Foundations of Quantum Mechanics

Lecture Notes
APM421

Max Lein

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Department of Mathematics
University of Toronto

Contents

Chapter 1

1 Introduction

At the end of the 19th up until the late 1920s three (!) revolutionary physical theories were developed: *statistical mechanics* which explains the physics of many particles in equilibrium, *general relativity* which governs the physics on the large scale and *quantum mechanics* which describes the physics on the microscopic scale. Einstein made seminal contributions to all three: he put statistical mechanics on firm grounds with his articles on Brownian motion, he invented general relativity and explained the photo electric effect. For the latter, the contribution to quantum mechanics, he received the Nobel Prize in 1921.

The aim of this course is to give an introduction to quantum mechanics with a focus on the underlying mathematical structures. That means we will dedicate one or more chapters to systematically study the notion of *states*, what *observables* are and the *dynamical equations*. Each of these chapters gives insight into some interesting aspects relevant to applications, e. g. we present some standard techniques to prove existence or absence of bound states in quantum systems as part of the discussion of observables.

This course is located at the intersection of mathematics and physics, so one of the tasks is to establish a dictionary between the mathematics and physics community. Both communities have benefitted from each other tremendously over the course of history: physicists would often generate new problems for mathematicians while mathematicians build and refine new tools to analyze problems from physics.

However, the course is *not* meant to be a comprehensive introduction to any of these fields in particular, but is intended to give an overview, elucidate some of the connections and whet the appetite for more.

Literature We make no attempts at completeness, and there are many very interesting aspects of quantum theory or mathematics which are not covered. For readers who are interested in the subject, a good standard physics textbook on the subject is [Sak94] while

the mathematics of quantum mechanics is covered in more depth in [Tes09; GS11] and the four-book Reed-Simon series [RS72; RS75; RS79; RS78]. In each of the chapters we will give additional references specific to the topic. However, many topics will not be discussed at all even though they are fascinating. One such omission is quantum electrodynamics, the theory of quantized light coupled to matter (cf. [Spo04, Part II]).

Chapter 2

2 Paradigms of quantum mechanics

The explanation of the photoelectric effect through light *quanta* is the name sake for quantum mechanics. Quantization here refers to the idea that energy stored in light comes in "chunks" known as *photons*, and that the energy per photon depends only on the frequency. This is quite a departure from the classical theory of light through Maxwell's equations (cf. [Jac98]).

2.1 Two archetypical quantum systems

The simplest *bona fide* quantum system is that of a quantum spin, and it can be used to give an effective description of the *Stern-Gerlach experiment* where a beam of neutral atoms with magnetic moment g is sent through a magnet with inhomogeneous magnetic field $B = (B_1, B_2, B_3)$. It was observed experimentally that the beam splits in two rather than fan out with continuous distribution. Hence, the system behaves as if only two spin configurations, spin-up $\uparrow$ and spin-down $\downarrow$, are realized. A simplified (effective) model neglects the translational degree of freedom and focusses only on the internal spin degree of freedom. Then the energy observable, the *hamiltonian*, is the matrix

$$H = gB \cdot S$$

which involves the spin operator $S_j := \frac{\hbar}{2}\sigma_j$ defined in terms of Planck's constant $\hbar$ and the three Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ +\mathrm{i} & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix},$$

and the magnetic moment g and the magnetic field B. The prefactor of the Pauli matrices are real, and thus $H = H^*$ is a hermitian matrix.

For instance, assume $B = (0, 0, b)$ points in the x_3-direction. Then spin-up and spin-down (seen from the x_3-direction) are the *eigenvectors* of

$$H = \begin{pmatrix} +\frac{\hbar g b}{2} & 0 \\ 0 & -\frac{\hbar g b}{2} \end{pmatrix},$$

i. e. $\psi_\uparrow = (1, 0)$ and $\psi_\downarrow = (0, 1)$. The dynamical equation is the *Schrödinger equation*

$$\mathrm{i}\,\hbar\,\frac{\partial}{\partial t}\psi(t) = H\psi(t), \qquad \psi(0) = \psi_0 \in \mathcal{H}. \tag{2.1.1}$$

The vector space $\mathcal{H} = \mathbb{C}^2$ becomes a Hilbert space if we equip it with the scalar product

$$\langle \psi, \varphi \rangle_{\mathbb{C}^2} := \sum_{j=1,2} \overline{\psi_j}\, \varphi_j.$$

Moreover, the hermitian matrix H can always be diagonalized (cf. exercises 1–2), and the eigenvectors to distinct eigenvalues are orthogonal. The complex-valued *wave function* ψ encapsulates probabilities: for any $\psi \in \mathbb{C}^2$ normalized to $1 = \|\psi\|_{\mathbb{C}^2}$, the probability to find the particle in the spin-up configuration is

$$\mathbb{P}(\mathsf{S}_3 = \uparrow) = |\psi_1|^2 = \big|\langle \psi_\uparrow, \psi \rangle\big|^2$$

since $\psi_\uparrow = (1, 0)$. The above notation comes from probability theory and means "the probability of finding the random observable spin S_3 in the spin-$\uparrow$ configuration $+\frac{\hbar}{2}$".

The second exemplary quantum system describes a non-relativistic particle of mass m subjected to an electric field generated by the potential V. The classical Hamilton *function* $h(q, p) = \frac{1}{2m}p^2 + V(q)$ is then "quantized" to

$$h\big(\hat{x}, -\mathrm{i}\hbar\nabla_x\big) = H = \frac{1}{2m}\big(-\mathrm{i}\hbar\nabla_x\big)^2 + V(\hat{x})$$

by replacing momentum p by the momentum *operator* $\mathsf{P} = -\mathrm{i}\hbar\nabla_x$ and position q by the multiplication operator $\mathsf{Q} = \hat{x}$.[1] The hamiltonian is now an operator on the Hilbert space $L^2(\mathbb{R}^d)$ whose action on suitable vectors ψ is

$$(H\psi)(x) = -\frac{\hbar^2}{2m}(\Delta_x\psi)(x) + V(x)\,\psi(x).$$

Quantum particles simultaneously have wave and particle character: the Schrödinger

[1] To find a consistent quantization procedure is highly non-trivial. One possibility is to use Weyl quantization [Wey27; Wig32; Moy49; Fol89; Lei10]. Such a quantization procedure also yields a formulation of a semiclassical limit, and the names for various operators (e. g. position, momentum and angular momentum) are then justified via a semiclassical limit. For instance, the momentum operator is $-\mathrm{i}\hbar\nabla_x$, because in the semiclassical limit it plays the role of the classical momentum observable p (cf. e. g. [Lei10, Theorem 1.0.1] and [Lei10, Theorem 7.0.1]).

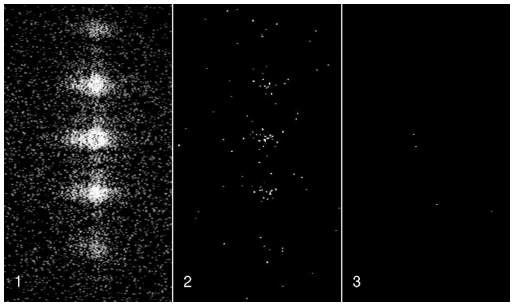

Figure 2.1.1: Images of a low-intensity triple slit experiment with photons (taken from [Cro08]).

equation (2.1.1) is structurally very similar to a wave equation. The physical constant $\hbar$ relates the energy of a particle with the associated wave length and has units [energy $\cdot$ time]. The particle aspects come into play when one measures outcomes of experiments: consider a version of the Stern-Gerlach experiment where the intensity of the atomic beam is so low that single atoms pass through the magnet. If the modulus square of the wave function $|\psi(t,x)|^2$ were to describe the intensity of a *matter* wave, then one expects that the two peaks build up slowly, but *simultaneously*. In actuality, one registers single impacts of atoms and only if one waits long enough, two peaks emerge (similar to what one sees in a low-intensity triple slit experiment in Figure 2.1.1). This is akin to tossing a coin: one cannot see the probabilistic nature in a few coin tosses, let alone a single one. Probabilities emerge only after repeating the experiment often enough. These experiments show that $|\psi(t,x)|^2$ is to be interpreted as a *probability distribution*, but more on that below.

Pure states are described by wave functions, i. e. complex-valued, square integrable functions. Put more precisely, we are considering $L^2(\mathbb{R}^d)$ made up of equivalence classes of functions with scalar product

$$\langle \varphi, \psi \rangle = \int_{\mathbb{R}^d} \mathrm{d}x \, \overline{\varphi(x)} \, \psi(x)$$

and norm $\|\psi\| := \sqrt{\langle \psi, \psi \rangle}$. In physics text books, one usually encounters the *bra-ket* notation: here $|\psi\rangle$ is a state and $\langle x|\psi\rangle$ stands for $\psi(x)$. The scalar product of $\phi, \psi \in L^2(\mathbb{R}^d)$ is denoted by $\langle \phi|\psi\rangle$ and corresponds to $\langle \phi, \psi\rangle$. Although bra-ket notation can be ambiguous, it is sometimes useful and is in fact used in mathematics every once in a while.

The fact that $L^2(\mathbb{R}^d)$ consists of *equivalence classes* of functions is only natural from a physical perspective: if $\psi_1 \sim \psi_2$ are in the same equivalence class (i. e. they differ on a set of measure 0), then the associated probabilities coincide: Physically, $|\psi(t,x)|^2$ is interpreted as the *probability to measure a particle at time t in (an infinitesimally small box located*

in) location x. If we are interested in the probability that we can measure a particle in a region $\Lambda \subseteq \mathbb{R}^d$, we have to integrate $|\psi(t,x)|^2$ over Λ,

$$\mathbb{P}(X(t) \in \Lambda) = \int_\Lambda \mathrm{d}x \ |\psi(t,x)|^2 \,. \tag{2.1.2}$$

If we want to interpret $|\psi|^2$ as *probability* density, then the wave function has to be *normalized*, i. e.

$$\|\psi\|^2 = \int_{\mathbb{R}^d} \mathrm{d}x \ |\psi(x)|^2 = 1.$$

This point of view is called *Born rule*: $|\psi|^2$ could either be a *mass* or *charge density* – or a *probability density*. To settle this, physicists have performed the double slit experiment with an electron source of low flux (cf. Figure 2.1.1). If $|\psi|^2$ were a density, one would see the whole interference pattern building up slowly. Instead, one *measures* "single impacts" of electrons and the result is similar to the data obtained from experiments in statistics (e. g. the Dalton board). Hence, we speak of *particles*.

2.2 The mathematical framework of quantum mechanics

To identify the structures common to all physical theories, let us study quantum mechanics in the abstract. We have to identify the notions of *states*, *observables* and *dynamical equations* in *Schrödinger* and *Heisenberg picture*. Here, Schrödinger and Heisenberg picture refer two equivalent formulations of the dynamics where on the one hand one can evolve states or on the other develop observables in time.

2.2.1 Quantum observables

Quantities that can be *measured* are represented by selfadjoint (hermitian in physics parlance) operators F on the Hilbert space $\mathcal{H}$ (typically $L^2(\mathbb{R}^d)$), i. e. special linear maps

$$F : \mathcal{D}(F) \subseteq \mathcal{H} \longrightarrow \mathcal{H}.$$

Here, $\mathcal{D}(F)$ is the *domain* of the operator since *typical* observables are not defined for all $\psi \in \mathcal{H}$. *This is not a mathematical subtlety with no physical content*, quite the contrary: consider the observable energy, typically given by

$$H = \frac{1}{2m}(-\mathrm{i}\hbar\nabla_x)^2 + V(\hat{x}),$$

then states in the domain

$$\mathcal{D}(H) := \left\{ \psi \in L^2(\mathbb{R}^d) \;\middle|\; H\psi \in L^2(\mathbb{R}^d) \right\} \subseteq L^2(\mathbb{R}^d)$$

are those of *finite energy*. For all ψ in the domain of the hamiltonian $\mathcal{D}(H) \subseteq L^2(\mathbb{R}^d)$, the energy expectation value

$$\langle \psi, H\psi \rangle < \infty$$

is bounded. Well-defined observables have domains that are *dense* in $\mathcal{H}$. Similarly, states in the domain $\mathcal{D}(\hat{x}_j)$ of the jth component of the position operator are those that are "localized in a finite region" in the sense of expectation values. Boundary conditions may also enter the definition of the domain: as seen in the example of the momentum operator on $[0, 1]$, different boundary conditions yield different momentum operators (see Chapter 4.3 for details).

The set of possible outcomes of measurements of H is its spectrum $\sigma(H)$, namely the set of complex numbers z so that $H - z$ is not invertible (cf. Definition 4.1.6). These can include eigenvalues, but also other types of spectra are possible if H is defined on an infinite-dimensional Hilbert space.

The energy observable is just a specific example, but it contains all the ingredients which enter the definition of a quantum observable:

Definition 2.2.1 (Observable) *A quantum observable F is a densely defined, selfadjoint operator on a Hilbert space. The spectrum $\sigma(F)$ (cf. Definition 4.1.6) is the set of outcomes of measurements.*

Physically, results of measurements are real which is reflected in the selfadjointness of operators (cf. Chapter 5), $H^* = H$, and one can show that spectra of selfadjoint operators are necessarily subsets of the reals (cf. Theorem 5.2.11). Typically one "guesses" quantum observables from classical observables: in $d = 3$, the angular momentum operator is given by

$$L = \hat{x} \times (-\mathrm{i}\hbar\nabla_x).$$

In the simplest case, one uses Dirac's recipe (replace x by $\hat{x}$ and p by $-\mathrm{i}\hbar\nabla_x$) on the classical observable angular momentum $L(x, p) = x \times p$. In other words, *many quantum observables are obtained as quantizations of classical observables*: examples are position, momentum and energy. Moreover, the *interpretation* of, say, $L = \hat{x} \times (-\mathrm{i}\hbar\nabla_x)$ as angular momentum is taken from classical mechanics.

In the definition of the domain, we have already used the definition of expectation value: the expectation value of an observable F with respect to a state ψ (which we assume to be normalized, $\|\psi\| = 1$) is given by

$$\mathbb{E}_\psi(F) := \langle \psi, F\psi \rangle. \tag{2.2.1}$$

The expectation value is finite if the state ψ is in the domain $\mathcal{D}(F)$. The Born rule of quantum mechanics tells us that if we repeat an experiment measuring the observable F many times for a particle that is prepared in the state ψ each time, the statistical average calculated according to the relative frequencies converges to the expectation value $\mathbb{E}_\psi(F)$.

Hence, quantum observables, selfadjoint operators on Hilbert spaces, are *bookkeeping devices* that have two components:

(i) a *set of possible outcomes* of measurements, the spectrum $\sigma(F)$, and

(ii) *statistics* contained in the spectral measure (cf. Chapter 6), i. e. how often a possible outcome occurs.

The uncertainty principle One of the fundamentals of quantum mechanics is *Heisenberg's uncertainty principle*, namely that one cannot arbitrarily localize wave functions in position *and* momentum space simultaneously. This is a particular case of a much more general fact about non-commuting (quantum) observables:

Theorem 2.2.2 (Heisenberg's uncertainty principle) *Let $A, B : \mathcal{H} \longrightarrow \mathcal{H}$ be two bounded selfadjoint operators on the Hilbert space $\mathcal{H}$. And we define the variance*

$$\sigma_\psi(A)^2 := \mathbb{E}_\psi\Big(\big(A - \mathbb{E}_\psi(A)\big)^2\Big)$$

with respect to $\psi \in \mathcal{H}$ with $\|\psi\| = 1$. Then Heisenberg's uncertainty relation holds:

$$\tfrac{1}{2}\big|\mathbb{E}_\psi\big(\mathrm{i}[A, B]\big)\big| \leq \sigma_\psi(A)\,\sigma_\psi(B) \tag{2.2.2}$$

Proof Let $\psi \in \mathcal{H}$ be an arbitrary normalized vector. Due to the selfadjointness of A and B, the expectation values are real,

$$\begin{aligned}\mathbb{E}_\psi(A) &= \big\langle \psi, A\psi\big\rangle = \big\langle A^*\psi, \psi\big\rangle = \big\langle A\psi, \psi\big\rangle \\ &= \overline{\big\langle \psi, A\psi\big\rangle} = \overline{\mathbb{E}_\psi(A)}.\end{aligned}$$

In general A and B will not have mean 0, but

$$\tilde{A} := A - \mathbb{E}_\psi(A)$$

and $\tilde{B} := B - \mathbb{E}_\psi(B)$ do. Hence, we can express the variance of A as an expectation value:

$$\sigma_\psi(A)^2 = \mathbb{E}_\psi\Big(\big(A - \mathbb{E}_\psi(A)\big)^2\Big) = \mathbb{E}_\psi\big(\tilde{A}^2\big)$$

Moreover, the commutator of $\tilde{A}$ and $\tilde{B}$ coincides with that of A and B,

$$\begin{aligned}\big[\tilde{A}, \tilde{B}\big] &= \big[A, B\big] - \big[\mathbb{E}_\psi(A), B\big] - \big[A, \mathbb{E}_\psi(B)\big] + \big[\mathbb{E}_\psi(A), \mathbb{E}_\psi(B)\big] \\ &= [A, B].\end{aligned}$$

Then expressing the left-hand side of (2.2.2) in terms of the shifted observables $\tilde{A}$ and $\tilde{B}$, and using the Cauchy-Schwarz inequality as well as the selfadjointness yields Heisenberg's inequality,

$$\begin{aligned}\big|\mathbb{E}_\psi\big(\mathrm{i}[A,B]\big)\big| &= \big|\mathbb{E}_\psi\big([\tilde{A},\tilde{B}]\big)\big| = \Big|\big\langle\psi,\tilde{A}\tilde{B}\psi\big\rangle - \big\langle\psi,\tilde{B}\tilde{A}\psi\big\rangle\Big| \\ &\leq \big|\big\langle\tilde{A}\psi,\tilde{B}\psi\big\rangle\big| + \big|\big\langle\tilde{B}\psi,\tilde{A}\psi\big\rangle\big| \leq 2\,\big\|\tilde{A}\psi\big\|\,\big\|\tilde{B}\psi\big\| \\ &= 2\sqrt{\big\langle\tilde{A}\psi,\tilde{A}\psi\big\rangle}\sqrt{\big\langle\tilde{B}\psi,\tilde{B}\psi\big\rangle} = 2\sqrt{\big\langle\psi,\tilde{A}^2\psi\big\rangle}\sqrt{\big\langle\psi,\tilde{B}^2\psi\big\rangle} \\ &= 2\,\sigma_\psi(A)\,\sigma_\psi(B).\end{aligned}$$

□

Often Heisenberg's inequality is just stated for the *position observable* x_j (multiplication by x_j) and the *momentum observable* $-\mathrm{i}\hbar\partial_{x_k}$: even though these are unbounded selfadjoint operators (cf. the discussion in Chapters 4.3 and 5), this introduces only technical complications on $\mathbb{R}^d$. For instance, the above arguments hold verbatim if we require in addition $\psi \in \mathcal{C}_\mathrm{c}^\infty(\mathbb{R}^d) \subset L^2(\mathbb{R}^d)$, and vectors of this type lie dense in $L^2(\mathbb{R}^d)$. Then the left-hand side of Heisenberg's inequality reduces to $\hbar/2$ because

$$\begin{aligned}\big[x_j,(-\mathrm{i}\hbar\partial_{x_k})\big]\psi &= x_j\,(-\mathrm{i}\hbar\partial_{x_k}\psi) - (-\mathrm{i}\hbar)\partial_{x_k}\big(x_j\,\psi\big) \\ &= \mathrm{i}\hbar\,\delta_{kj}\,\psi\end{aligned}$$

and ψ is assumed to have norm 1,

$$\sigma_\psi(x_j)\,\sigma_\psi\big(-\mathrm{i}\hbar\partial_{x_k}\big) \geq \tfrac{\hbar}{2}. \tag{2.2.3}$$

Skipping over some of the details (there are technical difficulties defining the commutator of two unbounded operators), we see that one cannot do better than $\hbar/2$ but there are cases when the left-hand side of (2.2.3) is not even finite.

The physical interpretation of (2.2.2) is that one cannot measure non-commuting observables simultaneously with arbitrary precision. In his original book on quantum mechanics [Hei30], Heisenberg spends a lot of care to explain why in specific experiments position and momentum along the same direction cannot be measured simultaneously with arbitrary precision, i. e. why increasing the resolution of the position measurement increases the error of the momentum measurement and vice versa.

2.2.2 Quantum states

Pure states are wave functions $\psi \in \mathcal{H}$ with $\|\psi\| = 1$, or rather, normalized wave functions up to a total phase: just like one can measure only energy *differences*, only phase *shifts* are accessible to measurements. Hence, one can think of pure states as orthogonal *projections*

$$P_\psi := |\psi\rangle\langle\psi| = \langle\psi,\cdot\rangle\,\psi.$$

Here, one can see the elegance of bra-ket notation vs. the notation that is "mathematically proper". A generalization of this concept are *density operators* ρ (often called density *matrices* with obvious abuse of terminology): density matrices are defined via the trace. If ρ is a suitable linear operator and $\{\varphi_n\}_{n\in\mathbb{N}}$ any orthonormal basis of $\mathcal{H}$, then we define

$$\mathrm{Tr}\ \rho := \sum_{n\in\mathbb{N}} \langle \varphi_n, \rho\varphi_n\rangle.$$

One can easily check that this definition is independent of the choice of basis (see homework problem 3). Clearly, P_ψ has trace 1 and it is also positive in the sense that

$$\big\langle \varphi, P_\psi \varphi\big\rangle \geq 0$$

for all $\varphi \in \mathcal{H}$. This is also the good definition for quantum states:

Definition 2.2.3 (Quantum state) *A quantum state (or density operator/matrix) $\rho = \rho^*$ is a non-negative selfadjoint operator of trace 1, i. e.*

$$\begin{aligned} \big\langle \psi, \rho\psi\big\rangle &\geq 0, && \forall \psi \in \mathcal{H}, \\ \mathrm{Tr}\ \rho &= 1. \end{aligned}$$

If ρ is also an orthogonal projection, i. e. $\rho^2 = \rho$, it is a pure state.[2] Otherwise ρ is a mixed state.

Density operators are projections if and only if they are rank-1 projections, i. e. $\rho = |\psi\rangle\langle\psi|$ for some $\psi \in \mathcal{H}$ of norm 1 (see problem 3).

Example Let $\psi_j \in \mathcal{H}$ be two wave functions normalized to 1. Then for any $0 < \alpha < 1$

$$\rho = \alpha P_{\psi_1} + (1-\alpha) P_{\psi_2} = \alpha |\psi_1\rangle\langle\psi_1| + (1-\alpha)|\psi_2\rangle\langle\psi_2|$$

is a mixed state as

$$\begin{aligned} \rho^2 = \alpha^2 |\psi_1\rangle\langle\psi_1| + (1-\alpha)^2 |\psi_2\rangle\langle\psi_2| + \\ + \alpha(1-\alpha)\big(|\psi_1\rangle\langle\psi_1|\psi_2\rangle\langle\psi_2| + |\psi_2\rangle\langle\psi_2|\psi_1\rangle\langle\psi_1|\big) \\ \neq \rho. \end{aligned}$$

Even if ψ_1 and ψ_2 are orthogonal to each other, since $\alpha^2 \neq \alpha$ and similarly $(1-\alpha)^2 \neq (1-\alpha)$, ρ cannot be a projection. Nevertheless, it is a state if $\psi_1 \perp \psi_2$ since $\mathrm{Tr}\ \rho = \alpha + (1-\alpha) = 1$. Keep in mind that ρ does not project on $\alpha\psi_1 + (1-\alpha)\psi_2$!

Also the expectation value of an observable F with respect to a state ρ is defined in terms of the trace,

$$\mathbb{E}_\rho(F) := \mathrm{Tr}\,(\rho\, F),$$

which for pure states $\rho = |\psi\rangle\langle\psi|$ reduces to $\big\langle \psi, F\psi\big\rangle$.

[2] Note that the condition $\mathrm{Tr}\ \rho = 1$ implies that ρ is a *bounded* operator while the positivity implies the selfadjointness. Hence, if ρ is a projection, i. e. $\rho^2 = \rho$, it is automatically also an orthogonal projection.

2.2.3 Time evolution

The time evolution is determined through the *Schrödinger equation*,

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi(t) = H\psi(t), \qquad \psi(t)\in\mathcal{H},\ \psi(0)=\psi_0,\ \|\psi_0\|=1. \tag{2.2.4}$$

Alternatively, one can write $\psi(t) = U(t)\psi_0$ with $U(0) = \mathrm{id}_{\mathcal{H}}$. Then, we have

$$\mathrm{i}\hbar\frac{\partial}{\partial t}U(t) = HU(t), \qquad U(0)=\mathrm{id}_{\mathcal{H}}.$$

If H *were* a number, one would immediately use the ansatz

$$U(t) = \mathrm{e}^{-\mathrm{i}\frac{t}{\hbar}H} \tag{2.2.5}$$

as solution to the Schrödinger equation. If H is a selfadjoint operator, this is *still true*, but takes a lot of work to justify (2.2.5) rigorously if the domain of H is not all of $\mathcal{H}$ (the case of unbounded operators, the *generic* case). We will do that in Chapter 6.

As has already been mentioned, we can evolve either states or observables in time and one speaks of the Schrödinger or Heisenberg picture, respectively. In the Schrödinger picture, pure states evolve according to

$$\psi(t) = U(t)\psi_0$$

while observables remain fixed. Conversely, in the Heisenberg picture, states are kept fixed in time and observables evolve according to

$$F(t) := U(t)^*\,F\,U(t) = \mathrm{e}^{+\mathrm{i}\frac{t}{\hbar}H}F\,\mathrm{e}^{-\mathrm{i}\frac{t}{\hbar}H}. \tag{2.2.6}$$

Heisenberg observables satisfy *Heisenberg's equation of motion*,

$$\frac{\mathrm{d}}{\mathrm{d}t}F(t) = \frac{\mathrm{i}}{\hbar}\big[H,F(t)\big], \qquad F(0)=F, \tag{2.2.7}$$

which can be checked by plugging in the definition of $F(t)$ and elementary *formal* manipulations. It is no coincidence that this equation looks structurally similar to the analogous equation in classical mechanics,

$$\frac{\mathrm{d}}{\mathrm{d}t}f(t) = \big\{h,f(t)\big\}, \qquad f(0)=f,$$

where $\{f,g\} = \nabla_p f\cdot\nabla_q g - \nabla_q f\cdot\nabla_p g$ is the Poisson bracket.

Density operators have to be evolved *backwards* in time, meaning that $\rho(t) = U(t)\,\rho\,U(t)^*$ satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = -\frac{\mathrm{i}}{\hbar}\big[H,\rho(t)\big], \qquad \rho(0)=\rho.$$

The equivalence of Schrödinger and Heisenberg picture is seen by comparing expectation values: the cyclicity of the trace, $\mathrm{Tr}\,(AB) = \mathrm{Tr}\,(BA)$, yields

$$\begin{aligned}\mathbb{E}_{\rho(t)}(F) &= \mathrm{Tr}\,\big(\rho(t)\,F\big) = \mathrm{Tr}\,\Big(U(t)\,\rho\,U(t)^*\,F\Big)\\ &= \mathrm{Tr}\,\Big(\rho\,U(t)^*\,F\,U(t)\Big) = \mathrm{Tr}\,\big(\rho\,F(t)\big) = \mathbb{E}_\rho\big(F(t)\big).\end{aligned}$$

As a last point, we mention the conservation of probability: if $\psi(t)$ solves the Schrödinger equation for some selfadjoint H, then we can check at least formally that the time evolution is unitary and thus preserves probability,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\big\|\psi(t)\big\|^2 &= \frac{\mathrm{d}}{\mathrm{d}t}\big\langle\psi(t),\psi(t)\big\rangle = \big\langle \tfrac{1}{\mathrm{i}\hbar}H\psi(t),\psi(t)\big\rangle + \big\langle\psi(t),\tfrac{1}{\mathrm{i}\hbar}H\psi(t)\big\rangle\\ &= \frac{\mathrm{i}}{\hbar}\Big(\big\langle\psi(t),H^*\psi(t)\big\rangle - \big\langle\psi(t),H\psi(t)\big\rangle\Big)\\ &= \frac{\mathrm{i}}{\hbar}\big\langle\psi(t),(H^*-H)\psi(t)\big\rangle = 0.\end{aligned}$$

We see that the condition $H^* = H$ is the key here: selfadjoint operators generate unitary evolution groups. As a matter of fact, there are cases when one *wants* to violate conservation of proability: one has to introduce so-called *optical potentials* which simulate particle creation and annihilation.

The time evolution $\mathrm{e}^{-\mathrm{i}\frac{t}{\hbar}H}$ is not the only unitary group of interest, other commonly used examples are *translations* in position or momentum which are generated by the momentum and position operator, respectively (the order is reversed!), as well as rotations which are generated by the angular momentum operators.

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2.2.4 Comparison to classical mechanics on $\mathbb{R}^d$

We have juxtaposed the framework of classical and quantum mechanics in Table 2.2.1, and we can elaborate on the differences and similarities of both theories. For instance, observables form an *algebra* (a vector space with multiplication): in classical mechanics, we use the *pointwise product* of functions,

$$\begin{aligned}&\cdot : \mathcal{C}^\infty(\mathbb{R}^{2n}) \times \mathcal{C}^\infty(\mathbb{R}^{2n}) \longrightarrow \mathcal{C}^\infty(\mathbb{R}^{2n}),\ (f,g) \mapsto f\cdot g\\ &(f\cdot g)(x,p) := f(x,p)\,g(x,p),\end{aligned}$$

which is obviously commutative. We also admit *complex*-valued functions and add *complex conjugation* as involution (i. e. $f^{**} = f$). Lastly, we add the Poisson bracket to make $\mathcal{C}^\infty(\mathbb{R}^{2n})$ into a so-called Poisson algebra. As we have seen, the notion of Poisson bracket gives rise to dynamics as soon as we choose an energy function (hamiltonian).

	Classical	*Quantum*
Observables	$f \in \mathcal{C}^\infty(\mathbb{R}^{2n}, \mathbb{R})$	selfadjoint operators acting on Hilbert space $\mathcal{H}$
Building block observables	position x and momentum p	position $\hat{x}$ and momentum $\hat{p}$ operators
Possible results of measurements	$\mathrm{im}(f)$	$\sigma(F)$
States	probability measures μ on phase space $\mathbb{R}^{2n}$	density operators ρ on $\mathcal{H}$
Pure states	points in phase space $\mathbb{R}^{2n}$	wave functions $\psi \in \mathcal{H}$
Generator of evolution	hamiltonian function $H : \mathbb{R}^{2n} \longrightarrow \mathbb{R}$	hamiltonian operator H
Infinitesimal time evolution equation	$\frac{\mathrm{d}}{\mathrm{d}t} f(t) = \{H, f(t)\}$	$\frac{\mathrm{d}}{\mathrm{d}t} F(t) = \frac{\mathrm{i}}{\hbar}[H, F(t)]$
Integrated time evolution	hamiltonian flow ϕ_t	$\mathrm{e}^{+\mathrm{i}\frac{t}{\hbar}H} \,\square\, \mathrm{e}^{-\mathrm{i}\frac{t}{\hbar}H}$

Table 2.2.1: Comparison of classical and quantum framework

On the quantum side, bounded operators (see Chapter 4.1) form an algebra. This algebra is *non-commutative*, i. e.

$$F \cdot G \neq G \cdot F.$$

Exactly this is what makes quantum mechanics different. Taking adjoints is the involution here and the commutator plays the role of the Poisson bracket. Again, once a hamiltonian (operator) is chosen, the dynamics of Heisenberg observables $F(t)$ is determined by the commutator of the $F(t)$ with the hamiltonian H. If an operator commutes with the hamiltonian, *it is a constant of motion*. This is in analogy with classical mechanics where an observable is a constant of motion if and only if its Poisson bracket with the hamiltonian (function) vanishes.

