{L}^2(\Omega)/\mathcal{N} \tag{1.26}$$

where

$$\mathcal{N} := \{f \in \mathcal{L}^2(\Omega) | \|f\|_2 = 0\} \tag{1.27}$$

Using measure theory, it can be shown that $f \in \mathcal{N}$ iff $f(x) = 0$ for all $x \in \Omega \backslash N$, where $N \subset \Omega$ is some set of measure zero. If f is continuous, this implies that $f(x) = 0$ for all $x \in \Omega$.

It is clear that $\|\cdot\|_2$ descends to a norm on $L^2(\Omega)$ by

$$\|[f]\|_2 := \|f\|_2 \tag{1.28}$$

where $[f]$ is the equivalence class of $f \in \mathcal{L}^2(\Omega)$ in the quotient space. However, we normally work with $\mathcal{L}^2(\Omega)$ and regard elements of $L^2(\Omega)$ as functions instead of equivalence classes thereof. So in what follows we should often write $[f] \in L^2(\Omega)$instead of $f \in \mathcal{L}^2(\Omega)$, but who cares.

We would now like to show that $L^2(\Omega)$ is the completion of $C_c(\Omega)$. The details of the proof require the theory of Lebesgue integration (see section 4.8), but the idea is similar to the case of ℓ^2.

Let (f_n) be Cauchy in $\mathcal{L}^2(\Omega)$. By definition of the norm in $L^2(\Omega)$, there is a sequence (h_n) in $C_c(\Omega)$ such that:

1. $\|f_n - h_n\|_2 \leq 2^n \;\; for \;\; all \;\; n$;
2. $|f_n(x) - h_n(x)| \leq 2^{-n} \;\; for \;\; all \;\; x \in \Omega \backslash A_n, \;\; where \;\; |A_n| \leq 2^{-n}$

By the first property one can prove that (h_n) is Cauchy, and by the second that $\lim_n h_n(x)$ exists for almost all $x \in \Omega$ (i.e. except perhaps at a set N of measure zero). This limit defines a function $f : \Omega \backslash N \to \mathbb{C}$ for which $h_n(x) \to f(x)$ Outside N, f can be defined in any way one likes. Hence $f \in \mathcal{L}^2(\Omega)$, and its equivalence class $[f] \in L^2(\Omega)$ is independent of the value of f on the null set N. It easily follows that $\lim_n f_n = f$ in $\|\cdot\|_2$, so that Cauchy sequence (f_n) converges to an element of $L^2(\Omega)$. Hence $L^2(\Omega)$ is complete.

The identification of $L^2(\Omega)$ with the formal completion of $C_c(\Omega)$ is done in the same way as before: we repeat (4.20), where this time the function $f \in CL^2(\Omega)$ is the one associated to the Cauchy sequence (f_n) in $C_c(\Omega)$ through Definition 4.2.7. As stated before, it would be really correct to write (4.20) as follows:

$$U([f_n]) := [f] = [\lim_n f_n] \tag{1.29}$$

where the square brackets on the left-hand side denote equivalence classes with respect to the equivalence relation $(f_n) \sim (g_n)$ when $\lim_n \|f_n - g_n\|_2 = 0$ between Cauchy sequences in $C_c(\Omega)$, whereas the square brackets on the right-hand side denote equivalence classes with respect to the equivalence relation $f \sim g$ when $\lim_n \|f - g\|_2 = 0$ between elements of $\mathcal{L}^2(\Omega)$.

We finally note a interesting result about $L^2(\Omega)$ without proof:

Theorem 4.2.8 *Every Cauchy sequence* (f_n) *in* $\mathcal{L}^2(\Omega)$ *has a subsequence that converges pointwise almost everywhere to somef* $\in \mathcal{L}^2(\Omega)$

The proof of this theorem yields an alternative approach to the completeness of $L^2(\Omega)$.

In many cases, all you need to know is the following fact about L^2 or $\mathcal{L}^2$, which follows from the fact that $L^2(\Omega)$ is indeed the completion of $C_c(\Omega)$ (and is a consequence of Definition 4.2.7) if enough measure theory is used):

Proposition 4.2.9 *For any* $f \in \mathcal{L}^2(\Omega)$ *there is a Cauchy sequence* (f_k) *in* $C_c(\Omega)$ *such that* $f_k \to f$ *in norm (ie.,* $\lim_{k\to\infty} \|f - f_k\|_2 = 0$*).*

Without creating confusion, one can replace $f \in \mathcal{L}^2(\Omega)$ by$f \in L^2(\Omega)$ in this statement, as long as one keeps the formal difference between L^2 and $\mathcal{L}^2$ in the back of ones mind.

1.2.3 Orthogonality and orthonormal bases

As stressed in the Introduction, Hilbert spaces are the vector spaces whose geometry is closest to that of $\mathbb{R}^3$. In particular, the inner product yields a notion of orthogonality. We say that two vectors $f, g \in H$ are orthogonal, written $f \perp g$, when $(f, g) = 0$[By definition of the norm, if $f \perp g$ one has Pythagoras theorem $\|f + g\|^2 = \|f\|^2 + \|g\|^2$]. Similarly, two subspaces $K \subset H$ and $L \subset H$ are said to be orthogonal ($K \perp L$) when $(f, g) = 0$ for all $f \in K$ and all $g \in L$. A vector f is called orthogonal to a subspace K, written $f \perp K$, when $(f, g) = 0$ for all $g \in K$, etc.

For example, if $H = L^2(\Omega)$ and $\Omega = \Omega_1 \cup \Omega_2$, elementary (Riemann) integration theory shows that the following subspaces are orthogonal:

$$K = \{f \in C_c(\Omega) | f(x) = 0 \ \forall x \in \Omega_1\} \tag{1.30}$$

$$L = \{f \in C_c(\Omega) | f(x) = 0 \ \forall x \in \Omega_2\} \tag{1.31}$$

We define the **orthogonal complement** $K^\perp$ of a subspace $K \subset H$ as

$$K^\perp := \{f \in H | f \perp K\} \tag{1.32}$$

This set is automatically linear, so that the map $K \mapsto K^\perp$, called **orthocomplementation**, is an operation from subspaces of H to subspaces of H. Clearly, $H^\perp = 0$ and $0^\perp = H$.

Now, a subspace of a Hilbert space may or may not be closed. A **closed subspace** $K \subset H$ of a Hilbert space H is by definition complete in the given norm on H(i.e. any Cauchy-sequence in K converges to an element of K [Since H is a Hilbert space we know that the sequence has a limit in H, but this limit may not lie in K even when all elements of the sequence lie in K. This possibility

arises precisely when K fails to be closed]). This implies that a closed subspace K of a Hilbert space H is itself a Hilbert space if one restricts the inner product from H to K. If K is not closed already, we define its **closure** $\bar{K}$ as the smallest closed subspace of H containing K.

For example, if $\Omega \subset \mathbb{R}^n$ then $C_c(\Omega)$ is a subspace of $L^2(\Omega)$ which is not closed; its closure is $L^2(\Omega)$.

Closure is an analytic concept, related to convergence of sequences. Orthogonality is a geometric concept. However, both are derived from the inner product. Hence one may expect certain connections relating analysis and geometry on Hilbert space.

Proposition 4.210 *Let $K \subset H$ be a subspace of a Hilbert space.*

1. *The subspace $K^\perp$ is closed, with*
$$K^\perp = \bar{K}^\perp = \bar{K^\perp} \tag{1.33}$$
2. *One has*
$$K^{\perp\perp} := (K^\perp)^\perp = \bar{K} \tag{1.34}$$
3. *Hence for closed subspaces K one has $K^{\perp\perp} = K$.*

We now turn to the concept of an **orthonormal basis** (o.n.b.) in a Hilbert space. First, one can:

1. Define a Hilbert space H to be finite-dimensional if has a finite o.n.b. (e_k) in the sense that $(e_k, e_l) = \delta_{kl}$ and any $v \in H$ can be written as $v = \sum_k v_k e_k$ for some $v_k \in$
2. Prove (by elementary linear algebra) that any o.n.b. in a finite-dimensional Hilbert space H has the same cardinality;
3. Define the dimension of H as the cardinality of an arbitrary o.n.b. of H.

It is trivial to show that if $v = \sum_k v_k e_k$, then
$$v_k = (e_k, v) \tag{1.35}$$
and
$$\sum_k |(e_k, v)|^2 = \|v\|^2 \tag{1.36}$$
This is called **Parsevals equality**; it is a generalization of Pythagorass Theorem. Note that if H is finite-dimensional, then any subspace is (automatically) closed.

Now what happens when H is not finite-dimensional? In that case, it is called

infinite-dimensional. The spaces ℓ^2 and $L^2(\Omega)$ are examples of infinite-dimensional Hilbert spaces. We call an infinite-dimensional Hilbert space separable when it contains a *countable* orthonormal set $(e_k)_{k\in\mathbb{N}}$ such that any $v \in H$ can be written as

$$v = \sum_{k=1}^{\infty} v_k e_k \tag{1.37}$$

for some $v_k \in \mathbb{C}$. By definition, this means that

$$v = \lim_{N\to\infty} \sum_{k=1}^{N} v_k e_k \tag{1.38}$$

where the limit means that

$$\lim_{N\to\infty} \|v - \sum_{k=1}^{N} v_k e_k\| = 0 \tag{1.39}$$

Here the norm is derived from the inner product in the usual way. Such a set is again called an orthonormal basis. It is often convenient to take $\mathbb{Z}$ instead of $\mathbb{N}$ as the index set of the basis, so that one has $(e_k)_{k\in\mathbb{Z}}$ and

$$v = \lim_{N\to\infty} \sum_{k=-N}^{N} v_k e_k \tag{1.40}$$

Also, the following lemma will often be used:

Lemma 4.2.11 *Let (e_k) be an o.n.b. in an infinite-dimensional separable Hilbert space H and let $f, g \in H$. Then*

$$\sum_k (f, e_k)(e_k, g) = (f, g) \tag{1.41}$$

This follows if one expands f and g on the right-hand side according to (4.37) and uses (4.35); one has to be a little bit careful with the infinite sums but these complications are handled in the same way as in the proof of (4.35) and (4.34).

The following result is spectacular:

Theorem 4.2.12

1. *Two finite-dimensional Hilbert spaces are isomorphic* iff *they have the same dimension.*

2. *Any two separable infinite-dimensional Hilbert spaces are isomorphic.*

The general statement is as follows. One can introduce the notion of an orthonormal basis for an arbitrary Hilbert space as a maximal orthonormal set

(i.e., a set of orthonormal vectors that is not properly contained in any other orthonormal set). It can then be shown that in the separable case, this notion of a basis is equivalent to the one introduced above. One then proves that any two orthonormal bases of a given Hilbert space have the same cardinality. Hence one may define the dimension of a Hilbert space as the cardinality of an arbitrary orthonormal basis. Theorem 4.2.12 then reads in full glory: *Two Hilbert spaces are isomorphic* iff *they have the same dimension.*

To illustrate the theorem, we show that $\ell^2(\mathbb{Z})$ and $L^2([-\pi,\pi])$ are isomorphic through the Fourier transform. Namely, using Fourier theory one can show that the functions $(e_k)_{k\in\mathbb{Z}}$ defined by

$$e_k(x) := \frac{1}{\sqrt{2\pi}} e^{ikx} \tag{1.42}$$

from an o.n.b. of $L^2([-\pi,\pi])$. Trivially, the functions $(\varphi_k)_{k\in\mathbb{Z}}$ defined by

$$\varphi_k(l) = \delta_{kl} \tag{1.43}$$

form an o.n.b of $\ell^2(\mathbb{Z})$. (If one regards an element of $\ell^2(\mathbb{Z})$ as a sequence instead of a function, f_k is the sequence with a 1 at position k and zeros everywhere else.) This shows that $\ell^2(\mathbb{Z})$and $L^2([-\pi,\pi])$ are both separable infinite-dimensional, and hence isomorphic by Theorem 4.2.12. Indeed, it is trivial to write down the unitary map $U : L^2([-\pi,\pi]) \to \ell^2(\mathbb{Z})$ that makes $\ell^2(\mathbb{Z})$ and $L^2([-\pi,\pi])$ isomorphic according to the definition of isomorphism: one simply puts

$$Uf(k) := (e_k, f)_{L^2} = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} dx\, e^{-ikx} f(x) \tag{1.44}$$

Here $f \in \mathcal{L}([-\pi,\pi])$. The second equality comes from the definition of the inner product in $L^2([-\pi,\pi])$. The inverse of U is $V : \ell^2(\mathbb{Z}) \to L^2([-\pi,\pi])$, given by

$$V\varphi := \sum_{k\in\mathbb{Z}} \varphi(k) e_k \tag{1.45}$$

where $\varphi \in \ell^2(\mathbb{Z})$. It is instructive to verify that $V = U^{-1}$:

$$\begin{aligned}(UV\varphi)(k) = (e_k, V\varphi)_{L^2} &= (e_k, \sum_l \varphi(l) e_l)_{L^2} \\ &= \sum_l \varphi(l)(e_k, e_l)_{L^2} = \sum_l \varphi(l)\delta_{kl} = \varphi(k)\end{aligned} \tag{1.46}$$

where one justifies taking the infinite sum over l out of the inner product by the Cauchy-Schwarz inequality (using the fact that $\sum_l \|\varphi(l)\|^2 < \infty$, since by assumption $\varphi \in \ell^2(\mathbb{Z})$. Similarly, for $f \in L^2([-\pi,\pi])$ one computes

$$VUf = \sum_k (Uf)(k) e_k = \sum_k (e_k, f)_{L^2} e_k = f \tag{1.47}$$

by (4.37) and (4.35). Of course, all the work is in showing that the functions e_k form an o.n.b. of $L^2([-\pi,\pi])$, which we have not done here!

Hence $V = U^{-1}$, so that (4.45) reads

$$U^{-1}\varphi(x) = \sum_{k\in\mathbb{Z}} \varphi(k)e_k(x) = \frac{1}{\sqrt{2\pi}} \sum_{k\in\mathbb{Z}} \varphi(k)e^{ikx} \tag{1.48}$$

Finally, the unitarity of U follows from the computation (where $f, g \in L^2$)

$$(Uf, Ug)^{\ell^2} = \sum_k (f, e_k)_{L^2}(e_k, g)_{L^2} = (f, g)_{L^2} \tag{1.49}$$

where we have used (4.41).

The choice of a basis in the argument that $\ell^2(\mathbb{Z}) \simeq L^2([-\pi,\pi])$ was clearly essential. There are pairs of concrete Hilbert spaces, however, which one can show to be isomorphic *without choosing bases*. A good example is provided by (4.20) and surrounding text, which proves the practical completion ℓ^2 of ℓ_c and the formal completion $\tilde{\ell}_c$ to be isomorphic. If one can find a unitary map $U : H_1 \to H_2$ without choosing bases, the two Hilbert spaces in question are called **naturally isomorphic**. As another example, the formal completion $\widetilde{C_c(\Omega)}$ of $C_c(\Omega)$ is naturally isomorphic to $L^2(\Omega)$.

1.3 Operators and Functionals

1.3.1 Bounded Operators

For the moment, we are finished with the description of Hilbert spaces on their own. Indeed, Theorem 4.2.12 shows that, taken by themselves, Hilbert spaces are quite boring. The subject comes alive when one studies operators on Hilbert spaces. Here an **operator** $a : H_1 \to H_2$ between two Hilbert spaces is nothing but a linear map (i.e., $a(\lambda v+\mu w) = \lambda a(v)+\mu a(w)$ for all $\lambda, \mu \in \mathbb{C}$ and $v, w \in H_1$. We usually write av for $a(v)$.

The following two special cases will occur time and again:

1. Let $H_1 = H$ and $H_2 = \mathbb{C}$: a linear map $\varphi : H \to \mathbb{C}$ is called a **functional** on H.

2. Let $H_1 = H_2 = H$: a linear map $a : H \to H$ is just called an **operator** on H.

To construct an example of a functional on H, take $f \in H$ and define $\varphi_f : H \to \mathbb{C}$ by

$$\varphi_f(g) := (f, g) \tag{1.50}$$

When H is finite-dimensional, any operator on H can be represented by a matrix and the theory reduces to linear algebra. For an infinite-dimensional example, take $H = \ell^2$ and $\hat{a} \in \ell^\infty$. It is easy to show that if $f \in \ell^2$, then $\hat{a}f \in \ell^2$. Hence we may define an operator $a : \ell^2 \to \ell^2$ by

$$\hat{a}f := af \tag{1.51}$$

We will often write a for this operator instead of $\hat{a}$. Similarly, take $H = L^2(\Omega)$ and $\hat{a} \in C_b(\Omega)$ (where $C_b(\Omega)$ is the space of bounded continuous functions on $\Omega \subset \mathbb{R}^n$, i.e., $\hat{a} : \Omega \to \mathbb{C}$ is continuous and $\|\hat{a}\|_\infty < \infty$. It is can then be shown that if $f \in L^2(\Omega)$ and $\hat{a} \in C_b(\Omega)$, then$\hat{a}f \in L^2(\Omega)$. Thus also in this case (4.51) defines an operator $a : L^2(\Omega) \to L^2(\Omega)$, called a **multiplication operator**.

Finally, the operators U and V constructed at the end of the previous section in the context of the Fourier transform give examples of operators between different Hilbert spaces.