2.2.5 Representations

Linear algebra distinguishes abstract linear maps $H : \mathcal{X} \longrightarrow \mathcal{Y}$ and their representations as matrices using a basis in initial and target space: any pair of bases $\{x_n\}_{n=1}^N$ and $\{y_k\}_{k=1}^K$ of $\mathcal{X} \cong \mathbb{C}^N$ and $\mathcal{Y} \cong \mathbb{C}^K$ induces a matrix representation $h = (h_{nk}) \in \mathrm{Mat}_{\mathbb{C}}(N, K)$ of H (called *basis representation*) via

$$Hx_n = \sum_{k=1}^{K} h_{nk}\, y_k.$$

The basis now identifies coordinates on the vector spaces: $x = \sum_{n=1}^{N} \xi_n \, x_n \in \mathcal{X}$ has the coordinate $\xi = (\xi_1, \ldots, \xi_n) \in \mathbb{C}^N$, and similarly $y = \sum_{k=1}^{K} \eta_k \, y_k \in \mathcal{Y}$ is expressed in terms of the coordinate $\eta \in \mathbb{C}^K$. Using these coordinates, the equation $Hx = y$ becomes the matrix equation $h\xi = \eta$.

A change in basis can now be described in the same way: if $\{x'_n\}_{j=1}^{N}$ and $\{y'_k\}_{k=1}^{K}$ are two other orthonormal bases, then the coordinate representations of the maps

$$U_{xx'} : x_n \mapsto x'_n$$
$$U_{yy'} : y_k \mapsto y'_k$$

are unitary matrices $u_{xx'} \in \mathcal{U}(\mathbb{C}^N)$ and $u_{yy'} \in \mathcal{U}(\mathbb{C}^K)$, and these matrices connect the coordinate representations of H with respect to $\{x_n\}_{n=1}^{N}$, $\{y_k\}_{k=1}^{K}$ and $\{x'_n\}_{n=1}^{N}$, $\{y'_k\}_{k=1}^{K}$,

$$h' = u_{yy'} \, h \, u_{xx'}^{-1}.$$

$u_{xx'}^{-1}$ maps ξ' onto ξ, h maps ξ onto η and $u_{yy'}$ maps η onto η'.

Similarly, we can represent operators on *infinite*-dimensional Hilbert spaces such as $L^2(\mathbb{R}^d)$ in much the same way: for instance, consider the free Schrödinger operator $H = -\frac{1}{2}\Delta_x : \mathcal{D} \subset L^2(\mathbb{R}^d_x) \longrightarrow L^2(\mathbb{R}^d_x)$. Then the Fourier transform $\mathcal{F} : L^2(\mathbb{R}^d_x) \longrightarrow L^2(\mathbb{R}^d_\xi)$ is such a unitary which changes from one "coordinate system" to another, and the free Schrödinger operator in this new representation becomes a simple multiplication operator

$$H^{\mathcal{F}} := \mathcal{F} \, H \, \mathcal{F}^{-1} = \tfrac{1}{2}\hat{\xi}^2.$$

Because initial and target space are one and the same, $\mathcal{F}$ appears twice.

Another unitary is a rescaling which can be seen as a change of units: for $\lambda > 0$ one defines

$$(U_\lambda \varphi)(x) := \lambda^{d/2} \, \varphi(\lambda x)$$

where the scaling factor λ relates the two scales. Similarly, other linear changes of the underlying configuration space $\mathbb{R}^d$ (e. g. rotations) induce a unitary operator on $L^2(\mathbb{R}^d)$.

One can exploit this freedom of representation to simplify a problem: Just like choosing spherical coordinates for a problem with spherical symmetry, we can work in a representation which simplifies the problem. For instance, the Fourier transform exploits the *translational symmetry* of the free Schrödinger operator (H commutes with translations).

Another example would be to use an *eigenbasis*: assume $H = H^* \geq 0$ as a set of eigenvectors $\{\psi_n\}_{n\in\mathbb{N}}$ which span all of $\mathcal{H}$, i. e. the ψ_n are linearly independent and $H\psi_n = E_n \, \psi_n$ where $E_n \in \mathbb{R}$ is the eigenvalue. The eigenvalues are enumerated by magnitude and repeated according to their multiplicity, i. e. $E_1 \leq E_2 \leq \ldots$. Just like in the case of hermitian

matrices, the eigenvectors to distinct eigenvalues of selfadjoint operators are trivial, and hence, we can choose the $\{\psi_n\}_{n\in\mathbb{N}}$ to be orthonormal. Then the suitable unitary is

$$U : \mathcal{H} \longrightarrow \ell^2(\mathbb{N}), \quad \psi = \sum_{n=1}^{\infty} \widehat{\psi}(n)\, \psi_n \mapsto \widehat{\psi} \in \ell^2(\mathbb{N})$$

where $\widehat{\psi} = \big(\widehat{\psi}(1), \widehat{\psi}(2), \ldots\big)$ is the sequence of coefficients and $\ell^2(\mathbb{N})$ is the prototypical Hilbert space defined in Definition 3.1.2; moreover, the definition of orthonormal basis (Definition 3.2.2) implies that $\widehat{\psi}$ is necessarily square summable.

In this representation, H can be seen as an "infinite diagonal matrix"

$$H = \sum_{n=1}^{\infty} E_n\, P_{\psi_n} \mapsto H^U = U\, H\, U^{-1} = \begin{pmatrix} E_1 & 0 & \cdots & \cdots \\ 0 & E_2 & 0 & \cdots \\ \vdots & & \ddots & \ddots \end{pmatrix}$$

where $P_\psi \varphi := \langle \psi, \varphi \rangle\ \psi$ are the rank-1 projections onto ψ. Put another way, H^U acts on $\widehat{\psi} \in \ell^2(\mathbb{N})$ as

$$H^U \widehat{\psi} = \big(E_1\, \widehat{\psi}(1), E_2\, \widehat{\psi}(2), \ldots\big).$$

The simple structure of this operator allows one to compute the unitary evolution group explicitly in terms of the projections P_{ψ_n},

$$\mathrm{e}^{-\mathrm{i}\frac{t}{\hbar}H} = \sum_{n=1}^{\infty} \mathrm{e}^{-\mathrm{i}\frac{t}{\hbar}E_n}\, P_{\psi_n}.$$

Sadly, most Schrödinger operators H do not have a basis of eigenvectors.

2.3 Magnetic fields

Classically, there are *two* ways to include magnetic fields: either by minimal substitution $p \mapsto p - A(x)$ which involves the magnetic vector *potential* A or one modifies the symplectic form to include the magnetic *field* $B = \nabla_x \times A$. Note that the physical observable is the magnetic *field* rather than the vector *potential*, because there are many vector potentials which represent the same magnetic field. For instance, if A is a vector potential to the magnetic field $B = \nabla_x \times A$, then also $A' = A + \nabla_x \phi$ is another vector potential to B, because $\nabla_x \times \nabla_x \phi = 0$. The scalar function ϕ generates a *gauge transformation*.

In contrast, one always needs to choose a vector potential in quantum mechanics, and the hamiltonian for a non-relativistic particle subjected to an external electromagnetic field $(E, B) = \big(-\nabla_x V, \nabla_x \times A\big)$ is obtained by minimal substitution as well,

$$H^A = \big(-\mathrm{i}\nabla_x - A\big)^2 + V. \tag{2.3.1}$$

What happens if we choose an *equivalent* gauge $A' = A + \nabla_x \phi$? It turns out that H^A and $H^{A+\nabla_x \phi}$ are *unitarily equivalent* operators, and the unitary which connects the two is $\mathrm{e}^{-\mathrm{i}\phi}$,

$$\mathrm{e}^{+\mathrm{i}\phi}\, H^A\, \mathrm{e}^{-\mathrm{i}\phi} = H^{A+\nabla_x \phi}$$

Using the lingo of Chapter 2.2.5, $\mathrm{e}^{-\mathrm{i}\phi}$ is a unitary that connects two different representations. This has several very important ramifications. The spectrum $\sigma(H^A)$, for instance, only depends on the magnetic field $B = \nabla_x \times A$ because unitarily equivalent operators necessarily have the same spectrum. Moreover, the gauge freedom is essential to solving problems, because *some gauges are nicer to work with than others*. One such condition is $\nabla_x \cdot A = 0$, known as Coulomb gauge.

2.4 Bosons vs. fermions

The extension of *single*-particle quantum mechanics to *multi*-particle quantum mechanics is highly non-trivial. To simplify the presentation, let us focus on the case of *two* identical particles moving in $\mathbb{R}^d$. Two options are arise: either the compound wave function Ψ is a function on $\mathbb{R}^d$, i. e. it acts like a *density*, or it is a function of $\mathbb{R}^d \times \mathbb{R}^d$ where each set of coordinates $x = (x_1, x_2)$ is associated to one particle. It turns out that wave functions depend on $\mathbb{R}^{Nd}$ where N is the number of particles.

However, that is not all, there is an added complication: classically, we can label identical particles by tracking their trajectory. This is impossible in the quantum framework, because the uncertainty principle forbids any such tracking procedure. Given that the probability density $\big|\Psi(x_1, x_2)\big|^2$ is a physical observable, the inability to distinguish particles implies

$$\big|\Psi(x_1, x_2)\big|^2 = \big|\Psi(x_2, x_1)\big|^2,$$

and hence, $\Psi(x_1, x_2) = \mathrm{e}^{+\mathrm{i}\theta}\, \Psi(x_2, x_1)$. However, seeing as exchanging variables twice must give the same wave function, the only two admissible phase factors are $\mathrm{e}^{+\mathrm{i}\theta} = \pm 1$.

Particles for which $\Psi(x_1, x_2) = \Psi(x_2, x_1)$ holds are *bosons* (integer spin) while those for which $\Psi(x_1, x_2) = -\Psi(x_2, x_1)$ are *fermions* (half-integer spin). Examples are bosonic photons and fermionic electrons. This innocent looking fact has very, very strong consequences on the physical and mathematical properties of quantum systems. The most immediate implication is *Pauli's exclusion principle* for fermions,

$$\Psi(x, x) = 0,$$

a fact that is colloquially summarized by saying that bosons are social (because they like to bunch together) while sociophobic fermions tend to avoid one another.

To make this more rigorous, let us consider the splitting

$$L^2(\mathbb{R}^d \times \mathbb{R}^d) \cong L^2_{\mathsf{s}}(\mathbb{R}^d \times \mathbb{R}^d) \oplus L^2_{\mathsf{as}}(\mathbb{R}^d \times \mathbb{R}^d)$$

into symmetric and antisymmetric part induced via $f = f_{\mathsf{s}} + f_{\mathsf{as}}$ where

$$\begin{aligned} f_{\mathsf{s}}(x_1, x_2) &:= \tfrac{1}{2}\big(f(x_1, x_2) + f(x_2, x_1)\big), \\ f_{\mathsf{as}}(x_1, x_2) &:= \tfrac{1}{2}\big(f(x_1, x_2) - f(x_2, x_1)\big). \end{aligned}$$

Then one can proceed and restrict the two-particle Schrödinger operator

$$H = \sum_{j=1,2} \big(-\Delta_{x_j} + V(x_j)\big)$$

to either the bosonic space $L^2_{\mathsf{s}}(\mathbb{R}^d \times \mathbb{R}^d)$. The kinetic energy $-\sum_{j=1,2} \Delta_{x_j}$ preserves the (anti-)symmetry, e. g. in the antisymmetric (fermionic case) it defines a bounded linear map

$$H : L^2_{\mathsf{as}}(\mathbb{R}^d \times \mathbb{R}^d) \cap H^2(\mathbb{R}^d \times \mathbb{R}^d) \longrightarrow L^2_{\mathsf{as}}(\mathbb{R}^d \times \mathbb{R}^d).$$

Chapter 3

3 Hilbert spaces

First, we take a closer mathematical look at the mathematical description of states. Standard courses on quantum mechanics often use Dirac's "bra-ket" notation [Sak94, Chapter 1.2] where states are "kets" $|\psi\rangle$ that are *elements of a complex* (as opposed to real) *Hilbert space*, and kets have a "dual" called "bras" $\langle\psi|$. Many details such as the "dual correspondence" $|\psi\rangle \leftrightarrow \langle\psi|$ between kets and bras is introduced in an ad-hoc manner. The abbreviation "bra(c)ket" $\langle\psi|\varphi\rangle$ comes from the fact that one encloses common expressions (scalar products, expectation values) in angular brackets. Bra-ket notation can by systematically transliterated to Hilbert space notation that is more common in mathematics and sometimes also used theoretical physics.

Hence, in order to elucidate the connection between bras and kets with Hilbert spaces, we will introduce Hilbert spaces in this chapter and study some of their basic properties. Note that this is not intended to be a replacement for a lecture on functional analysis. For a more in depth look on the subject, we refer to [RS72; Tes09; LL01].

So let us start with the basic definition: A Hilbert space is a vector space over $\mathbb{C}$ with inner product that is complete with respect to the induced norm.

Definition 3.0.1 (Pre-Hilbert space and Hilbert space) *A pre-Hilbert space is a complex vector space $\mathcal{H}$ with scalar product*

$$\langle\cdot,\cdot\rangle : \mathcal{H} \times \mathcal{H} \longrightarrow \mathbb{C},$$

i. e. a mapping with properties

(i) $\langle\varphi,\varphi\rangle \geq 0$ *and* $\langle\varphi,\varphi\rangle = 0$ *implies* $\varphi = 0$ *(positive definiteness),*

(ii) $\overline{\langle\varphi,\psi\rangle} = \langle\psi,\varphi\rangle$*, and*

(iii) $\langle\varphi,\alpha\psi+\chi\rangle = \alpha\langle\varphi,\psi\rangle + \langle\varphi,\chi\rangle$

for all $\varphi, \psi, \chi \in \mathcal{H}$ and $\alpha \in \mathbb{C}$. This induces a natural norm $\|\varphi\| := \sqrt{\langle \varphi, \varphi \rangle}$ and metric $d(\varphi, \psi) := \|\varphi - \psi\|$, $\varphi, \psi \in \mathcal{H}$. If $\mathcal{H}$ is complete with respect to the induced metric, it is a Hilbert space*.*

Let us proceed and study some examples in more detail.

3.1 Prototypical Hilbert spaces: $\mathbb{C}^n$, $L^2(\mathbb{R}^d)$ and $\ell^2(\mathbb{Z}^d)$

The simplest case of a Hilbert space is $\mathbb{C}^n$ with scalar product

$$\langle z, w \rangle := \sum_{j=1}^{n} \overline{z_j}\, w_j.$$

Not all inner product spaces need to be complete: $\mathcal{C}([a, b], \mathbb{C})$ with scalar product

$$\langle f, g \rangle := \int_a^b \mathrm{d}x\, \overline{f(x)}\, g(x)$$

is just a pre-Hilbert space, since it is not complete: L^2-limits of continuous functions need not be continuous.

Instead the space of square integrable functions on $\mathbb{R}^d$

$$\mathcal{L}^2(\mathbb{R}^d) := \Big\{ \varphi : \mathbb{R}^d \longrightarrow \mathbb{C} \;\Big|\; \varphi \text{ measurable}, \int_{\mathbb{R}^d} \mathrm{d}x\; |\varphi(x)|^2 < \infty \Big\},$$

which appears when talking about wave functions on $\mathbb{R}^d$ is well-defined for functions that are just *measurable*. The Born rule states that $|\psi(x)|^2$ is to be interpreted as a probability density on $\mathbb{R}^d$ for position. Hence, we are interested in solutions to the Schrödinger equation which are also square integrable with respect to the Lebesgue measure [LL01, p. 6 ff.]. $\mathcal{L}^2(\mathbb{R}^d)$ is a $\mathbb{C}$-vector space, but

$$\|\varphi\|^2 := \int_{\mathbb{R}^d} \mathrm{d}x\; |\varphi(x)|^2$$

does not define a norm: there are functions $\varphi \neq 0$ for which $\|\varphi\| = 0$. Instead, $\|\varphi\| = 0$ only ensures

$$\varphi(x) = 0 \text{ almost everywhere (with respect to the Lebesgue measure } \mathrm{d}x).$$

Almost everywhere is sometimes abbreviated with a. e. and the terms “almost surely” and “for almost all $x \in \mathbb{R}^d$” can be used synonymously. If we introduce the equivalence relation

$$\varphi \sim \psi :\Leftrightarrow \|\varphi - \psi\| = 0,$$

then we can define the vector space $L^2(\mathbb{R}^d)$:

Definition 3.1.1 ($L^2(\mathbb{R}^d)$) *We define $L^2(\mathbb{R}^d)$ as*

$$\mathcal{L}^2(\mathbb{R}^d)/\sim$$

where $\sim$ is the equivalence relation that identifies φ and ψ if $\|\varphi - \psi\| = 0$.

If $\varphi_1 \sim \varphi_2$ are two normalized functions in $\mathcal{L}^2(\mathbb{R}^d)$, then we get the same probabilities for both: if $\Lambda \subseteq \mathbb{R}^d$ is a measurable set, then

$$\mathbb{P}_1(X \in \Lambda) = \int_\Lambda \mathrm{d}x \; |\varphi_1(x)|^2 = \int_\Lambda \mathrm{d}x \; |\varphi_2(x)|^2 = \mathbb{P}_2(X \in \Lambda).$$

This is proven via the triangle inequality and the Cauchy-Schwartz inequality (we will prove the latter in the next chapter):

$$\begin{aligned}
0 \leq \big|\mathbb{P}_1(X \in \Lambda) - \mathbb{P}_2(X \in \Lambda)\big| &= \left| \int_\Lambda \mathrm{d}x \; |\varphi_1(x)|^2 - \int_\Lambda \mathrm{d}x \; |\varphi_2(x)|^2 \right| \\
&= \left| \int_\Lambda \mathrm{d}x \, \overline{\big(\varphi_1(x) - \varphi_2(x)\big)} \, \varphi_1(x) - \int_\Lambda \mathrm{d}x \, \overline{\varphi_2(x)} \, \big(\varphi_1(x) - \varphi_2(x)\big) \right| \\
&\leq \int_\Lambda \mathrm{d}x \, \big|\varphi_1(x) - \varphi_2(x)\big| \, \big|\varphi_1(x)\big| - \int_\Lambda \mathrm{d}x \, \big|\varphi_2(x)\big| \, \big|\varphi_1(x) - \varphi_2(x)\big| \\
&\leq \|\varphi_1 - \varphi_2\| \; \|\varphi_1\| + \|\varphi_2\| \; \|\varphi_1 - \varphi_2\| = 0
\end{aligned}$$

Very often, another space is used in applications (e. g. in tight-binding models):

Definition 3.1.2 ($\ell^2(S)$) *Let S be a countable set. Then*

$$\ell^2(S) := \Big\{ c : S \longrightarrow \mathbb{C} \;\Big|\; \textstyle\sum_{j \in S} \overline{c_j} \, c_j < \infty \Big\}$$

is the space of square-summable sequences.

On $\ell^2(S)$ the scalar product $\langle c, c' \rangle := \sum_{j \in S} \overline{c_j} \, c'_j$ induces the norm $\|c\| := \sqrt{\langle c, c' \rangle}$. With respect to this norm, $\ell^2(S)$ is complete.

3.2 Orthonormal bases and orthogonal subspaces

Hilbert spaces have the important notion of orthonormal vectors and sequences which do not exist in Banach spaces.

Definition 3.2.1 (Orthonormal set) *Let $\mathcal{I}$ be a countable index set. A family of vectors $\{\varphi_k\}_{k \in \mathcal{I}}$ is called orthonormal set if for all $k, j \in \mathcal{I}$*

$$\langle \varphi_k, \varphi_j \rangle = \delta_{kj}$$

holds.

As we will see, all vectors in a separable Hilbert spaces can be written in terms of a countable orthonormal basis. Especially when we want to approximate elements in a Hilbert space by elements in a proper closed subspace, the vector of best approximation can be written as a linear combination of basis vectors.

Definition 3.2.2 (Orthonormal basis) *Let $\mathcal{I}$ be a countable index set. An orthonormal set of vectors $\{\varphi_k\}_{k\in\mathcal{I}}$ is called orthonormal basis if and only if for all $\psi \in \mathcal{H}$, we have*

$$\psi = \sum_{k\in\mathcal{I}} \langle \varphi_k, \psi\rangle\, \varphi_k.$$

If $\mathcal{I}$ is countably infinite, $\mathcal{I} \cong \mathbb{N}$, then this means the sequence $\psi_n := \sum_{j=1}^{n} \langle \varphi_j, \psi\rangle\, \varphi_j$ of partial converges in norm to ψ,

$$\lim_{n\to\infty} \left\| \psi - \textstyle\sum_{j=1}^{n} \langle \varphi_j, \psi\rangle\, \varphi_j \right\| = 0$$

With this general notion of orthogonality, we have a Pythagorean theorem:

Theorem 3.2.3 (Pythagoras) *Given a finite orthonormal family $\{\varphi_1, \ldots, \varphi_n\}$ in a pre-Hilbert space $\mathcal{H}$ and $\varphi \in \mathcal{H}$, we have*

$$\|\varphi\|^2 = \textstyle\sum_{k=1}^{n} \left|\langle \varphi_k, \varphi\rangle\right|^2 + \left\|\varphi - \sum_{k=1}^{n} \langle \varphi_k, \varphi\rangle\, \varphi_k\right\|^2.$$

Proof It is easy to check that $\psi := \sum_{k=1}^{n} \langle \varphi_k, \varphi\rangle\, \varphi_k$ and $\psi^\perp := \varphi - \sum_{k=1}^{n} \langle \varphi_k, \varphi\rangle\, \varphi_k$ are orthogonal and $\varphi = \psi + \psi^\perp$. Hence, we obtain

$$\begin{aligned} \|\varphi\|^2 = \langle \varphi, \varphi\rangle &= \langle \psi + \psi^\perp, \psi + \psi^\perp\rangle = \langle \psi, \psi\rangle + \langle \psi^\perp, \psi^\perp\rangle \\ &= \left\|\textstyle\sum_{k=1}^{n} \langle \varphi_k, \varphi\rangle\, \varphi_k\right\|^2 + \left\|\varphi - \sum_{k=1}^{n} \langle \varphi_k, \varphi\rangle\, \varphi_k\right\|^2. \end{aligned}$$

This concludes the proof. □

A simple corollary are Bessel's inequality and the Cauchy-Schwarz inequality.

Theorem 3.2.4 *Let $\mathcal{H}$ be a pre-Hilbert space.*

(i) Bessel's inequality holds: let $\{\varphi_1, \ldots \varphi_n\}$ be a finite orthonormal sequence. Then

$$\|\psi\|^2 \geq \sum_{j=1}^{n} |\langle \varphi_j, \psi\rangle|^2.$$

holds for all $\psi \in \mathcal{H}$.

(ii) The Cauchy-Schwarz inequality holds, i. e.

$$|\langle \varphi, \psi \rangle| \leq \|\varphi\| \|\psi\|$$

is valid for all $\varphi, \psi \in \mathcal{H}$

Proof (i) This follows trivially from the previous Theorem as $\|\psi^{\perp}\|^2 \geq 0$.

(ii) Pick $\varphi, \psi \in \mathcal{H}$. In case $\varphi = 0$, the inequality holds. So assume $\varphi \neq 0$ and define

$$\varphi_1 := \frac{\varphi}{\|\varphi\|}$$

which has norm 1. We can apply (i) for $n = 1$ to conclude

$$\|\psi\|^2 \geq |\langle \varphi_1, \psi \rangle|^2 = \frac{1}{\|\varphi\|^2} |\langle \varphi, \psi \rangle|^2 .$$

This is equivalent to the Cauchy-Schwarz inequality. □

An important corollary says that the scalar product is continuous with respect to the norm topology. This is not at all surprising, after all the norm is induced by the scalar product!

Corollary 3.2.5 *Let* $\mathcal{H}$ *be a Hilbert space. Then the scalar product is continuous with respect to the norm topology, i. e. for two sequences* $(\varphi_n)_{n\in\mathbb{N}}$ *and* $(\psi_m)_{m\in\mathbb{N}}$ *that converge to* φ *and* ψ*, respectively, we have*

$$\lim_{n,m\to\infty} \langle \varphi_n, \psi_m \rangle = \langle \varphi, \psi \rangle.$$

Proof Let $(\varphi_n)_{n\in\mathbb{N}}$ and $(\psi_m)_{m\in\mathbb{N}}$ be two sequences in $\mathcal{H}$ that converge to φ and ψ, respectively. Then by Cauchy-Schwarz, we have

$$\begin{aligned}
\lim_{n,m\to\infty} \big|\langle \varphi, \psi \rangle - \langle \varphi_n, \psi_m \rangle\big| &= \lim_{n,m\to\infty} \big|\langle \varphi - \varphi_n, \psi \rangle - \langle \varphi_n, \psi_m - \psi \rangle\big| \\
&\leq \lim_{n,m\to\infty} \big|\langle \varphi - \varphi_n, \psi \rangle\big| + \lim_{n,m\to 0} \big|\langle \varphi_n, \psi_m - \psi \rangle\big| \\
&\leq \lim_{n,m\to\infty} \|\varphi - \varphi_n\| \, \|\psi\| + \lim_{n,m\to\infty} \|\varphi_n\| \, \|\psi_m - \psi\| = 0
\end{aligned}$$

since there exists some $C > 0$ such that $\|\varphi_n\| \leq C$ for all $n \in \mathbb{N}$. □

Definition 3.2.6 (Separable Hilbert space) *A Hilbert space* $\mathcal{H}$ *is called separable if there exists a countable dense subset.*

Before we prove that a Hilbert space is separable exactly if it admits a *countable* basis, we need to introduce the notion of orthogonal complement: if A is a subset of a pre-Hilbert space $\mathcal{H}$, then we define

$$A^\perp := \{\varphi \in \mathcal{H} \mid \langle \varphi, \psi \rangle = 0 \; \forall \psi \in A\}.$$

The following few properties of the orthogonal complement follow immediately from its definition:

(i) $\{0\}^\perp = \mathcal{H}$ and $\mathcal{H}^\perp = \{0\}$.

(ii) $A^\perp$ is a closed linear subspace of $\mathcal{H}$ for *any* subset $A \subseteq \mathcal{H}$.

(iii) If $A \subseteq B$, then $B^\perp \subseteq A^\perp$.

(iv) If we denote the sub vector space spanned by the elements in A by span A, we have

$$A^\perp = \big(\operatorname{span} A\big)^\perp = \big(\overline{\operatorname{span} A}\big)^\perp$$

2014.09.19 where $\overline{\operatorname{span} A}$ is the completion of span A with respect to the norm topology.

If $(\mathcal{H}, d)$ is a metric space, we can define the distance between a point $\varphi \in \mathcal{H}$ and a subset $A \subseteq \mathcal{H}$ as

$$d(\varphi, A) := \inf_{\psi \in A} d(\varphi, \psi).$$

If there exists $\varphi_0 \in A$ which minimizes the distance, i. e. $d(\varphi, A) = d(\varphi, \varphi_0)$, then φ_0 is called *element of best approximation* for φ in A. This notion is helpful to understand why and how elements in an infinite-dimensional Hilbert space can be approximated by finite linear combinations – something that is used in numerics all the time.

If $A \subset \mathcal{H}$ is a convex subset of a Hilbert space $\mathcal{H}$, then one can show that there always exists an element of best approximation. In case A is a linear subspace of $\mathcal{H}$, it is given by projecting an arbitrary $\psi \in \mathcal{H}$ down to the subspace A.

Theorem 3.2.7 *Let A be a closed convex subset of a Hilbert space $\mathcal{H}$. Then there exists for each $\varphi \in \mathcal{H}$ exactly one $\varphi_0 \in A$ such that*

$$d(\varphi, A) = d(\varphi, \varphi_0).$$

Proof We choose a sequence $(\psi_n)_{n \in \mathbb{N}}$ in A with $d(\varphi, \psi_n) = \|\varphi - \psi_n\| \to d(\varphi, A)$. This sequence is also a Cauchy sequence: we add and subtract φ to get

$$\big\|\psi_n - \psi_m\big\|^2 = \big\|(\psi_n - \varphi) + (\varphi - \psi_m)\big\|^2.$$

If $\mathcal{H}$ were a normed space, we could have to use the triangle inequality to estimate the right-hand side from above. However, $\mathcal{H}$ is a Hilbert space and by using the parallelogram identity,[1] we see that the right-hand side is actually *equal* to

$$\begin{aligned}\big\|\psi_n - \psi_m\big\|^2 &= 2\big\|\psi_n - \varphi\big\|^2 + 2\big\|\psi_m - \varphi\big\|^2 - \big\|\psi_n + \psi_m - 2\varphi\big\|^2 \\ &= 2\big\|\psi_n - \varphi\big\|^2 + 2\big\|\psi_m - \varphi\big\|^2 - 4\big\|\tfrac{1}{2}(\psi_n + \psi_m) - \varphi\big\|^2 \\ &\leq 2\big\|\psi_n - \varphi\big\|^2 + 2\big\|\psi_m - \varphi\big\|^2 - 4d(\varphi, A) \\ &\xrightarrow{n,m\to\infty} 2d(\varphi, A) + 2d(\varphi, A) - 4d(\varphi, A) = 0.\end{aligned}$$

By convexity, $\frac{1}{2}(\psi_n + \psi_m)$ is again an element of A. This is crucial once again for the uniqueness argument. Letting $n, m \to \infty$, we see that $(\psi_n)_{n\in\mathbb{N}}$ is a Cauchy sequence in A which converges in A as it is a closed subset of $\mathcal{H}$. Let us call the limit point $\varphi_0 := \lim_{n\to\infty} \psi_n$. Then φ_0 is *an* element of best approximation,

$$\big\|\varphi - \varphi_0\big\| = \lim_{n\to\infty} \big\|\varphi - \psi_n\big\| = d(\varphi, A).$$

To show uniqueness, we assume that there exists another element of best approximation $\varphi_0' \in A$. Define the sequence $(\tilde{\psi}_n)_{n\in\mathbb{N}}$ by $\tilde{\psi}_{2n} := \varphi_0$ for even indices and $\tilde{\psi}_{2n+1} := \varphi_0'$ for odd indices. By assumption, we have $\|\varphi - \varphi_0\| = d(\varphi, A) = \|\varphi - \varphi_0'\|$ and thus, by repeating the steps above, we conclude $(\tilde{\psi}_n)_{n\in\mathbb{N}}$ is a Cauchy sequence that converges to some element. However, since the sequence is alternating, the two elements $\varphi_0' = \varphi_0$ are in fact identical. □

As we have seen, the condition that the set is convex and closed is crucial in the proof. Otherwise the minimizer may not be unique or even contained in the set.

Corollary 3.2.8 *Let E be a closed subvector space of the Hilbert space $\mathcal{H}$. Then for any $\varphi \in \mathcal{H}$, there exists $\varphi_0 \in E$ such that $d(\varphi, E) = d(\varphi, \varphi_0)$.*

This is all very abstract. For the case of a closed subvector space $E \subseteq \mathcal{H}$, we can express the element of best approximation in terms of the basis: not surprisingly, it is given by the projection of φ onto E.

Theorem 3.2.9 *Let $E \subseteq \mathcal{H}$ be a closed subspace of a Hilbert space that is spanned by countably many orthonormal basis vectors $\{\varphi_k\}_{k\in\mathcal{I}}$. Then for any $\varphi \in \mathcal{H}$, the element of best approximation $\varphi_0 \in E$ is given by*

$$\varphi_0 = \sum_{k\in\mathcal{I}} \langle \varphi_k, \varphi \rangle \, \varphi_k.$$

[1] For all $\varphi, \psi \in \mathcal{H}$, the identity $2\|\varphi\|^2 + 2\|\psi\|^2 = \|\varphi + \psi\|^2 + \|\varphi - \psi\|^2$ holds.

Proof It is easy to show that $\varphi - \varphi_0$ is orthogonal to any $\psi = \sum_{k\in\mathcal{I}} \lambda_k \varphi_k \in E$: we focus on the more difficult case when E is not finite dimensional: then, we have to approximate φ_0 and ψ by finite linear combinations and take limits. We call $\varphi_0^{(n)} := \sum_{k=1}^{n} \langle \varphi_k, \varphi\rangle\, \varphi_k$ and $\psi^{(m)} := \sum_{j=1}^{m} \lambda_j \varphi_j$. With that, we have

$$\begin{aligned}\left\langle \varphi - \varphi_0^{(n)}, \psi^{(m)} \right\rangle &= \left\langle \varphi - \textstyle\sum_{k=1}^{n} \langle \varphi_k, \varphi\rangle\, \varphi_k, \sum_{j=1}^{m} \lambda_j \varphi_j \right\rangle \\ &= \sum_{j=1}^{m} \lambda_j \left\langle \varphi, \varphi_j \right\rangle - \sum_{k=1}^{n}\sum_{j=1}^{m} \lambda_j \overline{\langle \varphi_k, \varphi\rangle} \left\langle \varphi_k, \varphi_j \right\rangle \\ &= \sum_{j=1}^{m} \lambda_j \left\langle \varphi, \varphi_j \right\rangle \Big(1 - \textstyle\sum_{k=1}^{n} \delta_{kj}\Big).\end{aligned}$$

By continuity of the scalar product, Corollary 3.2.5, we can take the limit $n, m \to \infty$. The term in parentheses containing the sum is 0 exactly when $j \in \{1, \dots, m\}$ and 1 otherwise. Specifically, if $n \geq m$, the right-hand side vanishes identically. Hence, we have

$$\left\langle \varphi - \varphi_0, \psi \right\rangle = \lim_{n,m\to\infty} \left\langle \varphi - \varphi_0^{(n)}, \psi^{(m)} \right\rangle = 0,$$

in other words $\varphi - \varphi_0 \in E^\perp$. This, in turn, implies by the Pythagorean theorem that

$$\|\varphi - \psi\|^2 = \|\varphi - \varphi_0\|^2 + \|\varphi_0 - \psi\|^2 \geq \|\varphi - \varphi_0\|^2$$

and hence $\|\varphi - \varphi_0\| = d(\varphi, E)$. Put another way, φ_0 is *an* element of best approximation. Let us now show uniqueness. Assume, there exists another element of best approximation $\varphi_0' = \sum_{k\in\mathcal{I}} \lambda_k' \varphi_k$. Then we know by repeating the previous calculation backwards that $\varphi - \varphi_0' \in E^\perp$ and the scalar product with respect to any of the basis vectors φ_k which span E has to vanish,

$$\begin{aligned}0 = \left\langle \varphi_k, \varphi - \varphi_0' \right\rangle &= \langle \varphi_k, \varphi\rangle - \sum_{j\in\mathcal{I}} \lambda_j' \left\langle \varphi_k, \varphi_j \right\rangle = \langle \varphi_k, \varphi\rangle - \sum_{j\in\mathcal{I}} \lambda_j' \delta_{kj} \\ &= \langle \varphi_k, \varphi\rangle - \lambda_k'.\end{aligned}$$

This means the coefficients with respect to the basis $\{\varphi_k\}_{k\in\mathcal{I}}$ all agree with those of φ_0. Hence, the element of approximation is unique, $\varphi_0 = \varphi_0'$, and given by the projection of φ onto E. □

Theorem 3.2.10 *Let E be a closed linear subspace of a Hilbert space $\mathcal{H}$. Then*

(i) $\mathcal{H} = E \oplus E^\perp$, i. e. every vector $\varphi \in \mathcal{H}$ can be uniquely decomposed as $\varphi = \psi + \psi^\perp$ with $\psi \in E$, $\psi^\perp \in E^\perp$.

(ii) $E^{\perp\perp} = E$.

Proof (i) By Theorem 3.2.7, for each $\varphi \in \mathcal{H}$, there exists $\varphi_0 \in E$ such that $d(\varphi, E) = d(\varphi, \varphi_0)$. From the proof of the previous theorem, we see that $\varphi_0^\perp := \varphi - \varphi_0 \in E^\perp$. Hence, $\varphi = \varphi_0 + \varphi_0^\perp$ is *a* decomposition of φ. To show that it is unique, assume $\varphi_0' + {\varphi_0'}^\perp = \varphi = \varphi_0 + \varphi_0^\perp$ is another decomposition. Then by subtracting, we are led to conclude that

$$E \ni \varphi_0' - \varphi_0 = \varphi_0^\perp - {\varphi_0'}^\perp \in E^\perp$$

holds. On the other hand, $E \cap E^\perp = \{0\}$ and thus $\varphi_0 = \varphi_0'$ and $\varphi_0^\perp = {\varphi_0'}^\perp$, the decomposition is unique.

(ii) It is easy to see that $E \subseteq E^{\perp\perp}$. Let $\tilde{\varphi} \in E^{\perp\perp}$. By the same arguments as above, we can decompose $\tilde{\varphi} \in E^{\perp\perp} \subseteq \mathcal{H}$ into

$$\tilde{\varphi} = \tilde{\varphi}_0 + \tilde{\varphi}_0^\perp$$

with $\tilde{\varphi}_0 \in E \subseteq E^{\perp\perp}$ and $\tilde{\varphi}_0^\perp \in E^\perp$. Hence, $\tilde{\varphi} - \tilde{\varphi}_0 \in E^{\perp\perp} \cap E^\perp = (E^\perp)^\perp \cap E^\perp = \{0\}$ and thus $\tilde{\varphi} = \tilde{\varphi}_0 \in E$. □

Now we are in a position to prove the following important Proposition:

Proposition 3.2.11 *A Hilbert space $\mathcal{H}$ is separable if and only if there exists a countable orthonormal basis.*

Proof $\Leftarrow$: The set generated by the orthonormal basis $\{\varphi_j\}_{j\in\mathcal{I}}$, $\mathcal{I}$ countable, and coefficients $z = q + ip$, $q, p \in \mathbb{Q}$, is dense in $\mathcal{H}$,

$$\left\{\sum_{j=1}^n z_j\varphi_j \in \mathcal{H} \;\middle|\; \mathbb{N} \ni n \leq |\mathcal{I}|\,,\ \varphi_j \in \{\varphi_k\}_{k\in\mathbb{N}},\ z_j = q_j + ip_j,\ q_j, p_j \in \mathbb{Q}\right\}.$$

$\Rightarrow$: Assume there exists a countable dense subset $\mathcal{D}$, i. e. $\overline{\mathcal{D}} = \mathcal{H}$. If $\mathcal{H}$ is finite dimensional, the induction terminates after finitely many steps and the proof is simpler. Hence, we will assume $\mathcal{H}$ to be infinite dimensional. Pick a vector $\tilde{\varphi}_1 \in \mathcal{D} \setminus \{0\}$ and normalize it. The normalized vector is then called φ_1. Note that φ_1 need not be in $\mathcal{D}$. By Theorem 3.2.10, we can split any $\psi \in \mathcal{D}$ into ψ_1 and $\psi_1^\perp$ such that $\psi_1 \in \text{span}\,\{\varphi_1\} := E_1$, $\psi_1^\perp \in \text{span}\,\{\varphi_1\}^\perp := E_1^\perp$ and

$$\psi = \psi_1 + \psi_1^\perp.$$

pick a second $\tilde{\varphi}_2 \in \mathcal{D} \setminus E_1$ (which is non-empty). Now we apply Theorem 3.2.9 (which is in essence Gram-Schmidt orthonormalization) to $\tilde{\varphi}_2$, i. e. we pick the part which is orthogonal to φ_1,

$$\varphi_2' := \tilde{\varphi}_2 - \langle \varphi_1, \tilde{\varphi}_2 \rangle \, \varphi_2$$

and normalize to φ_2,

$$\varphi_2 := \frac{\varphi_2'}{\|\varphi_2'\|}.$$

This defines $E_2 := \operatorname{span}\{\varphi_1, \varphi_2\}$ and $\mathcal{H} = E_2 \oplus E_2^\perp$.

Now we proceed by induction: assume we are given $E_n = \operatorname{span}\{\varphi_1, \ldots, \varphi_n\}$. Take $\tilde{\varphi}_{n+1} \in \mathcal{D} \setminus E_n$ and apply Gram-Schmidt once again to yield φ_{n+1} which is the obtained from normalizing the vector

$$\varphi_{n+1}' := \tilde{\varphi}_{n+1} - \sum_{k=1}^{n} \langle \varphi_k, \tilde{\varphi}_{n+1} \rangle \, \varphi_k.$$

This induction yields an orthonormal sequence $\{\varphi_n\}_{n\in\mathbb{N}}$ which is by definition an orthonormal basis of $E_\infty := \overline{\operatorname{span}\{\varphi_n\}_{n\in\mathbb{N}}}$ a closed subspace of $\mathcal{H}$. If $E_\infty \subsetneq \mathcal{H}$, we can split the Hilbert space into $\mathcal{H} = E_\infty \oplus E_\infty^\perp$. Then either $\mathcal{D} \cap (\mathcal{H} \setminus E_\infty) = \emptyset$ – in which case $\mathcal{D}$ cannot be dense in $\mathcal{H}$ – or $\mathcal{D} \cap (\mathcal{H} \setminus E_\infty) \neq \emptyset$. But then we have terminated the induction prematurely. □

3.3 Direct sums ($\oplus$) and tensor products ($\otimes$) of Hilbert spaces

There are several ways to split Hilbert spaces: in direct sums and direct products. With the same techniques, we can construct new ones from existing Hilbert spaces. In Theorem 3.2.10, we have shown that if E is a closed subspace, then $\mathcal{H}$ decomposes into a direct sum

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

That means any vector $\varphi = \psi + \psi_\perp \in \mathcal{H}$ can be *uniquely* decomposed into $\psi \in E$ and $\psi^\perp \in E^\perp$. We now define the direct sum of two Hilbert spaces:

Definition 3.3.1 (Direct sum $\oplus$) *Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be Hilbert spaces with scalar products $\langle \cdot, \cdot \rangle_1$ and $\langle \cdot, \cdot \rangle_2$. Then we define $\mathcal{H}_1 \oplus \mathcal{H}_2$ as the carteisan product $\mathcal{H}_1 \times \mathcal{H}_2$ of vector spaces endowed with the structure of a vector space in the following way: for any $\varphi = (\varphi_1, \varphi_2), \psi = (\psi_1, \psi_2) \in \mathcal{H}_1 \times \mathcal{H}_2$ and $\alpha \in \mathbb{C}$, we define*

(i) addition component-wise, $\varphi + \psi = (\varphi_1, \varphi_2) + (\psi_1, \psi_2) := (\varphi_1 + \psi_1, \varphi_2 + \psi_2)$,

(ii) scalar multiplication component-wise, $\alpha\varphi = \alpha(\varphi_1, \varphi_2) := (\alpha\varphi_1, \alpha\varphi_2)$,

(iii) and the scalar product on $\mathcal{H}_1 \oplus \mathcal{H}_2$ *is the sum of the two scalar products,*

$$\langle \varphi, \psi \rangle := \langle \varphi_1, \psi_1 \rangle_1 + \langle \varphi_2, \psi_2 \rangle_2.$$

Proposition 3.3.2 *The direct sum* $\mathcal{H}_1 \oplus \mathcal{H}_2$ *of two Hilbert spaces is a Hilbert space.*

Proof One immediately checks that $\mathcal{H}_1 \oplus \mathcal{H}_2$ is a vector space. Completeness also follows from the completeness of the components: let $\{\varphi^{(n)}\}_{n\in\mathbb{N}}$ be a Cauchy sequence with respect to the norm induced by $\langle \cdot, \cdot \rangle$. Writing out the definition, it is clear that this also means each component $\{\varphi_j^{(n)}\}_{n\in\mathbb{N}}$, $j = 1, 2$, is a Cauchy sequence in $\mathcal{H}_j$ which converges to some $\varphi_j \in \mathcal{H}_j$. Hence, $\varphi^{(n)} \longrightarrow (\varphi_1, \varphi_2)$ as $n \to \infty$. □

The other way to construct new Hibert spaces is taking tensor products: if $\varphi_1 \in \mathcal{H}_1$ and $\varphi_2 \in \mathcal{H}_2$ are two vectors from two vector spaces, we can characterize $\varphi_1 \otimes \varphi_2$, the tensor product of φ_1 and φ_2, by the following defining properties: for any $\varphi_1, \psi_1 \in \mathcal{H}_1$ and $\varphi_2, \psi_2 \in \mathcal{H}_2$

$$\begin{aligned} \varphi_1 \otimes (\varphi_2 + \psi_2) &= \varphi_1 \otimes \varphi_2 + \varphi_1 \otimes \psi_2 \\ (\varphi_1 + \psi_1) \otimes \varphi_2 &= \varphi_1 \otimes \varphi_2 + \psi_1 \otimes \varphi_2 \end{aligned}$$

holds. Scalars can be pushed back and forth between factors,

$$\alpha(\varphi_1 \otimes \varphi_2) = (\alpha\varphi_1) \otimes \varphi_2 = \varphi_1 \otimes (\alpha\varphi_2).$$

The formal definition is a lot more complicated: one has to construct a big space where vectors such as $(\alpha\varphi_1) \otimes \varphi_2$ and $\varphi_1 \otimes (\alpha\varphi_2)$ are distinct and then use equivalence relations to implement the above characteristics. The constructed space is defined only up to isomorphism.

Definition 3.3.3 (Tensor product $\otimes$) *Let* $\mathcal{H}_1$ *and* $\mathcal{H}_2$ *be two Hilbert spaces with scalar products* $\langle \cdot, \cdot \rangle_1$ *and* $\langle \cdot, \cdot \rangle_2$*. Then the tensor product* $\mathcal{H}_1 \otimes \mathcal{H}_2$ *is defined as the completion of the algebraic tensor product*

$$\mathcal{H}_1 \odot \mathcal{H}_2 := \left\{ \textstyle\sum_{k=1}^{n} \lambda_k \varphi_{1\,k} \otimes \varphi_{2\,k} \;\middle|\; n \in \mathbb{N},\, \varphi_{1\,k} \in \mathcal{H}_1,\, \varphi_{2\,k} \in \mathcal{H}_2,\, \lambda_k \in \mathbb{C}\, \forall 1 \le k \le n \right\}$$

with respect to the norm induced by the scalar product

$$\left\langle \varphi_1 \otimes \varphi_2 \,,\, \psi_1 \otimes \psi_2 \right\rangle := \langle \varphi_1, \psi_1 \rangle_1 \, \langle \varphi_2, \psi_2 \rangle_2, \qquad \forall \varphi_1, \psi_1 \in \mathcal{H}_1,\ \varphi_2, \psi_2 \in \mathcal{H}_2.$$

If $\{\varphi_{1\,k}\}_{k\in\mathcal{I}_1}$ and $\{\varphi_{2\,j}\}_{j\in\mathcal{I}_2}$ are orthonormal bases of two separable Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively, then

$$\left\{\varphi_{1\,k}\otimes\varphi_{2\,j}\right\}_{k\in\mathcal{I}_1,j\in\mathcal{I}_2}$$

is an orthonormal basis in $\mathcal{H}_1\otimes\mathcal{H}_2$, i. e. every vector $\Psi\in\mathcal{H}_1\otimes\mathcal{H}_2$ can be written as

$$\sum_{\substack{k\in\mathcal{I}_1\\ j\in\mathcal{I}_2}}\left\langle\varphi_{1\,k}\otimes\varphi_{2\,j},\Psi\right\rangle\varphi_{1\,k}\otimes\varphi_{2\,j}.$$

Example (i) A non-relativistic spin-$1/2$ particle lives in the Hilbert space $L^2(\mathbb{R}^d,\mathbb{C}^2)$. An easy, but very helpful exercise is to show the following equivalence (which correspond to different physical points of views):

$$L^2(\mathbb{R}^d,\mathbb{C}^2)\cong L^2(\mathbb{R}^d)\oplus L^2(\mathbb{R}^d)\cong L^2(\mathbb{R}^d)\otimes\mathbb{C}^2$$

Depending on the physical situation, these identification may be very helpful in solving a problem.

(ii) Consider $L^2(\mathbb{R}^d)\otimes L^2(\mathbb{R}^d)$. This is the Hilbert space of two particles. If they are identical, we have to restrict ourselves to the symmetric and antisymmetric subspace, depending on whether the particle in question is a boson or a fermion. Keep in mind that in general, elements $\Psi\in L^2(\mathbb{R}^d)\otimes L^2(\mathbb{R}^d)$ cannot be written as the product of two wave functions $\varphi_1,\varphi_2\in L^2(\mathbb{R}^d)$,

$$\Psi\neq\varphi_1\otimes\varphi_2.$$

We will show in an exercise that $L^2(\mathbb{R}^d)\otimes L^2(\mathbb{R}^d)\cong L^2(\mathbb{R}^d\times\mathbb{R}^d)$.

3.4 Linear functionals, dual space and weak convergence

The two main points of this section is to properly introduce the notion of linear functionals and show the connection between functionals and the bra-ket notation introduced by Dirac [Dir30]. "Kets" $|\psi\rangle$ are elements of the Hilbert space $\mathcal{H}$ while "bras" $\langle\psi|$ are in the dual $\mathcal{H}^*$. We will explain this in more detail below.

Definition 3.4.1 (Bounded linear functional) *Let $\mathcal{X}$ be a normed space. Then a map*

$$L:\mathcal{X}\longrightarrow\mathbb{C}$$

is a bounded linear functional if and only if

(i) there exists $C > 0$ such that $|L(x)| \leq C \|x\|$ and

(ii) $L(x + \mu y) = L(x) + \mu L(y)$

hold for all $x, y \in \mathcal{X}$ and $\mu \in \mathbb{C}$.

A very basic fact is that boundedness of a linear functional is equivalent to its continuity.

Theorem 3.4.2 *Let $L : \mathcal{X} \longrightarrow \mathbb{C}$ be a linear functional on the normed space $\mathcal{X}$. Then the following statements are equivalent:*

(i) L is continuous at $x_0 \in \mathcal{X}$.

(ii) L is continuous.

(iii) L is bounded.

Proof (i) $\Leftrightarrow$ (ii): This follows immediately from the linearity.

(ii) $\Rightarrow$ (iii): Assume L to be continuous. Then it is continuous at 0 and for $\varepsilon = 1$, we can pick $\delta > 0$ such that

$$|L(x)| \leq \varepsilon = 1$$

for all $x \in \mathcal{X}$ with $\|x\| \leq \delta$. By linearity, this implies for any $y \in \mathcal{X} \setminus \{0\}$ that

$$\left|L\left(\tfrac{\delta}{\|y\|} y\right)\right| = \tfrac{\delta}{\|y\|} \left|L(y)\right| \leq 1.$$

Hence, L is bounded with bound $1/\delta$,

$$\left|L(y)\right| \leq \tfrac{1}{\delta} \|y\| .$$

(iii) $\Rightarrow$ (ii): Conversely, if L is bounded by $C > 0$,

$$\left|L(x) - L(y)\right| \leq C \|x - y\| ,$$

holds for all $x, y \in \mathcal{X}$. This means, L is continuous: for $\varepsilon > 0$ pick $\delta = \varepsilon/C$ so that

$$\left|L(x) - L(y)\right| \leq C \|x - y\| \leq C \tfrac{\varepsilon}{C} = \varepsilon$$

holds for all $x, y \in \mathcal{X}$ such that $\|x - y\| \leq \varepsilon/C$. □

Definition 3.4.3 (Dual space) *Let $\mathcal{X}$ be a normed space. The dual space $\mathcal{X}^*$ is the vector space of bounded linear functionals endowed with the norm*

$$\|L\|_* := \sup_{x \in \mathcal{X} \setminus \{0\}} \frac{|L(x)|}{\|x\|} = \sup_{\substack{x \in \mathcal{X} \\ \|x\| = 1}} |L(x)| .$$

Independently of whether $\mathcal{X}$ is complete, $\mathcal{X}^*$ is a Banach space.

Proposition 3.4.4 *The dual space to a normed linear space $\mathcal{X}$ is a Banach space.*

Proof Let $(L_n)_{n\in\mathbb{N}}$ be a Cauchy sequence in $\mathcal{X}^*$, i. e. a sequence for which

$$\|L_k - L_j\|_* \xrightarrow{k,j\to\infty} 0.$$

We have to show that $(L_n)_{n\in\mathbb{N}}$ converges to some $L \in \mathcal{X}^*$. For any $\varepsilon > 0$, there exists $N(\varepsilon) \in \mathbb{N}$ such that

$$\|L_k - L_j\|_* < \varepsilon$$

for all $k, j \geq N(\varepsilon)$. This also implies that for any $x \in \mathcal{X}$, $\big(L_n(x)\big)_{n\in\mathbb{N}}$ converges as well,

$$\big|L_k(x) - L_j(x)\big| \leq \big\|L_k - L_j\big\|_* \, \|x\| < \varepsilon \, \|x\| \, .$$

The field of complex numbers is complete and $\big(L_n(x)\big)_{n\in\mathbb{N}}$ converges to some $L(x) \in \mathbb{C}$. We now *define*

$$L(x) := \lim_{n\to\infty} L_n(x)$$

for any $x \in \mathcal{X}$. Clearly, L inherits the linearity of the $(L_n)_{n\in\mathbb{N}}$. The map L is also bounded: for any $\varepsilon > 0$, there exists $N(\varepsilon) \in \mathbb{N}$ such that $\|L_j - L_n\|_* < \varepsilon$ for all $j, n \geq N(\varepsilon)$. Then

$$\begin{aligned}\big|(L - L_n)(x)\big| &= \lim_{j\to\infty} \big|(L_j - L_n)(x)\big| \leq \lim_{j\to\infty} \big\|L_j - L_n\big\|_* \, \|x\| \\ &< \varepsilon \, \|x\|\end{aligned}$$

holds for all $n \geq N(\varepsilon)$. Since we can write L as $L = L_n + (L - L_n)$, we can estimate the norm of the linear map L by $\|L\|_* \leq \|L_n\|_* + \varepsilon < \infty$. This means L is a bounded linear functional on $\mathcal{X}$. □

In case of Hilbert spaces, the dual $\mathcal{H}^*$ can be canonically identified with $\mathcal{H}$ itself:

Theorem 3.4.5 (Riesz' Lemma) *Let $\mathcal{H}$ be a Hilbert space. Then for all $L \in \mathcal{H}^*$ there exist $\psi_L \in \mathcal{H}$ such that*

$$L(\varphi) = \langle \psi_L, \varphi \rangle.$$

In particular, we have $\|L\|_* = \|\psi_L\|$.

Riesz' Lemma justifies the bra-ket notation of physics: to translate between physics and math notation, let us consider a "ket" $|\psi\rangle$ which is an element in a Hilbert space $\mathcal{H}$. Mathematicians would write $\psi \in \mathcal{H}$. The associated "bra" $\langle\psi|$ is functional on $\mathcal{H}$, meaning that if a bra $\langle\psi|$ and a ket $|\varphi\rangle$ meet, $\langle\psi|\varphi\rangle \in \mathbb{C}$, one obtains a complex number. Put another way, $\langle\psi|$ is just the functional $L_\psi(\varphi) = \langle\psi, \varphi\rangle$.

Proof Let $\ker L := \{\varphi \in \mathcal{H} \mid L(\varphi) = 0\}$ be the kernel of the functional L and as such is a closed linear subspace of $\mathcal{H}$. If $\ker L = \mathcal{H}$, then $0 \in \mathcal{H}$ is the associated vector,

$$L(\varphi) = 0 = \langle 0, \varphi \rangle.$$

So assume $\ker L \subsetneq \mathcal{H}$ is a proper subspace. Then we can split $\mathcal{H} = \ker L \oplus (\ker L)^\perp$. Pick $\varphi_0 \in (\ker L)^\perp$, i. e. $L(\varphi_0) \neq 0$. Then define

$$\psi_L := \frac{\overline{L(\varphi_0)}}{\|\varphi_0\|^2}\, \varphi_0.$$

We will show that $L(\varphi) = \langle \psi_L, \varphi \rangle$. If $\varphi \in \ker L$, then $L(\varphi) = 0 = \langle \psi_L, \varphi \rangle$. One easily shows that for $\varphi = \alpha\, \varphi_0$, $\alpha \in \mathbb{C}$,

$$\begin{aligned} L(\varphi) &= L(\alpha\, \varphi_0) = \alpha\, L(\varphi_0) \\ &= \langle \psi_L, \varphi \rangle = \left\langle \tfrac{\overline{L(\varphi_0)}}{\|\varphi_0\|^2} \varphi_0, \alpha\, \varphi_0 \right\rangle \\ &= \alpha\, L(\varphi_0)\, \frac{\langle \varphi_0, \varphi_0 \rangle}{\|\varphi_0\|^2} = \alpha\, L(\varphi_0). \end{aligned}$$

Every $\varphi \in \mathcal{H}$ can be written as

$$\varphi = \left(\varphi - \frac{L(\varphi)}{L(\varphi_0)}\, \varphi_0 \right) + \frac{L(\varphi)}{L(\varphi_0)}\, \varphi_0.$$

Then the first term is in the kernel of L while the second one is in the orthogonal complement of $\ker L$. Hence, $L(\varphi) = \langle \psi_L, \varphi \rangle$ for all $\varphi \in \mathcal{H}$. If there exists a second $\psi'_L \in \mathcal{H}$, then for any $\varphi \in \mathcal{H}$

$$0 = L(\varphi) - L(\varphi) = \langle \psi_L, \varphi \rangle - \langle \psi'_L, \varphi \rangle = \langle \psi_L - \psi'_L, \varphi \rangle.$$

This implies $\psi'_L = \psi_L$ and thus the element ψ_L is unique.

To show $\|L\|_* = \|\psi_L\|$, assume $L \neq 0$. Then, we have

$$\begin{aligned} \|L\|_* &= \sup_{\|\varphi\|=1} \big|L(\varphi)\big| \geq \big|L\big(\tfrac{\psi_L}{\|\psi_L\|}\big)\big| \\ &= \big\langle \psi_L, \tfrac{\psi_L}{\|\psi_L\|} \big\rangle = \|\psi_L\|. \end{aligned}$$

On the other hand, the Cauchy-Schwarz inequality yields

$$\begin{aligned} \|L\|_* &= \sup_{\|\varphi\|=1} \big|L(\varphi)\big| = \sup_{\|\varphi\|=1} \big|\langle \psi_L, \varphi \rangle\big| \\ &\leq \sup_{\|\varphi\|=1} \|\psi_L\| \|\varphi\| = \|\psi_L\|. \end{aligned}$$

□

Putting these two together, we conclude $\|L\|_* = \|\psi_L\|$. 2014.09.26

Remark 3.4.6 The bidual of a Hilbert space $\mathcal{H}^{**}$ can be canonically identified with $\mathcal{H}$ itself, i. e. Hilbert spaces are reflexive.

Definition 3.4.7 (Weak convergence) *Let $\mathcal{X}$ be a Banach space. Then a sequence $(x_n)_{n\in\mathbb{N}}$ in $\mathcal{X}$ is said to converge weakly to $x \in \mathcal{X}$ if for all $L \in \mathcal{X}^*$*

$$L(x_n) \xrightarrow{n\to\infty} L(x)$$

holds. In this case, one also writes $x_n \rightharpoonup x$.

Weak convergence, as the name suggests, is really weaker than convergence in norm. The reason why "more" sequences converge is that, a sense, uniformity is lost. If $\mathcal{X}$ is a Hilbert space, then applying a functional is the same as computing the inner product with respect to some vector ψ_L. If the "non-convergent part" lies in the orthogonal complement to $\{\psi_L\}$, then this particular functional does not notice that the sequence has not converged yet.

The distinction between weak and ordinary convergence can become important when doing numerics: very often only expectation values $\langle\varphi_n, A\varphi_n\rangle$ converge as $n \to \infty$ while $\psi_n \not\to \psi_*$.

Example Let $\mathcal{H}$ be a separable infinite-dimensional Hilbert space and $\{\varphi_n\}_{n\in\mathbb{N}}$ an orthonormal basis. Then the sequence $(\varphi_n)_{n\in\mathbb{N}}$ does not converge in norm, for as long as $n \neq k$

$$\|\varphi_n - \varphi_k\| = \sqrt{2},$$

but it does converge weakly to 0: for any functional $L = \langle\psi_L, \cdot\rangle$, we see that $\big(|L(\varphi_n)|\big)_{n\in\mathbb{N}}$ is a sequence in $\mathbb{R}$ that converges to 0. Since $\{\varphi_n\}_{n\in\mathbb{N}}$ is a basis, we can write

$$\psi_L = \sum_{n=1}^{\infty} \langle\varphi_n, \psi_L\rangle\, \varphi_n$$

and for the sequence of partial sums to converge to ψ_L, the sequence of coefficients

$$\big(\langle\varphi_n, \psi_L\rangle\big)_{n\in\mathbb{N}} = \big(\overline{L(\varphi_n)}\big)_{n\in\mathbb{N}}$$

must converge to 0. Since this is true for any $L \in \mathcal{H}^*$, we have proven that $\varphi_n \rightharpoonup 0$ (i. e. $\varphi_n \to 0$ weakly).

3.5 Important facts on $L^p(\mathbb{R}^d)$

For future reference, we collect a few facts on $L^p(\mathbb{R}^d)$ spaces. In particular, we will make use of dominated convergence frequently. We will give them without proof, they can be found in standard text books on analysis, see e. g. [LL01].