As in elementary analysis, where one deals with functions $f : \mathbb{R} \to \mathbb{R}$, it turns out to be useful to single out functions with good properties, notably continuity. So what does one mean by a continuous operator $a : H_1 \to H_2$? One answer come from topology: the inner product on a Hilbert space defines a norm, the norm defines a metric, and finally the metric defines a topology, so one may use the usual definition of a continuous function $f : X \to Y$ between two topological spaces. Since not everyone is familiar with abstract topology, we use another definition, which turns out to be equivalent to the topological one. (In fact, the definition below is much more useful than the topological definition).

Definition 4.3.1 *Let $a : H_1 \to H_2$ be an operator. Define a positive number $\|a\|$ by*

$$\|a\| := \sup\{\|av\|_{H_2}, v \in H_1, \|v\|_{H_1} = 1\} \tag{1.52}$$

*where $\|v\|_{H_1} = \sqrt{(v,v)_{H_1}}$, etc. We say that a is **continuous** or **bounded** when $\|a\| < \infty$.*

For the benefit of those familiar with topology, we mention without proof that a is continuous according to this definition iff it is continuous in the topological sense, as explained above. This may be restated as follows: an operator $a : H_1 \to H_2$ is continuous (in the topological sense) iff it is bounded (in the sense of Definition 4.3.1).

Geometrically, the set $\{v \in H_1, \|v\|_{H_1} = 1\}$ is the unit ball in H_1, i.e. the set of vectors of length 1 in H_1. Hence $\|a\|$ is the supremum of the function $v \mapsto \|av\|_{H_2}$ from the unit ball in H_1 to $\mathbb{R}^+$. If H_1 is finite-dimensional the unit ball in H_1 is compact. Since the function just mentioned is continuous, it follows that any operator a on a finite-dimensional Hilbert space is bounded (as a continuous function from a compact set in $\mathbb{R}^n$ to $\mathbb{R}$ assumes a maximum somewhere).

If a is bounded, the number $\|a\|$ is called the **norm** of a. This terminology remains to be justified; for the moment it is just a name. It is easy to see that if $\|a\| < \infty$, the norm of a coincided with the constant

$$\|a\| = \inf\{C \geq 0 | \|av\|_{H_2} \leq C\|v\|_{H_1} \forall v \in H_1\} \tag{1.53}$$

Moreover, if a is bounded, then it is immediate that

$$\|av\|_{H_2} \leq \|a\|\|v\|_{H_1} \tag{1.54}$$

for all $v \in H_1$. This inequality is very important. For example, it trivially implies that

$$\|ab\| \leq \|a\|\|b\| \tag{1.55}$$

where $a : H \to H$ and $b : H \to H$ are any two bounded operators, and $ab := a \circ b$, so that $(ab)(v) := a(bv)$.

In the examples just considered, all operators turn out to be bounded. First take a functional $\varphi : H \to \mathbb{C}$; since $\|\cdot\|_{\mathbb{C}} = |\cdot|$, one has

$$\|\varphi\| := \sup\{|\varphi(v)|, v \in H, \|v\|_H = 1\} \tag{1.56}$$

If one uses Cauchy-Schwarz, it is clear from (4.50) that $\|\varphi_f\| \leq \|f\|_H$. In fact, an important result in Hilbert space theory says:

Theorem 4.3.2 *Let H be a Hilbert space. Any functional of the form φ_f for some $f \in H$ (see (4.50)) is continuous. Conversely, any continuous functional $\varphi : H \to \mathbb{C}$ is of the form $\varphi_f : g \mapsto (f, g)$ for some unique $f \in H$, and one has*

$$\|\varphi_f\| = \|f\|_H \tag{1.57}$$

The proof is as follows. First, given $f \in H$, as already mentioned, φ_f is bounded by Cauchy-Schwarz. Conversely, take a continuous functional $\varphi : H \to \mathbb{C}$, and let N be the kernel of φ. This is a closed subspace of H by the boundedness of φ. If $N = H$ then $\varphi = 0$ so we are ready, since $\varphi = \varphi_{f=0}$. Assume $N \neq H$. Since N is closed, $N^\perp$ is not empty, and contains a vector h with $\|h\| = 1$[To see this, pick an orthonormal basis (e_n) of N. Since N is closed, any f of the form $f = \sum_n c_n e_n$, $c_n \in \mathbb{C}$, that lies in H (which is the case iff $\sum_n |c_n|^2 < \infty$ actually lies in N. Since $N \neq H$, there exists $g \notin N$, which implies that $g \neq \sum_n (e_n, g)e_n$, or $h := g - \sum_n (e_n, g)e_n \neq 0$. Clearly, $h \in N^\perp$, and since $h \neq 0$ the vector has norm 1. This argument will become clearer after the introduction of projections later in this section]. For any $g \in H$, one has $\varphi(g)h - \varphi(h)g \in N$, so $(h, \varphi(g)h - \varphi(h)g = 0$, which means $\varphi(g)(h, h) = \varphi(h)(h, g)$, or $\varphi(g) = (f, g)$ with $f = \varphi(h)h$.

To prove uniqueness of f, suppose there is h with $h' \in \ker(\varphi)^\perp$ and $\|h'\| = 1$, and consequently also $\varphi(g) = (f', g)$ with $f' = \varphi(h)h'$. Then $\varphi(h) = \varphi(h)(h', h)$, so that $h - (h', h)h' \in \ker(\varphi)$. But $\ker(\varphi)^\perp$ is a linear subspace of H, so it must

be that $h - (h', h)h' \in \ker(\varphi)^\perp$ as well. Since $\ker(\varphi)^\perp \cap \ker(\varphi) = 0$, it follows that $h - (h', h)h' = 0$. Hence $h = (h', h)h'$ and therefore $\|h\| = 1$ and $\|h\| = 1$ yield $|(h, h')| = 1$, or $\overline{(h, h)}(h', h) = 1$. It follows that

$$f = \overline{\varphi(h)}h = \overline{(h', h)\varphi(h')}(h', h)h' = \overline{\varphi(h')}h' = f'$$

To compute$\|\varphi_f\|$, first use Cauchy-Schwarz to prove $\|\varphi_f\| \leq \|f\|$ and then apply φ_f to f to prove equality.

For an example of a bounded operator $a : H \to H$, note that on ℓ^2 as well as on $L^2(\Omega)$ the operator a defined by (4.51) is bounded, with

$$\|a\| = \|\hat{a}\|_\infty \tag{1.58}$$

A useful estimate

$$\|af\|_2 \leq \|\hat{a}\|_\infty \|f\|_2 \tag{1.59}$$

arises in the proof.

Finally, the operators U and V at the end of the previous section are unitary; it easily follows from the definition of unitarity that

$$\|U\| = 1 \tag{1.60}$$

for any unitary operator U.

What about discontinuous or unbounded operators? In view of (4.58), let us take an unbounded function $\hat{a} : \mathbb{Z} \to \mathbb{C}$ and attempt to define an operator $a : \ell^2 \to \ell^2$ by means of (4.51), hoping that $\|a\| = \infty$. The problem with this attempt is that in fact an unbounded function does not define a map from $\ell^2 \to \ell^2$ at all, since $\hat{a}f$ will not be in ℓ^2 for many choices of $f \in \ell^2$. (For example, consider $\hat{a}(k) = k$ and find such an f for which $\hat{a}f \notin \ell^2$ yourself). This problem is generic: as soon as one has a candidate for an unbounded operator $a : H_1 \to H_2$, one discovers that in fact a does not map H_1 into H_2.

Nonetheless, unbounded operators occur naturally in many examples and hence are extremely important in practice, especially in quantum mechanics and the theory of (partial) differential equations. But they are not constructed in the above manner as maps from H_1 to H_2. To prepare for the right concept of an unbounded operator, let us look at the bounded case once more. We restrict ourselves to the case $H_1 = H_2 = H$, as this is the relevant case for quantum mechanics.

As before, we denote the completion or closure of a subspace D of a Hilbert space H by $\bar{D} \subset V$.

Proposition 4.3.3 *Let $D \subset H$ be a subspace of a Hilbert space, and let $a : D \to H$ be a linear map. Define the positive number*

$$\|a\|_D := \sup\{\|av\|_H, v \in D, \|v\|_H = 1\} \tag{1.61}$$

If $\|a\|_D < \infty$, there exists a unique bounded extension of a to an operator $a^- : \bar{D} \to H$ with

$$\|a^-\| = \|a\|_D \tag{1.62}$$

In particular, when D is dense in H (in the sense that $\bar{D} = H$), the extension a^- is a bounded operator from H to H.

Conversely, a bounded operator $a : H \to H$ is determined by its restriction to a dense subspace $D \subset H$.

Hence in the above examples it suffices to compute the norm of a in order to find the norm of a^-. The point is now that unbounded operators are defined as linear maps $a : D \to H$ for which $\|a\|_D = \infty$. For example, take $\hat{a} \notin \ell^\infty$ and $f \in D = \ell_c$. Then $\hat{a}f \in \ell_c$, so that $a : \ell_c \to \ell^2$ is defined. One can also show that $\|a\|_{\ell_c} = \infty \text{iff} \hat{a} \notin \ell^\infty$ (i.e. $\hat{a}$ is unbounded). Another example is $af := df/dx$, defined on $f \in C^{(1)}([0,1]) \subset L^2([0,1])$. It can be shown that $\|df/dx\|_{C^{(1)}([0,1])} = \infty$. In quantum mechanics, operators like position, momentum and the Hamiltonian of a particle in a potential are unbounded, as we will see.

1.3.2 The Adjoint

Now let H be a Hilbert space, and let $a : H \to H$ be a bounded operator. The inner product on H gives rise to a map $a \mapsto a^*$, which is familiar from linear algebra: if $H = \mathbb{C}^n$, so that, upon choosing the standard basis (e_i), a is a matrix $a = (a_{ij})$ with $a_{ij} = (e_i, ae_j)$, then the adjoint is given by $a^* = (\bar{a_{ji}})$. In other words, one has

$$(a^* f, g) = (f, ag) \tag{1.63}$$

for all $f, g \in \mathbb{C}^n$. This equation defines the adjoint also in the general case. Note that the map $a \mapsto a^*$ is anti-linear: one has $(\lambda a)^* = \bar{\lambda} a$ for $\lambda \in \mathbb{C}$. One can also show that

$$\|a^*\| = \|a\| \tag{1.64}$$

$$\|a^* a\| = \|a\|^2 \tag{1.65}$$

A bounded operator $a : H \to H$ is called **self-adjoint** or **Hermitian** when $a^* = a$. It immediately follows form (4.63) that for self-adjoint a one has $(f, af) \in \mathbb{R}$.

One may also define self-adjointness in the unbounded case, in a way very similar to the story above. Namely, let $D \subset H$ be dense and let $a : D \to H$ be a possibly unbounded operator. We write $D(a)$ for D and define an operator $a^* : D(a^*) \to H$ as follows.

Definition 4.3.4

1. *The adjoint a^* of an unbounded operator $a : D(a) \to H$ has domain $D(a^*)$ consisting of all $f \in H$ for which the functional $g \mapsto \varphi_f^a(g) := (f, ag)$ is bounded. On this domain, a^* is defined by requiring $(a^*f, g) = (f, ag)$ for all $g \in D(a)$.*

2. *The operator a is called **self-adjoint** when $D(a^*) = D(a)$ and $a^* = a$.*

For example, a multiplication operator $\hat{a} \in C(\Omega)$ on $H = L^2(\Omega)$, defined on the domain $D(a) = C_c(\Omega)$ by $af = \hat{a}f$ as usual, has $a^* = \bar{a}$ (i.e., the complex conjugate of a seen as a multiplication operator) defined on the domain $D(a^*)$ given by

$$D(a^*) = \{f \in L^2(\Omega) | af \in L^2(\Omega)\} \tag{1.66}$$

Since $D(a) \subset D(a^*)$, the operator a cannot be self-adjoint. However, if we start again and define a on the domain specified by the right-hand side of (4.66), it turns out that this time one does have $a^* = a$. We will study such questions in detail later on, as they are very important for quantum mechanics. We return to the bounded case.

1.3.3 Projections

The most important examples of self-adjoint operators are projections.

Definition 4.3.5 *A **projection** on a Hilbert space H is a bounded operator $p \in H$ satisfying $p^2 = p^* = p$.*

To understand the significance of projections, one should first recall the discussion about orthogonality and bases in Hilbert spaces in section 4.2.3. Now let $K \subset H$ be a closed subspace of H ; such a subspace is a Hilbert space by itself, and therefore has an orthonormal basis (e_i). Applying (4.37) with (4.35) to K, it is easy to verify that

$$p : f \mapsto \sum_i (e_i, f) e_i \tag{1.67}$$

for each $f \in H$, where the sum converges in H, defines a projection. Clearly,

$$pf = \begin{cases} f & \text{for } f \in K \\ 0 & \text{for } f \in K^\perp \end{cases} \tag{1.68}$$

Proposition 4.3.6 *For each closed subspace $K \subset H$ one has $H = K \oplus K^\perp$. In other words, given any closed subspace $K \subset H$ each $f \in H$ has a unique decomposition $f = f^\parallel + f^\perp$, where $f^\parallel \in K$ and $f^\perp \in K^\perp$*

Theorem 4.3.7 *There is a bijective correspondence $p \leftrightarrow K$ between projections p on H and closed subspaces K of H: given a projection p one puts $K := pH$, and given a closed subspace $K \subset H$ one defines p by (4.67), where (e_i) is an arbitrary orthonormal basis of K*

An important special case of a projection is the unit operator $p = 1$, associated with $K = H$.

Projections are important in many ways. One is their occurrence in the spectral theorem, which will occupy us for the remainder of these notes. For the moment, let us mention that the spectral theorem of linear algebra has an elegant reformulation in terms of projections. In the usual formulation, a matrix $a : \mathbb{C}^n \to \mathbb{C}^n$ satisfying $a^*a = aa^*$ has an o.n.b. of eigenvectors $\{e_i\}_{i=1,.....,n}$, i.e., one has $ae_i = \lambda_i e_i$ for some $\lambda_i \in \mathbb{C}$. In the list of eigenvalues $\{\lambda_i\}i_{i=1,.....,n}$, some may coincide. Now make a list $\{\lambda_\alpha\}i_{\alpha=1,.....,m\leq n}$ where all the λ_α's are different. Let p_α be the projection onto the subspace $H_\alpha = p_\alpha\mathbb{C}^n$ of all $f \in \mathbb{C}^n$ for which $af = \lambda_\alpha f$; of course, H_α is the linear span of those e_i for which $\lambda_\alpha = \lambda_i$. The spectral theorem now states that $a = \sum_\alpha \lambda_\alpha p_|alpha$. In other words, each normal matrix is a linear combination of mutually orthogonal projections. We will see in due course what remains of this theorem if one passes from $\mathbb{C}^n$ to an arbitrary (separable) Hilbert space.

Furthermore, it follows from Proposition 4.3.6 that $f \in H$ is an eigenvector of p iff $f \in pH$ or $f \in (pH)^\perp$; in the first case the eigenvector is 1, and in the second case it is 0. Apart from projections, another important class of operators on a Hilbert space consists of the unitaries. An operator $u : H \to H$ is called **unitary** when $uu^* = u^*u = 1$. Equivalently, u is **isometric**, in that $(uf, uf) = (f, f)$ for all $f \in H$, and invertible (with inverse $u^{-1} = u^*$). For example, if (e_i) and (u_i) are two orthonormal bases of H, then the operator $u(\sum_i c_i e_i) := \sum_i ciu_i$ is unitary. In quantum mechanics, one usually encounters unitary operators of the form $u = \exp(ia)$, where a is self-adjoint and (for bounded a) the exponential is defined by its usual power series expansion, which converges in operator norm. Clearly, one has $u^* = \exp(-ia)$ and since for commuting a and b (that is, $ab = ba$) one has $\exp(a + b) = \exp(a)\exp(b)$, one sees immediately that u is indeed unitary.

A **partial isometry** is an operator v for which $v^*v = p$ is a projection. A special case is an **isometry**, characterized by $p = 1$, i.e., $v^*v = 1$. An invertible isometry is clearly unitary. The structure of partial isometries is as follows.

Proposition4.3.8 *If v is a partial isometry, then v^* is a partial isometry as well. Let the associated projection be $q := vv^*$. The kernel of v is $(pH)^\perp$, and its range is qH. The operator v is unitary from pH to its range qH and zero on $(pH)^\perp$. Conversely, any partial isometry has this form for projections p and q.*

1.4 Compact Operators

1.4.1 Linear algebra revisited

Compact operators on a Hilbert space (or, more generally, on a Banach space) are special bounded operators that behave like matrices on $\mathbb{C}^n$ in many ways. To make this point, we first recall the proof that any hermitian matrix (a_{ij}) (i.e., satisfying $\bar{a_{ji}} = a_{ij}$) can be diagonalized. In linear algebra this theorem is usually stated in a basis-dependent form. From our more abstract perspective of operators, the matrix (a_{ij}) arises from the operator $a : \mathbb{C}^n \to \mathbb{C}^n$ through the choice of an arbitrary orthonormal basis (e_i), in terms of which one has $a_{ij} = (e_i, ae_j)$. The spectral theorem then states that $\mathbb{C}^n$ has a (possibly) new basis of eigenvectors (u_i), in which a is diagonal: with respect to this basis one has $a_{ij} = (u_i, au_j) = (u_i, \lambda_j u_j) = \lambda_i \delta_{ij}$, where λ_i are the eigenvalues of a (possibly degenerate). Now, this result can be restated without any reference to the notion of a basis, as follows.

Proposition 4.4.1 *Let $H = \mathbb{C}^n$ be a finite-dimensional Hilbert space, and let $a : H \to H$ be a self-adjoint operator on H. There exists a family of mutually orthogonal projections (pa) (i.e., $p_\alpha H \perp p_\beta H$ for $\alpha \neq \beta$ or $p_\alpha p_\beta = \delta_{\alpha\beta}$) with $\sum_\alpha p_\alpha = 1$ and $a = \sum_\alpha \lambda_\alpha p_\alpha$, where λ_α are the eigenvalues of a. In other words, $_\alpha$ is the projection onto the eigenspace in H with eigenvalue λ_α; the dimension of $p_\alpha H$ is equal to the multiplicity of the eigenvalue λ_α.*

We also have the following lemmas.

Lemma 4.4.2 *Every self-adjoint operator a on $H = \mathbb{C}^n$ has an eigenvector with associated eigenvalue λ satisfying $|\lambda| = \|a\|$.*

Note that by definition of the operator norm an eigenvalue cannot possibly be any bigger!

Lemma4.4.3

1. *The image of a compact set in H under a continuous map into H or $\mathbb{C}$ is compact.*

2. *A continuous function $f : K \to \mathbb{R}$ on a compact set K attains a maximum and a minimum.*

1.4.2 The spectral theorem for self-adjoint compact operators

Let H be infinite-dimensional (and separable). Eigenvectors and eigenvalues of operators a on a Hilbert space H are defined in the same way as for $H = \mathbb{C}^n$: if $af = \lambda f$ for some $\lambda \in \mathbb{C}$ then$f \in H$ is called an eigenvector of a with eigenvalue λ. A crucial difference with the finite-dimensional situation is that

even a bounded self-adjoint operator on an infinite-dimensional Hilbert space may not have any eigenvectors (let alone a basis of them!). For example, on $H = L^2(\Omega)$ a multiplication operator defined by a nonzero continuous function has no eigenfunctions at all. The idea is now to define a class of operators on H for which the proof of Proposition 4.4.1 can be copied, so that the existence of a complete set of eigenvectors is guaranteed.

We will need some topology, but in our setting of separable Hilbert spaces we may keeps things simple: a set K in a separable Hilbert space H is compact when every sequence in K has a convergent subsequence, and a map $\alpha : H \to T$, where $T = \mathbb{C}$ or $T = H$, is **continuous** if it preserves limits, i.e., if $f_n \to f$ in H then $\alpha(f_n) \to \alpha(f)$ in T. For $H = \mathbb{C}^n$, this notion of compactness is equivalent to the Heine-Borel property; for separable infinite-dimensional H this equivalence no longer holds. Our notion of continuity is equivalent to the usual one in topology. The norm $f \mapsto \|f\|$ is continuous on H, which is tautological given our definition of continuity, because convergence in H has been defined in terms of the norm, i.e., $f_n \to f$ in H means $\|f_n - f\| \to 0$, which precisely expresses continuity of the norm. Similarly, according to our definition a bounded operator $a : H \to H$ is clearly continuous, too, for $\|af_n - af\| \to 0$ because $\|af_n - af\| \leq \|a\|\|f_n - f\|$ by (4.54). The main point is that Lemma 4.4.3 still applies.

Definition 4.4.4 *A compact operator on a Hilbert space H is a bounded operator that maps the unit ball $B_1 \subset H$ into a compact set.*

This is not the case for any bounded operator, for although such operators are continuous, the unit ball in H is not compact. If H is finite-dimensional, so that B_1 is compact, then any operator is compact. More generally, a finite-rank operator on an infinite-dimensional Hilbert space (i.e., an operator whose image is finite-dimensional) is compact.

Proposition 4.4.5 *A bounded operator on a separable Hilbert space is compact* iff *if is the norm-limit of a sequence of finite-rank operators.*

A consequence of the proposition is:

Corollary 4.4.6

1. *If a is compact then so is its adjoint a^**
2. *If a is compact and b is bounded then ab and ba are compact*
3. *A projection p is compact* iff *it is finite-dimensional.*

Using this corollary, it is easy to show that the set of all compact operators in $B(H)$ is a Banach space called $B_0(H)$ in the operator norm. Moreover, $B_0(H)$ is even an algebra under operator multiplication, closed under involution.

Integral operators form an important class of compact operators. We note that

if $\Omega \subset \mathbb{R}^n$ is compact, any operator of the form $af(x) = \int_\Omega d^n x a(x,y) f(y)$ is compact when the kernel $a(-,-)$ is continuous on $\Omega \times \Omega$. More generally, for any $\Omega \subset \mathbb{R}^n$ such an operator is compact when $a(-,-) \in L^2(\Omega \times \Omega)$, i.e., when $\int d^n x d^n y |a(x,y)|^2 < \infty$. The following theorem completely characterizes self-adjoint compact operators.

Theorem 4.4.7 *Let a be a self-adjoint compact operator on a Hilbert space H. Then H has an orthonormal basis (e_i) of eigenvectors of a, in terms of which*

$$a = \sum_i \lambda_i p_i \tag{1.69}$$

where p_i projects onto the span of e_i, and the sum converges in the sense that $af = \sum_i \lambda_i p_i f$ for each fixed $f \in H$. Moreover, the set (λ_i) of eigenvalues of a has the property that

$$\lim_{i \to \infty} |\lambda_i| = 0 \tag{1.70}$$

Conversely, a bounded self-adjoint operator on H of the form (4.69) where the eigenvalues satisfy (4.70) is compact. **Corollary 4.4.8** *Each eigenvalue of a self-adjoint compact operator except possibly 0 has finite multiplicity, and 0 is the only possible accumulation point of the set of eigenvalues. Hence we may rewrite (4.69) as*

$$a = \sum_\alpha \lambda_\alpha p_\alpha \tag{1.71}$$

where all eigenvalues λ_α, are different and p_α is the finite-dimensional projection $p_\alpha := \sum_{i|\lambda_i = \lambda_\alpha} e_i$.

This expansion has the advantage over (4.69) that it is unique; in (4.69) there is an arbitrariness in the choice of basis within the eigenspace of each eigenvalue with multiplicity greater than one.

In particular, the eigenvalues (λ_i) are uniquely determined by a.

Corollary 4.4.9 *An arbitrary compact operator a on a Hilbert space H has an expansion*

$$af = \sum_i \mu_i (e_i, f) u_i \tag{1.72}$$

where (e_i) and (u_i) are orthonormal bases of H, $\mu_i > 0$, and (μ_i^2) are the eigenvalues of $a^* a$. The μ_i are sometimes called the **singular values** of a.

1.5 Quantum Mechanics and Hilbert Space: States and Observables

We are now going to apply the previous machinery to quantum mechanics, referring to the Intro- duction for history and motivation. The mathematical

formalism of quantum mechanics is easier to understand if it is compared with classical mechanics, of which it is a modification. We therefore start with a rapid overview of the latter, emphasizing its mathematical structure.

1.5.1 Classical mechanics

The formalism of classical mechanics is based on the notion of a phase space M and time-evolution, going back to Descartes and Newton, and brought into its modern form by Hamilton. The phase space of a given physical system is a collection of points, each of which is interpreted as a possible state of the system. At each instance of time, a given state is supposed to completely characterize the state of affairs of the system, in that:

1. The value of any observable (i.e., any question that may possibly be asked about the system, such as the value of its energy, or angular momentum,.....) is determined by it[Philosophers would say that any quantity pertaining to the system supervenes on its states; this means that no change in a given quantity is possibly without a change in the state. For example, most scientists would agree that the mind supervenes on the brain (seen as a physical system)].

2. Together with the equations of motion, the state at $t = 0$ is the only required ingredient for the prediction of the future of the system[We do not say that such a prediction is always possible in practice. But *if* it is possible at all, it merely requires the state and the equations of motion].

Observables are given by functions f on M. The relationship between states (i.e., points of M) and observables is at follows:

The value of the observable f in the state x is $f(x)$

This may be reformulated in terms of questions and answers. Here an observable f is identified with the question: *what is the valve of f?* A state is then a list of answers to all such questions.

A very basic type of observable is defined by a subset $S \subset M$. This observable is the characteristic function χ_S of S, given by $\chi_S(x) = 1$ when $x \in S$ and $\chi_S(x) = 0$ when $x \notin S$. The corresponding question is: *is the system in some state lying in $S \subset M$?* The answer yes is identified with the value $\chi_S(x) = 1$ and the answer no corresponds to $\chi_S(x) = 0$. Such a question with only two possible answers is called a **yes-no question**. In these notes we only look at the special case $M = \mathbb{R}^{2n}$, which describes a physical system consisting of a point particles moving in $\mathbb{R}^n$. We use coordinates $(q, p) := (q^i, p_i)$, where $i = 1, ..., n$. The q variable (position) denotes the position of the particle, whereas the meaning of the p variable (momentum) depends on the time-evolution of the system. For example, for a free particle of mass m one has the relation $\vec{p} = m\vec{v}$, where v is the velocity of the particle (see below). Let us note that one may look at, say, q^i also as an observable: seen as a function on M, one simply has $q^i(q, p) = q^i$,

etc.

Given the phase space M, the specification of the system is completed by specifying a function h on M, called the **Hamiltonian** of the system. For $M = \mathbb{R}^{2n}$ we therefore have h as a function of (q, p), informally written as $h = h(q, p)$. The Hamiltonian plays a dual role:

- Regarded as an observable it gives the value of the energy;
- it determines the time-evolution of the system.

Indeed, given h the time-evolution is determined by **Hamiltons equations**

$$\begin{aligned} \dot{q}^i &:= \frac{dq^i}{dt} = \frac{\partial h}{\partial p_i} \\ \dot{p}_i &:= \frac{dp_i}{dt} = -\frac{\partial h}{\partial q^i} \end{aligned} \tag{1.73}$$

For example, a particle with mass m moving in a potential V has Hamiltonian

$$h(q, p) = \frac{p^2}{2m} + V(q) \tag{1.74}$$

where $p^2 := \sum_{i=1}^{n} (p_i)^2$. The equations (4.73) then read $\dot{q}^i = p_i/m$ and $\dot{p}_i = -\partial V/\partial q^1$. With the force defined by $F^i := -\partial V/\partial q^1$, these are precisely Newtons equations $d^2q^1/dt^2 = F^i/m$, or $\vec{F} = m\vec{a}$. In principle, h may explicitly depend on time as well.

1.5.2 Quantum Mechanics

Quantum mechanics is based on the postulate that the phase space is a Hilbert space H, with the additional stipulations that:

1. Only vectors of norm 1 correspond to physical states;
2. Vectors differing by a phase, i.e., by a complex number of modulus 1, correspond to the same physical state.

In other words, $\psi \in H$ and $z\psi$ with $z \in \mathbb{C}$ and $|z| = 1$ give the same state[It follows that the true state space of a quantum-mechanical system is the **projective** Hilbert space $\mathbb{P}H$, which may be defined as the quotient $SH/\sim$, where $SH := \{f \in H | \|f\| = 1\}$ and $f \sim g \text{iff} f = zg \text{for some } x \in \mathbb{C} \text{ with } |z| = 1]$. We here stick to the physicists convention of denoting elements of Hilbert spaces by Greek letters[This notation was initially used by Schrodinger in order to make his wave mechanics, a precursor of quantum mechanics, look even more mysterious than it already was].

The reason for the first point lies in the probability interpretation of quantum mechanics. The simplest example of this interpretation is given by the quantum

mechanics of a particle moving in $\mathbb{R}^3$. In that case the Hilbert space may be taken to be $H = L^2(\mathbb{R}^3)$, and Born and Pauli claimed in 1926 that the meaning of the wavefunction $\psi \in L^2(\mathbb{R}^3)$ was as follows: *the probability* $P(\psi, x \in \Delta)$ *that the particle in state* ψ *is found to be in a region* $\Delta \subseteq \mathbb{R}^3$ *is*

$$P(x \in \Delta|\psi) = (\psi\chi_\Delta\psi) = \int_\Delta d^3x \|\psi(x)\|^2 \tag{1.75}$$

Here χ_Δ is the characteristic function of Δ, given by $\chi_\Delta = 1$ when $x \in \Delta$ and $\chi_\Delta = 0$ when $x \notin \Delta$. It follows that

$$P(x \in \mathbb{R}^n|\psi) = \|\psi\|^2 = (\psi, \psi) = 1 \tag{1.76}$$

since by definition of the physical system in question we assume that the particle is somewhere.

More generally, observables are represented in quantum mechanics by self-adjoint operators a on H. In the bounded case ($\|a\| < \infty$) this means $a^* = a$, and the meaning of self-adjointness for unbounded operators will be taken up later. As in classical physics, observables define questions: *what is the value of* a*?* And once again, a state $\psi \in H$ with $\|\psi\| = 1$ is nothing but a list of answers to such questions. Indeed, the answer to the above question in the state ψ is as follows:

- *The value of the observable* a *in the state* ψ *is* $(\psi, a\psi)$.

Although this is a real number, like in classical physics (thanks to $a^* = a$), it now has the interpretation of the **expectation value** of the observable a, rather than its exact value[What this really means is a matter of ongoing debate. For example, do expectation values refer to outcomes of a long series of measurements? Or to propensities of the observable to have the given expectation value? Or to averages with respect to some unknown theory underlying quantum mechanics? Etcetera]. In quantum mechanics any projection p defines a so-called yes-no question: *is the system in some state in* pH*?* Thus projections are the quantum analogues of characteristic functions in classical physics. The fundamental difference between classical and quantum physics, namely the intrinsically statistical character of the latter, is beautifully illustrated by yes-no questions. In the classical case the possible values of χ_S are 0 (no) and 1 (yes). In quantum mechanics the answer to the question p in the state ψ is $(\psi, a\psi)$. If $\psi \in (pH)^\perp$ one has $(\psi, a\psi) = 0$ and if $\psi \in pH$ one has $(\psi, a\psi) = 1$. Indeed, in the former case (no) one can maintain that the state is not in pH, and in the latter case (yes) one can safely say that the state is in pH. In classical physics these are the only possibilities: either $x \in S$ or $x \notin S$. But in quantum mechanics $\psi \in (pH)^\perp$ and $\psi \in pH$ are not the only possibilities! In general, one has the decomposition $\psi = \psi^\parallel + \psi^\perp$ as explained in Proposition4.3.6, with both $\psi^\parallel$ and $\psi^\perp$ nonzero. Using $p^2 = p^* = p$, one finds

$$(\psi, p\psi) = (\psi^\parallel, p\psi^\parallel) \in [0, 1]$$

the fact that $(\psi, p\psi) \in [0,1]$ follows from $\|p\| = 1$ from projections (which in turn follows from (4.63)) and (4.54) and Cauchy-Schwarz. Generalizing the interpretation Born and Pauli gave to wavefunctions, we say that:

The number $(\psi, p\psi)$ is the probability that the state ψ lies in pH.

Alternatively:

The probability of the answer yes to the question p in the state ψ is $(\psi, p\psi)$.

1.5.3 Trace-class operators and mixed states

To be honest, we have only discussed a limited class of states so far, namely the pure states. These are states containing maximum information about the system. Hence in classical physics pure states are points in phase space, whereas in quantum mechanics they are unit vectors in Hilbert space. However, in some cases a physics student may not know the precise state of the system, for example because he is drunk. A professor of experimental physics may be in the same situation, this time because he does not know enough theoretical physics to figure out which state he has prepared in the lab. In either case one is unable to distinguish a number of candidate states.

The way out is to make a list of possible pure states (x_k), $x_k \in M$ (in classical physics) or (ψ_k), $\psi_k \in H$ (in quantum physics and assign each state a probability P_k. Of course, one should have $P_k \in [0,1]$ for each k and $\sum_k P_k = 1$. In classical physics the answer to the question what the value of f is, is then given by

$$\langle f \rangle = \sum_k P_k f(x_k)$$

In quantum physics, the value of a in the given state ρ is

$$\langle a \rangle = \sum_k P_k (\psi_k, a\psi_k) \tag{1.77}$$

In textbooks on quantum mechanics one here introduces a **density matrix**

$$\rho = \sum_k P_k \left|\psi_k\right\rangle \left\langle\psi_k\right| \tag{1.78}$$

where $[\psi_k] = \left|\psi_k\right\rangle \left\langle\psi_k\right|$ is the projection onto the one-dimensional subspace spanned by ψ_k or $|\psi_k\rangle$, i.e. (for general unit vectors ψ or $|\psi\rangle$) in the one-dimensional case

$$[\psi]\varphi := (\psi, \varphi)\psi \quad or \quad \left|\psi\right\rangle \left\langle\psi \,|\, \varphi\right\rangle |\varphi\rangle \tag{1.79}$$

This a tautology; it coincides with (4.67) since $\langle \psi \,|\, \varphi \rangle = (\psi, \varphi)$. This is one of the many instances where the Dirac language used in quantum mechanics is actually better than the one in math books.