Definition 3.5.1 ($L^p(\mathbb{R}^d)$) *Let $1 \leq p < \infty$. Then we define*

$$\mathcal{L}^p(\mathbb{R}^d) := \left\{ f : \mathbb{R}^d \longrightarrow \mathbb{C} \;\middle|\; f \text{ measurable, } \int_{\mathbb{R}^d} \mathrm{d}x \; |f(x)|^p < \infty \right\}$$

as the vector space of functions whose pth power is integrable. Then $L^p(\mathbb{R}^d)$ is the vector space

$$L^p(\mathbb{R}^d) := \mathcal{L}^p(\mathbb{R}^d) / \sim$$

consisting of equivalence classes of functions that agree almost everywhere. With the p norm

$$\|f\|_p := \left(\int_{\mathbb{R}^d} \mathrm{d}x \; |f(x)|^p \right)^{1/p}$$

it forms a normed space.

In case $p = \infty$, we have to modify the definition a little bit.

Definition 3.5.2 ($L^\infty(\mathbb{R}^d)$) *We define*

$$\mathcal{L}^\infty(\mathbb{R}^d) := \left\{ f : \mathbb{R}^d \longrightarrow \mathbb{C} \;\middle|\; f \text{ measurable, } \exists 0 < K < \infty : |f(x)| \leq K \text{ almost everywhere} \right\}$$

to be the space of functions that are bounded almost everywhere and

$$\|f\|_\infty := \operatorname{ess\,sup}_{x \in \mathbb{R}^d} \big| f(x) \big| := \inf \big\{ K \geq 0 \;\big|\; |f(x)| \leq K \text{ for almost all } x \in \mathbb{R}^d \big\}.$$

Then the space $L^\infty(\mathbb{R}^d) := \mathcal{L}^\infty(\mathbb{R}^d) / \sim$ is defined as the vector space of equivalence classes where two functions are identified if they agree almost everywhere.

Theorem 3.5.3 (Riesz-Fischer) *For any $1 \leq p \leq \infty$, $L^p(\mathbb{R}^d)$ is complete with respect to the $\|\cdot\|_p$ norm and thus a Banach space. If $p = 2$, $L^2(\mathbb{R}^d)$ is also a Hilbert space with scalar product*

$$\langle f, g \rangle = \int_{\mathbb{R}^d} \mathrm{d}x \, \overline{f(x)} \, g(x).$$

Theorem 3.5.4 *For any $1 \leq p \lneq \infty$, the Banach space $L^p(\mathbb{R}^d)$ is separable.*

Proof We refer to [LL01, Lemma 2.17] for an explicit construction. The idea is to approximate arbitrary functions by functions which are constant on cubes and take only values in the rational complex numbers. □

Theorem 3.5.5 (Monotone Convergence) *Let $(f_k)_{k \in \mathbb{N}}$ be a sequence of non-decreasing functions in $L^1(\mathbb{R}^d)$ with pointwise limit f defined almost everywhere. Define $I_k := \int_{\mathbb{R}^d} \mathrm{d}x \, f_k(x)$;*

then the sequence (I_k) is non-decreasing as well. If $I := \lim_{k\to\infty} I_k < \infty$, then $I = \int_{\mathbb{R}^d} \mathrm{d}x\, f(x)$, i. e.

$$\lim_{k\to\infty} \int_{\mathbb{R}^d} \mathrm{d}x\, f_k(x) = \int_{\mathbb{R}^d} \mathrm{d}x \lim_{k\to\infty} f_k(x) = \int_{\mathbb{R}^d} \mathrm{d}x\, f(x)$$

holds.

Theorem 3.5.6 (Dominated Convergence) *Let $(f_k)_{k\in\mathbb{N}}$ be a sequence of functions in $L^1(\mathbb{R}^d)$ that converges almost everywhere pointwise to some $f : \mathbb{R}^d \longrightarrow \mathbb{C}$. If there exists a non-negative $g \in L^1(\mathbb{R}^d)$ such that $|f_k(x)| \leq g(x)$ holds almost everywhere for all $k \in \mathbb{N}$, then g also bounds $|f|$, i. e. $|f(x)| \leq g(x)$ almost everywhere, and $f \in L^1(\mathbb{R}^d)$. Furthermore, the limit $k \to \infty$ and integration with respect to x commute and we have*

$$\lim_{k\to\infty} \int_{\mathbb{R}^d} \mathrm{d}x\, f_k(x) = \int_{\mathbb{R}^d} \mathrm{d}x \lim_{k\to\infty} f_k(x) = \int_{\mathbb{R}^d} \mathrm{d}x\, f(x).$$

In case of $L^p(\mathbb{R}^d)$, there are three basic mechanisms for when a sequence of functions $(f_k)_{\in\mathbb{N}}$ does not converge in norm, but only weakly:

(i) *f_k oscillates to death:* take $f_k(x) = \sin(kx)$ for $0 \leq x \leq 1$ and zero otherwise.

(ii) *f_k goes up the spout:* pick $g \in L^p(\mathbb{R})$ and define $f_k(x) := k^{1/p}\, g(kx)$. This sequence explodes near $x = 0$ for large k.

(iii) *f_k wanders off to infinity:* this is the case when for some $g \in L^p(\mathbb{R})$, we define $f_k(x) := g(x + k)$.

All of these sequences converge weakly to 0, but do not converge in norm.

Chapter 4

4 Bounded linear operators

The previous chapter concerned itself with what states are, now we shift our attention to observables. Observables are selfadjoint operators which are a special case of *linear* operators. While most physically relevant observables are *unbounded* operators, we postpone the technical complications associated to the unboundedness and try to understand *bounded* operators first.

4.1 Bounded operators

The simplest operators are bounded operators.

Definition 4.1.1 (Bounded operator) *Let $\mathcal{X}$ and $\mathcal{Y}$ be normed spaces. A linear operator $T : \mathcal{X} \longrightarrow \mathcal{Y}$ is called bounded if there exists $M \geq 0$ with $\|Tx\|_{\mathcal{Y}} \leq M \|x\|_{\mathcal{X}}$ for all $x \in \mathcal{X}$.*

Just as in the case of linear functionals, we have

Theorem 4.1.2 *Let $T : \mathcal{X} \longrightarrow \mathcal{Y}$ be a linear operator between two normed spaces $\mathcal{X}$ and $\mathcal{Y}$. Then the following statements are equivalent:*

(i) *T is continuous at $x_0 \in \mathcal{X}$.*

(ii) *T is continuous.*

(iii) *T is bounded.*

Proof We leave it to the reader to modify the proof of Theorem 3.4.2. □

We can introduce a norm on the operators which leads to a natural notion of convergence:

Definition 4.1.3 (Operator norm) *Let $T : \mathcal{X} \longrightarrow \mathcal{Y}$ be a bounded linear operator between normed spaces. Then we define the operator norm of T as*

$$\|T\| := \sup_{\substack{x \in \mathcal{X} \\ \|x\|=1}} \|Tx\|_{\mathcal{Y}} .$$

The space of all bounded linear operators between $\mathcal{X}$ and $\mathcal{Y}$ is denoted by $\mathcal{B}(\mathcal{X}, \mathcal{Y})$.

One can show that $\|T\|$ coincides with

$$\inf\{ M \geq 0 \mid \|Tx\|_{\mathcal{Y}} \leq M \|x\|_{\mathcal{X}} \ \forall x \in \mathcal{X} \} = \|T\| .$$

The product of two bounded operators $T \in \mathcal{B}(\mathcal{Y}, \mathcal{Z})$ and $S \in \mathcal{B}(\mathcal{X}, \mathcal{Y})$ is again a bounded operator and its norm can be estimated from above by

$$\|TS\| \leq \|T\| \, \|S\| .$$

If $\mathcal{Y} = \mathcal{X} = \mathcal{Z}$, this implies that the product is jointly continuous with respect to the norm topology on $\mathcal{X}$.

The set of bounded operators naturally forms a normed vector space: Let T, S be bounded linear operators between the normed spaces $\mathcal{X}$ and $\mathcal{Y}$. If we define

$$(T + S)x := Tx + Sx$$

as addition and

$$\big(\lambda \cdot T\big)x := \lambda T x$$

as scalar multiplication, the set of bounded linear operators forms a vector space.

Proposition 4.1.4 *The vector space $\mathcal{B}(\mathcal{X}, \mathcal{Y})$ of bounded linear operators between normed spaces $\mathcal{X}$ and $\mathcal{Y}$ with operator norm forms a normed space. If $\mathcal{Y}$ is complete, $\mathcal{B}(\mathcal{X}, \mathcal{Y})$ is a Banach space.*

Proof The fact $\mathcal{B}(\mathcal{X}, \mathcal{Y})$ is a normed vector space follows directly from the definition. To show that $\mathcal{B}(\mathcal{X}, \mathcal{Y})$ is a Banach space whenever $\mathcal{Y}$ is, one has to modify the proof of Theorem 3.4.4 to suit the current setting. This is left as an exercise. □

Very often, it is easy to *define* an operator T on a "nice" dense subset $\mathcal{D} \subseteq \mathcal{X}$. Then the next theorem tells us that if the operator is bounded, there is a unique bounded extension of the operator to the whole space $\mathcal{X}$. For instance, this allows us to instantly extend the Fourier transform from Schwartz functions to $L^2(\mathbb{R}^d)$ functions [Lei10, Proposition 5.1.9].

Theorem 4.1.5 *Let $\mathcal{D} \subseteq \mathcal{X}$ be a dense subset of a normed space and $\mathcal{Y}$ be a Banach space. Furthermore, let $T : \mathcal{D} \longrightarrow \mathcal{Y}$ be a bounded linear operator. Then there exists a unique bounded linear extension $\tilde{T} : \mathcal{X} \longrightarrow \mathcal{Y}$ and $\|\tilde{T}\| = \|T\|_{\mathcal{D}}$.*

Proof We construct $\tilde{T}$ explicitly: let $x \in \mathcal{X}$ be arbitrary. Since $\mathcal{D}$ is dense in $\mathcal{X}$, there exists a sequence $(x_n)_{n\in\mathbb{N}}$ in $\mathcal{D}$ which converges to x. Then we set

$$\tilde{T}x := \lim_{n\to\infty} Tx_n.$$

First of all, $\tilde{T}$ is linear. It is also well-defined: $(Tx_n)_{n\in\mathbb{N}}$ is a Cauchy sequence in $\mathcal{Y}$,

$$\left\|Tx_n - Tx_k\right\|_{\mathcal{Y}} \leq \|T\|_{\mathcal{D}} \|x_n - x_k\|_{\mathcal{X}} \xrightarrow{n,k\to\infty} 0,$$

where the norm of T is defined as

$$\|T\|_{\mathcal{D}} := \sup_{x\in\mathcal{D}\setminus\{0\}} \frac{\|Tx\|_{\mathcal{Y}}}{\|x\|_{\mathcal{X}}}.$$

This Cauchy sequence in $\mathcal{Y}$ converges to some unique $y \in \mathcal{Y}$ as the target space is complete. Let $(x'_n)_{n\in\mathbb{N}}$ be a second sequence in $\mathcal{D}$ that converges to x and assume the sequence $(Tx'_n)_{n\in\mathbb{N}}$ converges to some $y' \in \mathcal{Y}$. We define a third sequence $(z_n)_{n\in\mathbb{N}}$ which alternates between elements of the first sequence $(x_n)_{n\in\mathbb{N}}$ and the second sequence $(x'_n)_{n\in\mathbb{N}}$, i. e.

$$\begin{aligned} z_{2n-1} &:= x_n \\ z_{2n} &:= x'_n \end{aligned}$$

for all $n \in \mathbb{N}$. Then $(z_n)_{n\in\mathbb{N}}$ also converges to x and $\left(Tz_n\right)$ forms a Cauchy sequence that converges to, say, $\zeta \in \mathcal{Y}$. Subsequences of convergent sequences are also convergent and they must converge to the same limit point. Hence, we conclude that

$$\begin{aligned} \zeta &= \lim_{n\to\infty} Tz_n = \lim_{n\to\infty} Tz_{2n} = \lim_{n\to\infty} Tx_n = y \\ &= \lim_{n\to\infty} Tz_{2n-1} = \lim_{n\to\infty} Tx'_n = y' \end{aligned}$$

holds and $\tilde{T}x$ does not depend on the particular choice of sequence which approximates x in $\mathcal{D}$. It remains to show that $\|\tilde{T}\| = \|T\|_{\mathcal{D}}$: we can calculate the norm of $\tilde{T}$ on the dense subset $\mathcal{D}$ and use that $\tilde{T}|_{\mathcal{D}} = T$ to obtain

$$\begin{aligned} \|\tilde{T}\| &= \sup_{\substack{x\in\mathcal{X} \\ \|x\|=1}} \|\tilde{T}x\| = \sup_{x\in\mathcal{X}\setminus\{0\}} \frac{\|\tilde{T}x\|}{\|x\|} = \sup_{x\in\mathcal{D}\setminus\{0\}} \frac{\|\tilde{T}x\|}{\|x\|} \\ &= \sup_{x\in\mathcal{D}\setminus\{0\}} \frac{\|Tx\|}{\|x\|}. \end{aligned}$$

□

Hence, the norm of the extension $\tilde{T}$ is equal to the norm of the original operator T. 2014.09.30

The spectrum of an operator has been related to the set of possible outcomes of measurements (if the operator is selfadjoint).

Definition 4.1.6 (Spectrum) *Let $T \in \mathcal{B}(\mathcal{X})$ be a bounded linear operator on a Banach space $\mathcal{X}$. We define:*

(i) The resolvent of T is the set $\rho(T) := \{z \in \mathbb{C} \mid T - z \text{ is bijective}\}$.

(ii) The spectrum $\sigma(T) := \mathbb{C} \setminus \rho(T)$ is the complement of $\rho(T)$ in $\mathbb{C}$.

(iii) The set of all eigenvalues is called point spectrum

$$\sigma_{\mathrm{p}}(T) := \{z \in \mathbb{C} \mid T - z \text{ is not injective}\}.$$

(iv) The continuous spectrum *is defined as*

$$\sigma_{\mathrm{cont}}(T) := \{z \in \mathbb{C} \mid T - z \text{ is injective, } \operatorname{im}(T - z) \subseteq \mathcal{X} \text{ dense}\}.$$

(v) The remainder of the spectrum is called residual spectrum,

$$\sigma_{\mathrm{r}} := \{z \in \mathbb{C} \mid T - z \text{ is injective, } \operatorname{im}(T - z) \subseteq \mathcal{X} \text{ not dense}\}$$

One can show that for all $z \in \rho(T)$, the map $(T - z)^{-1}$ is a *bounded* operator (this is a non-trivial fact and follows from the Open Mapping Theorem [RS72, Theorem III.10]) and the spectrum is a closed subset of $\mathbb{C}$. Moreover, $\sigma(T)$ is *compact* and contained in $\{z \in \mathbb{C} \mid |z| \leq \|T\|\} \subset \mathbb{C}$.

4.2 Adjoint operator

If $\mathcal{X}$ is a normed space, then we have defined $\mathcal{X}^*$, the space of bounded linear functionals on $\mathcal{X}$. If $T : \mathcal{X} \longrightarrow \mathcal{Y}$ is a bounded linear operator between two normed spaces, it naturally defines the *adjoint operator* $T' : \mathcal{Y}^* \longrightarrow \mathcal{X}^*$ via

$$(T'L)(x) := L(Tx) \tag{4.2.1}$$

for all $x \in \mathcal{X}$ and $L \in \mathcal{Y}^*$. In case of Hilbert spaces, one can associate the *Hilbert space adjoint*. We will almost exclusively work with the latter and thus drop "Hilbert space" most of the time.

Definition 4.2.1 (Hilbert space adjoint) *Let $\mathcal{H}$ be a Hilbert space and $T \in \mathcal{B}(\mathcal{H})$ be a bounded linear operator on $\mathcal{H}$. The antilinear isomorphism $C : \mathcal{H} \longrightarrow \mathcal{H}^*$ taken from Theorem 3.4.5 maps*

functionals on $\mathcal{H}$ onto the corresponding vectors, i. e. $C\psi := \langle \psi, \cdot \rangle = L_\psi$. Then the Hilbert space adjoint is defined as

$$T^* := C^{-1} T' C,$$

or put differently

$$\langle T^* \varphi, \psi \rangle := \langle \varphi, T\psi \rangle$$

for all $\varphi, \psi \in \mathcal{H}$.

Proposition 4.2.2 *Let $A, B \in \mathcal{B}(\mathcal{H})$ be two bounded linear operators on a Hilbert space $\mathcal{H}$ and $\alpha \in \mathbb{C}$. Then, we have:*

(i) $(A+B)^* = A^* + B^*$

(ii) $(\alpha A)^* = \overline{\alpha}\, A^*$

(iii) $(AB)^* = B^* A^*$

(iv) $\|A^*\| = \|A\|$

(v) $A^{**} = A$

(vi) $\|A^* A\| = \|A A^*\| = \|A\|^2$

(vii) $\ker A = (\operatorname{ran} A^*)^\perp$, $\ker A^* = (\operatorname{ran} A)^\perp$

Proof Properties (i)-(iii) follow directly from the defintion.

To show (iv), we note that $\|A\| \leq \|A^*\|$ follows from

$$\begin{aligned} \|A\varphi\| = \left| \left\langle \tfrac{A\varphi}{\|A\varphi\|}, A\varphi \right\rangle \right| &\overset{*}{=} \sup_{\|L\|_*=1} |L(A\varphi)| \\ &= \sup_{\|\psi_L\|=1} |\langle A^* \psi_L, \varphi \rangle| \leq \|A^*\|\, \|\varphi\| \end{aligned}$$

where in the step marked with $*$, we have used that we can calculate the norm from picking the functional associated to $\frac{A\varphi}{\|A\varphi\|}$: for a functional with norm 1, $\|L\|_* = 1$, the norm of $L(A\varphi)$ cannot exceed that of $A\varphi$

$$|L(A\varphi)| = |\langle \psi_L, A\varphi \rangle| \leq \|\psi_L\| \|A\varphi\| = \|A\varphi\|.$$

Here, ψ_L is the vector such that $L = \langle \psi_L, \cdot \rangle$ which exists by Theorem 3.4.5. This theorem also ensures $\|L\|_* = \|\psi_L\|$. On the other hand, from

$$\begin{aligned} \left\| A^* \psi_L \right\| = \left\| L_{A^* \psi_L} \right\|_* &= \sup_{\|\varphi\|=1} \left| \left\langle A^* \psi_L, \varphi \right\rangle \right| \\ &\leq \sup_{\|\varphi\|=1} \|\psi_L\|\, \|A\varphi\| = \|A\|\, \|L\|_* = \|A\|\, \|\psi_L\| \end{aligned}$$

we conclude $\|A^*\| \leq \|A\|$. Hence, $\|A^*\| = \|A\|$.

(v) is clear. For (vi), we remark

$$\begin{aligned}\|A\|^2 &= \sup_{\|\varphi\|=1} \|A\varphi\|^2 = \sup_{\|\varphi\|=1} \langle \varphi, A^*A\varphi \rangle \\ &\leq \sup_{\|\varphi\|=1} \|A^*A\varphi\| = \|A^*A\| .\end{aligned}$$

This means

$$\|A\|^2 \leq \|A^*A\| \leq \|A^*\| \, \|A\| = \|A\|^2 .$$

which combined with (iv),

$$\|A\|^2 = \|A^*\|^2 \leq \|AA^*\| \leq \|A\| \, \|A^*\| = \|A\|^2$$

implies $\|A^*A\| = \|A\|^2 = \|AA^*\|$. (vii) is left as an exercise. □

Definition 4.2.3 *Let $\mathcal{H}$ be a Hilbert space and $T \in \mathcal{B}(\mathcal{H})$. Then T is called*

(i) normal if $T^* T = T T^*$.

(ii) selfadjoint (or hermitian) if $T^* = T$.

(iii) unitary if $T^* T = \mathrm{id}_{\mathcal{H}} = T T^*$.

(iv) an orthogonal projection if $T^2 = T$ and $T^* = T$.

(v) positive if $\langle \varphi, T\varphi \rangle \geq 0$ for all $\varphi \in \mathcal{H}$.

4.3 Unitary operators

More generally, unitary operators $U : \mathcal{H}_1 \longrightarrow \mathcal{H}_2$ between two Hilbert spaces are characterized by

$$\langle U\varphi, U\psi \rangle_{\mathcal{H}_2} = \langle \varphi, U^*U\psi \rangle_{\mathcal{H}_1} = \langle \varphi, \psi \rangle_{\mathcal{H}_1} , \qquad \varphi, \psi \in \mathcal{H},$$

combined with the fact $U\mathcal{H}_1 = \mathcal{H}_2$. Note that here, the adjoint $U^* : \mathcal{H}_2 \longrightarrow \mathcal{H}_1$ maps onto $\mathcal{H}_1$, so that the definition of a unitary is still $U^* = U^{-1}$. This more general definition is necessary to understand common unitary operators such as the discrete Fourier transform

$$\begin{aligned}\mathcal{F} &: L^2([0, 2\pi]^d) \longrightarrow \ell^2(\mathbb{Z}^d), \\ (\mathcal{F}\psi)(k) &:= \frac{1}{(2\pi)^d} \int_{[0,2\pi]^d} \mathrm{d}x \, \mathrm{e}^{-\mathrm{i}k\cdot x} \, \psi(x).\end{aligned}$$

Physically, one important consequence is the conservation of probability under unitary maps.

4.3.1 Representations and bra-ket notation

Let us reconsider the bra-ket notation physicists use and the topic of *representations* which is the generalization of a *choice of basis* in linear algebra (see also the discussion in Chapter 2.2.5). Let us start with a few examples: for a particle on $\mathbb{R}^d$, the most common representation is the *position representation* where position operator Q and momentum operator P are

$$\begin{aligned}(\mathsf{Q}\psi)(x) &= x\,\psi(x),\\ (\mathsf{P}\psi)(x) &= -\mathrm{i}\hbar\nabla_x\psi(x),\end{aligned}$$

i. e. the position operator is multiplication by x and while momentum is $-\mathrm{i}\hbar$ times the gradient. These two operators are characterized by algebraic relations called *commutation relations*,

$$[\mathsf{Q}_j,\mathsf{Q}_k]=0,\qquad [\mathsf{P}_j,\mathsf{P}_k]=0,\qquad [\mathsf{Q}_j,\mathsf{P}_k]=\mathrm{i}\hbar\delta_{jk}.$$

Here, $|\psi(x)|^2$ is a probability density on (real) space, i. e. the units of $\psi(x)$ are $1/[\text{length}]^{d/2}$.

Position representation is the "eigenbasis representation" of the position operator, meaning Q_j is *multiplication by* x_j. However, Q_j seen as an operator on $L^2(\mathbb{R}^d)$ has *purely continuous spectrum*,

$$\sigma(\mathsf{Q}_j)=\sigma_{\text{cont}}(\mathsf{Q}_j)=\mathbb{R},$$

meaning that to each $\lambda\in\mathbb{R}$ the tempered distribution $\delta\big(x-\lambda\,e_j\big)$ is a *pseudo*eigenfunction – it is a *bona fide* tempered distribution, and thus, cannot be an element of $L^2(\mathbb{R}^d)$ (see [Lei13, Chapter 7]).

While position Q_j is diagonal in position representation, momentum $\mathsf{P}_j=-\mathrm{i}\hbar\partial_{x_j}$ is not. However, one can change to the *momentum representation* via the Fourier transform

$$\begin{aligned}\mathcal{F}&: L^2(\mathbb{R}^d_x)\longrightarrow L^2(\mathbb{R}^d_\xi),\\ (\mathcal{F}\psi)(\xi)&:=\frac{1}{(2\pi)^{d/2}}\int_{\mathbb{R}^d}\mathrm{d}x\,\mathrm{e}^{-\mathrm{i}\xi\cdot x}\,\psi(x).\end{aligned}\tag{4.3.1}$$

The indices in the L^2-spaces mean nothing mathematically, they are included to emphasize that the variables x in the original space are spatial variables while the ones in the target space are momenta ξ. A note to mathematicians: The integral expression is first defined on the dense subspace $L^1(\mathbb{R}^d)\cap L^2(\mathbb{R}^d)$ and then extended by continuity (see [LL01, Chapter 5.4] for a more "hands-on" way to implement the extension). Formally, (4.3.1) can be written as

$$\text{“}\widehat{\psi}(\xi)=\big\langle \mathrm{e}^{+\mathrm{i}\xi\cdot x},\psi\big\rangle=\langle\xi|\psi\rangle\text{ ”},$$

and it is this what physicists mean when they write $\widehat{\psi}(\xi) = \langle \xi | \psi \rangle$, because $|\xi\rangle$ is understood to be the (pseudo)eigenvector of $-\mathrm{i}\hbar\nabla_x$, namely $\mathrm{e}^{+\mathrm{i}\xi\cdot x}$. However, plane waves $\mathrm{e}^{+\mathrm{i}\xi\cdot x}$ are not square-integrable, and thus, they are not elements of $L^2(\mathbb{R}^d)$ and the associated spectrum is purely continuous,

$$\sigma\big(-\mathrm{i}\hbar\partial_{x_j}\big) = \sigma_{\mathrm{cont}}\big(-\mathrm{i}\hbar\partial_{x_j}\big).$$

One can show that $\mathcal{F}$ is a unitary (Parseval formula) and thus, norm-preserving (Plancherel identity). Moreover, for suitable functions (e. g. $\mathcal{C}_{\mathrm{c}}^{\infty}(\mathbb{R}^d)$) for all multiindices $a, \alpha \in \mathbb{N}_0^d$

$$\mathcal{F}\big(x^a(-\mathrm{i}\partial_x)^\alpha \psi\big) = (+\mathrm{i}\partial_\xi)^a \xi^\alpha \mathcal{F}\psi$$

holds. We can use the Fourier transform to switch from position to momentum representation: here, the momentum operator

$$\mathsf{P}^{\mathcal{F}} := \mathcal{F}\,\mathsf{P}\,\mathcal{F}^{-1} = \hbar\widehat{\xi}$$

becomes just multiplication with ξ while the position operator

$$\mathsf{Q}^{\mathcal{F}} := \mathcal{F}\,\mathsf{Q}\,\mathcal{F}^{-1} = +\mathrm{i}\nabla_\xi$$

involves the derivative now. Note that the commutation relations of position and momentum operators in momentum representation are *identical*,

$$[\mathsf{Q}_j^{\mathcal{F}}, \mathsf{Q}_k^{\mathcal{F}}] = 0, \qquad [\mathsf{P}_j^{\mathcal{F}}, \mathsf{P}_k^{\mathcal{F}}] = 0, \qquad [\mathsf{Q}_j^{\mathcal{F}}, \mathsf{P}_k^{\mathcal{F}}] = \mathrm{i}\hbar\delta_{jk},$$

unitary transformations cannot change these algebraic relations. In fact, physically relevant quantities cannot depend on the representation, e. g. the spectrum of an operator is independent of it:

Lemma 4.3.1 *Let T be a bounded operator on a Hilbert space $\mathcal{H}_1$ and $U : \mathcal{H}_1 \longrightarrow \mathcal{H}_2$ a unitary. Then $\sigma(T) = \sigma\big(U\,T\,U^{-1}\big)$ and similarly $\sigma_\sharp(T) = \sigma_\sharp\big(U\,T\,U^{-1}\big)$ where $\sharp = \mathrm{c}, \mathrm{p}, \mathrm{r}$*

Proof This is left as an exercise. □

One last thing about notation: if $\mathcal{H}$ is a separable, infinite-dimensional Hilbert space and $\{\varphi_n\}_{n\in\mathbb{N}}$ an orthonormal basis, then one can show

$$\mathrm{id}_{\mathcal{H}} = \sum_{n\in\mathbb{N}} |\varphi_n\rangle\langle\varphi_n|$$

since any vector $\psi = \sum_{n\in\mathbb{N}} \langle\varphi_n, \psi\rangle\ \varphi_n$ can be expressed in terms of the basis $\{\varphi_n\}_{n\in\mathbb{N}}$. Such an expression is known as a *resolution of the identity*. Analogously, physicists also write

$$\mathrm{id}_{L^2(\mathbb{R})} = \int_{\mathbb{R}} \mathrm{d}x\, |x\rangle\langle x|$$

where $|x\rangle = \delta(\cdot - x)$ are the pseudoeigenvectors of the position operator $\hat{x}$ on $L^2(\mathbb{R})$ and the sum is replaced by an integral. The purpose of this is to expand vectors in $L^2(\mathbb{R})$ in terms of the "eigenbasis" of the position operator. For instance, $\langle x|\psi\rangle$ stands for $\psi(x)$. To define this expression mathematically requires a lot more machinery and will require *functional calculus* (see Chapter 6). It turns out that $|x\rangle\langle x|$ stands for a *projection-valued measure*.

Similarly, expansions into plane waves ("eigenfunctions" of the momentum operator) also exists,

$$\mathrm{id}_{L^2(\mathbb{R})} = \int_{\mathbb{R}} \mathrm{d}\xi \, |\xi\rangle\langle\xi|,$$

and corresponds to a plane wave expansion, $\widehat{\psi}(\xi) = \langle\xi|\psi\rangle$.

4.3.2 Unitary evolution groups

In case of quantum mechanics, we are interested in solutions to the Schrödinger equation

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\psi(t) = H\psi(t), \qquad \psi(t) = \psi_0,$$

for a hamilton operator which satisfies $H^* = H$. Assume that H is bounded (this is really the case for many simple quantum systems). Then the unitary group generated by H,

$$U(t) = \mathrm{e}^{-\mathrm{i}tH},$$

can be written as a power series,

$$\mathrm{e}^{-\mathrm{i}tH} = \sum_{n=0}^{\infty} \frac{1}{n!}(-\mathrm{i}t)^n \, H^n$$

where $H^0 := \mathrm{id}$ by convention. The sequence of partial sums converges in the operator norm to $\mathrm{e}^{-\mathrm{i}tH}$,

$$\sum_{n=0}^{N} \frac{1}{n!}(-\mathrm{i}t)^n \, H^n \xrightarrow{N\to\infty} \mathrm{e}^{-\mathrm{i}tH},$$

since we can make the simple estimate

$$\begin{aligned}\left\| \sum_{n=0}^{\infty} \frac{1}{n!}(-\mathrm{i}t)^n \, H^n\psi \right\| &\leq \sum_{n=0}^{\infty} \frac{1}{n!} \, |t|^n \, \|H^n\psi\| \leq \sum_{n=0}^{\infty} \frac{1}{n!} \, |t|^n \, \|H\|^n \, \|\psi\| \\ &= \mathrm{e}^{|t|\|H\|} \, \|\psi\| < \infty.\end{aligned}$$

This shows that the power series of the exponential converges in the operator norm independently of the choice of ψ to a bounded operator. Given a unitary evolution group, it is suggestive to obtain the hamiltonian which generates it by deriving $U(t)\psi$ with respect to time. This is indeed the correct idea. The left-hand side of the Schrödinger equation (modulo a factor of i) can be expressed as a limit

$$\frac{\mathrm{d}}{\mathrm{d}t}\psi(t) = \lim_{\delta\to 0} \tfrac{1}{\delta}\big(\psi(t+\delta) - \psi(t)\big).$$

This limit really exists, but before we compute it, we note that since

$$\psi(t+\delta) - \psi(t) = \mathrm{e}^{-\mathrm{i}(t+\delta)H}\psi_0 - \mathrm{e}^{-\mathrm{i}tH}\psi_0 = \mathrm{e}^{-\mathrm{i}tH}\big(\mathrm{e}^{-\mathrm{i}\delta H} - 1\big)\psi_0,$$

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it suffices to consider differentiability at $t = 0$: taking limits in norm of $\mathcal{H}$, we get

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\psi(0) &= \lim_{\delta\to 0} \tfrac{1}{\delta}\big(\psi(\delta) - \psi_0\big) = \lim_{\delta\to 0} \frac{1}{\delta}\left(\sum_{n=0}^{\infty} \frac{(-\mathrm{i})^n}{n!}\delta^n H^n\psi_0 - \psi_0\right)\\ &= \lim_{\delta\to 0}\sum_{n=1}^{\infty}\frac{(-\mathrm{i})^n}{n!}\delta^{n-1}H^n\psi_0 = -\mathrm{i}H\psi_0.\end{aligned}$$

Hence, we have established that $\mathrm{e}^{-\mathrm{i}tH}\psi_0$ solves the Schrödinger condition with $\psi(0) = \psi_0$,

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\psi(t) = H\psi(t).$$

However, this procedure *does not work* if H is unbounded (i. e. the generic case)! Before we proceed, we need to introduce several different notions of convergence of sequences of operators which are necessary to define derivatives of $U(t)$.