In any case, one now writes (4.77) as

$$\langle a \rangle = Tr(\rho a) \tag{1.80}$$

Here the **trace** of a (bounded) operator b is defined as follows: take any orthonormal basis (e_i) of H and put

$$Tr\, b := \sum_i (e_i, be_i) \tag{1.81}$$

This is supposed to be independent of the chosen basis. So if ρ is given by (4.78) and the vectors ψ_k, are mutually orthogonal, one may choose a basis that contains all of them. In that case one easily shows that

$$Tr(\rho a) = \sum_k P_k(\psi_k, a\psi_k) \tag{1.82}$$

so that (4.77) and (4.81) are the same.

In quantum mechanics density matrices are often called **mixed states**. If (4.78) contains only one term $\rho = [\psi]$, one has $Tr(\rho a) = (\psi, a\psi)$ and the state is actually pure.

We now present the general theory of the trace; this is more complicated than the physics literature suggests. For example, the independence of the trace on the basis chosen is delicate. If $dim(H) < \infty$ there is no problem; a simple computation shows that

$$\sum_i (e_i, ae_i) = \sum_i (u_i, au_i) \tag{1.83}$$

for any two o.n.b. (e_i) and (u_i) (just expand u_i in terms of the e_i and interchange summations). However, if $dim(H) = \infty$ one can find bounded operators $b : H \to H$ and orthonormal bases (u_k) and (e_i) such that $\sum_i (e_i, be_i) = \infty$ and $\sum_k (u_k, be_k) = \infty$.

To avoid this, in order to make sense of the trace when H is infinite-dimensional one needs a class of operators a for which (4.81) is (i) finite and (ii) independent of the basis. This class can be constructed in (at least) two different but equivalent ways. The simplest way is as follows.

1. In order to have a well-defined trace, an operator b needs to be bounded and compact.

2. If b is compact, then so is b^*b. Morever, b^*b is self-adjoint, since

$$(b^*b)^* = b^*b^{**} = b^*b$$

3. So we can apply Theorem 4.4.7 with $a = b^*b$. This yields

$$b^*b = \sum_k \mu_k p_k$$

for certain $\mu_\in\mathbb{R}$ and projection $p_k : H \to H$. Now, if $\psi \in p_k H$, so that $b^*b\psi = \mu_k\psi$, taking the inner product with ψ one has, $(\psi, n^*b\psi) = \mu_k(\psi,\psi)$, i.e., $\|b\psi\|^2 = \mu_k\|\psi\|^2$. Hence $\mu_k \geq 0$.

Definition 4.5.1 *We say that a bounded operator $b : H \to H$ is **trace-class** when b is compact and $\sum_k \sqrt{\mu_k} < \infty$. Here the μ_k are the eigenvalues of b^*b. If b is trace-class we write $b \in B_1(H)$.*

Another approach to the trace is based on the notion of the square root of the operator b^*b itself (instead of on the square root of its eigenvalues, as above). Let us call an operator $b : H \to H$ positive when $(f, bf) \geq 0$ for all $f \in H$. We write $b \geq 0$. We will often use the simple property that if b is positive, then $b^* = b$. It turns out that if b is positive, then (4.81) is independent of the orthonormal basis (e_i), so it is either finite or infinite. If it is finite this defines the trace of b, and we say b is trace-class. This defines the trace for positive operators.

To define the trace in general, one uses the square-root of a positive operator. Namely, one can show that if b is positive, then there exists a unique operator $\sqrt{b}$ with the properties $\sqrt{b}^2 = ben\sqrt{b} > 0$. In particular, the **absolute value**

$$|b| := \sqrt{b^*b} \tag{1.84}$$

is defined, as we have just seen that $b * b$ is positive. We now say that an arbitrary bounded operator b is trace-class if $Tr\,|b| < \infty$, where the trace is given by (4.81). It turns out that b is trace-class in this sense $mathrmiff$ it is trace-class according to Definition 4.5.1.

In any case, the most important properties of the trace are:

Theorem 4.5.2 *Suppose b is trace-class, or $b \in B_1(H)$ Then:*

1. *The expression (4.81), called the trace of b, is absolutely convergent and independent of the orthonormal basis (e_i).*

2. *If a is bounded, then $ab \in B_1(H)$ and $ba \in B_1(H)$ and*

$$Tr(ab) = Tr(ba) \tag{1.85}$$

3. *If u is unitary then*

$$Tr(ubu^{-1}) = Tr(b) \tag{1.86}$$

This theorem is easy to use but by no means easy to prove. We return to quantum mechanics.

Definition 4.5.3 *An bounded operator $\rho : H \to H$ is called a* ***density operator*** *or* ***density matrix*** *if:*

1. ρ is positive
2. ρ is trace-class
3. $Tr\,\rho = 1$

By part 2 of Theorem 4.5.2, for any bounded operator a the expectation value (4.80) is well defined. Furthermore, since ρ is compact (cf. Definition 4.5.1) and self-adjoint (as follows from its positivity), we may apply Theorem 4.4.7 with $a = \rho$. This yields the expansion (4.78) and we have come full circle.

The above mathematical model of quantum mechanics is too limited, however. The states are OK, but most observables in quantum mechanics turn out to be unbounded. Position and momentum are examples. We now turn to the theory of such unbounded observables.

1.6 Closed Unbounded Operators

1.6.1 The closure

We are now familiar with two classes of operators on a Hilbert space: bounded ones, and compact ones. As we have seen, the latter are precisely those bounded operators for which a spectral theory analogous to that for matrices exists. It would be possible to develop the spectral theory of general bounded (self-adjoint)operators at this point, but in fact it turns out that this theory can be written down almost without extra effort for the far wider class of closed (self-adjoint) operators.

To come to grips with the notion of un unbounded operator, we note the following.

Theorem 4.6.1 *An operator on a Hilbert space H is bounded* iff *it is continuous in the sense that $f_n \to f$ implies $af_n \to af$ for all convergent sequences (f_n) in H.*

Let $a : H \to H$ be bounded. By (4.54), if $f_n -> f$ in H, that is, $\|f_n - f\| \to 0$, then $af_n \to af$ in H, since $\|af_n - af\| \leq \|a\|\|f_n - f\|$. Conversely, if a is not bounded, then for each $n \in N$ there is $f_n \in H$ with $\|f_n\| = 1$ and $\|af_n\| \geq n$. The sequence $(g_n = f_n/n)$ converges to 0, but since $\|ag_n\| \geq 1$, the sequence (ag_n) does not converge to $a0 = 0$. Hence a is not continuous, and the implication continuous $\Rightarrow$ bounded has been proved by *reductio ad absurdum.*

It follows that unbounded operators are discontinuous: if $f_n \to f$ it is not guaranteed that a $af_n \to af$; indeed, it is not guaranteed that (af_n) converges at all! Hence an essential difference between the bounded and the unbounded case is that whereas for bounded operators a Proposition 4.3.3 states that even if a is initially defined on some dense subspace D of H, it can uniquely be extended to H by continuity, for unbounded operators a such an extension by continuity will not in general exist. Although a discontinuous extension to H might exist, in practice it is very unusual to talk about unbounded operators a defined on H. This is because interesting unbounded operators tend to be defined on $D \subset H$ by some natural expression, which simply does not make sense on all of H. Consequently, the specification of the subspace D on which a is defined, called the domain of a, denoted by $D(a)$ is absolutely essential when a is an unbounded operator.

Recall that a subspace $K \subset H$ is called dense in H when for each $f \in H$ there is a sequence (f_n) in K converging to f.

> *Unless explicitly stated otherwise, we always assume that the domain of an operator is dense in H.*

For example, we have seen that $a \in C(\mathbb{R})$ defines a bounded operator on $H = L^2(\mathbb{R})$ by multiplication when $\|f\| < \infty$, i.e., when a is bounded. When a is unbounded as a function, we cannot really make the natural claim that consequently a is unbounded as a multiplication operator on H, since a does not map H to itself as soon as it is unbounded. What we can say, however, is that a is unbounded as a multiplication operator on the subspace $D(a) = C_c(\mathbb{R})$, which (by our definition of L^2) is dense in H. Other examples are given by differential operators: whereas one cannot really say that $a = id/dx$ is unbounded on $L^2(\mathbb{R})$ since the derivative of most functions in L^2 is not even defined, one can say that a is unbounded on, say, $D(a) = C_c^1(\mathbb{R}) := C_c(\mathbb{R}) \cap C^1(\mathbb{R})$.

There is some flexibility in the choice of the domain, and the theory of unbounded operators of closable type even largely revolves around the business of enlarging a given domain. Here we define an extension of a given operator $a : D(a) \to H$ as an operator $a_1 : D(a_1) \to H$ where $D(a) \subset D(a_1)$ and $a_1 = a$ on $D(a)$; we write $a \subset a_1$. As we have seen, if a is bounded there is only one interesting extension, namely the one defined on any larger domain (including H) by continuity, but in the unbounded case the theory of extension of operators turns out to be very rich indeed. As a rather trivial example, we could have defined $a = id/dx$ initially on $D(a) = C_c^1(\mathbb{R}) := C_c(\mathbb{R}) \cap C^1(\mathbb{R})$; the same expression $a_1 = id/dx$ but now defined on $D(a_1) = C_c(\mathbb{R})$ is formally an extension of a. Similarly, an unbounded multiplication operator $a \in C(\mathbb{R})$ may initially be defined on $D(a) = C_c^\infty(\mathbb{R})$, to be extended by the same expression defined on $D(a_1) = C_c(\mathbb{R})$, as above. Clearly, the largest possible domain on which a

multiplication operator $a \in C(\Omega)$ can be defined in the natural way is

$$D(a) = \{f \in L^2(\Omega) | af \in L^2(\Omega)\} \tag{1.87}$$

The particular unbounded operators that one can deal with satisfy a relic of continuity. To explain this, we define the **graph** of a as the subset $\{f, af\} \subset H \times H$. To define the notion of closedness in $H \times H$ we equip this set with the structure of a Hilbert space in the following way: we first equip $H \times H$ with the structure of a vector space by defining $\langle f_1, f_2\rangle + \langle g_1, g_2\rangle := \langle f_1 + g_1 f_2 + g_2\rangle$ and $\lambda\langle f_1, f_2\rangle := \langle \lambda f_1, \lambda f_2\rangle$, and subsequently putting an inner product on it by $(\langle f_1, f_2\rangle, \langle g_1, g_2\rangle) := (f_1, g_1) + (f_2, g_2)$. With this structure, $H \times H$ is a Hilbert space called $H \oplus H$, for it is precisely the direct sum of H with itself.

Definition 4.6.2 *A **closed operator** A closed operator $a : D(a) \to H$ is a linear map from a dense subspace $D(a) \subset H$ to H for which either of the following equivalent conditions holds:*

- *If $f_n \to f$ in H for a sequence(f_n) in $D(a$ and (af_n) converges in H, then $f \in D(a)$ and $af_n \to af$ in H.*
- *The graph of a is closed.*
- *The domain $D(a)$ is closed in the norm $\|f\|_a^2 := \|f\|^2 + \|af\|^2$.*

Note that the norm $\|\cdot\|_a$ comes from the new inner product $(f, g)_a := (f, g) + (af, ag)$ on $D(a)$. Hence $D(a)$ is a Hilbert space in the new inner product when a is closed.

It is quite unusual for an operator to be closed in the form initially given. For example, a multiplication operator a in $L^2(\Omega)$s not closed on $C_c(\Omega)$; in fact, a turns out to be closed only on the domain (4.87). Fortunately, an operator a that is not closed may often be extended into a closed one. The condition for this to be possible is as follows.

Definition 4.6.3 *A **closable operator** $a : D(a) \to H$ is a linear map from a dense subspace $D(a) \subset H$ to H with the property that the closure $G(a)^-$ of its graph is itself the graph $G(a^-)$ of some operator a^- (called the **closure** of a*

In other words, a^- is a closed extension of a. It is clear that a^- is uniquely defined by its graph $G(a^-) = G(a)^-$.

Proposition 4.6.4 *An operator a is closable* iff *either of the following equivalent conditions holds:*

- *If $f_n \to 0$ for a sequence (f_n) in $D(a)$ and if (af_n) converges, then (af_n) must converge to 0.*
- *The closure $G(a)^-$ of the graph of a does not contain any element of the form $(0, g)$ for $g \neq 0$.*

In that case, the domain of the closure a^- of a is the set of all $f \in H$ to which some sequence (f_n) in $D(a)$ converges and for which (af_n) converges as well. Its action is given by $a^- f := \lim_n af_n$. Finally, the operator a^- is the smallest closed extension of a.

To verify that a^- is indeed closed, suppose $f_n \to f$ and $af_n \to g$, with (f_n) in $D(a^-)$. Since $f_n \in D(a^-)$ for fixed n, there exists $(f_{m,n})$ in $D(a)$ such that $\lim_M f_{m,n} = f_n$ and $\lim_m af_{m,n} =: g_n$ exists. Then clearly $\lim_{m,n} f_{m,n} = f$, and we claim that

$$\lim_{m,n} af_{m,n} = g \tag{1.88}$$

Namely, $\|af_{m,n} - g\| \leq \|af_{m,n} - af_n\| + \|af_n - g\|$ For $\epsilon > 0$ take n so that the second term is $< \epsilon/2$. For that fixed n, $a(f_{m,n} - f_n)$ converges as $m \to \infty$ because $af_{m,n} \to g_n$ and af_n is independent of m. Also, recall that $f_{m,n} - f_n \to 0$ as $m \to \infty$. By assumption, a is closable, hence by definition one must have $a(f_{m,n} - f_n) \to 0$ in m. Hence we may find m so that $\|af_{m,n} - af_n\| < \epsilon/2$, so that $\|af_{m,n} - g\| < \epsilon$, and (4.88) follows. Hence $f \in D(a^-)$. Finally, since $a^- f := \lim_{m,n} af_{m,n}$ one has $a^- f = g$ by (4.88), or $a^- f = \lim_n af_n$ by definition of g. It follows that a^- is closed. This extension of a is clearly the minimal closed one.

This argument shows that for a^- to be closed it is sufficient that a is closable. Conversely, if a fails to be closable it cannot have any closed extension whatsoever, since a^- is by definition linear, and $a^- 0 = 0$ for any operator. The second condition for closability is then clearly equivalent to the first.

For example, a multiplication operator a in $H = L^2(\Omega)$ is closable on $C_c(\Omega)$: in both cases the closure has domain (4.87). On the other hand, an example of a non-closable operator is given by $H = L^2(\Omega)$, $D(a) = C_c(\Omega)$, and $af := f(0)g$, where $g \in H$ is arbitrary.

In general, even closed unbounded operators may have closed extensions, a phenomenon which is particular important in connection with the theory of self-adjointness; see below.

This section would not be complete without mentioning a special case of one of the most famous theorems in functional analysis, namely the **closed graph theorem** (for Hilbert spaces):

Theorem 4.6.5 *If $a : H \to H$ has a closed graph, then it is bounded. In other words, a closed operator defined on all of H is necessarily bounded.*

We will use this theorem only once, since in applications an operator defined on H is usually already known to be bounded, whereas unbounded operators are never defined on H, so that their graph cannot be studied in any case[On the theoretical side, however, an important consequence of the closed graph theorem

is another famous result known as the **open mapping theorem**: a bounded surjective operator on a Hilbert space H is open (in that the image of an open set in H is open; the boundedness of H implies the opposite, namely that the inverse image of an open set in H is open)].

1.6.2 Symmetric and self-adjoint operators

The most important closed operators, not just for quantum mechanics also but for mathematics as a whole, are the self-adjoint ones. To define these, first recall the definition of the adjoint a* in the unbounded case: see Definition 4.3.4.

Although it may even happen that $D(a^*)$ is zero, this is pretty pathological, and in most natural examples $D(a^*)$ turns out to be dense. For example, a multiplication operator $a \in C(\Omega)$ on $H = L^2(\Omega)$, defined on any of the domains we have considered (i.e., $D(a) = C_c^\infty(\Omega)$, $D(a) = C_c(\Omega)$, or (4.66)), has $a^* = \bar{a}$ (i.e., the complex conjugate of a seen as a multiplication operator) defined on $D(a^*)$ given by the right-hand side of (4.66). The following important result shows when $D(a^*)$ is dense.

Proposition 4.6.6 *Let $a : D(a) \to H$ (where $D(a)$ is dense) be an operator on a Hilbert space H.*

1. *The adjoint a^* is closed.*
2. *The operator a is closable* iff *$D(a^*)$ is dense.*
3. *In that case, one has $a^- = a^{**}$ and $(a^-)^* = a^*$.*

We now come to the central definition of this section. An equality $a = b$ between unbounded operators always stand for $D(a) = D(b)$ and $a = b$. Similarly, $a \subset b$ means $D(a) \subset D(b)$ and $b = a$ on $D(a)$.

Definition 4.6.7 *Let $a : D(a) \to H$ (where $D(a)$ is dense) be an operator on a Hilbert space H.*

- *If $a = a^*$, i.e., if $D(a^*) = D(a)$ and $(af, g) = (f, ag)$ for all $f, g \in D(a)$, then a is called* ***self-adjoint****.*
- *If $a^{**} = a^*$ (equivalently, if a is closable and $a^- = a^*$ or $(a^-)^* = a^*$), then a is called* ***essentially self-adjoint****.*
- *If $a \subset a^*$ i.e., if $(af, g) = (f, ag)$ for all $f, g \in D(a)$, then a is called* ***symmetric****.*

It follows Proposition 4.6.6 that a self-adjoint operator is closed, and that a symmetric operator is closable (because $D(a^*)$, containing $D(a)$, is dense). For a symmetric operator one has $a \subseteq a^- = a^{**} \subseteq a^*$, with equality at the first position when a is closed, and equality at the second position when a is essentially self-adjoint; when both equalities hold, a is self-adjoint. Conversely, an

essentially self-adjoint operator is, of course, symmetric. A symmetric operator may or may not have self-adjoint extensions; we will deal with this problem in detail later on. Without proof we quote the **Hellinger-Toeplitz theorem**: *If a is self-adjoint on $D(a) = H$, then a is bounded.* This confirms the idea that it is pointless to try to define unbounded operators on all of H in some manifestly discontinuous way. All this is very subtle, but the following example illustrates at least the easy part of the theory:

Proposition 4.6.8 *A real-valued multiplication operator $a \in C(\Omega)$ on $H = L^2(\Omega)$ is essentially self-adjoint on $D(a) = C_c^\infty(\Omega)$, and on $D(a) = C_c(\Omega)$, and is self-adjoint on*

$$D(a) = \{f \in L^2(\Omega) | af \in L^2(\Omega)\} \tag{1.89}$$

Cf. (4.66)). Of course, $D(a) = H$ when $\|a\|_\infty < \infty$, since in that case a is a bounded operator, as we have seen.

1.7 Spectral Theory for Self-Adjoint Operators

We denote the kernel or null space of a map a by $N(a)$ and its range or image by $R(a)$. As before, $D(a)$ denotes the domain of a. Also, $a - z$ for $z \in \mathbb{C}$ denotes the operator $a - z$.

1.7.1 Resolvent and spectrum

The theory of the spectrum of a closed operator on a Hilbert space (which may be bounded or unbounded) is a generalization of the theory of eigenvalues of a matrix. From linear algebra we recall:

Proposition 4.7.1 *Let $a : \mathbb{C}^n \to \mathbb{C}^n$ be a linear map. Then a is injective* iff *it is surjective.*

Corollary 4.7.2 *Let $a : \mathbb{C}^n \to \mathbb{C}^n$ be a linear map. Then $a - z$ is invertible (i.e., injective and surjective)* iff *z is not an eigenvalue of a, i.e., if there exists no $f \in \mathbb{C}^n$ such that $af = zf$.* Defining the spectrum $\sigma(a)$ of $a : \mathbb{C}^n \to \mathbb{C}^n$ as the set of eigenvalues of a and the **resolvent** $\rho(a)$ as the set of all $z \in \mathbb{C}$ for which $a - z$ is invertible, we therefore have

$$\sigma(a) = \mathbb{C} \backslash \rho(a) \tag{1.90}$$

If $z \in \rho(a)$, the equation $(a - z)f = g$ for the unknown $f \in \mathbb{C}^n$ has a unique solution for any g; existence follows from the surjectivity of $a - z$, whereas uniqueness follows from its *injectivity* (if $a - z$ fails to be injective then any element of its kernel can be added to a given solution).

Now, if a is an operator on an infinite-dimensional Hilbert space, it may not have any eigenvalues, even when it is bounded and self-adjoint. For example, if

$a(x) = \exp(-x^2)$ the associated multiplication operator $a : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ is bounded and self-adjoint, but it has no eigenvalues at all: the equation $af = \lambda f$ for eigenvectors is $\exp(-x^2)f = \lambda f$ for (almost) all $x \in \mathbb{R}$, which holds only if f is nonzero at a single point. But in that case f is not an element of L^2. However, the situation is not hopeless. More generally, let any $a \in C_b(\mathbb{R})$, interpreted as a multiplication operator $a : L^2(\mathbb{R}) \to L^2(\mathbb{R})$. If $x_0 \in \mathbb{R}$ one may find approximate eigenvectors of a in the following sense: take

$$f_n(x) := \left(\frac{n}{\pi}\right)^{1/4} e^{-n(x-x_0)^2/2} \tag{1.91}$$

Then $\|f_n\| = 1$ and $\lim_{n\to\infty}(a(x) - a(x_0))f_n = 0$, although the sequence f_n itself has no limit in $L^2(\mathbb{R})$. Thus we may call $\lambda = a(x_0)$ something like a generalized eigenvalue of a for any $x_0 \in \mathbb{R}$, and define the spectrum accordingly: let $a : D(a) \to H$ be a (possibly unbounded) operator on a Hilbert space. We say that $\lambda \in \sigma(a)$ when there exists a sequence (f_n) in $D(a)$ for which $\|f_n\| = 1$ and

$$\lim_{n\to\infty}(a - \lambda)f_n = 0 \tag{1.92}$$

Of course, when λ is an eigenvalue of a with eigenvector f, we may take $f_n = f$ for all n. However, this is not the official definition of the spectrum, which is as follows.

Definition 4.7.3 *Let $a : D(a) \to H$ be a (possibly unbounded) operator on a Hilbert space. The resolvent $\rho(a)$ is the set of all $z \in \mathbb{C}$ for which $a - z : D(a) \to H$ is lnjectlve and surjectlve (l.e., lnvertlble). The **spectrum** $\sigma(a)$ of a is defined by $\sigma(a) := \mathbb{C}\backslash\rho(a)$.*

Hence the property (4.90) has been turned into a definition! We will prove the equivalence of this definition of the spectrum with the definition above later on. In the example just given, one has $\sigma(a) = a(\mathbb{R})$ if the right domain of a is used, namely (III.17). Thus the spectrum can be nonempty even if there arent any eigenvalues. The subsequent theory shows that these are precisely the right definitions for spectral theory.

The following result explains the role of closedness[Some books define the resolvent of a, as the set of those $z \in \mathbb{C}$ for which $(a - z)$ is invertible and has bounded inverse. In that case, the resolvent is empty when a, is not closed].

Proposition 4.7.4 *If an operator $a : D(a) \to R(a) = H$ has an inverse, then a^{-1} is bounded* iff *a is closed.*

Returning to the equation $(a - z)f = g$, it now follows that when $z \in \rho(a)$, the solution f depends continuously on the initial data g iff a is closed. To avoid pathologies, we therefore assume that a is closed in what follows. Furthermore, as we shall see, practically every argument below breaks down when $(a - z)^{-1}$ is unbounded. This also explains why as far as spectral theory is concerned

there isnt much difference between bounded operators and closed unbounded operators: in both cases $(a-z)^{-1}$ is bounded for $z \in \rho(a)$.

One then easily shows:

Proposition 4.7.5 *Let a be a closed operator.*

1. $\rho(a)$ is open (and hence $\sigma(a)$ is closed) in $\mathbb{C}$.
2. $\rho(a^*) = \overline{\rho(a)}$; $\sigma(a^*) = \overline{\sigma(a)}$

For unbounded operators the spectrum can (literally) be any subset of $\mathbb{C}$, including the empty set.

1.7.2 The spectrum of self-adjoint operators

For a general closed operator a, we may decompose the spectrum as

$$\sigma(a) = \sigma_d(a) \cup \sigma_c(a) \tag{1.93}$$

where the **discrete spectrum** $\sigma_d(a)$ consists of all eigenvalues of a, and the continuous spectrum $\sigma_c(a)$ is the remainder of $\sigma(a)$. Recall that eigenvalues lie in $\sigma(a)$, for if $(a-\lambda)f = 0$ for some nonzero f then $a - \lambda$ cannot be injective. The spectrum of self-adjoint operators has a particularly transparent structure.

Theorem 4.7.6 *Let a be a self-adjoint operator (i.e., $a^* = a$), and let $z \in \mathbb{C}$. Then one of the following possibilities occurs:*

1. $R(a-z) = H$ iff $z \in \rho(a)$
2. $R(a-z)^- = H$ *but* $R(a-z) \neq H$ iff $z \in \sigma_c(a)$
3. $R(a-z)^- \neq H$ iff $z \in \sigma_d(a)$

with associated lemmas:

Lemma 4.7.7 *If a is closable (equivalently, if $D(a^*)$ is dense), then $R(a-z)^- = N(a^* - \bar{z})^\perp$ and $N(a^* - \bar{z} = R(a-z)^\perp$*

Lemma 4.7.8 *Let a be symmetric. Then $\|(a-z)f\| \geq |Im(z)|\|f\|$*

Lemma 4.7.9 *Let a be any densely defined operator. If $\|af\| \geq C\|f\|$ for some $C > 0$ and all $f \in D(a)$, then a is injective and $a^{-1} : R(a) \to D(a)$ is bounded with bound $\|a^{-1}\| \leq C^{-1}$*

Lemma 4.7.10 *If b is closed and injective, then $b^{-1} : R(b) \to D(b)$ is closed*

Lemma 4.7.11 *If b is closed and bounded, then $D(b)$ is closed*

with the corollary

Theorem 4.7.12 *Let a be a symmetric operator. Then the following properties are equivalent:*

1. $a^* = a$, *i.e., a is self-adjoint*
2. a *is closed and* $N(a^* \pm i) = 0$
3. $R(a \pm i) = H$
4. $R(a - z) = h$ *for all* $z \in \mathbb{C}\backslash\mathbb{R}$
5. $\sigma(a^-) \subset \mathbb{R}$

Similarly, the following properties are equivalent:

1. $a^* = a^{**}$, *i.e., a is essentially self-adjoint*
2. $N(a^* \pm i) = 0$
3. $R(a \pm i)^- = H$
4. $R(a - z)^- = H$ *for all* $z \in \mathbb{C}\backslash\mathbb{R}$
5. $\sigma(a^-) \subset \mathbb{R}$

Corollary 4.7.132 *Let $a^* = a$. Then $\sigma(a) \subset \mathbb{R}$. In other words, the spectrum of a self-adjoint operator is real*

Finally we have the proposition:

Proposition 4.7.14 *Let $a \in C(\Omega)$ define a real-valued multiplication operator on*

$$D(a) = \{f \in L^2(\Omega) | af \in L^2(\Omega)\} \subset H = L^2(\Omega)$$

so that $a^* = a$ (cf. Proposition 4.6.8.) Then the operator a is injective iff $a(x) \neq 0$ *for all $x \in \Omega$, and surjective* iff *there exists $\epsilon > 0$ so that $|a(x)| \geq \epsilon$ for all $x \in \Omega$; in that case a is injective and has bounded inverse. Consequently, $\sigma(a) = a(\Omega)^-$ with $a(\Omega) := \{a(x), x \in \Omega\}$*

which leads to the theorem:

Theorem 4.7.15 *Let a be self-adjoint. Then $\lambda \in \sigma(a)$* iff *there exists a sequence (f_n) in $D(a)$ with $\|f_n\| = 1$ for all n such that $\lim_n (a - \lambda) f_n = 0$*

1.7.3 Application to quantum mechanics

The theory of self-adjoint operators has many applications, for example to the theory of boundary value problems for linear partial differential equations. In these notes we focus on applications to quantum mechanics.

In section 4.5 we initially assumed that observables in quantum mechanics are mathematically represented by bounded self-adjoint operators, i.e. linear maps $a : B(H) \to B(H)$ such that $\|a\| < \infty$ and $a^* = a$. As already mentioned at the end of that section, however, this model is too limited. For example, in physics textbooks you will find the position and momentum operators

$$\begin{aligned} \hat{q}^i &= x^i \\ \hat{p}_i &= -i\hbar \frac{\partial}{\partial x^i} \end{aligned} \tag{1.94}$$

Here h $\hbar \in \mathbb{R}^+$ is a constant of nature, called Plancks constant, and $i = 1, 2, 3$. These operators are allegedly defined on $H = L^2(\mathbb{R}^3)$, but we know from the previous work that at least $\hat{q}^i$ is unbounded. It is a multiplication operator of the form $a\psi(x) = \hat{a}\psi(x)$ with $\hat{a} \in C(\mathbb{R}^3)$, in this case $\hat{a}(x) = x^i$. As we have seen, a is bounded iff $\|a\|_\infty < \infty$, and this clearly not the case for x^i. Hence the position operator is unbounded. It follows from Proposition 4.6.8 that $\hat{q}^i$ is self-adjoint on the domain

$$D(\hat{q}^i) = \{\psi \in L^2(\mathbb{R}^3) | x^i\psi \in L^2(\mathbb{R}^3)\} \tag{1.95}$$

where $x^i\psi$ is shorthand for the function $x \mapsto x^i\psi(x)$.

Although we have not had the opportunity to develop the necessary machinery, the story of the momentum operator $\hat{p}_i$ is similar. If we denote the Fourier transform of $\psi \in L^2(\mathbb{R}^3)$ by $\hat{\psi}$, and call its argument $k = (k_1, k_2, k_3) \in \mathbb{R}^3$, we can write

$$\hat{\psi}(k) = \int_{\mathbb{R}^3} d^3x \psi(x) e^{-ikx} \tag{1.96}$$

where $kx = x^1k_1 + x^2k_2 + x^3k_3$. This improper integral is defined as follows.

1. Approximate ψ by a sequence (ψ_n) in $C_c(\mathbb{R}^3)$ (i.e. $\lim_{n\to\infty} \psi_n = \psi$ in the norm of $L^2(\mathbb{R}^3)$). This is possible by Proposition 4.2.9.

2. Put
$$\hat{\psi}_n(k) := \int_{\mathbb{R}^3} d^3x \psi_n(x) e^{-ikx} \tag{1.97}$$
as proper Riemann integrals (the integrand is continuous and since ψ_n has compact support the integral is proper, i.e. over a finite region).

3. It turns out that $\hat{\psi}_n$ is a Cauchy sequence in $L^2(\mathbb{R}^3)$, so we may finally define
$$\hat{\psi} := \lim_{n\to\infty} \hat{\psi}_n \tag{1.98}$$
where the limit is taken in $L^2(\mathbb{R}^3)$.

It turns out that $\psi \in L^2(\mathbb{R}^3)$ iff $\hat{\psi} \in L^2(\mathbb{R}^3)$, and that one can reconstruct ψ from $\hat{\psi}$ by

$$\psi(x) = \int_{\mathbb{R}^3} \frac{d^3k}{(2\pi)^3} \hat{\psi}(k) e^{ikx} \tag{1.99}$$

which is defined by the same procedure as (4.96). This reconstruction is as an element of L^2; we cannot recover ψ as an element $0\mathcal{L}^2$ from its Fourier transform. Thus (4.99) holds *almost everywhere* but not for all x.

The correct domain of the momentum operator $\hat{p}_i$, is then as follows:

$$D(\hat{p}_i) = \{\psi \in L^2(\mathbb{R}^3) | k_i \hat{\psi} \in L^2(\mathbb{R}^3)\} \tag{1.100}$$

On this domain one has $\hat{p}_i^* = \hat{p}_i$, i.e. the momentum operator is self-adjoint.

In general, any quantum-mechanical observable a should be a self-adjoint operator on some Hilbert space. By Corollary 4.7.13, this implies that the spectrum of a is real, and we will see later that the spectral theorem for self-adjoint operators enables one to construct yes-no questions similar to χ_Δ for the position operator (as discussed earlier).

1.7.4 The Hamiltonian

In case that the observable is the Hamiltonian, more detailed statements can be made, as follows.

Hamiltons equations of motion for classical mechanics were given in (4.73) and (4.74). Quantum mechanics has a single equation of motion, known as the Schrodinger equation. The role of the classical Hamiltonian $h = h(p, q)$ (i.e. a function on phase space) is now played by a certain operator h on a Hilbert space H, whose specification is part of the definition of a given physical system. The precise form of this operator is usually guessed from the form of the classical Hamiltonian. For example, if $H = L^2(\mathbb{R}^3)$ and the classical Hamiltonian is (4.74), Schrodinger took the quantum Hamiltonian to be

$$h = -\frac{\hbar^2}{2m} \sum_{i=1}^{3} \frac{\partial^2}{\partial x_i^2} + V \tag{1.101}$$

Here m is the mass of a particle moving in a potential V, seen as a a multiplication operator. For example, if the particle is an electron in a hydrogen atom, the potential is given by $V(x) = -e/|x|$ It is clear that h cannot be defined on all of $L^2(\mathbb{R}^3)$: the partial derivatives of an arbitrary $\psi \in L^2(\mathbb{R}^3)$ will not be defined (and even if they are defined the result may not be square-integrable), and the product $V\Psi$ may not lie in $L^2(\mathbb{R}^3)$ either, especially when the potential is singular (as is the case for the hydrogen atom and many other examples). Hence h is an unbounded operator, and we have to find a domain on which it is

self-adjoint. Even for $V = 0$ this is a nontrivial problem. The solution is similar to the case of the momentum operator: it turns out that the free Hamiltonian

$$h_0 = -\frac{\hbar^2}{2m} \sum_{i=1}^{3} \frac{\partial^2}{\partial x_i^2} \tag{1.102}$$

is self-adjoint on the domain

$$D(h_0) = \{\psi \in L^2(\mathbb{R}^3) | k^2 \hat{\psi} \in L^2(\mathbb{R}^3)\} \tag{1.103}$$

with $k^2 = k_1^2 + k_2^2 + k_3^2$. For nonzero potential the problem is very difficult, although most realistic cases have been completely understood now. All known examples support the following interpretation of the spectrum of the Hamiltonian:

- The discrete spectrum $\sigma_d(h)$ corresponds to the bound states of the system
- The continuous spectrum $\sigma_c(h)$ corresponds to the scattering states

To clarify this, first note that if $E \in \sigma_d(h)$, by definition there is an eigenvector ψ_E such that $h\psi_E = E\psi_E$. Hence ψ_E is a solution to the time-independent Schrodinger equation with energy E. For example, for the hydrogen atom one has $E_n = -m_e e^4/2\hbar^2 n^2$, where m_e is the mass of the electron and e is its charge, with the well-known eigenfunctions $\psi_{n,\ell,m}$. Such an eigenfunction describes a bound state, in which the electron forms a standing wave around the nucleus.