Definition 4.3.2 (Convergence of operators) *Let $A_n \in \mathcal{B}(\mathcal{H})$ be a sequence of bounded operators. We say that the sequence converges to $A \in \mathcal{B}(\mathcal{H})$*

(i) uniformly/in norm if $\lim_{n\to\infty}\big\|A_n - A\big\| = 0$.

(ii) strongly if $\lim_{n\to\infty}\big\|A_n\psi - A\psi\big\| = 0$ for all $\psi \in \mathcal{H}$.

(iii) weakly if $\lim_{n\to\infty}\big\langle\varphi, A_n\psi - A\psi\big\rangle = 0$ for all $\varphi, \psi \in \mathcal{H}$.

Convergence of a sequence of operators in norm implies strong and weak convergence, but not the other way around. In the tutorials, we will also show explicitly that weak convergence does not necessarily imply strong convergence.

Example With the arguments above, we have shown that if $H = H^*$ is selfadjoint and bounded, then $t \mapsto \mathrm{e}^{-\mathrm{i}tH}$ is *uniformly* continuous.

If $\|H\| = \infty$ on the other hand, uniform continuity is too strong a requirement. If $H = -\frac{1}{2}\Delta_x$ is the free Schrödinger operator on $L^2(\mathbb{R}^d_x)$, then the Fourier transform $\mathcal{F}$ links the position representation on $L^2(\mathbb{R}^d_x)$ to the momentum representation on $L^2(\mathbb{R}^d_\xi)$. In this representation, the free Schrödinger operator H simplifies to the multiplication operator

$$\hat{H} = \tfrac{1}{2}\hat{\xi}^2$$

acting on $L^2(\mathbb{R}^d_\xi)$. More elaborate mathematical arguments show that for any $t \in \mathbb{R}$, the norm of the difference between $\hat{U}(t) = \mathrm{e}^{-\mathrm{i}t\frac{1}{2}\hat{\xi}^2}$ and $\hat{U}(0) = \mathrm{id}$

$$\left\|\hat{U}(t) - \mathrm{id}\right\| = \sup_{\xi\in\mathbb{R}^d_\xi} \left|\mathrm{e}^{-\mathrm{i}t\frac{1}{2}\xi^2} - 1\right| = 2$$

is exactly 2 and $\hat{U}(t)$ *cannot* be uniformly continuous in t. However, if $\hat{\psi} \in L^2(\mathbb{R}^d_\xi)$ is a wave function, the estimate

$$\begin{aligned}\left\|\hat{U}(t)\hat{\psi} - \hat{\psi}\right\|^2 &= \int_{\mathbb{R}^d_\xi} \mathrm{d}\xi \left|\mathrm{e}^{-\mathrm{i}t\frac{1}{2}\xi^2} - 1\right|^2 \left|\hat{\psi}(\xi)\right|^2 \\ &\leq 2^2 \int_{\mathbb{R}^d_\xi} \mathrm{d}\xi \left|\hat{\psi}(\xi)\right|^2 = 4\left\|\hat{\psi}\right\|^2\end{aligned}$$

shows we can invoke the Theorem of Dominated Convergence to conclude $\hat{U}(t)$ is *strongly continuous* in $t \in \mathbb{R}$.

Definition 4.3.3 (Strongly continuous one-parameter unitary group) *A family of unitary operators $\{U(t)\}_{t\in\mathbb{R}}$ on a Hilbert space $\mathcal{H}$ is called a strongly continuous one-parameter unitary group – or unitary group for short – if*

(i) $t \mapsto U(t)$ *is strongly continuous and*

(ii) $U(t)\,U(t') = U(t+t')$ *as well as* $U(0) = \mathrm{id}_{\mathcal{H}}$

hold for all $t, t' \in \mathbb{R}_t$.

This is again a *group representation of* $\mathbb{R}_t$ just as in the case of the classical flow Φ. The form of the Schrödinger equation,

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\psi(t) = H\psi(t),$$

also suggests that strong continuity/differentiability is the correct notion. Let us once more consider the free hamiltonian $H = -\frac{1}{2}\Delta_x$ on $L^2(\mathbb{R}^d_x)$. We have shown in the tutorials that its domain is

$$\mathcal{D}(H) = \left\{\varphi \in L^2(\mathbb{R}^d_x) \mid -\Delta_x\varphi \in L^2(\mathbb{R}^d_x)\right\}.$$

Using $\big(\mathcal{F}\big((-\mathrm{i}\partial_x)^\alpha f\big)\big)(\xi) = \xi^\alpha\,(\mathcal{F}f)(\xi)$, $\alpha \in \mathbb{N}_0^d$, we see that $\mathcal{D}(H)$ is mapped by the Fourier transform onto

$$\mathcal{D}(\hat{H}) = \big\{\hat{\psi} \in L^2(\mathbb{R}^d_\xi) \mid \hat{\xi}^2\hat{\psi} \in L^2(\mathbb{R}^d_\xi)\big\}.$$

Dominated Convergence can once more be used to make the following claims rigorous: for any $\hat{\psi} \in \mathcal{D}(\hat{H})$, we have

$$\lim_{t\to 0}\big\|\tfrac{\mathrm{i}}{t}\big(\hat{U}(t) - \mathrm{id}\big)\hat{\psi} - \tfrac{1}{2}\hat{\xi}^2\hat{\psi}\big\| \leq \lim_{t\to 0}\big\|\tfrac{\mathrm{i}}{t}\big(\hat{U}(t) - \mathrm{id}\big)\hat{\psi}\big\| + \big\|\tfrac{1}{2}\hat{\xi}^2\hat{\psi}\big\|. \tag{4.3.2}$$

The second term is finite since $\hat{\psi} \in \mathcal{D}(\hat{H})$ and we have to focus on the first term. On the level of functions,

$$\lim_{t\to 0}\tfrac{\mathrm{i}}{t}\big(\mathrm{e}^{-\mathrm{i}t\frac{1}{2}\xi^2} - 1\big) = \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{-\mathrm{i}t\frac{1}{2}\xi^2}\Big|_{t=0} = \tfrac{1}{2}\xi^2$$

holds pointwise. Furthermore, by the mean value theorem, for any finite $t \in \mathbb{R}$ with $|t| \leq 1$, for instance, then there exists $0 \leq t_0 \leq t$ such that

$$\tfrac{1}{t}\big(\mathrm{e}^{-\mathrm{i}t\frac{1}{2}\xi^2} - 1\big) = \partial_t\mathrm{e}^{-\mathrm{i}t\frac{1}{2}\xi^2}\big|_{t=t_0} = -\mathrm{i}\tfrac{1}{2}\xi^2\,\mathrm{e}^{-\mathrm{i}t_0\frac{1}{2}\xi^2}.$$

This can be bounded uniformly in t by $\frac{1}{2}\xi^2$. Thus, also the first term can be bounded by $\big\|\frac{1}{2}\hat{\xi}^2\hat{\psi}\big\|$ uniformly. By Dominated Convergence, we can interchange the limit $t \to 0$ and integration with respect to ξ on the left-hand side of equation (4.3.2). But then the integrand is zero and thus the domain where the free evolution group is differentiable coincides with the domain of the Fourier transformed hamiltonian,

$$\lim_{t\to 0}\Big\|\tfrac{\mathrm{i}}{t}\big(\hat{U}(t) - \mathrm{id}\big)\hat{\psi} - \tfrac{1}{2}\hat{\xi}^2\hat{\psi}\Big\| = 0.$$

This suggests to use the following definition:

Definition 4.3.4 (Generator of a unitary group) *A densely defined linear operator on a Hilbert space $\mathcal{H}$ with domain $\mathcal{D}(H) \subseteq \mathcal{H}$ is called generator of a unitary evolution group $U(t)$, $t \in \mathbb{R}$, if*

(i) the domain coincides with

$$\widetilde{\mathcal{D}(H)} = \Big\{\varphi \in \mathcal{H} \;\Big|\; t \mapsto U(t)\varphi \textit{ differentiable}\Big\} = \mathcal{D}(H)$$

(ii) and for all $\psi \in \mathcal{D}(H)$, the Schrödinger equation holds,

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}U(t)\psi = HU(t)\psi.$$

This is only one of the two implications: usually we are given a hamiltonian H and we would like to know under which circumstances this operator generates a unitary evolution group. We will answer this question conclusively in the next section with Stone's Theorem.

Theorem 4.3.5 *Let H be the generator of a strongly continuous evolution group $U(t)$, $t \in \mathbb{R}$. Then the following holds:*

(i) *$\mathcal{D}(H)$ is invariant under the action of $U(t)$, i. e. $U(t)\mathcal{D}(H) = \mathcal{D}(H)$ for all $t \in \mathbb{R}$.*

(ii) *H commutes with $U(t)$, i. e. $[U(t), H]\psi := U(t)\,H\psi - H\,U(t)\psi = 0$ for all $t \in \mathbb{R}$ and $\psi \in \mathcal{D}(H)$.*

(iii) *H is symmetric, i. e. $\langle H\varphi, \psi\rangle = \langle \varphi, H\psi\rangle$ holds for all $\varphi, \psi \in \mathcal{D}(H)$.*

(iv) *$U(t)$ is uniquely determined by H.*

(v) *H is uniquely determined by $U(t)$.*

Proof (i) Let $\psi \in \mathcal{D}(H)$. To show that $U(t)\psi$ is still in the domain, we have to show that the norm of $HU(t)\psi$ is finite. Since H is the generator of $U(t)$, it is equal to

$$H\psi = \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}s}U(s)\psi\bigg|_{s=0} = \lim_{s\to 0}\tfrac{\mathrm{i}}{s}\big(U(s) - \mathrm{id}\big)\psi.$$

Let us start with $s > 0$ and omit the limit. Then

$$\Big\|\tfrac{\mathrm{i}}{s}\big(U(s) - \mathrm{id}\big)U(t)\psi\Big\| = \Big\|U(t)\tfrac{\mathrm{i}}{s}\big(U(s) - \mathrm{id}\big)\psi\Big\| = \Big\|\tfrac{\mathrm{i}}{s}\big(U(s) - \mathrm{id}\big)\psi\Big\| < \infty$$

holds for all $s > 0$. Taking the limit on left and right-hand side yields that we can estimate the norm of $HU(t)\psi$ by the norm of $H\psi$ – which is finite since ψ is in the domain. This means $U(t)\mathcal{D}(H) \subseteq \mathcal{D}(H)$. To show the converse, we repeat the proof for $U(-t) = U(t)^{-1} = U(t)^*$ to obtain

$$\mathcal{D}(H) = U(-t)U(t)\mathcal{D}(H) \subseteq U(t)\mathcal{D}(H).$$

Hence, $U(t)\mathcal{D}(H) = \mathcal{D}(H)$.

(ii) This follows from an extension of the proof of (i): since the domain $\mathcal{D}(H)$ coincides with the set of vectors on which $U(t)$ is strongly differentiable and is left invariant by $U(t)$, taking limits on left- and right-hand side of

$$\Big\|\tfrac{\mathrm{i}}{s}\big(U(s) - \mathrm{id}\big)U(t)\psi - U(t)\tfrac{\mathrm{i}}{s}\big(U(s) - \mathrm{id}\big)\psi\Big\| = 0$$

leads to $[H, U(t)]\psi = 0$.

(iii) This follows from differentiating $\langle U(t)\varphi, U(t)\psi\rangle$ for arbitrary $\varphi, \psi \in \mathcal{D}(H)$ and using $\big[U(t), H\big] = 0$ as well as the unitarity of $U(t)$ for all $t \in \mathbb{R}$.

(iv) Assume that both unitary evolution groups, $U(t)$ and $\tilde{U}(t)$, have H as their generator. For any $\psi \in \mathcal{D}(H)$, we can calculate the time derivative of $\big\|(U(t) - \tilde{U}(t))\psi\big\|^2$,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\big\|(U(t) - \tilde{U}(t))\psi\big\|^2 &= 2\frac{\mathrm{d}}{\mathrm{d}t}\Big(\|\psi\|^2 - \mathrm{Re}\,\big\langle U(t)\psi, \tilde{U}(t)\psi\big\rangle\Big)\\ &= -2\mathrm{Re}\,\Big(\big\langle -\mathrm{i}HU(t)\psi, \tilde{U}(t)\psi\big\rangle + \big\langle U(t)\psi, -\mathrm{i}H\tilde{U}(t)\psi\big\rangle\Big)\\ &= 0.\end{aligned}$$

Since $U(0) = \mathrm{id} = \tilde{U}(0)$, this means $U(t)$ and $\tilde{U}(t)$ agree at least on $\mathcal{D}(H)$. Using the fact that there is only bounded extension of a bounded operator to all of $\mathcal{H}$, Theorem 4.1.5, we conclude they must be equal on all of $\mathcal{H}$.

(v) This follows from the definition of the generator and the density of the domain. □

Now that we have collected a few facts on unitary evolution groups, one could think that *symmetric* operators generate evolution groups, but *this is false!* The standard example to showcase this fact is the group of translations on $L^2([0,1])$. Since we would like $T(t)$ to conserve "mass" – or more accurately, probability, we define for $\varphi \in L^2([0,1])$ and $0 \leq t < 1$

$$\big(T(t)\varphi\big)(x) := \begin{cases} \varphi(x-t) & x - t \in [0,1] \\ \varphi(x-t+1) & x - t + 1 \in [0,1] \end{cases}.$$

For all other $t \in \mathbb{R}$, we extend this operator periodically, i. e. we plug in the fractional part of t. Clearly, $\big\langle T(t)\varphi, T(t)\psi\big\rangle = \big\langle \varphi, \psi\big\rangle$ holds for all $\varphi, \psi \in L^2([0,1])$. Locally, the infinitesimal generator is $-\mathrm{i}\partial_x$ as a simple calculation shows:

$$\left(\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\big(T(t)\varphi\big)\right)(x)\bigg|_{t=0} = \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\varphi(x-t)\bigg|_{t=0} = -\mathrm{i}\partial_x\varphi(x)$$

However, $T(t)$ does not respect the maximal domain of $-\mathrm{i}\partial_x$,

$$\mathcal{D}_{\max}(-\mathrm{i}\partial_x) = \big\{\varphi \in L^2([0,1]) \mid -\mathrm{i}\partial_x\varphi \in L^2([0,1])\big\}.$$

Any element of the maximal domain has a continuous representative, but if $\varphi(0) \neq \varphi(1)$, then for $t > 0$, $T(t)\varphi$ will have a discontinuity at t. We will denote the operator $-\mathrm{i}\partial_x$ on $\mathcal{D}_{\max}(-\mathrm{i}\partial_x)$ with $\mathsf{P}_{\max}$. Let us check whether $\mathsf{P}_{\max}$ is symmetric: for any $\varphi, \psi \in \mathcal{D}_{\max}(-\mathrm{i}\partial_x)$,

we compute

$$\begin{aligned}\langle\varphi, -\mathrm{i}\partial_x\psi\rangle &= \int_0^1 \mathrm{d}x\, \overline{\varphi(x)}\,(-\mathrm{i}\partial_x\psi)(x) = \Big[-\mathrm{i}\,\overline{\varphi(x)}\,\psi(x)\Big]_0^1 - \int_0^1 \mathrm{d}x\,(-\mathrm{i})\,\overline{\partial_x\varphi(x)}\,\psi(x)\\ &= \mathrm{i}\big(\overline{\varphi(0)}\,\psi(0) - \overline{\varphi(1)}\,\psi(1)\big) + \int_0^1 \mathrm{d}x\,\overline{(-\mathrm{i}\partial_x\varphi)(x)}\,\psi(x)\\ &= \mathrm{i}\big(\overline{\varphi(0)}\,\psi(0) - \overline{\varphi(1)}\,\psi(1)\big) + \big\langle -\mathrm{i}\partial_x\varphi, \psi\big\rangle. \qquad (4.3.3)\end{aligned}$$

In general, the boundary terms do not disappear and the maximal domain is "too large" for $-\mathrm{i}\partial_x$ to be symmetric. Thus it is not at all surprising, $T(t)$ does not leave $\mathcal{D}_{\max}(-\mathrm{i}\partial_x)$ invariant. Let us try another domain: one way to make the boundary terms disappear is to choose

$$\mathcal{D}_{\min}(-\mathrm{i}\partial_x) := \Big\{\varphi \in L^2([0,1]) \;\Big|\; -\mathrm{i}\partial_x\varphi \in L^2([0,1]),\ \varphi(0) = 0 = \varphi(1)\Big\}.$$

We denote $-\mathrm{i}\partial_x$ on this "minimal" domain with $\mathsf{P}_{\min}$. In this case, the boundary terms in equation (4.3.3) vanish which tells us that $\mathsf{P}_{\min}$ is symmetric. Alas, the domain is still not invariant under translations $T(t)$, even though $\mathsf{P}_{\min}$ is symmetric. This is an example of a symmetric operator which *does not* generate a unitary group.

There is another thing we have missed so far: the translations allow for an additional phase factor, i. e. for $\varphi, \psi \in L^2([0,1])$ and $\vartheta \in [0, 2\pi)$, we define for $0 \le t < 1$

$$\big(T_\vartheta(t)\varphi\big)(x) := \begin{cases} \varphi(x-t) & x - t \in [0,1] \\ \mathrm{e}^{\mathrm{i}\vartheta}\varphi(x-t+1) & x - t + 1 \in [0,1] \end{cases}.$$

while for all other t, we plug in the fractional part of t. The additional phase factor cancels in the inner product, $\langle T_\vartheta(t)\varphi, T_\vartheta(t)\psi\rangle = \langle\varphi,\psi\rangle$ still holds true for all $\varphi, \psi \in L^2([0,1])$. In general $T_\vartheta(t) \neq T_{\vartheta'}(t)$ if $\vartheta \neq \vartheta'$ and the unitary groups are genuinely different. Repeating the simple calculation from before, we see that the local generator still is $-\mathrm{i}\partial_x$ and it would seem we can generate a family of unitary evolutions from a *single* generator. The confusion is resolved if we focus on *invariant domains*: choosing $\vartheta \in [0, 2\pi)$, we define P_ϑ to be the operator $-\mathrm{i}\partial_x$ on the domain

$$\mathcal{D}_\vartheta(-\mathrm{i}\partial_x) := \Big\{\varphi \in L^2([0,1]) \;\Big|\; -\mathrm{i}\partial_x\varphi \in L^2([0,1]),\ \varphi(0) = \mathrm{e}^{-\mathrm{i}\vartheta}\varphi(1)\Big\}.$$

A quick look at equation (4.3.3) reassures us that P_ϑ is symmetric and a quick calculation shows it is also *invariant* under the action of $T_\vartheta(t)$. Hence, P_ϑ is the generator of T_ϑ, and the *definition of an unbounded operator is incomplete without spelling out its domain.*

Example Another example where the domain is crucial in the properties is the wave equation on $[0, L]$,

$$\partial_t^2 u(x,t) - \partial_x^2 u(x,t) = 0, \qquad\qquad u \in \mathcal{C}^2([0,L] \times \mathbb{R}_t).$$

Here, u is the amplitude of the vibration, i. e. the lateral deflection. If we choose Dirichlet boundary conditions at both ends, i. e. $u(0) = 0 = u(L)$, we model a closed pipe, if we choose Dirichlet boundary conditions on one end, $u(0) = 0$, and von Neumann boundary conditions on the other, $u'(L) = 0$, we model a half-closed pipe. Choosing domains is a question of physics!

Chapter 5

5 Unbounded selfadjoint operators

Most physical observables, e. g. standard Schrödinger operators of the form $H = -\Delta_x + V$, are *unbounded* selfadjoint operator, so in order to understand even the simplest physical observables such as position $\hat{x}$, momentum $-\mathrm{i}\nabla_x$ and energy H we need to define and understand unbounded operators first, extend the definition of adjoint and finally define selfadjointness properly.

5.1 Unbounded operators

Akin to Chapter 4.1, we first need to introduce the notion of unbounded operators and their adjoints. For the purpose of this chapter, a densely defined operator T always denotes a linear operator $T : \mathcal{D}(T) \subseteq \mathcal{H} \longrightarrow \mathcal{H}$ defined on a separable Hilbert space $\mathcal{H}$ with *domain* $\mathcal{D}(T)$.

Definition 5.1.1 (Extension of an operator) *Let T be a densely defined linear operator. Then an extension $S : \mathcal{D}(S) \subseteq \mathcal{H} \longrightarrow \mathcal{H}$ is an operator such that $S \supset T$, meaning $\mathcal{D}(S) \supset \mathcal{D}(T)$ and $S|_{\mathcal{D}(T)} = T$.*

The use of $\subset$ in $T \subset S$ also motivates calling T *smaller* than S.

Example We have discussed several candidates for the generator of translations on the Hilbert space $L^2([0,1])$ in Chapter 4.3.2, and one can see from the definitions that $P_{\min} \subset P_\vartheta \subset P_{\max}$, i. e. P_ϑ and $P_{\max}$ are two extensions of $P_{\min}$.

An important properties with which to distinguish some unbounded operators from others is *closedness*:

Definition 5.1.2 (Closed and closable operators) *Let $T : \mathcal{D}(T) \subseteq \mathcal{H} \longrightarrow \mathcal{H}$ be a densely defined linear operator.*

(i) The graph of T *is the linear subset*

$$\Gamma(T) := \big\{(\varphi, T\varphi) \mid \varphi \in \mathcal{D}(T)\big\} \subset \mathcal{H} \oplus \mathcal{H}.$$

(ii) T *is called* closed *if* $\Gamma(T)$ *is a closed subset of* $\mathcal{H} \oplus \mathcal{H}$*.*

(iii) T *is called* closable *if there exists a closed extension of* T*. In this case, the smallest closed extension* $\overline{T}$ *is the* closure of T *which satisfies* $\Gamma(\overline{T}) = \overline{\Gamma(T)}$*.*

An important example of closed operators are adjoints of densely defined operators.

Definition 5.1.3 (Adjoint operator) *Let* T *be a densely defined operator. Let* $\mathcal{D}(T^*)$ *be the set of* $\varphi \in \mathcal{H}$ *for which there exists* $\phi \in \mathcal{H}$ *with*

$$\langle T\psi, \varphi\rangle = \langle \psi, \phi\rangle \qquad\qquad \forall \psi \in \mathcal{D}(T).$$

For each $\varphi \in \mathcal{D}(T^*)$*, we define* $T^*\varphi := \phi$ *and* T^* *is called the adjoint of* T*.*

Remark 5.1.4 By Riesz Lemma, φ belongs to $\mathcal{D}(T^*)$ if and only if

$$\big|\langle T\psi, \varphi\rangle\big| \leq C\,\|\psi\| \qquad\qquad \forall \psi \in \mathcal{D}(T).$$

This is equivalent to saying $\varphi \in \mathcal{D}(T^*)$ if and only if $\psi \mapsto \langle T\psi, \varphi\rangle$ is continuous on $\mathcal{D}(T)$. As a matter of fact, we could have used to latter to *define* the adjoint operator.

One word of caution: although adjoint operators are always closed, their domain may be too small, i. e. even if T is densely defined, T^* need not be:

Example Let $f \in L^\infty(\mathbb{R})$, but $f \notin L^2(\mathbb{R})$, and pick $\psi_0 \in L^2(\mathbb{R})$. Define

$$\mathcal{D}(T_f) := \Big\{\psi \in L^2(\mathbb{R}) \;\Big|\; \int_{\mathbb{R}} \mathrm{d}x\; |f(x)\,\psi(x)| < \infty\Big\}.$$

Then the adjoint of the operator

$$T_f\psi := \langle f, \psi\rangle\,\psi_0, \qquad\qquad \psi \in \mathcal{D}(T_f),$$

has domain $\mathcal{D}(T_f^*) = \{0\}$. Let $\psi \in \mathcal{D}(T_f)$. Then for any $\varphi \in \mathcal{D}(T_f^*)$

$$\begin{aligned}\big\langle T_f\psi, \varphi\big\rangle &= \big\langle \langle f, \psi\rangle\,\psi_0, \varphi\big\rangle = \big\langle \psi, f\big\rangle\,\big\langle \psi_0, \varphi\big\rangle \\ &= \big\langle \psi, \langle \psi_0, \varphi\rangle f\big\rangle.\end{aligned}$$

Hence $T_f^*\varphi = \langle \psi_0, \varphi\rangle f$. However $f \notin L^2(\mathbb{R})$ and thus $\varphi = 0$ is the only possible choice for which $T_f^*\varphi$ is well defined.

Definition 5.1.5 (Symmetric operator) *A densely defined operator T is called* symmetric *if and only if*

$$\langle T\psi, \varphi\rangle = \langle \psi, T\varphi\rangle$$

holds for all $\varphi, \psi \in \mathcal{D}(T)$.

Theorem 5.1.6 *Let T be a densely defined linear operator. Then T^* is closed.*

Proof According to Definition 5.1.3, the condition $(\psi, \phi) \in \Gamma(T^*)$ is in fact equivalent to

$$\langle \psi, T\varphi\rangle - \langle \phi, \varphi\rangle = 0 \qquad \forall \varphi \in \mathcal{D}(T).$$

However, seeing as $\langle \psi, T\varphi\rangle - \langle \phi, \varphi\rangle = \big\langle (\psi, \phi), (-T\varphi, \varphi)\big\rangle_{\mathcal{H}\oplus\mathcal{H}}$, we introduce the unitary map

$$W : \mathcal{H} \oplus \mathcal{H} \longrightarrow \mathcal{H} \oplus \mathcal{H}, \quad (\varphi_1, \varphi_2) \mapsto (-\varphi_2, \varphi_1)$$

and rewrite the graph of T^* as

$$\Gamma(T^*) = W\big(\Gamma(T)\big)^{\perp}. \tag{5.1.1}$$

Since unitaries are bounded, it maps the *closed* set $\big(\Gamma(T)\big)^{\perp}$ (orthogonal complements of sets are always *closed* subspaces) onto a closed set. Hence, T^* is closed. □

Corollary 5.1.7 *Let T be a densely defined operator and $T \subset S$. Then $S^* \subset T^*$.*

Proof This follows directly from (5.1.1), because $\Gamma(T) \subset \Gamma(S)$ implies

$$\Gamma(S^*) = W\big(\Gamma(S)\big)^{\perp} \subset W\big(\Gamma(T)\big)^{\perp} = \Gamma(T^*).$$ □

Corollary 5.1.8 *Let T be densely defined and closable, and assume that also T^* is densely defined.*

(i) $\overline{T} = T^{**} =: \big(T^*\big)^*$

(ii) $\big(\overline{T}\big)^* = T^* = T^{***}$

Proof (i) First of all, it is easy to show that for any subspace $\mathcal{K} \subset \mathcal{H} \oplus \mathcal{H}$ we have

$$W\big(\mathcal{K}^{\perp}\big) = \big(W\mathcal{K}\big)^{\perp}.$$

Now using (5.1.1) repeatedly, we can express $\Gamma(T^{**})$ in terms of $\Gamma(T)$,

$$\begin{aligned}\Gamma(T^{**}) &= W\big(\Gamma(T^*)\big)^{\perp} = W\Big(W\big(\Gamma(T)\big)^{\perp}\Big)^{\perp} \\ &= W\Big(W\big(\Gamma(T)^{\perp}\big)^{\perp}\Big) = W^2\Big(\big(\Gamma(T)^{\perp}\big)^{\perp}\Big).\end{aligned}$$

Evidently, $W^2 = -\mathrm{id}_{\mathcal{H}\oplus\mathcal{H}}$ and seeing as $\left(\mathcal{K}^\perp\right)^\perp = \overline{\mathcal{K}}$, we deduce

$$\Gamma(T^{**}) = \overline{\Gamma(T)}.$$

But this implies (i) as T is closable by assumption, and its smallest closed extension satisfies $\overline{\Gamma(T)} = \Gamma(\overline{T})$.

(ii) This follows from

$$\Gamma\left(\left(\overline{T}\right)^*\right) = \Gamma(T^{***}) = \overline{\Gamma(T^*)} = \Gamma(T^*)$$

2014.10.10 since T^* is closed by (i). Hence, also (ii) holds true. □

Corollary 5.1.9 *Let T be densely defined and symmetric. Then T is closable and T^* is densely defined, and we have $T \subseteq \overline{T} = T^{**} \subseteq T^*$ and $\left(\overline{T}\right)^* = T^*$.*

Proof Since T is symmetric, T^* is densely defined as well as $\mathcal{D}(T) \subseteq \mathcal{D}(T^*)$ implies the latter is dense in $\mathcal{H}$. Thus, Corollary 5.1.8 applies. □

5.2 Selfadjoint operators

We are finally in a position to define unbounded selfadjoint operators properly, and we see that in large part, selfadjointness is a matter of domains. Very often, though, it is not easy (or possible) to compute the domain explicitly. That is why the notion of *essential* selfadjointness is useful where one gives a smaller symmetric operator which has a unique selfadjoint extension.

Definition 5.2.1 (Selfadjoint operator) *Suppose H is a symmetric, densely defined.*

(i) H is called selfadjoint *if and only if $H = H^*$.*

(ii) H is called essentially selfadjoint *with* core $\mathcal{D}(H)$ *if its closure $\overline{H}$ is selfadjoint.*

Selfadjointness is not just a matter of an operator being symmetric, the crucial bit concerns the *domain*.

Corollary 5.2.2 *A symmetric, densely defined operator H is essentially selfadjoint if and only if H^* is symmetric. Then the selfadjoint extension is $\overline{H} = H^*$.*

Proof "⇒:" Essentially selfadjoint operators are symmetric by definition and closable by Corollary 5.1.9, and hence, the unique selfadjoint extension $\overline{H} = \overline{H}^* = H^{***} = H^*$ (Corollary 5.1.8) is symmetric.

"⇐:" Assume H^* is symmetric. Then the combination of the two inclusions from Corollary 5.1.9, $H^* \subseteq H^{**} = \overline{H}$ and $H \subseteq \overline{H} = H^{**} \subseteq H^*$, yields $H^* = \overline{H}^* = \overline{H}$, i. e. H is essentially selfadjoint. □

Selfadjointness is not just important to have well-defined observables, but also *existence of the dynamics* as a unitary evolution group.