There is an interesting difference between the classical and the quantum-mechanical description of bound states: a planet revolving around the sun is in a bound state, but it clearly displays time-dependent behavior (it moves around)! An electron in a bound state, on the other hand, evolves according to the time-dependent Schrodinger equation. We will turn to the precise mathematical meaning of this equation in the next section, but for the moment we just write it down:

$$h\psi(t) = i\hbar \frac{d\psi(t)}{dt} \tag{1.104}$$

This equation should be seen as the quantum-mechanical analogue of Hamiltons equations (4.101). If $E \in \sigma_d(h)$, a possible solution of (4.104) is

$$\psi_E(t) = e^{-itE/\hbar} \psi_E \tag{1.105}$$

Although formally $\psi_E(t)$ changes in time, physically nothing really happens, as $\psi_E(s)$ and $\psi_E(t)$ for $s \neq t$ merely differ by a phase factor. Hence any expectation value $(\psi_E(t), a\psi_E(t))$ is independent of t. So bound states in quantum mechanics are static, whereas in classical mechanics they are dynamical. This makes the transition from quantum mechanics to classical mechanics in the limit $\hbar \to 0$ very difficult.

In any case, given $h = h^*$ we may split up the Hilbert space H on which h acts

by $H = H_d \oplus H_c$, where H_d contains all eigenvectors of h and $H_c = H_d^{\perp}$. States in H_c really move in time, and physically turn out to describe situations in which a particle moves in space in a non-closed trajectory. For example, think of a comet moving into the solar system with such a speed that it is not captured by the gravitational pull of the sun, but moves out again. In atomic physics, think of an electron shot into an atom and, after being scattered, moving out again.

1.7.5 Stones theorem

The time-dependent Schrodinger equation (4.104) is very delicate, mathematically speaking. Let us start with the left-hand side. The Hamiltonian h is generally an unbounded operator, so we should worry about its domain and possible self-adjointness (in order to qualify as an observable). The right-hand side involves a limit, since by definition

$$\frac{d\psi(t)}{dt} := \lim_{s \to 0} \frac{\psi(t+s) - \psi(t)}{s} \tag{1.106}$$

Since for fixed t the object $\psi(t)$ is an element of a Hilbert space H, the natural meaning of this limit is to take it in the natural norm of H (i.e., as always, the one derive from the inner product). The existence of the limit then means: for each fixed t there is a vector $\dot{\psi}(t) \in H$ such that

$$\lim_{s \to 0} \| \frac{\psi(t+s) - \psi(t)}{s} - \dot{\psi}(t) \| = 0 \tag{1.107}$$

If it exists, the vector $\dot{\psi}(t)$ is by definition the time-derivative $d\psi(t)/dt$ (as the notation already suggests). But why should this limit exist?

Hence both the left-hand side and the right-hand side of the time-dependent Schrodinger equation (4.104) are problematic. Stones Theorem provides a complete mathematical meaning of the time-dependent Schrodinger equation and in fact relates the problem on one side to that on the other. In doing so, it provides an explanation of self-adjointness as well. Stones Theorem is generally regarded as a highlight in the interaction between Hilbert space theory and quantum mechanics (although it may be considered a theorem in pure mathematics if so desired).

Stones theorem can be read in two directions:

1. Given the Hamiltonian h as a self-adjoint operator, it defines the time-evolution $\psi(t)$

2. Given the time-evolution $\psi(t)$, it defines the Hamiltonian h as a self-adjoint operator

Thus the theorem provides a relationship between the global time-evolution and the *infinitesimal* time-evolution given by the Hamiltonian and the Schrodinger

equation.

We already know what a self-adjoint operator is. To state the theorem, we need to define the notion of time-evolution on a Hilbert space. We motivate this definition by some intuition from quantum mechanics. Physicists solve the time-dependent Schrodinger equation with initial value $\psi(0) = \psi$ by

$$\psi(t) = u(t)\psi \tag{1.108}$$

where

$$u(t) = e^{-ith/\hbar} \tag{1.109}$$

Here we assume that the Hamiltonian h is time-independent. Indeed, if h is bounded (a situation that rarely occurs in practice except when H is finite-dimensional) the exponential in (4.109) can simply be defined by a norm-convergent power-series. When h is not bounded the exponential cannot be defined in this way. We will define the exponential of an unbounded operator in the next section using spectral calculus.

Some desirable properties of $u(t)$ may be read off nonetheless from *Australian style* formal computation with the motto *no worries* about any mathematical problem that might arise. We then take these heuristic properties as axioms.

First, we expect that $(\psi(s))(t) = \psi(s + t)$, and this indeed follows from (4.109) and the formal computation $exp(ta)exp(sa) = exp((s + t)a)$, where a is any operator. Indeed, this is rigorously true when a is bounded. This translates into the property

$$u(s)u(t) = u(s + t) \tag{1.110}$$

for all $s, t \in \mathbb{R}$. Furthermore, one clearly has

$$u(0) = 0 \tag{1.111}$$

and the strong continuity property

$$\lim_{t\to 0} u(t)\psi = \psi \tag{1.112}$$

for each $\psi \in H$. Finally, each $u(t)$ is unitary. This follows from (4.109) by a formal computation:

$$u(t)u(t)^* = e^{-ith/\hbar}(e^{ith/\hbar})^* = e^{-ith/\hbar}e^{ith^*/\hbar} = e^{ith/\hbar} = 1$$

and similarly for $u(t)^*u(t) = 1$. Here we have used $h^* = h$.

To some up, intuition based on the Schrodinger equation suggests the following idea[Those familiar with groups and representations will recognize that this is just the definition of a continuous unitary representation of $\mathbb{R}$ as a topological group. Condition (4.112) can be shown to be equivalent to the continuity of the

map $\langle t, \psi \rangle \mapsto u(t)\psi$ from $\mathbb{R} \times H$ to H].

Definition 4.7.16 *A time-evolution on H is a map $R \to B(H)$, $t \mapsto u(t)$, with the properties (4.110), (4.111) and (4.113) and where $u(t)$ is unitary for each t*

We now state Stones theorem. We put $\hbar = 1$ for simplicity

Theorem 4.7.17

1. *Let $t \mapsto u(t)$ be a time-evolution on H. Define an operator h by the domain*
$$D(h) : \{\psi \in H | \lim_{s \to 0} \frac{u(s) - 1}{s} \psi \; exists\} \tag{1.113}$$
and the action
$$h\psi := i \lim_{s \to 0} \frac{u(s) - 1}{s} \psi \tag{1.114}$$
The $D(h)$ is dense in H and h is self-adjoint.

2. *Provided $\psi \in D(h)$, for each $t \in \mathbb{R}$ the vector $\psi(t) = u(t0\psi$ lies in $D(h)$ and satisfies the time-dependent Schrodinger equation*
$$h\psi(t) = i\frac{d\psi(t)}{dt} \tag{1.115}$$

3. *Given a (densely defined) self-adjoint operator h on H there exists a unique time-evolution on H that is related to h in the way just specified. Explicitly, one has*
$$u(t) = e^{-ith} \tag{1.116}$$
where the exponential function is defined by the spectral calculus.

We also have the associated lemma:

Lemma 4.7.18 *Suppose h is a symmetric operator, i.e. $D(h)$ is dense and*
$$(h\varphi, \psi) = (\varphi, h\psi) \tag{1.117}$$
for all $\varphi, \psi \in D(h)$. If $R(h + i) = H$ and $R(h - i) = H$, then h is self-adjoint.

So far, we have thought of $t \mapsto u(t)\psi$ as the time-evolution of ψ. But nothing has relied on this interpretation (this is the power of abstraction in mathematicsl). Consider the following example. Take $H = L^2(\mathbb{R})$ and define the map $t \mapsto u(t)$ by
$$(u(t)\psi)(x) := \psi(x - t) \tag{1.118}$$
which satisfies Definition 4.7.16. Using superior foresight, we now rename the operator h defined in Part 1 of Theorem 4.7.17 as $\hat{p}$. Then (4.113) is just
$$D(\hat{p}) := \{\psi \in L^2(\mathbb{R}) | \psi' \in L^2(\mathbb{R})\} \tag{1.119}$$

where the derivative ψ' is defined as follows:

$$\psi'(x) := \lim_{s \to 0} \frac{\psi(x+s) - \psi(x)}{s} \tag{1.120}$$

the limit not being meant pointwise in x but in the norm of $L^2(\mathbb{R})$. Reinserting h, the action (4.114) of $\hat{p}$ is

$$\hat{p}\psi = -i\hbar \frac{d\psi}{dx} \tag{1.121}$$

This is indeed the usual momentum operator, and Stones theorem states that it is self-adjoint on the domain (4.121). The theory of the Fourier transform finally shows that the domains (4.121) and (4.100) coincide.

More generally, the domains of many operators of interest in quantum theory can be determined through Stones theorem.

1.8 The Spectral Theorem

In this section we prove the spectral theorem for self-adjoint operators a. This theorem generalizes the expansion or spectral decomposition (see Theorem 4,4.7)

$$a = \sum_i \lambda_i p_i \tag{1.122}$$

of a self-adjoint compact operator (such as a hermitian matrix) in terms of its eigenvalues λ_i and the projections p_i of the corresponding eigenspaces (i.e., if $\psi \in p_i H$ then $a\psi = \lambda_i \psi$. Let us note the properties

$$p_i \perp p_j \quad (i \neq j) \tag{1.123}$$

(since the eigenvectors belonging to different eigenvalues are orthogonal) and

$$\sum_i p_i = 1 \tag{1.124}$$

(for the eigenvectors form an orthonormal basis).

This spectral decomposition plays a leading role in the probability interpretation of quantum mechanics, which reads as follows *in case the observable $a = a^*$ is a compact operator*:

1. The possible values of the observable $a : H \to H$ that may be found when it is measured are its eigenvalues $\lambda_i \in \mathbb{R}$;

2. The probability that λ_i occurs when a is measured when the system is in a state $\psi \in H$ (i.e. a unit vector) is

$$P(a = \lambda_i | \psi) = (\psi, p_i \psi) = \|p_i \psi\|^2 \tag{1.125}$$

Here we have used the standard notation for conditional probabilities. In particular, when p_i is one-dimensional and $e_i \in p_i H$ is a unit vector one has the Born rule

$$P(a = \lambda_i|\psi) = |(e_i, \psi)|^2 \tag{1.126}$$

As we have pointed out before, in general a self-adjoint operator need not have any eigenvalues at all (recall the example of the multiplication operator $a(x) = exp(-x^2)$ on $H = L^2(\mathbb{R})$), or may have mixed spectrum consisting of both eigenvalues and continuous spectrum (for example, a multiplication operator $a \in C(\Omega)$ on $L^2(\Omega)$ with compact support has eigenvalue 0 with infinite multiplicity, since any ψ with support disjoint from a satisfies $a\psi = 0$, whereas the remainder of the range of a will form its continuous spectrum).

Hence, given $a = a^*$, we need to generalize:

- The map $\lambda_i \mapsto p_i \equiv p(\{\lambda_i\})$ from the spectrum of a to the set of projections on H
- The expansion (4.122).

1.8.1 Spectral measures

We start with the former. The appropriate generalization turns out to be a map $B \mapsto p(B)$ from the Borel subsets[If you are unfamiliar with this concept, think of just any *reasonable* subset of $\mathbb{R}$. For example, all open subsets of $\mathbb{R}$ as well as all countable intersections of open sets are Borel, as are all closed subsets of $\mathbb{R}$ and all countable unions thereof. In fact, it is practically (though not logically) impossible to construct a subset of R that is not Borel!] of $\mathbb{R}$ to the set of projections on H. This map, called the spectral measure on R defined by a, will have the following properties.

Definition 4.8.1 *A map $B \mapsto p(B)$ from the Borel subsets of $\mathbb{R}$ to the set of projections on H is called a* ***spectral measure*** *when*:

1. $p(\emptyset) = 0$
2. $p(\mathbb{R}) = 1$
3. $p(A \cap B) = p(A)p(B)$
4. $p(A \cup B) = p(A) + p(B)$ when $A \cap B = 0$
5. $p(\cup_n B_n) = \wedge p(B_n)$, where $\wedge p_n$ is the smallest projection p such that $p_n \leq p$ for all n

Note that 1. follows from 4. It follows from the third item that all $p(B)$ commute among each other when B varies, since $A \cap B = B \cap A$. It also follows that

$$p(A)p(B) = 0 \; if \; A \cap B = \emptyset \tag{1.127}$$

It will also turn out that $p(B) = 0$ if $B \cap \sigma(a) = \emptyset$) (see Corollary. 4.8.10), so that the spectral measure of a may be regarded as a map from the Borel sets in $\sigma(a)$ to the set of projections on H. This property allows us to write down the map $B \mapsto p(B)$ for compact self-adjoint operators: if a is compact and $a^* = a$ one has

$$p(B) = \sum_{i|\lambda_i \in B} p_i \tag{1.128}$$

In particular, $p_i = p(\{\lambda_i\})$ as already mentioned. The property (4.123) is then a special case of (4.127), and (4.124) follows from properties 2, 4 and 5 in Definition 4.8.1.

Given a self-adjoint operator a, we will construct a spectral measure $B \mapsto p(B)$ by means of

$$p(B) = \chi_B(a) \tag{1.129}$$

Here $\chi_B : \mathbb{R} \to \{0, 1\}$ is the characteristic function of B, but we will show how to define it with a self-adjoint operator instead of a real number as its argument. In terms of this spectral measure associated with a, the probability interpretation of quantum mechanics for arbitrary self-adjoint operators is as follows:

1. The possible values of $a : D(a) \to H$ that may be found when it is measured are the elements of its spectrum $\sigma(a)$;
2. The probability that some value within $B \subset \sigma(a)$ occurs when a is measured when the system is in a state $\psi \in H$ is

$$P(a \in B|\psi) = (\psi, p(B)\psi) = \|p(B)\psi\|^2 \tag{1.130}$$

For example, take the position operator $\hat{q}$ on $L^2(\mathbb{R})$ with domain

$$D(\hat{q}) = \{\psi \in L^2(\mathbb{R}) | x\psi \in L^2(\mathbb{R})\} \tag{1.131}$$

and action $\hat{q}\psi(x) = x\psi(x)$; see (4.94) and (4.95). This operator is self-adjoint; see Proposition 4.6.8. It turns out that

$$p(B) = \chi_B \tag{1.132}$$

as a multiplication operator on $L^2(\mathbb{R})$. Hence (4.130) becomes

$$P(\hat{q} \in B|\psi) = \int_{\mathbb{R}} dx \chi_B(x)|\psi(x)|^2 = \int_B dx|\psi(x)|^2 \tag{1.133}$$

See also (4.75). More generally, the multiplication operator a on $L^2(\Omega$ defined by $\hat{a} \in C(\Omega)$ (i.e., $a\psi = \hat{a}\psi$) gives rise to the spectral measure

$$p(B) = \chi_{\hat{a}^{-1}(B)} \tag{1.134}$$

where $\hat{a}^{-1}(B) = \{x \in \Omega | \hat{a}(x) \in B\}$. Hence

$$P(\hat{q} \in B|\psi) = \int_{\hat{a}^{-1}(B)} d^n x|\psi(x)|^2 \tag{1.135}$$

A completely different example is provided by the unit operator $a = 1 = id$, which leads to

$$p(B) = \begin{cases} 1 & \text{if } 1 \in B \\ 0 & \text{if } 1 \notin B \end{cases} \tag{1.136}$$

Hence

$$p(id \in B|\psi) = \begin{cases} 1 & \text{if } 1 \in B \\ 0 & \text{if } 1 \notin B \end{cases} \tag{1.137}$$

In other words, the unit operator assumes the value 1 with probability one.

More generally, suppose $\sigma(a)$ is discrete. In that case the spectral theorem below will take the same form (4.122) as for compact operators. One then recovers (4.128), so that

$$P(a \in B|\psi) = \sum_{i|\lambda_i \in B} (\psi, p_i \psi) \tag{1.138}$$

Let us write

$$P_\psi(B) := (\psi, p(B)\psi) \tag{1.139}$$

for the probabilities defined by a given spectral measure on H and a unit vector $\psi \in H$; if the spectral measure is derived from a self-adjoint operator a one of course has $P_\psi(B) = P(a \in B|\psi)$ as in (4.130). It now follows from Definition 4.8.1 and $\|\psi\| = 1$ that the numbers$P_\psi(B)$ define a probability measure on $\mathbb{R}$ in the following sense.

Definition 4.8.2 *A map $B \mapsto P(B)$ from the Borel subsets of $\mathbb{R}$ to $[0, 1]$ is called a* ***probability measure*** *when*:

1. $P(\mathbb{R}) = 1$

2. $P(\cup_n B_n) = \sum_n P(B_n)$ whenever $B_i \cap B_j = \emptyset$ for $i \neq j$

Note that $P(A \cup B) = P(A) + P(B)$ when $A \cap B = \emptyset$ is a special case of the second property, from which $P(\emptyset) = 0$ follows by taking $A = \emptyset$).

This shows that a quantum-mechanical observable (i.e. a self-adjoint operator) a and a state (i.e. a unit vector) ψ in a Hilbert space H together define a probability measure on $\mathbb{R}$ through (4.129) and (4.139). This should be compared with the classical situation, in which one starts with a measure space X, a probability measure μ on X, and a measurable function $f : X \to R$. From these data, one obtains a probability measure P on $\mathbb{R}$ by $P(B) := \mu(f^{-1}(B))$. Clearly, X, μ and f play the roles of H, ψ and a, respectively. Here $\mathbb{R}$ may be replaced by $f(X) \subset \mathbb{R}$, just as $\mathbb{R}$ may be replaced by $\sigma(a) \in \mathbb{R}$ in the Hilbert space situation.

1.8.2 Construction of spectral measures

Now that we know the goal, we are going to make sense of (4.129). We do this for bounded self-adjoint operators a; the unbounded case will be dealt with later. The idea is this. For a polynomial $p(x) = \sum_{k=1}^{n} c_k x^k$ on $\mathbb{R}$, it is clear what $p(a)$ should mean, namely $p(a) = \sum_{k=1}^{n} c_k a^k$. We now approximate χ_B by polynomials $(p)_n$ pointwise, $p_n(x) \to \chi_B$ for all $x \in \mathbb{R}$ (see below for a caveat and a precise version). We then define $\chi_B(a)$ and hence $p(B)$ by $\lim_n p_n(a)$, where the limit has to be taken in a certain way (see below). This procedure is justified by the following lemmas.

Lemma 4.8.3 *Let $K = [-k, k] \subset \mathbb{R}$, $k \in \mathbb{R}^+$. For each positive bounded (Borel) function $f : K \to R$ there exists a bounded monotone increasing sequence (p_k) of polynomials on K that converges pointwise to f.*

This means that

$$0 \leq p_0(x) \leq p_1(x) \leq .....p_n(x) \leq p_{n+1}(x) \leq ..... \leq c$$

for some $c > 0$ and all $x \in K$, and

$$\lim_{n\to\infty} p_n(x) = f(x) \tag{1.140}$$

for all $x \in K$.

Lemma 4.8.4

1. *If p is a real polynomial on K and $p(x) \geq 0$ for all $x \in K$, then $p(a) \geq 0$.*
2. *Consequently, if (p_n) is a monotone increasing sequence (p_n) of real polynomials on K bounded by c, then the sequence of operators $(a_n := p_n(a))$ satisfies*

$$0 \leq p_0(a) \leq p_1(a) \leq .....p_n(a) \leq p_{n+1}(a) \leq ..... \leq c \tag{1.141}$$

Recall that $a \leq b$ for two bounded operators means that $(\psi, a\psi) \leq (\psi, b\psi)$ for all $\psi \in H$.

Lemma 4.8.5 *If pq is the pointwise product of two (possibly complex-valued) polynomials p and q, then $(pq)(a) = p(a)q(a)$, and similarly for $p + q$ and cp, $c \in \mathbb{R}$. Moreover, one has $p(a)^* = \bar{p}(a)$ (where $\bar{p}$ is the complex conjugate of p*

We say that a sequence (a_n) of bounded self-adjoint operators is monotone increasing bounded when

$$a_0 \leq a_1 \leq .....a_n \leq a_{n+1} \leq ..... \leq c \tag{1.142}$$

for some constant c.

Lemma 4.8.6 *Each monotone increasing bounded sequence (an) of bounded self-adjoint operators converges strongly to a bounded self-adjoint operator. This means that for any fixed $\psi \in H$ one has*

$$\lim_n a_n\psi = a\psi \tag{1.143}$$

for some bounded self-adjoint operator a. We write this as

$$a = \lim_n a_n \tag{1.144}$$

Now take K such that $[-\|a\|, \|a\|] \subset K$ (see below why) and use Lemma 4.8.3 to find a bounded monotone increasing sequence (p_n) of polynomials on K that converges pointwise to a given positive bounded Borel function f. We then put

$$f(a) := \lim p_n(a) \;\; where \;\; p_n(x) \to f(x) \forall x 6 \in K \tag{1.145}$$

This is independent of the approximating sequence (p_n).

We are now in a position to make sense of (4.129) for a bounded and self-adjoint; just take $f = \chi_B$ in (4.145) to define

$$\chi_B(a) := \lim p_n(a) \;\; where \;\; p_n(x) \to \chi_B \forall x \in K \tag{1.146}$$

To show that the ensuing map $B \mapsto p(B)$ is indeed a spectral measure, we need a strengthening of Lemma 4.8.1. First, note that any bounded Borel function $f : R \to \mathbb{C}$ can be decomposed as

$$f = f_0 - f_1 + i(f_2 - f_3) \tag{1.147}$$

with all $f_i \geq 0$. Definition (4.145) then applies to each of the four terms in the decomposition of f, and we can define

$$f(a) := f_0(a) - f_1(a) + i(f_2(a) - f_3(a)) \tag{1.148}$$

Theorem 4.8.7 *Let $a^* = a$ be a bounded operator on H. Let again $K = [-k, k] \subset \mathbb{R}$ be such that $[-\|a\|, \|a\|] \subset K$.*

1. *The map $f \mapsto f(a)$ from the space of bounded Borel functions $f : K \to \mathbb{C}$ to the bounded operators on H is an algebra homomorphism in the sense that*

$$(t_1 f + t_2 g)(a) = t_1 f(a) + t_2 g(a) \tag{1.149}$$
$$(fg)(a) = f(a)g(a) \tag{1.150}$$
$$\bar{f}(a) = f(a)^* \tag{1.151}$$

   Here fg is the pointwise product of f and g and $t_i \in \mathbb{R}$.

2. *The map$f \mapsto f(a)$ preserves positivity in the sense that*

$$f(x) \leq g(x) \, \forall x \in K \Rightarrow f(a) \leq g(a) \tag{1.152}$$

3. *If (f_n) is a bounded monotone increasing sequence of (Borel) functions on K converging pointwise to f, then $f(a) = \lim_n f_n(a)$ (strong limit, i.e., $f(a)\psi = \lim_n f_n(a)\psi$ for each $\psi \in H$*

4. *One has*
$$\|f(a)\| \leq \|f\|_\infty = \sup_{x \in K} |f(x)| \tag{1.153}$$

Corollary 4.8.8 *The map $B \mapsto p(B)$ defined by (4.129) in terms of a bounded self-adjoint operator a is a spectral measure (cf, Definition 4.8.1).*

Indeed, the properties 1-5 in Definition 4.8.1 faithfully reflect the following properties of characteristic functions:

1. $\chi_\emptyset = 0$
2. $\chi_{\mathbb{R}} = 1$
3. $\chi_{A \cap B} = \chi_A \chi_B$
4. $\chi_{A \cup B} = \chi_A + \chi_B$ *when* $A \cap B = \emptyset$
5. $\chi_{\cup_n B_n} = \sup\{\chi_{B_n}\}$

Finally, the spectral measure associated with a is related to the spectrum $\sigma(a)$ of a in the following way.

Proposition 4.8.9 *One has $\lambda \in \sigma(a)$ iff $p(\lambda - \epsilon, \lambda + \epsilon) \neq 0$ for all $\epsilon > 0$*

Corollary 4.8.10 *Let $B \mapsto p(B)$ be defined by (4.129). If $B \cap \sigma(a) = \emptyset$, then $p(B) = 0$*

Now notice that for bounded $a = a^*$ one has $\sigma(a) \subseteq [-\|a\|, \|a\|]$. We note that, if $z \notin [-\|a\|, \|a\|]$ then $a - z$ is invertible, hence $z \in \rho(a)$. Hence everything we have done so far is independent of the choice of K, as long as it is compact (so that every polynomial $p : K \to \mathbb{R}$ is bounded) and contains $[-\|a\|, \|a\|]$.

1.8.3 The spectral theorem for bounded operators

The map $B \mapsto P(B)$ defined by (4.129) generalizes the projections p_i in the spectral theory of compact operators. We now turn to the generalization of the expansion (4.122). To state this, we first define a map $t \mapsto E(t)$ from $\mathbb{R}$ to the set of projections on H by

$$E(t) := p((-\infty, t]) = \lim_{s \to \infty} p((-s, t]) \tag{1.154}$$

where $p(B)$ for $B \subset \mathbb{R}$ is given by (4.129). In other words,

$$E(t) = \chi_{(-\infty, t]}(a) \tag{1.155}$$

Using part 1 of Theorem 4.8.7, it is easily shown that $E(t)$ is a projection, since

$$E(t)^2 = chi_{(-\infty,t]}(a)^2 = chi^2_{(-\infty,t]}(a) = chi_{(-\infty,t]}(a) = E(t)$$

and

$$E(t)^* = chi_{(-\infty,t]}(a)^* = \overline{chi_{(-\infty,t]}}(a) = chi_{(-\infty,t]}(a) = E(t)$$

For example, combining (4.128) and (4.154), we have, for compact $a = a^*$,

$$E(t) = \sum_{i|\lambda_i \leq t} p_i \tag{1.156}$$

Similarly, from (4.134) and (4.154) we obtain

$$E(t) = \chi_{a \leq t} := \chi x \in \mathbb{R}^n | a(x) \leq t \tag{1.157}$$

The map $t \mapsto E(t)$ defines a so-called spectral density in the sense that the following properties hold.

1. E is monotone increasing, that is, $E(s) \leq E(t)$ if $s \leq t$. For projections, this is equivalent to $E(s)H \subseteq E(t)H$
2. E is strongly right-continuous, that is, $\lim_{\epsilon \to 0^+} E(t + \epsilon) = E(t)$
3. $\lim_{t \to -\infty} E(t) = 0$ and $\lim_{t \to +\infty} E(t) = 1$.

The spectral theorem now has the following form.

Theorem 4.8.11 *Let a be a bounded self-adjoint operator on H and let $f : \mathbb{R} \to \mathbb{R}$ be a bounded (Borel) function. Then*

$$f(a) = \int dE(t) f(t) \tag{1.158}$$

In particular, the cases $f(t) = t$ and $f(t) = 1$ generalize (4.122) and (4.124), respectively:

$$a = \int dE(t) t \tag{1.159}$$

$$1 = \int dE(t) \tag{1.160}$$

To make sense of this theorem, we need to define the integral. As we shall see, defining it already proves the theorem. We proceed in four steps.

1. For $f = \chi_B$ we put

$$\int dE(t) \chi_B(t) := p(B) = \chi_B(a) \tag{1.161}$$

2. For a simple function $f = \sum_k c_k \chi_{B_k}$ (finite sum) with $c_k \geq 0$ we define the integral by extending the previous case by linearity, i.e.

$$\int dE(t) \sum_k c_k \chi_{B_k} := \sum_k c_k p(B_k) = \sum_k c_k \chi_{B_k}(a) \tag{1.162}$$

This already proves the spectral theorem for simple functions, since if f is simple, then (4.162) coincides with (4.159).

3. For general bounded positive (Borel) functions f, we use Lemma 4.8.12 to find a sequence (s_n) of simple functions (subject to the conditions stated in the lemma) converging pointwise to f to define

$$\int dE(t) f(t) \equiv \int dE(t) \lim_n s_n(t) := \lim_n \int dE(t) s_n(t) \tag{1.163}$$

By (4.162), this equals

$$\int dE(t) f(t) = \lim_n s_n(a) \tag{1.164}$$

The existence of this limit follows in the same way as in (4.145), with polynomials replaced by simple functions.

4. Finally, the general (i.e. complex) case follows as in (4.147) and defining the integral by linearity, i.e. if $f = f_0 - f_1 + i(f_2 - f_3)$ with all $f_i \geq 0$, then

$$\begin{aligned} \int dE(f) f(t) := & \int dE(f) f_0(t) - \int dE(t) f_1(t) \\ & + i \left(\int dE(t) f_2(t) - \int dE(t) f_3(t) \right) \end{aligned} \tag{1.165}$$

If we now use the the third claim in Theorem 4.8.7, we see that the right-hand side of (4.164) is just $f(a)$. This proves Theorem 4.8.11.

As we have seen, proving the spectral theorem is just a matter of defining the integral in the right way! The only substantial result on which the proof relies is this:

Lemma 4.8.12 *Let $K = [-k, k] \subset \mathbb{R}$, $k \in \mathbb{R}^+$. For each positive bounded (Borel) function $f : K \to \mathbb{R}$ there exists a bounded monotone increasing sequence (s_n) of simple functions on K that converges pointwise to f*

An important proposition is

Proposition 4.8.13 *One has $\lambda \in \sigma_d(a)$ iff $p(\{\lambda\}) \neq 0$, in which case $p(\{\lambda\})$ equals the projection onto the eigenspace H_λ of a.*

Consequently, if $\sigma(a) = \sigma_d(a)$ the integral in (4.159) only picks up contributions from $t = \lambda_i \in \sigma_d(a)$. Approximating the function $f(t) = t$ in the appropriate way then yields (4.122).

1.8.4 The spectral theorem for unbounded operators

The spectral Theorem 4.8.11 is valid when a and f are bounded. If both are possibly unbounded, the claim is as follows.

Theorem 4.8.14 *Let $a : D(a) \to H$ be a self-adjoint operator on H and let $f : \mathbb{R} \to \mathbb{R}$ be a (Borel) function. Then*

$$f(a) = \int dE(t) f(t) \tag{1.166}$$

is self-adjoint on

$$D(f(a)) = \{\psi \in H | \int dP|psi(t)|f(t)|^2 < \infty\} \tag{1.167}$$

In particular,

$$a = \int dE(t) t \tag{1.168}$$

and

$$D(a) = \{\psi \in H | \int dP|psi(t)t^2 < \infty\} \tag{1.169}$$

Finally we have,

Theorem 4.8.15 *Let u be a unitary operator on H. Then there exists a unique spectral density E on H with the properties $E(0) = 0$ (hence $E(t) = 0$ for all $t \leq 0$), $E(2\pi) = 1$ (hence $E(t) = 1$ for all $t \geq 2\pi$), and*

$$u = \int_0^{2\pi} dE(t) e^{it} \tag{1.170}$$

Furthermore, for bounded measurable functions $f : T \to \mathbb{C}$ (where T is the unit circle in $\mathbb{C}$ one has

$$f(u) = \int_0^{2\pi} dE(t) f(e^{it}) \tag{1.171}$$

1.8.5 Bibliography

1. E.G. Beltrametti & G. Gassinelli, The logic of quantum mechanics (Addison-Wesley, Reading, MA, 1981).
2. G. Birkhoff & E. Kreyszig, The establishment of functional analysis, Historia Mathematica 11, 258f321 (1984).
3. A. Connes, Noncommutative Geometry (Academic Press, San Diego, 1994).

4. J. Dieudonne, History of functional analysis (North-Holland, Amsterdam, 1981).

5. Gustafson, S.J. & Sigal, I.M. (2003). Mathematical concepts of quantum mechanics. Berlin: Springer.

6. P.R. Halmos, The legend of John von Neumann, The American Mathematical Monthly 80, 382-394 (1973).

7. S.J. Heims, John von Neumann and Norbert Wiener: From Mathematics to the Technologies of Life and Death (MIT Press, Cambridge, Mass., 1980).

8. P.D. Hislop & I.M. Sigal, Introduction to Spectral Theory, Springer, New York, 1996.

9. M. Jammer, The Conceptual Development of Quantum Mechanics (McGraw-Hill, New York, 1966).

10. N.P. Landsman, Mathematical Topics Between Classical and Quantum Mechanics (Springer, New York, 1998).

11. Klaas Landsman, Requiem voor Newton (Contact, Amsterdam, 2005).

12. N.P. Landsman, Lecture Notes on C*-algebras and K-theory, http://remote.science.uva.nl/ npl/CK.html, Part I.

13. N. Macrae, John von Neumann: The Scientific Genius Who Pioneered the Modern Computer, Game Theory, Nuclear Deterrence, and Much More (Pantheon Books, 1992).

14. J. Mehra & H. Rechenberg, The Historical Development of Quantum Theory, Vol. 6: The Completion of Quantum Mechanics 1926-1941 (Springer-Verlag, New York, 1982).

15. J. von Neumann, Mathematische Grundlagen der Quantenmechanik (Springer, Berlin, 1932).

16. G.K. Pedersen, Analysis Now (Springer, New York, 1989 and 1995).

17. J. Pier, Mathematical analysis during the 20th century (Oxford University Press, New York, 2001).

18. M. Reed and B. Simon, Methods of Modern Mathematical Physics, Vol. I: Functional Analysis (Academic Press, San Diego, 1980).

19. M. Reed and B. Simon, Methods of Modern Mathematical Physics. Vol II. Fourier Analysis, Self-adjointness. (Academic Press, San Diego, 1975). 63

20. M. Reed and B. Simon, Methods of Modern Mathematical Physics. Vol III. Scattering Theory. (Academic Press, San Diego, 1979).