Theorem 5.2.3 (Stone) *To every strongly continuous one-parameter unitary group U on a Hilbert space $\mathcal{H}$, there exists a selfadjoint operator $H = H^*$ which generates $U(t) = \mathrm{e}^{-\mathrm{i}tH}$. Conversely, every selfadjoint operator H generates the unitary evolution group $U(t) = \mathrm{e}^{-\mathrm{i}tH}$.*

This is a very deep result of functional analysis, and a proof is beyond out capabilities at this point (see e. g. [RS72, Chapter VIII.3]). However, we will at least prove one of the two implications when we discuss how to define $\mathrm{e}^{-\mathrm{i}tH}$ rigorously in Chapter 6.

5.2.1 Fundamental criterion for selfadjointness

While we now know how to define selfadjointness properly in case an operator is unbounded, the definition is too unwieldy to be able to prove selfadjointness. There are a few ways to decide whether an operator is selfadjoint the most basic one is the

Theorem 5.2.4 (Fundamental criterion for selfadjointness) *Let H be a symmetric, densely defined operator. Then the following are equivalent:*

(i) *H is selfadjoint.*

(ii) *H is closed and* $\ker(H^* \pm \mathrm{i}) = \{0\}$.

(iii) $\operatorname{ran}(H \pm \mathrm{i}) = \mathcal{H}$.

The proof is split in two parts, first we state and show this auxiliary result:

Lemma 5.2.5 *Let T be a densely defined operator. Then we have:*

(i) $\ker(T^* \mp \mathrm{i}) = \operatorname{ran}(T \pm \mathrm{i})^\perp$

(ii) $\ker(T^* \mp \mathrm{i}) = \{0\} \Leftrightarrow \operatorname{ran}(T \pm \mathrm{i}) \subseteq \mathcal{H}$ *dense*

(iii) *If in addition T is closed and symmetric, then* $\operatorname{ran}(T \pm \mathrm{i})$ *are closed.*

Proof (i) First of all, we note that $(T \pm \mathrm{i})^* = T^* \mp \mathrm{i}$. The following equivalences hold true:

$$\begin{aligned}
\psi \in \operatorname{ran}(T + \mathrm{i})^\perp &\Leftrightarrow \langle \psi, (T + \mathrm{i})\varphi \rangle = 0 \ \forall \varphi \in \mathcal{D}(T) \\
&\Leftrightarrow \psi \in \mathcal{D}(T^*) \text{ and } \langle (T^* - \mathrm{i})\psi, \varphi \rangle = 0 \ \forall \varphi \in \mathcal{D}(T) \\
&\Leftrightarrow \psi \in \mathcal{D}(T^*) \text{ and } (T^* - \mathrm{i})\psi = 0 \\
&\Leftrightarrow \psi \in \ker(T^* - \mathrm{i})
\end{aligned}$$

The proof for the other sign is analogous.

(ii) This follows immediately from (i).

(iii) For symmetric operators T and $\varphi \in \mathcal{D}(T)$ the expectation value $\langle T\varphi, \varphi\rangle = \langle \varphi, T\varphi\rangle$ is necessarily real, and consequently, it follows that

$$\big\|(T+\mathrm{i})\varphi\big\|^2 = \big\|T\varphi\big\|^2 + \|\varphi\|^2 + 2\mathrm{Re}\ \langle \mathrm{i}\varphi, T\varphi\rangle = \big\|T\varphi\big\|^2 + \|\varphi\|^2 \geq \|\varphi\|^2. \qquad \square$$

Hence, $T+\mathrm{i}$ is injective and the inverse $(T+\mathrm{i})^{-1} : \mathrm{ran}\,(T+\mathrm{i}) \longrightarrow \mathcal{D}(T)$ exists as a *bounded* operator. To see that $\mathrm{ran}\,(T+\mathrm{i})$ is closed, pick a Cauchy sequence $\{\psi_n\}_{n\in\mathbb{N}}$ in the range. The image of this Cauchy sequence under $(T+\mathrm{i})^{-1}$ is another Cauchy sequence $\psi_n := (T+\mathrm{i})^{-1}\varphi_n$ in $\mathcal{D}(T)$ ($(T+\mathrm{i})^{-1}$ is bounded!). Also $\big(\psi_n, T\psi_n\big)$ is a Cauchy sequence with respect to the norm on $\mathcal{H}\oplus\mathcal{H}$ because $T\,(T+\mathrm{i})^{-1} = \mathrm{id} - \mathrm{i}\,(T+\mathrm{i})^{-1}$ is bounded. That means $\big(\psi_n, T\psi_n\big)$ converges to some $(\phi,\eta) \in \mathcal{H}\oplus\mathcal{H}$. In fact, this sequence converges in $\Gamma(T)$ as T is closed. But then $(T+\mathrm{i})\phi$ is the limit point in $\mathrm{ran}\,(T+\mathrm{i})$, and the range is closed.

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Proof (Theorem 5.2.4) "(i) ⇒ (ii):" Suppose $H = H^*$ is selfadjoint. Then it is closed by Theorem 5.1.6. A vector $\varphi_\pm$ is an element of $\ker(H^* \pm \mathrm{i}) = \ker(H \pm \mathrm{i})$ if and only if $H\varphi_\pm = \mp\mathrm{i}\varphi_\pm$. Put another way, $\varphi_\pm$ is an eigenvector of H to the eigenvalue $\mp\mathrm{i}$. However, eigenvalues of symmetric operators are necessarily real: assume $\varphi_\lambda \in \mathcal{D}(H)$ is an eigenvector of H to $\lambda\in\mathbb{C}$, then a quick computation

$$\begin{aligned}\lambda\,\langle\varphi_\lambda,\varphi_\lambda\rangle &= \langle\varphi_\lambda, H\varphi_\lambda\rangle = \langle H\varphi_\lambda,\varphi_\lambda\rangle\\ &= \bar\lambda\,\langle\varphi_\lambda,\varphi_\lambda\rangle\end{aligned}$$

reveals $\lambda = \overline{\lambda}$. Thus, only $\varphi_\pm = 0$ satisfies $H\varphi_\pm = \mp\mathrm{i}\varphi_\pm$ and $\ker(H^*\pm\mathrm{i}) = \{0\}$.

"(ii) ⇒ (iii):" This follows from Lemma 5.2.5 above.

"(iii) ⇒ (i):" Assume $\mathrm{ran}\,(H\pm\mathrm{i}) = \mathcal{H}$. We will need to show $H = H^*$. The inclusion $H\subseteq H^*$ follows from Corollary 5.1.9, and we are left to show $H\supseteq H^*$. To unburden the notation, let us consider $H-\mathrm{i}$. The surjectivity of $H-\mathrm{i}$ yields that for any $\psi\in\mathcal{D}(H^*)$ there exists a $\varphi\in\mathcal{D}(H)$ so that

$$(H^*-\mathrm{i})\psi = (H-\mathrm{i})\varphi = (H^*-\mathrm{i})\varphi$$

where in the last step we have used $H^*\supseteq H$. But that means $\psi-\varphi\in\ker(H^*-\mathrm{i})$, and $\mathrm{ran}\,(H+\mathrm{i}) = \mathcal{H}$ (note the difference in sign!) combined with Lemma 5.2.5 (ii) implies $\psi=\varphi$. Given that $\psi\in\mathcal{D}(H^*)$ was chosen arbitrarily, we infer $\mathcal{D}(H^*) = \mathcal{D}(H)$. $\square$

Corollary 5.2.6 (Fundamental criterion for selfadjointness) *Let H be a symmetric, densely defined operator. Then the following are equivalent:*

(i) H is essentially selfadjoint.

(ii) $\ker(H^* \pm \mathrm{i}) = \{0\}$

(iii) $\operatorname{ran}(H \pm \mathrm{i}) \subseteq \mathcal{H}$ *is dense.*

Proof To see (i) $\Leftrightarrow$ (ii), we note that Theorem 5.2.4 applies for H^{**}, because according to Corollary 5.1.8 (i) $H^{**} = \overline{H}$ is the selfadjoint closure of H and $H^{***} = H^*$ by Corollary 5.1.8 (ii). Consequently, we have the following equivalences:

$$\begin{aligned} H \text{ essentially selfadjoint} &\Leftrightarrow \overline{H} = H^{**} \text{ selfadjoint} \\ &\Leftrightarrow H^{**} \text{ closed and } \ker\big(H^{***} \pm \mathrm{i}\big) = \{0\} \\ &\Leftrightarrow \ker\big(H^* \pm \mathrm{i}\big) = \{0\} \end{aligned}$$

The equivalence (ii) $\Leftrightarrow$ (iii) is the content of Lemma 5.2.5 (i). □

Usually it is simpler to check whether an operator is *essentially* selfadjoint. However, in certain cases, proving such statements can be hard work and require highly non-trivial machinery.

The corollary implies that an operator *cannot* be selfadjoint if the *deficiency indices*

$$\begin{aligned} N_+(H) &:= \dim\ker(H^* + \mathrm{i}), \\ N_-(H) &:= \dim\ker(H^* - \mathrm{i}), \end{aligned}$$

take different values, $N_+(H) \neq N_-(H)$. However, if the two are equal, one can always find a selfadjoint extension:

Theorem 5.2.7 *A densely defined, symmetric operator H has at least one selfadjoint extension if and only if $N_-(H) = N_+(H)$ holds.*

The proof is a bit technical, and will be skipped during the lecture. The interested reader can find it in [RS75, p. 141].

During the exercises, you are asked to compute the defect indices of $P_{\min}$ from Chapter 4.3.2. It turns out that $N_\pm(P_{\min}) = 1$, and this one-dimensional degree of freedom is connected to the freedom to choose a phase during the gluing procedure. In other words, for any value of $\vartheta \in \mathbb{R}$ the operator P_ϑ is a selfadjoint extension of $P_{\min}$.

5.2.2 Spectral properties

The spectrum of an operator is the generalization of the set of eigenvalues for matrices. According to Definition 4.1.6 the spectrum can be divided into three parts, the *point spectrum*

$$\sigma_{\mathrm{p}}(H) := \big\{z \in \mathbb{C} \mid H - z \text{ is not injective}\big\},$$

the *continuous spectrum*

$$\sigma_{\text{cont}}(H) := \big\{ z \in \mathbb{C} \mid H - z \text{ is injective, } \operatorname{im}(H-z) \subseteq \mathcal{H} \text{ dense} \big\},$$

and the *residual spectrum*

$$\sigma_{\text{r}}(H) := \big\{ z \in \mathbb{C} \mid H - z \text{ is injective, } \operatorname{im}(H-z) \subseteq \mathcal{H} \text{ not dense} \big\}.$$

Point spectrum is due to eigenvalues with eigenvector. Compared to matrices, the occurrence of continuous and residual spectra is new. The residual spectrum is not important for our discussion as it is empty for selfadjoint operators.

The continuous spectrum can be attributed to cases where the eigenvectors are not elements of the Hilbert space. For instance, in case of the free Schrödinger operator $H = -\frac{1}{2}\Delta_x$ on $L^2(\mathbb{R}^d)$, the spectrum is $\sigma(H) = \sigma_{\text{cont}}(H) = [0, +\infty)$. Here, the eigenvectors are plane waves, $\mathrm{e}^{+\mathrm{i}\xi\cdot x}$ which are smooth, bounded functions; however, plane waves are not square integrable. Similarly, multiplication operators have Dirac distributions as eigen"functions".

Note that this distinction between the spectral components goes further than looking at the spectrum as a set: for instance, it is known that certain random Schrödinger operators have dense point spectrum which "looks" the same as continuous spectrum.

There is also a second helpful classification of spectrum which cannot be made rigorous with the tools we have at hand, and that is the distinction between *essential* spectrum $\sigma_{\text{ess}}(H)$ and *discrete* spectrum $\sigma_{\text{disc}}(H)$. The essential spectrum is stable under local, short-range perturbations while the discrete spectrum may change. One has the following characterization for the essential spectrum:

Theorem 5.2.8 (Theorem VII.10 in [RS72]) *$\lambda \in \sigma_{\text{ess}}(H)$ if and only if* one or more *of the following holds:*

(i) *$\lambda \in \sigma_{\text{cont}}(H)$*

(ii) *λ is a limit point of $\sigma_{\text{p}}(H)$.*

(iii) *λ is an eigenvalue of infinite multiplicity.*

Similarly, the discrete spectrum has a similar characterization:

Theorem 5.2.9 (Theorem VII.11 in [RS72]) *$\lambda \in \sigma_{\text{disc}}(H)$ if and only if* both *of the following hold:*

(i) *λ is an isolated point of $\sigma(H)$, i. e. for some $\varepsilon > 0$ we have $\big(\lambda - \varepsilon, \lambda + \varepsilon\big) \cap \sigma(H) = \{\lambda\}$.*

(ii) *λ is an eigenvalue of* finite *multiplicity.*

The spectrum can be probed by means of approximate eigenfunctions ("Weyl's Criterion", see [RS72, Theorem VII.12]):

Theorem 5.2.10 (Weyl's criterion) *Let H be a bounded selfadjoint operator on a Hilbert space $\mathcal{H}$. Then $\lambda \in \sigma(H)$ holds if and only if there exists a sequence $\{\psi_n\}_{n\in\mathbb{N}}$ so that $\|\psi_n\| = 1$ and*

$$\lim_{n\to\infty} \left\| H\psi_n - \lambda\,\psi_n \right\|_{\mathcal{H}} = 0.$$

We have $\lambda \in \sigma_{\text{ess}}(H)$ if and only if we can choose the sequence $\{\psi_n\}_{n\in\mathbb{N}}$ to be orthonormal.

Example (Weyl's criterion for $H = -\partial_x^2$ on $L^2(\mathbb{R})$) For any $\lambda^2 \in [0, +\infty)$, one can choose a sequence $\{\psi_n\}_{n\in\mathbb{N}}$ of normalized and cut off plane waves $e^{\pm i\lambda x}$. To make sure they are normalized, we know that pointwise $\psi_n(x) \to 0$ as $n \to \infty$.

5.2.2.1 The spectrum of selfadjoint operators is real

As a side note, let us show that the spectrum of selfadjoint operators is purely real.

Theorem 5.2.11 *Let $H = H^*$ be a selfadjoint operator on the Hilbert space $\mathcal{H}$. Then the following holds true:*

(i) $\sigma(H) \subseteq \mathbb{R}$

(ii) $H \geq 0 \Rightarrow \sigma(H) \subseteq [0, +\infty)$

To prove this, we use the following

Lemma 5.2.12 *Let $\mathcal{H}_j$, $j = 1, 2$, be Hilbert spaces. Then an operator $T \in \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2)$ is invertible if and only if there exists a constant $C > 0$ such that $T^*\,T \geq C\,\mathrm{id}_{\mathcal{H}_1}$ and $T\,T^* \geq C\,\mathrm{id}_{\mathcal{H}_2}$ hold.*

Proof "⇒:" Assume T is invertible. Then $T^* : \mathcal{H}_2 \longrightarrow \mathcal{H}_1$ is also invertible with inverse $T^{*-1} = T^{-1^*}$. Set $C := \left\|T^{-1}\right\|^{-2} = \left\|T^{*-1}\right\|^{-2}$. Then the inequality

$$\|\psi\| = \left\|T^{-1}T\psi\right\| \leq \left\|T^{-1}\right\|\,\|T\psi\|$$

proves $\|T\psi\| \geq \left\|T^{-1}\right\|^{-1}$, and thus also

$$\langle\psi, T^*T\psi\rangle = \|T\psi\|^2 \geq \left\|T^{-1}\right\|^{-2}\,\|\psi\|^2 = C\,\|\psi\|^2\,, \tag{5.2.1}$$

i. e. we have shown $T^*\,T \geq C\,\mathrm{id}_{\mathcal{H}_1}$. The non-negativity of $T\,T^*$ is shown analogously.

"⇐:" Suppose there exists $C > 0$ such that $T^*\,T \geq C\,\mathrm{id}_{\mathcal{H}_2}$ and $T\,T^* \geq C\,\mathrm{id}_{\mathcal{H}_2}$. Then from (5.2.1) we deduce $\|T\psi\| \geq \sqrt{C}\,\|\psi\|$ holds for all $\psi \in \mathcal{H}_1$. First of all, this proves that

T is injective, and secondly T has closed range in $\mathcal{H}_2$ (one can see the latter by considering convergence of $T\psi_n$ for any Cauchy sequence $\{\psi_n\}_{n\in\mathbb{N}}$). Moreover, one can easily see

$$\operatorname{ran} T = \overline{\operatorname{ran} T} = \left(\ker T^*\right)^\perp.$$

Since we can make the same arguments for T^*, we also know that T^* is injective, and thus $\ker T^* = \{0\}$. This shows that T is surjective, i. e. it is bijective, and hence, invertible. □

With the proof of the Lemma complete, we can now prove the statement:

Proof (Theorem 5.2.11) (i) Let $H = H^*$ be selfadjoint and $z = \lambda + \mathrm{i}\mu \in \mathbb{C} \setminus \mathbb{R}$ be a complex number with non-vanishing imaginary part μ. We will show that $z \notin \sigma(H)$, i. e. that $H - \lambda$ is invertible: a quick computation shows

$$\begin{aligned}\left(H - z\right)^* \left(H - z\right) &= H^2 - 2\left(\operatorname{Re} z\right) H + |z|^2 = H^2 - 2\lambda H + (\lambda^2 + \mu^2)\\ &= \mu^2 + \left(H - \lambda\right)^2.\end{aligned}$$

The last term is non-negative, and thus, we have shown

$$\left(H - z\right)^* \left(H - z\right) \geq \mu^2. \tag{5.2.2}$$

By the Lemma, this means $H - \lambda$ is necessarily invertible, and $z \notin \sigma(H)$.

(ii) We have to show that for $\lambda \in (-\infty, 0)$, the operator $H - \lambda$ is invertible. This follows as before from

$$\left(H - \lambda\right)^* \left(H - \lambda\right) = H^2 - 2\lambda H + \lambda^2 \geq \lambda^2,$$

the non-negativity of $-2\lambda H = 2|\lambda| H$ and the Lemma. □

Equation (5.2.2) also yields a very useful estimate on the norm of the resolvent $(H - z)^{-1}$:

Corollary 5.2.13 *Let H be a selfadjoint operator and $z \in \mathbb{C} \setminus \mathbb{R}$. Then we have the following estimate for the norm of the resolvent:*

$$\left\|(H - z)^{-1}\right\| \leq \frac{1}{|\operatorname{Im} z|} \tag{5.2.3}$$

Proof As H is selfadjoint and $\operatorname{Im} z \neq 0$ the Fundamental Criterion of Selfadjointness 5.2.4 tells us that $\operatorname{ran}(H - z) = \mathcal{H}$. That means to any $\psi \in \mathcal{H}$ we can find $\varphi \in \mathcal{D}(H)$ such that $(H - z)\varphi = \psi$, and consequently, (5.2.2) yields

$$\begin{aligned}\left\|(H - z)\varphi\right\|^2 &= \|\psi\|^2\\ &\geq |\operatorname{Im} z|^2 \left\|\varphi\right\|^2 = |\operatorname{Im} z|^2 \left\|(H - z)^{-1}\psi\right\|^2.\end{aligned}$$

This is equivalent to equation (5.2.3). □

5.2.2.2 Spectra of common selfadjoint operators

Quite generally, the spectrum of selfadjoint operators is purely real. But before we prove that, let us discuss some examples from physics:

Multiplication operators The spectrum of the multiplication operator

$$\big(f(\hat{x})\psi\big)(x) := f(x)\,\psi(x)$$

is given by the range, $\sigma\big(f(\hat{x})\big) = \overline{\operatorname{ran} f}$, where $f : \mathbb{R}^d \longrightarrow \mathbb{R}$ is a piecewise-continuous function.[1]

To see this claim, we rely on the Weyl criterion: in order to show $\sigma\big(f(\hat{x})\big) \supseteq \overline{\operatorname{ran} f}$, pick any $\lambda \in \overline{\operatorname{ran} f}$. Then there exists a sequence x_n such that $|\lambda - f(x_n)| < 1/n$. Then by shifting an L^2-Dirac sequence by x_n (e. g. scaled Gaußians), we obtain a sequence of vectors ψ_n with $\big\|\big(f(\hat{x}) - \lambda\big)\psi_n\big\| \xrightarrow{n\to\infty} 0$. Hence, this reasoning shows $\overline{\operatorname{ran} f} \subseteq \sigma\big(f(\hat{x})\big)$.

To show the converse inclusion, let $\lambda \in \sigma\big(f(\hat{x})\big)$. Then there exists a Weyl sequence $\{\psi_n\}_{n\in\mathbb{N}}$ with $\big\|\big(f(\hat{x}) - \lambda\big)\psi_n\big\| \to 0$ as $n \to \infty$. Assume $\inf_{x\in\mathbb{R}^d}\big|f(x) - \lambda\big| = c > 0$, i. e. $\lambda \notin \overline{\operatorname{ran} f}$, then $\{\psi_n\}$ cannot be a Weyl sequence to λ,

$$\big\|\big(f(\hat{x}) - \lambda\big)\psi_n\big\| \geq \inf_{x\in\mathbb{R}^d}\big|f(x) - \lambda\big|\,\|\psi_n\| \geq c > 0,$$

which is absurd.

Should f be constant and equal to λ_0 on a set of positive measure, there are infinitely many eigenfunctions associated to the eigenvalue λ_0. Otherwise, f has continuous spectrum. In any case, the spectrum of $f(\hat{x})$ is purely essential.

Clearly, this takes care of any operator which is unitarily equivalent to a multiplication operator, e. g. the free Laplacian on $\mathbb{R}^d$ or $\mathbb{T}^d$.

The hydrogen atom One of the most early celebrated successes of quantum mechanics is the explanation of the spectral lines by Schrödinger [Sch26b; Sch26d; Sch26a; Sch26c]. Here, the operator

$$H_C := -\frac{\hbar^2}{2m}\Delta_x - \frac{e^2}{|\hat{x}|} \tag{5.2.4}$$

acts on a dense subspace of $L^2(\mathbb{R}^3)$. A non-obvious fact is that this operator is bounded from below, i. e. there exits a constant $c > 0$ such that $H \geq -c$. This is false for the corresponding classical system, because the function $h(q,p) = \frac{1}{2m}p^2 - \frac{e}{|q|}$ is *not* bounded from below.

[1] This condition can be relaxed and is chosen just for ease of use.

The reason for that is that states of low potential energy (i. e. wave functions which are sharply peaked around 0) must pay an ever larger price in kinetic energy (sharply peaked means large gradient). One heuristic way to see that is to compute the energy expectation value of $\psi_\lambda := \lambda^{3/2}\,\psi(\lambda x)$ for $\lambda \gg 1$ where $\psi \in \mathcal{S}(\mathbb{R}^d)$:

$$\begin{aligned}\mathbb{E}_{\psi_\lambda}(H) &= \frac{\hbar^2}{2m}\left\langle \psi_\lambda, -\Delta_x \psi_\lambda\right\rangle - e\left\langle \psi_\lambda, |\hat{x}|^{-1}\psi_\lambda\right\rangle \\ &= \frac{\hbar^2}{2m}\,\lambda^2 \int_{\mathbb{R}^3} \mathrm{d}x\,\lambda^3 \left|\nabla_x \psi(\lambda x)\right|^2 - e\,\lambda \int_{\mathbb{R}^3} \mathrm{d}x\,\lambda^3\,\frac{|\psi(\lambda x)|}{\lambda\,|x|} \\ &= \lambda^2 \left\langle \psi, -\tfrac{\hbar^2}{2m}\Delta_x \psi\right\rangle - \lambda\left\langle \psi, e\,|\hat{x}|^{-1}\psi\right\rangle \end{aligned} \tag{5.2.5}$$

Clearly, if one replaces the Coulomb potential by $-|x|^{-3}$, the kinetic energy wins and the quantum particle can "fall down the well".

The negative potential gives rise to a family of eigenvalues (the spectral lines) while 2014.10.17 $-\Delta_x$ contributes continuous spectrum $[0,+\infty)$,

$$\begin{aligned}\sigma(H) &= \{E_n\}_{n\in\mathbb{N}} \cup [0,+\infty), \\ \sigma_{\text{cont}}(H) &= [0,+\infty) = \sigma_{\text{ess}}(H), \\ \sigma_{\text{p}}(H) &= \{E_n\}_{n\in\mathbb{N}} = \sigma_{\text{disc}}(H).\end{aligned}$$

5.2.2.3 Eigenvalues and bound states

The hydrogen atom is a prototypical example of the type of problem we are interested in, namely Schrödinger operators on $L^2(\mathbb{R}^d)$ of the form

$$H = -\Delta_x + V$$

where $V \le 0$ is a non-positive potential decaying at infinity ($\lim_{|x|\to\infty} V(x) = 0$). Under suitable technical conditions on the potential, H defines a selfadjoint operator which is bounded from below, that is $H \ge c$ holds for some $c \in \mathbb{R}$, and we have

$$\sigma_{\text{ess}}(H) = \sigma(-\Delta_x) = [0,+\infty).$$

We will come back to the question of selfadjointness of $H = -\Delta_x + V$ later in Chapter 5.2.3. Now the question is whether $\sigma_{\text{p}}(H) = \emptyset$ or

$$\sigma_{\text{p}}(H) = \{E_n\}_{n=0}^{N} \subset (-\infty, 0)$$

for some $N \in \mathbb{N}_0 \cup \{\infty\}$. We shall always assume that the eigenvalues are ordered by magnitude,

$$E_0 \le E_1 \le \dots$$

The *ground state* ψ_0 is the eigenfunction to the lowest eigenvalue E_0. Eigenfunctions ψ are localized: the weakest form of localization is $\psi \in L^2(\mathbb{R}^d)$, but usually one can expect *exponential* localization.

So there are two natural questions which we will answer in turn:

(1) Do eigenvalues below the essential spectrum *exist*?

(2) Can we give *estimates* on their numerical values?

The Birman-Schwinger principle We begin with the Birman-Schwinger principle which gives a criterion for the existence and absence of eigenvalues at a specific energy level. It is *the* standard tool for showing the existence or absence of eigenvalues. Assume φ is an eigenvector of H to the eigenvalue $-E < 0$. Then the eigenvalue equation is equivalent to

$$\big(-\Delta_x + E\big)\varphi = -V\varphi = |V|\,\varphi.$$

If we define the vector $\psi := |V|^{1/2}\,\varphi$ and use that $-E \notin \sigma(-\Delta_x) = [0, +\infty)$, we obtain

$$|V|^{1/2}\,\big(-\Delta_x + E\big)^{-1}\,|V|^{1/2}\,\psi = \psi.$$

In other words, we have just shown the

Theorem 5.2.14 (Birman-Schwinger principle) *The function $\varphi \in L^2(\mathbb{R}^d)$ is an eigenvector of $H = -\Delta_x + V$ to the eigenvalue $-E < 0$ if and only if $\psi = |V|^{1/2}\,\varphi$ is an eigenvector of the Birman-Schwinger operator*

$$K_E := |V|^{1/2}\,\big(-\Delta_x + E\big)^{-1}\,|V|^{1/2} \tag{5.2.6}$$

to the eigenvalue 1.

The only assumption we have glossed over is the boundedness of K_E. One may think that solving $K_E\psi = \psi$ is just as difficult as $H\varphi = -E\varphi$, but it is not. For instance, we immediately obtain the following

Corollary 5.2.15 *Assume the Birman-Schwinger operator $K_E \in \mathcal{B}\big(L^2(\mathbb{R}^d)\big)$ is bounded. Then for λ_0 small enough, $H_\lambda = -\Delta_x + \lambda V$ has no eigenvalue at $-E$ for all $0 \leq \lambda < \lambda_0$.*

Proof Replacing V with λV in equation (5.2.6) yields that the Birman-Schwinger operator for H_λ is λK_E. Thus, for λ small enough, we can make $\lambda\,\|K_E\| < 1$ arbitrarily small and since $\sup\big|\sigma\big(K_E\big)\big| \leq \|K_E\|$,[2] this means 1 cannot be an eigenvalue. Hence, by the Birman-Schwinger principle there cannot exist an eigenvalue at $-E$. □

[2] This is a general fact: if $T \in \mathcal{B}(\mathcal{X})$ is an operator on a Banach space, then $\sup|\sigma(T)| \leq \|T\|$ holds [Yos80, Chapter VIII.2, Theorems 3 and 4].

Another advantage is that we have an explicit expression for the *operator kernel* of K_E, the *Birman-Schwinger kernel*, which allows us to make explicit estimates. In general, an operator kernel K_T for an operator T is a distribution on $\mathbb{R}^d \times \mathbb{R}^d$ so that

$$(T\psi)(x) = \int_{\mathbb{R}^d} \mathrm{d}y\, K_T(x,y)\, \psi(y).$$

For the sake of brevity, we will also write $T(x,y)$ for $K_T(x,y)$. One specific example are Green's functions G which are the operator kernel to L^{-1}, i. e. if we assume the operator L is invertible and $Lu = f$, then we have

$$u(x) = \int_{\mathbb{R}^d} \mathrm{d}y\, G(x,y)\, f(y) = \big(L^{-1} f\big)(x).$$

Seeing as K_E is the product of the multiplication operator $|V|^{1/2}$ and $\big(-\Delta_x + E\big)^{-1}$, the dimension-dependent, explicit expression of Birman-Schwinger kernel involves only the Green's function of $-\Delta_x + E$ in that particular dimension,

$$K_E(x,y) = |V(x)|^{1/2} \big(-\Delta_x + E\big)^{-1}(x,y)\, |V(y)|^{1/2}.$$

In odd dimension, there exist closed expressions for $\big(-\Delta_x + E\big)^{-1}(x,y)$ while for even d, no neat formulas for it exist. Nevertheless, its behavior can be characterized.

Let us return to the original question: Can we show the *existence* of eigenvalues as well via the Birman-Schwinger principle? The answer is yes, and we will treat a particular case:

Theorem 5.2.16 ([Sim76]) *Consider the Schrödinger operator $H_\lambda = -\partial_x^2 + \lambda V$ on $L^2(\mathbb{R})$ where $\lambda > 0$ and the potential $V \neq 0$ satisfies $V \leq 0$ and*

$$\int_{\mathbb{R}} \mathrm{d}x\, \big(1 + x^2\big)\ |V(x)| < \infty.$$

Then there exists $\lambda_0 > 0$ small enough so that H_λ has exactly one eigenvalue

$$E_\lambda = -\frac{\lambda^2}{4} \left(\int_{\mathbb{R}} \mathrm{d}x\ |V(x)| \right)^2 + \mathcal{O}(\lambda^4) \tag{5.2.7}$$

for all $\lambda \in (0, \lambda_0)$.

The eigenvalue gives an intuition on the shape of the eigenfunction: it has few oscillations to minimize kinetic energy and is approximately constant in the region where V is appreciably different from 0 (this region is not too large because of the decay assumption $\int_{\mathbb{R}} \mathrm{d}x\, x^2\ |V(x)| < \infty$). Hence, the eigenfunction sees only the average value of the potential.

This intuition neither explains why other eigenvalues may appear nor that for $d \geq 3$, the theorem is false.

Proof The arguments in [Sim76, Section 2] ensure the boundedness of the Birman-Schwinger operator. Moreover, in one dimension the Green's function for $-\partial_x^2 + E$ exists ($-E \notin \sigma(-\partial_x^2)$) and can be computed explicitly, namely

$$\big(-\partial_x^2 + E\big)^{-1}(x,y) = \sqrt{2\pi}\,\big(\mathcal{F}(\xi^2+E)^{-1}\big)(x-y) = \frac{\mathrm{e}^{-\sqrt{E}|x-y|}}{2\sqrt{E}}.$$

To simplify notation, let us define $\mu := \sqrt{E}$. Thus, the Birman-Schwinger kernel is the function

$$K_{\mu^2}(x,y) = \frac{1}{2\mu}\,|V(x)|^{1/2}\,\mathrm{e}^{-\mu|x-y|}\,|V(y)|^{1/2}\,.$$

In addition, define the operators

$$L_\mu := \frac{1}{2\mu}\,\big||V|^{1/2}\big\rangle\big\langle|V|^{1/2}\big|$$

and $M_\mu := K_{\mu^2} - L_\mu$. Clearly, given that $V \in L^1(\mathbb{R})$, its square root is L^2 and L_E is a bounded rank-1 operator. Moreover, the operator kernel

$$M_\mu(x,y) = |V(x)|^{1/2}\,\frac{\mathrm{e}^{-\mu|x-y|}-1}{2\mu}\,|V(y)|^{1/2}$$

is well-defined in the limit $\mu \to 0$ and analytic for $\mu \in \mathbb{C}$ with $\operatorname{Re}\mu > 0$.

The Birman-Schwinger principle tells us that H_λ has an eigenvalue at $-\mu^2$ if and only if $1 \in \sigma_{\mathrm{p}}(K_{\mu^2})$: for $\lambda \ll 1$ small enough we have $\big\|\lambda\, M_\mu\big\| < 1$ which means the Neumann series[3]

$$\big(1-\lambda\, M_\mu\big)^{-1} = \sum_{n=0}^{\infty} \lambda^n\, M_\mu^n = 1 + \lambda\, M_\mu + \mathcal{O}(\lambda^2) \tag{5.2.8}$$

exists in $\mathcal{B}\big(L^2(\mathbb{R})\big)$. Hence, the invertibility of

$$\begin{aligned} 1 - \lambda\, K_{\mu^2} &= 1 - \lambda\, M_\mu - \lambda\, L_\mu \\ &= \big(1-\lambda\, M_\mu\big)\,\Big(1 - \lambda\,\big(1-\lambda\, M_\mu\big)^{-1}\, L_\mu\Big) \end{aligned}$$

hinges on whether 1 is an eigenvalue of

$$\lambda\,\big(1-\lambda\, M_\mu\big)^{-1}\, L_\mu = \Big|\tfrac{\lambda}{2\mu}\big(1-\lambda\, M_\mu\big)^{-1}\,|V|^{1/2}\Big\rangle\,\Big\langle|V|^{1/2}\Big|\,.$$

[3] In this context, the geometric series is usually referred to as Neumann series.

This is again a rank-1 operator, and thus, we can read off the eigenvector

$$\psi_{\lambda,\mu} = \frac{\lambda}{2\mu}\big(1-\lambda\, M_\mu\big)^{-1}\ |V|^{1/2} \in L^2(\mathbb{R})$$

to its only non-zero eigenvalue. Moreover, we can compute this eigenvalue,

$$\Big\langle |V|^{1/2},\ \tfrac{\lambda}{2\mu}\big(1-\lambda\, M_\mu\big)^{-1}\ |V|^{1/2}\Big\rangle,$$

and this is equal to 1 if and only if μ satisfies the self-consistent equation

$$\mu = G(\mu) := \frac{\lambda}{2}\,\Big\langle |V|^{1/2},\ \big(1-\lambda\, M_\mu\big)^{-1}\ |V|^{1/2}\Big\rangle.$$

Given that $\|\lambda\, M_\mu\| < 1$ for $\lambda \ll 1$ small enough, we can express $\big(1-\lambda\, M_\mu\big)^{-1}$ in terms of (5.2.8). Keeping only the first term of the expansion (5.2.8), we approximate G by the average of the potential

$$G(\mu) = \tfrac{\lambda}{2}\,\big\langle |V|^{1/2}, |V|^{1/2}\big\rangle + \mathcal{O}(\lambda^2) = \frac{\lambda}{2}\int_{\mathbb{R}} \mathrm{d}x\ |V(x)| + \mathcal{O}(\lambda^2). \tag{5.2.9}$$

Hence, $G(\mu) = \mu$ has *a* solution μ_* provided λ is small enough; additionally *any* solution to this equation satisfies $\mu^{-1} \leq C_1\,\lambda^{-1}$ for some constant $C_1 > 0$ and λ small.

Now that we know that *a* solution exists, we need to show uniqueness: Suppose we have found two solutions $\mu_1 \leq \mu_2$. Then they both solve the self-consistent equation $G(\mu_j) = \mu_j$, and assuming for a moment that G is continuously differentiable in μ, we use the fundamental theorem of calculus to obtain

$$\begin{aligned}\big|\mu_2-\mu_1\big| = \big|G(\mu_2)-G(\mu_1)\big| &= \Big|\int_{\mu_1}^{\mu_2} \mathrm{d}\mu\, \partial_\mu G(\mu)\Big| \\ &\leq \sup_{\mu\in[\mu_1,\mu_2]} \big|\partial_\mu G(\mu)\big|\,\big|\mu_2-\mu_1\big|.\end{aligned}$$

If we can show G is continuously differentiable *and* its derivative is bounded by $1/2$ for λ small enough, then the above inequality reads $\big|\mu_2-\mu_1\big| \leq \frac{1}{2}\big|\mu_2-\mu_1\big|$. This is only possible if $\mu_1 = \mu_2$, and the solution is unique.

To show the last bit, we note that M_μ and $(1-z)^{-1}$ are real-analytic in μ so that their composition $\big(1-\lambda\, M_\mu\big)^{-1}$ is also real-analytic. The analyticity of M_μ for $\mu \in \mathbb{C}$, $\operatorname{Re}\mu > 0$, also yields the bound

$$\big\|\partial_\mu M_\mu\big\| \leq C_2\,\mu^{-1} \tag{5.2.10}$$

via the Cauchy integral formula, because the maximal radius of the circular contour is less than μ.

The derivative of the resolvent can be related to $\partial_\mu M_\mu$ via the useful trick

$$\begin{aligned} 0 = \partial_\mu(\mathrm{id}) &= \partial_\mu\Big(\big(1-\lambda\, M_\mu\big)^{-1}\,\big(1-\lambda\, M_\mu\big)\Big) \\ &= \partial_\mu\big(1-\lambda\, M_\mu\big)^{-1}\,\big(1-\lambda\, M_\mu\big) + \lambda\,\big(1-\lambda\, M_\mu\big)^{-1}\,\partial_\mu M_\mu \end{aligned}$$

which yields

$$\big|\partial_\mu G(\mu)\big| = \left|\frac{\lambda^2}{2}\left\langle |V|^{1/2},\ \big(1-\lambda\, M_\mu\big)^{-1}\,\partial_\mu M_\mu\,\big(1-\lambda\, M_\mu\big)^{-1}\ |V|^{1/2}\right\rangle\right|.$$

The right-hand side can be estimated with the help of the Cauchy-Schwarz inequality

$$\ldots \leq \lambda^2\,\big\||V|^{1/2}\big\|^2_{L^2(\mathbb{R})}\,\Big\|\big(1-\lambda\, M_\mu\big)^{-1}\Big\|^2\,\big\|\partial_\mu M_\mu\big\| =: C_3\,\lambda^2\,\big\|\partial_\mu M_\mu\big\|.$$

Combining (5.2.10) with $\mu^{-1} \leq C_1\,\lambda^{-1}$ (which we obtained from $\mu = G(\mu)$), we find

$$C_3\,\lambda^2\,\big\|\partial_\mu M_\mu\big\| \leq C_3\,\lambda^2\,C_2\,\mu^{-1} \leq C_1 C_2 C_3\,\lambda.$$

Put another way, we have deduced the bound $\big|\partial_\mu G(\mu)\big| \leq C\,\lambda$ which means that for λ small enough, we can ensure that the derivative is less than $1/2$. Thus, the eigenvalue is unique and we have shown the theorem. □

The min-max principle Now that we have established criteria for the *existence* of bound states below the continuous spectrum for operators of the form $H = -\Delta_x + V$, we proceed to find other ways to give estimates of their numerical values. Crucially, we shall always assume $H \geq c$ for some $c \in \mathbb{R}$. Most of the methods of this chapter do not depend on the particular form of the hamiltonian.

So let us assume we have established the existence of a *ground state* ψ_0, i. e. there exists an eigenvalue $E_0 = \inf\sigma(H) < 0 = \inf\sigma_{\mathrm{ess}}(H)$ at the bottom of the spectrum, the *ground state energy*, whose eigenfunction is ψ_0. Then simplest estimate is obtained by minimizing the *Rayleigh quotient*

$$\frac{\mathbb{E}_\psi(H)}{\|\psi\|^2} = \frac{\langle\psi, H\psi\rangle}{\|\psi\|^2}$$

for a family of trial wave functions (see also homework problem 54). Clearly, the Rayleigh quotient is bounded from below by E_0 for otherwise, E_0 is not the infimum of the spectrum.

Proposition 5.2.17 (The Rayleigh-Ritz principle) *Let H with a densely defined, selfadjoint operator which is bounded from below, i. e. there exists $c \in \mathbb{R}$ such that $H \geq c$. Then*

$$\inf \sigma(H) \leq \frac{\langle \psi, H\psi \rangle}{\|\psi\|^2} \tag{5.2.11}$$

holds for all $\psi \in \mathcal{H} \setminus \{0\}$.

A rigorous proof of this innocent-looking fact (see e. g. [RS78, Theorem XIII.1]) requires machinery that is not yet available to us.

A non-obvious fact is that we can also give a *lower* bound on the ground state energy:

Theorem 5.2.18 (Temple's inequality, Theorem XIII.5 in [RS78]) *Let H be a selfadjoint operator that is bounded from below with ground state $E_0 \in \sigma_{\text{disc}}(H)$. Suppose in addition $E_0 < E_1$ where E_1 is either the second eigenvalue (in case more eigenvalues exist) or the bottom of the essential spectrum. Then for $\mu \in (E_0, E_1)$ and ψ with $\|\psi\| = 1$ and $\langle \psi, H\psi \rangle < \mu$, Temple's inequality holds:*

$$E_0 \geq \langle \psi, H\psi \rangle - \frac{\langle \psi, H^2\psi \rangle - \langle \psi, H\psi \rangle^2}{\mu - \langle \psi, H\psi \rangle} = \langle \psi, H\psi \rangle - \frac{\mathrm{Var}_\psi(H)}{\mu - \langle \psi, H\psi \rangle}$$

Temple's inequality gives an energy window for the ground state energy: if ψ is close to the ground state wave function, then the right-hand side is also close to E_0. On the other hand, one needs to know a lower bound on the *second* eigenvalue E_1.

Proof By assumption, E_0 is an isolated eigenvalue of finite multiplicity (otherwise $E_0 = E_1 = E_n$ for all $n \in \mathbb{N}$), and thus the operator $(H - E_0)(H - \mu) \geq 0$ is non-negative: the product is $= 0$ if applied to the ground state and > 0 otherwise because $\mu < E_1$. Consequently,

$$\big\langle \psi, (H - \mu)H\psi \big\rangle \geq E_0 \big\langle \psi, (H - \mu)\psi \big\rangle \tag{5.2.12}$$

holds which, combined with the hypothesis $\big\langle \psi, (H - \mu)\psi \big\rangle < 0$, yields

$$E_0 \geq \frac{\mu \, \langle \psi, H\psi \rangle - \big\langle \psi, H^2\psi \big\rangle}{\mu - \langle \psi, H\psi \rangle}. \qquad \square$$

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What about other bound states below the essential spectrum (the ionization threshold)? Usually, we do not know *whether* and *how many* eigenvalues exist. Nevertheless, we can define a sequence of non-decreasing real numbers that coincides with the eigenvalues if they exist: the Rayleigh quotient suggests to use

$$E_0 := \inf_{\varphi \in \mathcal{D}(H), \|\varphi\| = 1} \langle \varphi, H\varphi \rangle$$

as the definition of the ground state energy. Note that even if H does not have eigenvalues, E_0 is still well-defined and yields $\inf \sigma(H)$ (use a Weyl sequence). A priori, we do *not* know whether a E_0 is an eigenvalue, so we do not know whether an eigenvector exists. However, *if* E_0 is an eigenvalue, then the eigenvector ψ_1 to the next eigenvalue E_1 (if it exists) would necessarily have to be orthogonal to ψ_0. Then the next eigenvalue satisfies

$$E_1 = \sup_{\varphi_0 \in \mathcal{D}(H)\setminus\{0\}} \inf_{\substack{\varphi \in \mathcal{D}(H), \|\varphi\|=1 \\ \varphi \in \{\varphi_0\}^\perp}} \langle \varphi, H\varphi \rangle \,.$$

It turns out that this is the good definition even if $E_0 \notin \sigma_{\text{disc}}(H)$ is not an eigenvalue of finite multiplicity, because then $E_0 = E_1$. Quite generally, the candidate for the nth eigenvalue is

$$E_n := \sup_{\substack{\varphi_1,\ldots,\varphi_n \in \mathcal{D}(H) \\ \langle \varphi_j, \varphi_k \rangle = \delta_{jk}}} \inf_{\substack{\varphi \in \mathcal{D}(H), \|\varphi\|=1 \\ \varphi \in \{\varphi_1,\ldots,\varphi_n\}^\perp}} \langle \varphi, H\varphi \rangle \,.$$

Thus, we obtain a sequence of non-decreasing real numbers

$$E_0 \leq E_1 \leq E_2 \leq \ldots$$

which – if they exist – are the eigenvalues repeated according to their multiplicities. One can show rigorously that if $E_n = E_{n+1} = E_{n+2} = \ldots$, then $E_n = \inf \sigma_{\text{ess}}(H)$ is the bottom of the essential spectrum. Otherwise, the $E_n < \inf \sigma_{\text{ess}}(H)$ are *eigenvalues of finite multiplicity*. In that case, there are at most n eigenvalues below the essential spectrum.

One may object that quite generally, it is impossible to evaluate E_n. Here is where the *min-max principle* comes into play: assume we have chosen n trial wave functions. Then this family of trial wave functions is a good candidate for the first few eigenfunctions if the eigenvalues λ_j of the matrix $h := \Big(\big\langle \varphi_j, H\varphi_k \big\rangle\Big)_{0 \leq j,k \leq n-1}$ (ordered by size) are close to the E_j.

Theorem 5.2.19 (The min-max principle) *Suppose H is a selfadjoint operator on the Hilbert space $\mathcal{H}$ with domain $\mathcal{D}(H)$. Moreover, assume H is bounded from below. Let $\{\varphi_0, \ldots, \varphi_{n-1}\} \subset \mathcal{D}(H)$ be an orthonormal system of n functions and consider the $n \times n$ matrix*

$$h := \Big(\big\langle \varphi_j, H\varphi_k \big\rangle\Big)_{0 \leq j,k \leq n-1}$$

with eigenvalues $\lambda_0 \leq \lambda_1 \leq \ldots \leq \lambda_{n-1}$. Then we have that

$$E_j \leq \lambda_j \qquad \forall j = 0, \ldots, n-1.$$

Proof We proceed by induction over k (which enumerates the eigenvalues of h): denote the normalized eigenvector to the lowest eigenvalue λ_0 with $v_0 = \big(v_{0,0}, \dots v_{0,n-1}\big)$. Then the normalized vector $\chi_0 := \sum_{j=0}^{n-1} v_{0,j}\, \varphi_j$ satisfies

$$\lambda_0 = \big\langle v_0, h v_0 \big\rangle_{\mathbb{C}^n} = \big\langle \chi_0, H \chi_0 \big\rangle \geq E_0$$

by the Rayleigh-Ritz principle.

Now assume we have shown that $E_l \leq \lambda_l$ holds for all $l = 0, \dots, k \leq n-2$. Clearly, the eigenvectors $v_0, \dots, v_k$ to h, and the space spanned by the corresponding normalized $\chi_l = \sum_{j=0}^{n-1} v_{l,j}\, \varphi_j$ is $k+1$-dimensional. Hence, for any

$$\chi = \sum_{j=0}^{n-1} w_j\, \chi_j \in \big\{\chi_0, \dots, \chi_k\big\}^\perp$$

with coefficients $w \in \{v_0, \dots, v_k\}^\perp$ we obtain

$$\langle w, h w \rangle = \langle \chi, H \chi \rangle \geq E_{k+1}$$

because χ is orthogonal to a $k+1$-dimensional subspace of $\mathcal{D}(H)$. The left-hand side can be minimized by setting $w = v_{k+1}$, the eigenvector to λ_{k+1}, and thus, $E_{k+1} \leq \lambda_{k+1}$. This concludes the proof. □

One can use the min-max principle to make the following intuition rigorous: Assume one is given an operator $H(V) = -\Delta_x + V$ whose potential vanishes sufficiently rapidly at ∞, and one knows that $H(V)$ has a certain number of negative eigenvalues $\{E_j(V)\}_{j \in \mathcal{I}}$, $\mathcal{I} \subseteq \mathbb{N}_0$. The decay conditions on V ensure $\sigma_{\text{ess}}\big(H(V)\big) = [0, +\infty)$. Then if $W \leq V$ is a second potential of the same type, the min-max principle implies

$$E_j(W) \leq E_j(V).$$

In particular, $H(W)$ has *at least* as many eigenvalues as $H(V)$. This fact combined with Theorem 5.2.16 immediately yields

Corollary 5.2.20 *Suppose we are in the setting of Theorem 5.2.16. Then even if V does not have a fixed sign, as long as $\int_{\mathbb{R}} \mathrm{d}x\, V(x) \leq 0$ for all $\lambda > 0$ the Schrödinger operator $H = -\partial_x^2 + \lambda V$ has at least one eigenvalue $E_0 < 0$.*

5.2.3 Perturbations of selfadjoint operators

Earlier, we have discussed the spectral properties of the hamiltonian H_C (5.2.4) which describes a hydrogen atom. We have pretended to know that the hamilton operator for

the hydrogen atom is selfadjoint – as if that is a foregone conclusion. So let us investigate this question, and consider the operator

$$H_C := -\tfrac{1}{2}\Delta_x - \tfrac{1}{|x|}$$

equipped with domain $\mathcal{D}(H_C) := \mathcal{C}_c^\infty(\mathbb{R}^3 \setminus \{0\})$. Here, we have excluded the origin because the Coulomb potential diverges at this point. So is H_C essentially selfadjoint? Before we proceed, let us note that we can rewrite H_C in polar coordinates, and given that the potential depends only on $|x|$, we obtain a free angular part and a Schrödinger operator $-\frac{1}{2}\partial_r^2 - r^{-1}\,\partial_r - r^{-1}$ on the line $\mathbb{R}^+$ for the radial part – and the definition of operators on the half line depends very delicately on the behavior at the boundary point 0.

Instead of checking the essential selfadjointness of H_C, we look at the simpler problem of the selfadjointness of $H_0 := -\frac{1}{2}\Delta_x$ on $\mathcal{C}_c^\infty(\mathbb{R}^3 \setminus \{0\})$ – and if that operator is not essentially selfadjoint, then this indicates that H_C cannot be essentially selfadjoint either. According to the fundamental criterion we need to solve

$$-\tfrac{1}{2}\Delta_x \phi_\pm = \mp \mathrm{i}\phi_{pm},$$

because surely $H_0^* = -\frac{1}{2}\Delta_x$ should hold in a suitable sense. Later on, we need to show that the solutions $\phi_\pm$ lie in the domain $\mathcal{D}(H_0^*)$. Rewriting the above in polar coordinates yields the equation

$$\big(-\tfrac{1}{2}\partial_r^2 - r^{-1}\,\partial_r\big)\phi_\pm(r) = \mp\mathrm{i}\phi_\pm(r),$$

and one can check that

$$\phi_\pm(r) = \frac{\mathrm{e}^{-(1\mp\mathrm{i})r}}{r}$$

are solutions. Evidently, $\phi_\pm \in L^2(\mathbb{R}^3)$ holds since the Coulomb singularity is locally L^2 in three dimensions and the functions decay exponentially at ∞. However, we still need to verify that $\phi_\pm \in \mathcal{D}(H_0^*)$: keeping in mind $\psi(0) = 0$ for $\psi \in \mathcal{C}_c^\infty(\mathbb{R}^3 \setminus \{0\})$ we can use partial integration to obtain

$$\begin{aligned}
\big\langle \phi_\pm, H_0\psi\big\rangle &= -\frac{1}{2}\int_{\mathbb{R}^3} \mathrm{d}x\, \overline{\phi_\pm(x)}\,\Delta_x\psi(x) \\
&= -\frac{1}{2}\int_{\mathbb{S}^2} \mathrm{d}\omega \int_0^{+\infty} \mathrm{d}r\, \overline{\phi_\pm(r)}\,\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{2}{r}\,\frac{\mathrm{d}}{\mathrm{d}r} + \frac{1}{r^2}\Delta_\omega\right)\psi(r,\omega) \\
&= -\frac{1}{2}\int_{\mathbb{S}^2} \mathrm{d}\omega \int_0^{+\infty} \mathrm{d}r\, \overline{\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{2}{r}\,\frac{\mathrm{d}}{\mathrm{d}r} + \frac{1}{r^2}\Delta_\omega\right)\phi_\pm(r)}\,\psi(r,\omega) \\
&= -\frac{1}{2}\int_{\mathbb{S}^2} \mathrm{d}\omega \int_0^{+\infty} \mathrm{d}r\, \overline{\mp\mathrm{i}\,\phi_\pm(r)}\,\psi(r,\omega) = \big\langle \mp\mathrm{i}\phi_\pm, \psi\big\rangle.
\end{aligned}$$

That means $\phi_\pm$ lie in the domain of the adjoint H_0^* and $H_0^*\phi_\pm = \mp \mathrm{i}\phi_\pm$. Hence, the defect indices $N_\pm \geq 1$ are non-zero and the operator cannot be essentially selfadjoint. Consequently, we reckon that also H_C is not essentially selfadjoint, and a more careful analysis bears this out. However, there exists a whole *family* of selfadjoint extensions, each of which generates its own dynamics – and one can show that only one generates the dynamics observed in nature.

The correct idea here is to think of the Coulomb potential as a *perturbation* of the kinetic energy $H_0 = -\frac{1}{2}\Delta_x$ with domain

$$H^2(\mathbb{R}^d) = \left\{\varphi \in L^2(\mathbb{R}^d) \;\middle|\; -\Delta_x\varphi \in L^2(\mathbb{R}^d)\right\}.$$

For two reasons, this is problematic: first of all, we are adding the two unbounded operators H_0 and $-1/|x|$, and we inevitably have to deal with domain questions. The second one is of physical significance: we are adding the non-negative kinetic energy operator $H_0 \geq 0$ to the *non-positive* attractive Coulomb potential $-1/|x| \leq 0$, will the sum be bounded from below, i. e. $H_C \geq -K$ for some $K > 0$? Physically, that is important, because if H_C were not bounded from below, the hydrogen atom *would not be stable!* The hydrogen atom could lose energy by radiating off photons *ad infinitum*, and the electron falls down the well. In fact, this is what happens classically! Fortunately, the (quantum) hydrogen atom is stable, because states with low potential energy (i. e. those increasingly localized around the origin) have to pay an increasing price in kinetic energy. One can see that the sum should be bounded from below by the simple scaling argument made around equation (5.2.5): for λ the kinetic energy scales as λ^2 while the potential energy scales as λ, i. e. $k\lambda^2 - p\lambda \geq$ const.

The way to solve both problems at the same time is as follows:

Definition 5.2.21 (Relative boundedness) *Let A and B be two densely defined operators, and suppose*

(i) $\mathcal{D}(A) \subseteq \mathcal{D}(B)$ *and*

(ii) there are constants $a, b \in \mathbb{R}$ so that for all $\varphi \in \mathcal{D}(A)$ we have

$$\|B\varphi\| \leq a\, \|A\varphi\| + b\, \|\varphi\| \tag{5.2.13}$$

for all $\varphi \in \mathcal{D}(A)$.

Then B is A-bounded, and the infimum over all a which satisfy (5.2.13) *is called the* relative bound*. In case the relative bound is 0, then B is called* infinitesimally A-bounded*.*

2014.10.31 Note that in the above reducing the size of a usually requires one to make b larger.

Remark 5.2.22 Instead of (5.2.13), one can also use the equivalent condition

$$\|B\varphi\|^2 \leq \tilde{a}^2\, \|A\varphi\|^2 + \tilde{b}^2\, \|\varphi\|^2$$

to define relative boundedness, and yield also the same relative bound.

Theorem 5.2.23 (Kato-Rellich) *Let H be selfadjoint, and V be symmetric and H-bounded with relative bound $a < 1$. Then $H + V$ equipped with domain $\mathcal{D}(H + V) = \mathcal{D}(H)$ is selfajoint and essentially selfadjoint on any core of H.*

Proof We will show that ran $\big(H + V \pm \mathrm{i}\mu_0\big) = \mathcal{H}$ holds for some $\mu_0 > 0$ and use the fundamental criterion of selfajointness. Then the selfadjointness of $\frac{1}{\mu_0}\big(H + V\big)$ on $\mathcal{D}(H)$ follows from the fundamental criterion of selfadjointness (Theorem 5.2.4), meaning that in this case also $H + V$ is selfadjoint on $\mathcal{D}(H)$.

For $\varphi \in \mathcal{D}(H)$ and $\mu > 0$ we have again

$$\big\|(H + \mathrm{i}\mu)\varphi\big\|^2 = \big\|H\varphi\big\|^2 + \mu^2\|\varphi\|^2.$$

Since H is selfadjoint, the vector $\varphi = (H + \mathrm{i}\mu)^{-1}\psi$ exists for all $\psi \in \mathcal{H}$, which leads to $\big\|H\,(H + \mathrm{i}\mu)^{-1}\big\| \leq 1$ and $\big\|(H + \mathrm{i}\mu)^{-1}\big\| \leq \mu^{-1}$ (Corollary 5.2.13). Plugging $\varphi = (H + \mathrm{i}\mu)^{-1}\psi$ into (5.2.13) yields the estimate

$$\big\|V(H + \mathrm{i}\mu)^{-1}\psi\big\| \leq a\,\big\|H\,(H + \mathrm{i}\mu)^{-1}\psi\big\| + b\,\big\|(H + \mathrm{i}\mu)^{-1}\psi\big\| \leq \big(a + {}^{b}\!/_{\mu}\big)\,\|\psi\|.$$

Given that $a < 1$ and b is fixed we know that for sufficiently large μ the operator norm of $T := V(H + \mathrm{i}\mu)^{-1}$ is necessarily less than 1. Hence, the inverse of $\mathrm{id} + T$ exists as the bounded operator $(\mathrm{id} + T)^{-1} = \sum_{n=0}^{\infty}(-1)^n\,T^n$ (cf. problem 18 (iii)). That also means ran $(\mathrm{id} + T) = \mathcal{H}$. Combined with one of the consequences of $H^* = H$, namely ran $(H + \mathrm{i}\mu) = \mathcal{H}$, and with the equation

$$\big(\mathrm{id} + T\big)\,\big(H + \mathrm{i}\mu\big)\varphi = \big(H + V + \mathrm{i}\mu\big)\varphi, \qquad\qquad \forall\varphi \in \mathcal{D}(H),$$

we conclude ran $(H + V + \mathrm{i}\mu) = \mathcal{H}$. Analogously, we show ran $(H + V - \mathrm{i}\mu) = \mathcal{H}$.

It remains to show that $H + V$ with domain $\mathcal{D}(H)$ is closed. But this follows from a Cauchy sequence argument, the closedness of H and (5.2.13). Thus, $H + V$ is selfadjoint on $\mathcal{D}(H)$ by the Fundamental Criterion of Selfajointness 5.2.4.

Now let $\mathcal{D}_0 \subseteq \mathcal{D}(H)$ be a core of H. Then using (5.2.13) it is easy to show that $\overline{\Gamma\big(H|_{\mathcal{D}_0}\big)} = \Gamma(H)$ implies $\overline{\Gamma\big((H + V)|_{\mathcal{D}_0}\big)} = \Gamma\big((H+V)|_{\mathcal{D}(H)}\big)$. And hence, any core of H is also a core of $H + V$. □

We will apply the Kato-Rellich Theorem to Schrödinger operators. While there are many more general results than this one, these are usually harder to prove and – in view of the hydrogen atom hamiltonian – not necessary here. Here, we view $H = -\Delta_x + V$ as perturbations of the free Schrödinger operator $H_0 := -\Delta_x$ whose domain $\mathcal{D}(H_0) := H^2(\mathbb{R}^d)$ is the 2nd *Sobolev space*:

Definition 5.2.24 (Sobolev space) *We define $H^m(\mathbb{R}^d)$ as the Hilbert space*

$$H^m(\mathbb{R}^d) := \Big\{\varphi \in L^2(\mathbb{R}^d) \;\Big|\; \mathcal{F}^{-1}\,\sqrt{1 + \xi^2}^{\,m}\,\mathcal{F}\varphi \in L^2(\mathbb{R}^d)\Big\}$$

endowed with scalar product

$$\langle \varphi, \psi \rangle_{H^m} := \int_{\mathbb{R}^d} \mathrm{d}\xi \left(1 + |\xi|^2\right)^m \overline{\mathcal{F}\varphi(\xi)}\, \mathcal{F}\psi(\xi)$$

where $\mathcal{F} : L^2(\mathbb{R}^d) \longrightarrow L^2(\mathbb{R}^d)$ is the Fourier transform.

In three dimensions, we will now prove a selfadjointness result which includes the Coulomb potential:

Theorem 5.2.25 *Suppose $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ (meaning $V = V_1 + V_2$ where $V_1 \in L^2(\mathbb{R}^3)$ and $V_2 \in L^\infty(\mathbb{R}^3)$) is a real-valued function. Then V is infinitesimally H_0-bounded and hence, the operator*

$$H = -\Delta_x + V$$

equipped with domain $\mathcal{D}(H) = \mathcal{D}(H_0) = H^2(\mathbb{R}^3)$ is selfadjoint.

The crucial estimate is the content of the following

Lemma 5.2.26 *For every $a > 0$ there exists $b > 0$ such that*

$$\|\varphi\|_{L^\infty} \leq a \left\|\Delta_x \varphi\right\|_{L^2} + b \|\varphi\|_{L^2} \tag{5.2.14}$$

holds for all $\varphi \in H^2(\mathbb{R}^3)$.