21. M. Reed and B. Simon, Methods of Modern Mathematical Physics. Vol IV. Analysis of Operators. (Academic Press, San Diego, 1978).

22. R. Siegmund-Schultze, The origins of functional analysis. H. N. Jahnke (ed.), A History of Analysis, pp. 385-408 (AMS, Providence, 2003).

23. F. Riesz and B. Sz.-Nagy, Functional Analysis Ungar, New York, 1955).

24. Thirring, W. (1981). A Course in Mathematical Physics. Vol. 3: Quantum Mechanics of Atoms and Molecules. New York: Springer-Verlag.

25. S.M. Ulam et al., John von Neumann 1903-1957, Bulletin of the American Mathematical Society 64 (3), 1958.

26. J. Weidmann, Lineare Operatoren in Hilbertraumen, Vol. I (Teubner, Stuttgart, 2000).

27. J. Weidmann, Lineare Operatoren in Hilbertraumen, Vol. II (Teubner, Stuttgart, 2003).

28. V.A. Zorich, Mathematical Analysis II (Springer, Berlin, 2004).

1.9 Lebesgue Integration

1.9.1 Introduction

In mathematics, Lebesgue integration, named after French mathematician Henri Lebesgue, refers to both the general theory of integration of a function with respect to a general measure, and to the specific case of integration of a function defined on a sub-domain of the real line or a higher dimensional Euclidean space with respect to the Lebesgue measure.

Before proceeding we digress to learn about the concept of **measure**.

Measure

In the mathematical branch measure theory, a **measure** on a set is a systematic way to assign to each suitable subset a number, intuitively interpreted as the size of the subset. In this sense, a measure is a generalization of the concepts of length, area, volume. A particularly important example is the Lebesgue measure on a Euclidean space, which assigns the conventional length, area and volume of Euclidean geometry to suitable subsets of an $n-$dimensional Euclidean space $\mathbb{R}^n$, $n = 1, 2, 3, ...$ For instance, the Lebesgue measure of the interval $[0, 1]$ in the real numbers is its length in the everyday sense of the word, specifically 1.

To qualify as a measure (see Definition below), a function that assigns a non-negative real number or $+\infty$ to a set's subsets must satisfy a few conditions. One important condition is countable additivity. This condition states that the

size of the union of a sequence of disjoint subsets is equal to the sum of the sizes of the subsets. However, it is in general impossible to associate a consistent size to each subset of a given set and also satisfy the other axioms of a measure. This problem was resolved by defining measure only on a sub-collection of all subsets; the subsets on which the measure is to be defined are called measurable and they are required to form a $\sigma-$algebra[the collection of sets over which a measure is defined], meaning that unions, intersections and complements of sequences of measurable subsets are measurable. Non-measurable sets in a Euclidean space, on which the Lebesgue measure cannot be defined consistently, are necessarily complicated, in the sense of being badly mixed up with their complements; indeed, their existence is a non-trivial consequence of the axiom of choice.

Measure theory was developed in successive stages during the late 19th and early 20th centuries by Emile Borel, Henri Lebesgue, Johann Radon and Maurice Fréchet, among others. The main applications of measures are in the foundations of the Lebesgue integral, in Andrey Kolmogorov's axiomatization of probability theory and in ergodic theory. In integration theory, specifying a measure allows one to define integrals on spaces more general than subsets of Euclidean space; moreover, the integral with respect to the Lebesgue measure on Euclidean spaces is more general and has a richer theory than its predecessor, the Riemann integral. Probability theory considers measures that assign to the whole set the size 1, and considers measurable subsets to be events whose probability is given by the measure. Ergodic theory considers measures that are invariant under, or arise naturally from, a dynamical system.

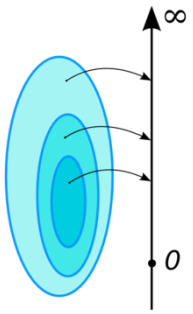

Figure 1.1: Informally, a measure has the property of being monotone in the sense that if A is a subset of B, the measure of A is less than or equal to the measure of B. Furthermore, the measure of the empty set is required to be 0.

Definition: Let Σ be a $\sigma-$algebra over a set X. A function μ from Σ to the extended real number line(contains $\pm\infty$) s called a **measure** if it satisfies the following properties:

- **Non-negativity**:
$$\mu(E) \geq 0 \ \ for \ \ all \ \ E \in \Sigma$$
- **Countable additivity**: For all countable collections $\{E_i\}_{i\in\mathbb{I}}$ of pairwise disjoint sets in Σ:
$$\mu\left(\bigcup_{i\in\mathbb{I}} E_i\right) = \sum_{i\in\mathbb{I}} \mu(E_i)$$
- **Null empty set**:
$$\mu(\emptyset) = 0$$

Requiring the empty set to have measure zero can be viewed a special case of countable additivity, if one regards the union over an empty collection to be the empty set $\bigcup_{\emptyset} = \emptyset$ and the sum over an empty collection to be zero $\sum_{\emptyset} = 0$.

A measure that takes values in the set of self-adjoint projections on a Hilbert space is called a *projection-valued measure*(PV or PVM); these are used mainly in functional analysis for the spectral theorem.

Returning to the discussion of Lebesgue integration.

Lebesgue integration plays an important role in real analysis, the axiomatic theory of probability, and many other fields in the mathematical sciences. The integral of a non-negative function can be regarded in the simplest case as the area between the graph of that function and the $x-$axis. The Lebesgue integral is a construction that extends the integral to a larger class of functions defined over spaces more general than the real line. For non-negative functions with a smooth enough graph (such as continuous functions on closed bounded intervals), the area under the curve is defined as the integral and computed using techniques of approximation of the region by polygons. For more irregular functions (such as the limiting processes of mathematical analysis and probability theory), better approximation techniques are required in order to define a suitable integral.

The integral of a function f between limits a and b can be interpreted as the area under the graph of f. This is easy to understand for familiar functions such as polynomials, but what does it mean for more exotic functions? In general, what is the class of functions for which "area under the curve" makes sense? The answer to this question has great theoretical and practical importance.

As part of a general movement toward rigor in mathematics in the nineteenth century, attempts were made to put the integral calculus on a firm foundation. The Riemann integral, proposed by Bernhard Riemann (18261866), is a

broadly successful attempt to provide such a foundation. Riemann's definition starts with the construction of a sequence of easily-calculated areas which converge to the integral of a given function. This definition is successful in the sense that it gives the expected answer for many already-solved problems, and gives useful results for many other problems.

However, Riemann integration does not interact well with taking limits of sequences of functions, making such limiting processes difficult to analyze. This is of prime importance, for instance, in the study of Fourier series, Fourier transforms and other topics. The Lebesgue integral is better able to describe how and when it is possible to take limits under the integral sign. The Lebesgue definition considers a different class of easily-calculated areas than the Riemann definition, which is the main reason the Lebesgue integral is better behaved. The Lebesgue definition also makes it possible to calculate integrals for a broader class of functions. For example, the Dirichlet function, which is 0 where its argument is irrational and 1 otherwise, has a Lebesgue integral, but it does not have a Riemann integral.

1.9.2 Construction of the Lebesgue integral

The discussion that follows parallels the most common expository approach to the Lebesgue integral. In this approach, the theory of integration has two distinct parts:

1. A theory of measurable sets and measures on these sets.
2. A theory of measurable functions and integrals on these functions.

Measure Theory

Measure theory was initially created to provide a useful abstraction of the notion of length of subsets of the real line and, more generally, area and volume of subsets of Euclidean spaces. In particular, it provided a systematic answer to the question of which subsets of $\mathbb{R}$ have a length. As was shown by later developments in set theory, it is actually impossible to assign a length to all subsets of $\mathbb{R}$ in a way which preserves some natural additivity and translation invariance properties. This suggests that picking out a suitable class of measurable subsets is an essential prerequisite.

The Riemann integral uses the notion of length explicitly. Indeed, the element of calculation for the Riemann integral is the rectangle $[a, b] \times [c, d]$, whose area is calculated to be $(b - a)(d - c)$. The quantity $b - a$ is the length of the base of the rectangle and $d - c$ is the height of the rectangle. Riemann could only use planar rectangles to approximate the area under the curve because there was no adequate theory for measuring more general sets.

In the development of the theory in most modern textbooks (after 1950), the

approach to measure and integration is axiomatic. This means that a measure is any function μ defined on a certain class X of subsets of a set E, which satisfies a certain list of properties. These properties can be shown to hold in many different cases.

Integration

We start with a measure space (E, X, μ) where E is a set, X is a $\sigma-$algebra of subsets of E and μ is a (non-negative) measure on X of subsets of E.

For example, E can be Euclidean $n-$space $\mathbb{R}^n$ or some Lebesgue measurable subset of it, X will be the $\sigma-$algebra of all Lebesgue measurable subsets of E, and μ will be the Lebesgue measure. In the mathematical theory of probability, we confine our study to a probability measure μ, which satisfies $\mu(E) = 1$.

In Lebesgue's theory, integrals are defined for a class of functions called measurable functions. A function f is measurable if the pre-image[In mathematics, the image of a subset of a function's domain under (or through) the function is the set of all outputs obtained when the function is evaluated at each element of the subset. The inverse image or preimage of a particular subset S of the codomain of a function is the set of all elements of the domain that map to the members of S] of every closed interval is in X:

$$f^{-1}([a, b]) \in X \quad for \quad all \quad a < b$$

It can be shown that this is equivalent to requiring that the pre-image of any Borel subset of $\mathbb{R}$ be in X. We will make this assumption henceforth. The set of measurable functions is closed under algebraic operations, but more importantly the class is closed under various kinds of pointwise sequential limits:

$$\sup_{k\in\mathbb{N}} f_k \quad , \quad \liminf_{k\in\mathbb{N}} f_k \quad , \quad \limsup_{k\in\mathbb{N}} f_k$$

are measurable if the original sequence $(f_k)_k$, where $k \in \mathbb{N}$, consists of measurable functions.

We build up an integral

$$\int_E f \, d\mu = \int_E f(x)\mu(dx)$$

or measurable real-valued functions f defined on E in stages:

Indicator functions: To assign a value to the integral of the *indicator function* 1_S of a measurable set S consistent with the given measure μ, the only reasonable choice is to set:

$$\int 1_S d\mu = \mu(S)$$

Notice that the result may be equal to $+\infty$, unless μ is a finite measure.

Simple functions: A finite linear combination of indicator functions

$$\sum_k a_k 1_{S_k}$$

where the coefficients a_k are real numbers and the sets S_k are measurable, is called a measurable simple function. We extend the integral by linearity to non-negative measurable simple functions. When the coefficients a_k are non-negative, we set

$$\int \left(\sum_k a_k 1_{S_k} \right) d\mu = \sum_k a_k \int 1_{S_k} d\mu = \sum_k a_k \mu(S_k)$$

The convention $0 \times \infty = 0$ must be used, and the result may be infinite. Even if a simple function can be written in many ways as a linear combination of indicator functions, the integral will always be the same; this can be shown using the additivity property of measures.

Some care is needed when defining the integral of a real-valued simple function, in order to avoid the undefined expression $(\infty - \infty)$: one assumes that the representation

$$f = \sum_k a_k 1_{S_k}$$

is such that $\mu(S_k) < \infty$ whenever $a_k \neq 0$. Then the above formula for the integral of f makes sense, and the result does not depend upon the particular representation of f satisfying the assumptions. If B is a measurable subset of E and s a measurable simple function one defines

$$\int_B s d\mu = \int 1_B s d\mu = \sum_k a_k \mu(S_k \cap B)$$

Non-negative functions: Let f be a non-negative measurable function on E which we allow to attain the value $+\infty$, in other words, f takes non-negative values in the extended real number line. We define

$$\int_E f d\mu = \sup \left\{ \int_E s d\mu : 0 \leq s \leq f,\ s \ \ simple \right\}$$

We need to show this integral coincides with the preceding one, defined on the set of simple functions. When E is a segment $[a, b]$, there is also the question of whether this corresponds in any way to a Riemann notion of integration. It is possible to prove that the answer to both questions is yes.

We have defined the integral of f for any non-negative extended real-valued measurable function on E. For some functions, this integral $\int_E f \, d\mu$ will be

infinite.

Signed functions: To handle signed functions, we need a few more definitions. If f is a measurable function of the set E to the reals (including $\pm\infty$), then we can write

$$f = f^+ + f^-$$

where

$$f^+(x) = \begin{cases} f(x) & \text{if } f(x) > 0 \\ 0 & \text{otherwise} \end{cases}$$

$$f^-(x) = \begin{cases} -f(x) & \text{if } f(x) < 0 \\ 0 & \text{otherwise} \end{cases}$$

Note that both f^+ and f^- are non-negative measurable functions. Also note that

$$|f| = f^+ + f^-$$

if

$$\int |f| d\mu < \infty$$

then f is called *Lebesgue integrable*. In this case, both integrals satisfy

$$\int f^+ d\mu < \infty \quad , \quad \int f^- d\mu < \infty$$

and it makes sense to define

$$\int f d\mu = \int f^+ d\mu - \int f^- d\mu$$

It turns out that this definition gives the desirable properties of the integral.

Complex valued functions can be similarly integrated, by considering the real part and the imaginary part separately.

Intuitive interpretation

To get some intuition about the different approaches to integration, let us imagine that it is desired to find a mountain's volume (above sea level).

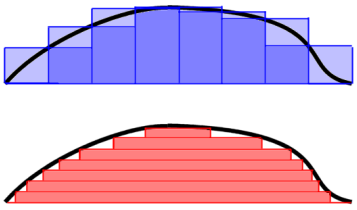

Figure 1.2: Riemann-Darboux's integration (in blue) and Lebesgue integration (in red)

The **Riemann-Darboux approach**: Divide the base of the mountain into a grid of 1 meter squares. Measure the altitude of the mountain at the center of each square. The volume on a single grid square is approximately $1 \times 1 \times$(altitude), so the total volume is the sum of the altitudes.

The **Lebesgue approach**: Draw a contour map of the mountain, where each contour is 1 meter of altitude apart. The volume of earth contained in a single contour is approximately that contour's area times its height. So the total volume is the sum of these volumes.

We can summarize the difference between the Riemann and Lebesgue approaches thus: "to compute the Riemann integral of f, one partitions the domain $[a, b]$ into subintervals", while in the Lebesgue integral, "one is in effect partitioning the range of f".

Example

Consider the indicator function of the rational numbers, $1_{\mathbb{Q}}$. This function is nowhere continuous.

- $1_{\mathbb{Q}}$ **is not Riemann-integrable** on $[0, 1]$: No matter how the set $[0, 1]$ is partitioned into subintervals, each partition will contain at least one rational and at least one irrational number, since rationals and irrationals are both dense in the reals. Thus the upper Darboux sums will all be one, and the lower Darboux sums will all be zero.

- $1_{\mathbb{Q}}$ **is Lebesgue-integrable** on $[0, 1]$ using the Lebesgue measure: Indeed it is the indicator function of the rationals so by definition

$$\int_{[0,1]} 1_{\mathbb{Q}} d\mu = \mu(\mathbb{Q} \cap [0, 1]) = 0$$

  since $\mathbb{Q}$ is countable.

Domain of Integration

A technical issue in Lebesgue integration is that the domain of integration is defined as a set (a subset of a measure space), with no notion of orientation. In elementary calculus, one defines integration with respect to an orientation:

$$\int_a^b f := -\int_a^b f$$

Generalizing this to higher dimensions yields integration of differential forms. By contrast, Lebesgue integration provides an alternative generalization, integrating over subsets with respect to a measure; this can be notated as

$$\int_A f d\mu = \int_{[a,b]} f d\mu$$

to indicate integration over a subset A.

1.9.3 Limitations of the Riemann integral

Here we discuss the limitations of the Riemann integral and the greater scope offered by the Lebesgue integral. We presume a working understanding of the Riemann integral.

With the advent of Fourier series, many analytical problems involving integrals came up whose satisfactory solution required interchanging limit processes and integral signs. However, the conditions under which the integrals

$$\sum_k \int f_k(x)dx \quad and \quad \int \left[\sum_k f_k(x)\right] dx$$

are equal proved quite elusive in the Riemann framework. There are some other technical difficulties with the Riemann integral. These are linked with the limit-taking difficulty discussed above.

Failure of monotone convergence. As shown above, the indicator function $1_{\mathbb{Q}}$ on the rationals is not Riemann integrable. In particular, the Monotone convergence theorem fails. To see why, let $\{a_k\}$ be an enumeration of all the rational numbers in $[0, 1]$ (they are countable so this can be done.) Then let

$$g_k(x) = \begin{cases} 1 & \text{if } x = a_j,\ j \leq k \\ 0 & \text{otherwise} \end{cases}$$

The function g_k is zero everywhere except on a finite set of points, hence its Riemann integral is zero. The sequence g_k is also clearly non-negative and monotonically increasing to $1_{\mathbb{Q}}$, which is not Riemann integrable.

Unsuitability for unbounded intervals. The Riemann integral can only

integrate functions on a bounded interval. It can however be extended to unbounded intervals by taking limits, so long as this doesn't yield an answer such as $\infty - \infty$.

Integrating on structures other than Euclidean space. The Riemann integral is inextricably linked to the order structure of the line.