Proof Using the Riemann-Lebesgue Lemma and the Cauchy-Schwarz inequality, we deduce

$$\begin{aligned} \|\varphi\|_{L^\infty} &\leq (2\pi)^{+3/2} \left\|\mathcal{F}\varphi\right\|_{L^1} = (2\pi)^{+3/2} \left\|(1+\xi^2)^{-1}\,(1+\xi^2)\mathcal{F}\varphi\right\|_{L^1} \\ &\leq (2\pi)^{+3/2} \left\|(1+\xi^2)^{-1}\right\|_{L^2} \left\|(1+\xi^2)\mathcal{F}\varphi\right\|_{L^2}. \end{aligned}$$

Given that we are in three dimensions, $\left\|(1+\xi^2)^{-1}\right\|_{L^2}$ is finite. Moreover, the other factor is finite by definition of $H^2(\mathbb{R}^3)$. Overall, we have shown

$$\|\varphi\|_{L^\infty} \leq c\big(\left\|\xi^2\,\mathcal{F}\varphi\right\|_{L^2} + \left\|\mathcal{F}\varphi\right\|_{L^2}\big) \tag{5.2.15}$$

where c is independent of φ. Now define $\hat{\varphi}_\lambda(\xi) := \lambda^3\,\mathcal{F}\varphi(\lambda\xi)$ for $\lambda > 0$. Then this scaling preserves the L^1-norm, $\|\hat{\varphi}_\lambda\|_{L^1} = \|\mathcal{F}\varphi\|_{L^1}$, but the two terms to the right of the inequality scale differently, namely

$$\begin{aligned} \|\hat{\varphi}_\lambda\|_{L^2} &= \lambda^{3/2} \|\mathcal{F}\varphi\|_{L^2}, \\ \left\|\xi^2\,\hat{\varphi}_\lambda\right\|_{L^2} &= \lambda^{-1/2} \left\|\xi^2\,\mathcal{F}\varphi\right\|_{L^2}. \end{aligned}$$

Plugged into (5.2.15) we obtain

$$\|\varphi\|_{L^\infty} \leq (2\pi)^{-3/2} \|\hat{\varphi}_\lambda\| \leq c\lambda^{-1/2} \left\|\xi^2 \mathcal{F}\varphi\right\|_{L^2} + c\lambda^{3/2} \|\mathcal{F}\varphi\|_{L^2},$$

and consequently, we can make the first constant $c\lambda^{-1/2}$ as small as we would like (at the expense of the second constant) by choosing λ large enough. This finishes the proof. □

Proof (Theorem 5.2.25) As a real-valued multiplication operator, V defined on the maximal domain

$$\mathcal{D}(V) = \left\{\varphi \in L^2(\mathbb{R}^3) \;\middle|\; V\varphi \in L^2(\mathbb{R}^3)\right\}$$

is symmetric (even selfadjoint). So let $V = V_1 + V_2$ with $V_1 \in L^2(\mathbb{R}^3)$ and $V_2 \in L^\infty(\mathbb{R}^3)$. Then for any $\varphi \in H^2(\mathbb{R}^3)$ we can use the splitting of the potential to obtain the estimate

$$\|V\varphi\|_{L^2} \leq \|V_1\|_{L^2} \|\varphi\|_{L^\infty} + \|V_2\|_{L^\infty} \|\varphi\|_{L^2},$$

which in view of Lemma 5.2.26 yields $H^2(\mathbb{R}^3) \subseteq \mathcal{D}(V)$. In fact, for any $a > 0$ there exists $b > 0$ such that

$$\|V\varphi\|_{L^2} \leq a\|V_1\|_{L^2} \|H_0\varphi\|_{L^2} + \left(b + \|V_2\|_{L^\infty}\right) \|\varphi\|_{L^2}$$

holds true, i. e. V is infinitesimally H_0-bounded. Then Kato-Rellich's theorem 5.2.23 implies $H = -\Delta_x + V$ defines a selfadjoint operator on $\mathcal{D}(H) = H^2(\mathbb{R}^3)$. □

Corollary 5.2.27 (Selfadjointness of hydrogen hamiltonian H_C) *In three dimensions the operator $H_C = -\frac{\hbar^2}{2m}\Delta_x - \frac{e^2}{|x|}$ defines a selfadjoint operator on $\mathcal{D}(H_C) = H^2(\mathbb{R}^3)$.*

Proof We merely have to split the Coulomb potential into a contribution around the origin,

$$V_1(x) := \begin{cases} -\frac{e}{|x|} & |x| \leq 1 \\ 0 & |x| > 1 \end{cases},$$

and a remainder $V_2 := V - V_1$. Clearly, V_2 is bounded and V_1 is square-integrable in three dimensions. That means Theorem 5.2.25 applies and H_C is selfadjoint on $\mathcal{D}(H_C) = H^2(\mathbb{R}^3)$. □

Chapter 6

6 Functional calculus and applications

The main purpose of this chapter is to attribute meaning to the expression $f(H)$ for self-adjoint operators H and suitable functions $f : \mathbb{R} \longrightarrow \mathbb{C}$. For hermitian $n \times n$ matrices H with eigenvalues $E_j \in \sigma(H)$ and associated projections P_j onto the eigenspaces, the answer is

$$f(H) := \sum_j f(E_j)\, P_j.$$

There are several complications we need to overcome:

(i) The spectrum of hermitian $n \times n$ matrices is finite and purely discrete, i. e. finitely many eigenvalues of finite multiplicity.

(ii) Matrices define bounded operators.

(iii) Operators on infinite-dimensional spaces may have continuous spectrum, meaning there exist no eigenfunctions in the Hilbert space. Hence, it is not clear in what sense the associated projections exist.

The most important examples for functions are $f(\lambda) = \mathrm{e}^{-\mathrm{i}t\lambda}$ to define the unitary evolution group. Spectral projections are defined in terms of characteristic functions

$$1_\Lambda(x) := \begin{cases} 1 & x \in \Lambda \\ 0 & x \notin \Lambda \end{cases}$$

which are constant and equal to 1 on some $\Lambda \subset \mathbb{R}$ and are 0 outside of Λ. And often smoothened characteristic functions are considered.

6.1 Functional calculus

Before we begin with the functional calculus itself, we will briefly recap measure theory, a necessary prerequisite if one wants to correctly understand all the mathematical objects.

6.1.1 Primer on measure theory

To understand functional calculus, one needs a bit of measure theory. So we will give a very quick primer on measure theory, partly to fix notation, partly to introduce the most important concepts. For a proper introduction we refer the interested reader to [LL01, Chapter 1] and references therein.

Definition 6.1.1 (σ algebra and measurable space) *Let Ω be a set and $\Sigma \subset P(\Omega)$ where $P(\Omega)$ is the power set of Ω, i. e. the set of all subsets. If*

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

(ii) $\Lambda \in \Sigma \Rightarrow \Omega \setminus \Lambda \in \Sigma$, *and*

(iii) $\Lambda_1, \Lambda_2, \ldots \in \Sigma \Rightarrow \bigcup_{n=1}^{\infty} \Lambda_n \in \Sigma$,

then Σ is called a σ algebra. *The pair (Ω, Σ) is called* measurable space, *and elements of Σ are* measurable sets.

One easily sees from the definition that countable intersections of measurable sets are again measurable, and that $\Omega \in \Sigma$. Moreover, arbitrary intersections $\bigcap_{n\in\mathcal{I}} \Sigma_n$ of σ algebras $\Sigma_n \subset P(\Omega)$ are again σ algebras. Since the power set $P(\Omega)$ itself is a σ algebra, to each $E \in P(\Omega)$ there exists a smallest σ algebra $\sigma(E)$ which contains E. This is the σ algebra generated by E. In case Ω is a *metric* space, the σ algebra generated by the open sets is called *Borel-σ algebra*.

A measure μ on a measurable space (Ω, Σ) associates a non-negative number to each measurable set $\Lambda \in \Sigma$:

Definition 6.1.2 (Measure and measure space) *Let (Ω, Σ) be a measurable space. A map $\mu : \Sigma \longrightarrow [0, +\infty) \cup \{+\infty\}$ is called* measure *if*

(i) $\mu(\emptyset) = 0$ *and*

(ii) μ *is σ-additive, i. e. for all pairwise disjoint $\Lambda_1, \Lambda_2, \ldots \in \Sigma$ we have*

$$\mu\Big(\bigcup_{n=1}^{\infty} \Lambda_n\Big) = \sum_{n=1}^{\infty} \mu(\Lambda_n).$$

The triple (Ω, Σ, μ) is called measure space. *In case $\mu(\Omega) < \infty$, the measure is called finite, and if $\mu(\Omega) = 1$, μ is a* probability measure.

If $\Omega = \bigcup_{n=1}^{\infty} \Lambda_n$ can be seen as the countable union of sets of finite measure, $\mu(\Lambda_n) < \infty$ for all $n \in \mathbb{N}$, then μ is called σ-finite. The prototypical example is the measure space $\big(\mathbb{R}, \mathcal{B}(\mathbb{R}), \lambda\big)$ where $\mathcal{B}(\mathbb{R})$ is the Borel-σ algebra on $\mathbb{R}$ and λ the Lebesgue measure. Obviously, λ is not finite, but it is σ-finite.

Definition 6.1.3 (Measurable function) *Let (Ω_j, Σ_j), $j = 1, 2$, be measurable spaces. A function $f : \Omega_1 \longrightarrow \Omega_2$ is called measurable if and only if preimages of measurable sets are measurable, i. e. $f^{-1}(B) \in \Sigma_1$ for all $B \in \Sigma_2$.*

For a given measure space (Ω, Σ, μ) one can construct a notion of integration, and the construction mimics that of $L^1(\mathbb{R}^d)$: first, one defines simple functions

$$f(\omega) = \sum_{j=1}^{n} c_j \, 1_{\Lambda_j}(\omega)$$

where the $\Lambda_j \in \Sigma$ are measurable sets and 1_{Λ_j} the indicator function for Λ_j, and then defines

$$\int_\Omega \mathrm{d}\mu \, f := \sum_{j=1}^{n} c_j \, \mu(\Lambda_j).$$

Because any *measurable* function f can be approximated arbitrarily well by simple functions from below, we can define the integral via the limit procedure

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

where each of the f_n is a simple function. That gives rise to spaces such as $L^1(\Omega)$, $L^2(\Omega)$ and $L^\infty(\Omega)$, e. g. a measurable function $f : \Omega \longrightarrow \mathbb{C}$ is in $L^1(\Omega)$ if and only if

$$\|f\|_{L^1(\Omega)} := \int_\Omega \mathrm{d}\mu \, |f| < \infty.$$

Similarly, one can define

$$L^2(\Omega) := \Big\{ f : \Omega \longrightarrow \mathbb{C} \text{ measurable } \Big| \int_\Omega \mathrm{d}\mu \, |f(\mu)|^2 < \infty \Big\}$$

and endow it with a scalar product

$$\langle f, g \rangle_{L^2(\Omega)} := \int_\Omega \mathrm{d}\mu \, \overline{f(\omega)} \, g(\omega).$$

In case μ is σ-finite, one can show that $L^2(\Omega)$ is separable. 2014.11.07

There is a very fundamental theorem about Borel measures on $\mathbb{R}$:

Theorem 6.1.4 (Decomposition of Borel measures) *Any Borel measure μ on $\mathbb{R}$ can be uniquely decomposed*

$$\mu = \mu_{\mathrm{pp}} + \mu_{\mathrm{ac}} + \mu_{\mathrm{sc}}$$

into a point measure μ_{pp}, an absolutely continuous measure μ_{ac} and a singularly continuous measure μ_{sc}.

The prototypical point measure is the Dirac measure $\delta(\cdot - y)$ for which

$$\int_{\mathbb{R}} \mathrm{d}\delta(x-y)\, f(x) = f(y).$$

A measure is absolutely continuous if there exists a *density* $\rho(x)$ (which is an absolutely continuous function, cf. [Tes09, Chapter 2.7]) so that

$$\mathrm{d}\mu_{\mathrm{ac}}(x) = \rho(x)\,\mathrm{d}x.$$

Finally, singularly continuous measures are those which are not point measures (meaning $\mu_{\mathrm{sc}}(\{x\}) = 0$ for all $x \in \mathbb{R}$) and for which there exists a measurable set $S \in \mathcal{B}(\mathbb{R})$ so that $\mu_{\mathrm{sc}}(S) = 0$ but $\lambda(\mathbb{R} \setminus S) = 0$ (λ being the Lebesgue measure). For most physical application, though, $\mu_{\mathrm{sc}} = 0$.

6.1.2 Herglotz functions

One way to define functional calculus is by means of *Herglotz functions*, i. e. holomorphic functions $F : \mathbb{C}^+ \longrightarrow \mathbb{C}^+$ which map the upper complex half plane into itself. This is because the expectation values of *resolvents of selfadjoint operators* H are Herglotz functions: clearly, the function

$$F_\psi(z) := \big\langle \psi, (H-z)^{-1}\psi \big\rangle \tag{6.1.1}$$

is holomorphic on the upper half plane $\mathbb{C}^+$ because $\sigma(H) \subseteq \mathbb{R}$ (Theorem 5.2.11) and $(H - z)^{-1}$ can be locally expanded around a $z_0 \in \mathbb{C}^+$ in terms of $(H - z_0)^{-1}$. Hence, for $z \in \mathbb{C}^+$ (i. e. $\operatorname{Im} z > 0$), we deduce that F_ψ is well-defined on $\mathbb{C}^+$

$$\big|F_\psi(z)\big| \leq \big\|(H-z)^{-1}\big\|\, \|\psi\|^2 \leq \frac{\|\psi\|^2}{\operatorname{Im} z}$$

where the last equality is due to the resolvent estimate (5.2.3). Moreover, $\big((H-z)^{-1}\big)^* = (H - \bar{z})^{-1}$ implies

$$\begin{aligned}\overline{F_\psi(z)} &= \overline{\langle \psi, (H-z)^{-1}\psi\rangle} = \big\langle (H-z)^{-1}\psi, \psi\big\rangle \\ &= \big\langle \psi, (H-\bar{z})^{-1}\psi\big\rangle = F_\psi(\bar{z}).\end{aligned}$$

This, combined with the resolvent identity

$$(H-z)^{-1}-(H-z')^{-1}=(z-z')\,(H-z)^{-1}\,(H-z')^{-1}$$

yields that F_ψ maps $\mathbb{C}^+$ to $\mathbb{C}^+$ as long as $\psi\neq 0$,

$$\operatorname{Im} F_\psi(z)=\frac{1}{\mathrm{i}2}\big(F_\psi(z)-\overline{F_\psi(z)}\big)=\operatorname{Im} z\,\big\|(H-z)^{-1}\psi\big\|^2>0.$$

Now the representation theorem for Herglotz functions (see Theorem 6.1.6 below) entails that there exists a unique Borel measure $\mu_\psi(z)$ on $\mathbb{R}$ called the *spectral measure* of H associated with ψ such that

$$F_\psi(z)=\int_{\mathbb{R}}\mathrm{d}\mu_\psi(\lambda)\,(\lambda-z)^{-1}.$$

We will give two different representation theorems for Herglotz functions, the first of which can be found in [DK05, Chapter 1.4].

Theorem 6.1.5 (Representation theorem 1 for Herglotz functions) *Any Herglotz function $F:\mathbb{C}^+\longrightarrow\mathbb{C}^+$ admits the representation*

$$F(z)=a\,z+b+\int_{\mathbb{R}}\mathrm{d}\mu(\lambda)\,\left(\frac{1}{\lambda-z}-\frac{\lambda}{1+\lambda^2}\right)$$

with some $a>0$, $b\in\mathbb{R}$, and a Borel measure μ on $\mathbb{R}$ satisfying $\int_{\mathbb{R}}\mathrm{d}\mu(\lambda)\,(1+\lambda^2)^{-1}<\infty$. The measure can be recovered from F via

$$\frac{1}{2}\Big(\mu\big(\lambda_1,\lambda_2\big)+\mu\big([\lambda_1,\lambda_2]\big)\Big)=\lim_{\varepsilon\searrow 0}\frac{1}{\pi}\int_{\lambda_1}^{\lambda_2}\mathrm{d}\lambda\operatorname{Im}F(\lambda+\mathrm{i}\varepsilon)$$

Herglotz functions naturally arise in spectral theory as the *Borel-Stieltjes transformation*

$$F(z):=\int_{\mathbb{R}}\frac{\mathrm{d}\mu(\lambda)}{\lambda-z}\tag{6.1.2}$$

of finite Borel measures μ on $\mathbb{R}$, and the relation between the two can be summed up as follows: 2014.11.11

Theorem 6.1.6 (Representation theorem 2 for Herglotz functions ([Tes09])) *The Borel-Stieltjes transform of any finite Borel measure μ is a Herglotz function satisfying*

$$|F(z)|\leq\frac{\mu(\mathbb{R})}{\operatorname{Im}z},\qquad\qquad z\in\mathbb{C}^+.$$

Conversely, if F is a Herglotz function satisfying

$$|F(z)| \leq \frac{C}{\operatorname{Im} z}$$

on $\mathbb{C}^+$ for some $C > 0$, then there exists a unique Borel measure μ with $\mu(\mathbb{R}) \leq C$ and F is its Borel-Stieltjes transform.

With these pieces in hand, we can proceed to define functional calculus.

6.1.3 Functional calculus and the spectral theorem

This subsection will introduce and prove the *two main theorems* of this Chapter: *functional calculus* for selfadjoint operators and the *spectral theorem*. From the previous Chapter, we know that to any selfadjoint operator H and $\psi \in \mathcal{H}$ there exists a bounded Borel measure μ_ψ on $\mathbb{R}$ which is related to $F_\psi(z) = \langle \psi, (H-z)^{-1}\psi \rangle$ via the Borel-Stieltjes transform (6.1.2). With the help of the polarization identity,

$$\begin{aligned}\big\langle \varphi, (H-z)^{-1}\psi \big\rangle &= \\ &= \frac{1}{4}\Big(\Big\langle (\varphi+\psi), (H-z)^{-1}(\varphi+\psi) \Big\rangle + \Big\langle (\varphi-\psi), (H-z)^{-1}(\varphi-\psi) \Big\rangle + \\ &\qquad -\mathrm{i}\Big\langle (\varphi+\mathrm{i}\,\psi), (H-z)^{-1}(\varphi+\mathrm{i}\psi) \Big\rangle - \mathrm{i}\Big\langle (\varphi-\mathrm{i}\,\psi), (H-z)^{-1}(\varphi-\mathrm{i}\psi) \Big\rangle \Big),\end{aligned} \tag{6.1.3}$$

we can define a complex finite Borel measure $\mu_{\varphi,\psi}$ such that

$$\big\langle \varphi, (H-z)^{-1}\psi \big\rangle = \int_{\mathbb{R}} \mathrm{d}\mu_{\varphi,\psi}(\lambda)\, (\lambda - z)^{-1}.$$

For any bounded Borel function $f : \mathbb{R} \longrightarrow \mathbb{C}$ this complex finite Borel measure, in turn, uniquely defines a bounded operator $f(H)$: given that for bounded Borel functions the integral

$$s_f(\psi) := \int_{\mathbb{R}} \mathrm{d}\mu_\psi(\lambda)\, f(\lambda)$$

exists, we can use polarization to define

$$\langle \varphi, f(H)\psi \rangle = \int_{\mathbb{R}} \mathrm{d}\mu_{\varphi,\psi}(\lambda)\, f(\lambda) \tag{6.1.4}$$

where $\mu_{\varphi,\psi}$ is the complex finite Borel measure defined above. As indicated by the notation, the existence of the matrix elements combined with an estimate of the form

$$\big|\langle \varphi, f(H)\psi \rangle\big| \leq C\, \|\varphi\|\, \|\psi\| \tag{6.1.5}$$

suffices to show the existence of $f(H)$ as a bounded operator (see e. g. [Tes09, Corollary 1.9]):

Lemma 6.1.7 *To each bounded Borel function $f : \mathbb{R} \longrightarrow \mathbb{C}$ there exists a unique bounded operator $f(H)$ such that* (6.1.4) *holds. Moreover, we can bound the operator norm by $\|f(H)\| \leq \|f\|_{L^\infty}$.*

Proof First of all, operators $f(H)$ are uniquely determined by their "diagonal matrix elements", meaning if we can show $|s_f(\psi)| \leq C\|\psi\|^2$ for some $C > 0$, then also the sesquilinear form $s_f(\varphi, \psi)$ obtained by polarization (see (6.1.3)) satisfies

$$\left|s_f(\varphi, \psi)\right| \leq C'\|\varphi\| \, \|\psi\|$$

for some constant $C' > 0$. The estimate for diagonal elements is straightforward, though, because the Representation Theorem 6.1.6 tells us that $\mu_\psi(\mathbb{R}) = \|\psi\|^2$ and thus, we obtain

$$|s_f(\psi)| \leq \int_{\mathbb{R}} \mathrm{d}\mu_\psi(\lambda) \; |f(\lambda)| \leq \|f\|_{L^\infty} \, \mu_\psi(\mathbb{R}) = \|f\|_{L^\infty} \, \|\psi\|^2$$

for all $\psi \in \mathcal{H}$. Then [Tes09, Corollary 1.9] states there exists a *unique* and *bounded* operator which we will denote with $f(H)$ so that

$$s_f(\varphi, \psi) = \langle \varphi, f(H)\psi \rangle \, .$$

This finishes the proof. □

The first main theorem, the *functional calculus* characterizes properties of this operator $f(H)$:

Theorem 6.1.8 (Functional Calculus for selfadjoint operators) *Let H be a selfadjoint operator on a Hilbert space $\mathcal{H}$, and suppose f and g are bounded Borel functions. Then the operator $f(H)$ constructed in Lemma 6.1.7 has the following properties:*

(i) The map $f \mapsto f(H)$ from the bounded Borel functions to $\mathcal{B}(\mathcal{H})$ is a $*$-homomorphism, i. e.

$$\begin{aligned} (f + \alpha g)(H) &= f(H) + \alpha \, g(H), \\ (f \, g)(H) &= f(H) \, g(H), \\ 1_{\mathbb{R}}(H) &= \mathrm{id}_{\mathcal{H}}, \\ f(H)^* &= \bar{f}(H). \end{aligned}$$

(ii) If $f_n(x) \to f(x)$ pointwise, and if the sequence $\|f_n\|_{L^\infty(\mathbb{R})}$ is bounded, then $f_n(H)$ converges to $f(H)$ strongly (cf. Definition 4.3.2).

(iii) If $H\psi = E\psi$, then $f(H)\psi = f(E)\,\psi$.

(iv) $f \geq 0 \Rightarrow f(H) \geq 0$

(v) If in addition $f \in \mathcal{C}\big(\sigma(H)\big)$*, then* $\big\|f(H)\big\| = \sup\limits_{\lambda\in\sigma(H)} \big|f(\lambda)\big|$.

There are many ways to prove this theorem, and we will choose one which only relies on the representation theorem for Herglotz functions and the second main result, the *Spectral Theorem*. The important ingredient is the notion of *projection-valued measure*.

Definition 6.1.9 (Projection-valued measure) *A family of orthogonal projection* $\{P(\Lambda)\}$ *indexed by the Borel measurable sets* $\Lambda \in \mathcal{B}(\mathbb{R})$ *on a Hilbert space* $\mathcal{H}$ *is called* projection-valued measure *(or PVM for short) if and only if the following hold:*

(i) $P(\emptyset) = 0$ *and* $P(\mathbb{R}) = 1$

(ii) $P(\Lambda_1)\,P(\Lambda_2) = P\big(\Lambda_1 \cap \Lambda_2\big)$

(iii) If $\Lambda = \bigcup_{n=1}^{\infty} \Lambda_n$ *is the union of pairwise disjoint Borel measurable sets* Λ_n*, then we have*

$$P(\Lambda) = s\text{-}\lim_{N\to\infty} \sum_{n=1}^{N} P(\Lambda_n)$$

where s-lim *denotes the strong limit of operators (cf. Definition 4.3.2).*

Given a projection-valued measure, we will see (as part of the Spectral Theorem) that we can *define* a selfadjoint operator

$$H := \int_{\mathbb{R}} \mathrm{d}P(\Lambda)\,\lambda \tag{6.1.6}$$

with domain

$$\mathcal{D}(H) = \Big\{\varphi \in \mathcal{H} \;\Big|\; \int_{\mathbb{R}} \langle\varphi, \mathrm{d}P(\Lambda)\varphi\rangle\;\lambda^2 < \infty\Big\}. \tag{6.1.7}$$

On the other hand, a selfadjoint operator uniquely defines a projection-valued measure via equation (6.1.4): Let Λ be any Borel set and 1_Λ the associated characteristic function. Evidently, 1_Λ is bounded, and consequently, the operator

$$P(\Lambda) := 1_\Lambda(H) \tag{6.1.8}$$

exists and is bounded by Lemma 6.1.7.

Lemma 6.1.10 *The family of operators* $P(\Lambda)$ *defined by equation* (6.1.8) *is a projection-valued measure.*

Proof Let us abbreviate the resolvent with $R(z) := (H - z)^{-1}$ and pick $\Lambda_1, \Lambda_2 \in \mathcal{B}(\mathbb{R})$ as well as two vectors $\varphi, \psi \in \mathcal{H}$. We will prove $P(\Lambda_1)\,P(\Lambda_2) = P\big(\Lambda_1 \cap \Lambda_2\big)$ in two steps: first of all, relying on Representation Theorem 6.1.6 and the first resolvent identity

$$(H - z)^{-1} - (H - z') = (z - z')\,(H - z)^{-1}\,(H - z')^{-1},$$

we obtain

$$\begin{aligned}\int_{\mathbb{R}} \mathrm{d}\mu_{R(\bar{z})\varphi,\psi}(\lambda)\,(\lambda - z')^{-1} &= \big\langle R(\bar{z})\varphi, R(z')\psi\big\rangle = \big\langle \varphi, R(z)\,R(z')\psi\big\rangle \\ &= \frac{1}{z - z'}\Big(\big\langle \varphi, R(z)\psi\big\rangle - \big\langle \varphi, R(z')\psi\big\rangle\Big) \\ &= \int_{\mathbb{R}} \mathrm{d}\mu_{\varphi,\psi}(\lambda)\,\frac{1}{z - z'}\left(\frac{1}{\lambda - z} - \frac{1}{\lambda - z'}\right) \\ &= \int_{\mathbb{R}} \mathrm{d}\mu_{\varphi,\psi}(\lambda)\,(\lambda - z)^{-1}\,(\lambda - z')^{-1}.\end{aligned}$$

This implies that

$$\mathrm{d}\mu_{R(\bar{z})\varphi,\psi}(\lambda) = (\lambda - z)^{-1}\,\mathrm{d}\mu_{\varphi,\psi}(\lambda). \tag{6.1.9}$$

So the idea is to insert resolvents in order to be able to invoke the Representation Theorem 6.1.6 again: for any Borel measurable set Λ, we can now use the relation (6.1.9) once more to deduce $1_\Lambda(\lambda)\,\mathrm{d}\mu_{\varphi,\psi}(\lambda) = \mathrm{d}\mu_{\varphi,P(\Lambda)\psi}(\lambda)$ from

$$\begin{aligned}\int_{\mathbb{R}} \mathrm{d}\mu_{\varphi,P(\Lambda)\psi}(\lambda)\,(\lambda - z')^{-1} &= \big\langle \varphi, R(z)\,P(\Lambda)\psi\big\rangle = \big\langle R(\bar{z})\varphi, P(\Lambda)\psi\big\rangle \\ &= \int_{\mathbb{R}} \mathrm{d}\mu_{R(\bar{z})\varphi,\psi}(\lambda)\,1_\Lambda(\lambda) = \int_{\mathbb{R}} \mathrm{d}\mu_{\varphi,\psi}(\lambda)\,1_\Lambda(\lambda)\,(\lambda - z)^{-1}.\end{aligned}$$

Now $P(\Lambda_1)\,P(\Lambda_2) = P\big(\Lambda_1 \cap \Lambda_2\big)$ follows from the obvious equality $1_{\Lambda_1}\,1_{\Lambda_2} = 1_{\Lambda_1 \cap \Lambda_2}$ on the level of functions. Moreover, choosing $\Lambda = \Lambda_1 = \Lambda_2$ tells us that $P(\Lambda)$ is a projection.

To see $P(\mathbb{R}) = \mathrm{id}_{\mathcal{H}}$, pick $\psi \in \ker P(\mathbb{R})$. But then from $\mu_\psi(\mathbb{R}) = \|\psi\|^2$ (Theorem 6.1.6) and

$$0 = \langle \psi, P(\mathbb{R})\psi\rangle = \mu_\psi(\mathbb{R}) = \|\psi\|^2$$

we deduce $\psi = 0$, and consequently, $P(\mathbb{R}) = \mathrm{id}_{\mathcal{H}}$.

Suppose $\Lambda = \bigcup_{n=1}^{\infty} \Lambda_n$ is the union of mutually disjoint sets, $\Lambda_j \cap \Lambda_n = \emptyset$ for all $j \neq n$. Then

$$\sum_{n=1}^{N} \big\langle \psi, P_{\Lambda_n}\psi\big\rangle = \sum_{n=1}^{N} \mu_\psi(\Lambda_n) \xrightarrow{N\to\infty} \big\langle \psi, P(\Lambda)\psi\big\rangle = \mu_\psi(\Lambda)$$

converges to $\mu_\psi(\Lambda)$ by the σ-additivity of μ_ψ. Hence, $P(\Lambda)$ is weakly σ-additive, and thus, also strongly σ-additive since

$$\big\langle \psi, P(\Lambda)\psi \big\rangle = \big\langle P(\Lambda)\psi, P(\Lambda)\psi \big\rangle. \qquad \square$$

The Spectral Theorem states that there is a one-to-one correspondence between selfadjoint operators and projection-valued measures:

Theorem 6.1.11 (Spectral theorem) *There is a one-to-one correspondence between selfadjoint operators H and projection-valued measures $P(\Lambda) = 1_\Lambda(H)$, $\Lambda \in \mathcal{B}(\mathbb{R})$, called the* spectral measure*, and we have*

$$H = \int_{\mathbb{R}} \mathrm{d}P(\lambda)\, \lambda \tag{6.1.10}$$

where $\mathcal{D}(H)$ coincides with the right-hand side of equation (6.1.7)*.*

On the other hand, any projection-valued measure defines a selfadjoint operator via (6.1.6) *whose domain $\mathcal{D}(H)$ is given by* (6.1.7)*.*

Proof "⇒:" Assume we are given a selfadjoint operator $H = H^*$. Then by Lemma 6.1.10 $P(\Lambda) := 1_\Lambda(H)$ defines a projection-valued measure. Moreover, $\mathcal{D}(H)$ coincides with the right-hand side of (6.1.7): if

$$g_n(\lambda) = \sum_{j=1}^{n} c_j\, 1_{\Lambda_j}(\lambda)$$

is a non-decreasing sequence of simple functions which converges to $g(\lambda) = \lambda$ from below, i. e. $0 \le g_n(\lambda) \le g_{n+1}(\lambda) \le \lambda$ and $\lim_{n\to\infty} g_n(\lambda) = \lambda$, then

$$\langle \varphi, g_n(H)\varphi \rangle = \sum_{j=1}^{n} c_j\, \big\langle \varphi, 1_{\Lambda_j}(H)\varphi \big\rangle = \int_{\mathbb{R}} \langle \varphi, \mathrm{d}P(\lambda)\varphi \rangle\; g_n(\lambda) \xrightarrow{n\to\infty} \int_{\mathbb{R}} \langle \varphi, \mathrm{d}P(\lambda)\varphi \rangle\; \lambda$$

by Monotone Convergence for $\varphi \in \mathcal{D}(H)$. Consequently, the two definitions of the domain coincide.

"⇐:" Now suppose we are given a projection-valued measure $\Lambda \mapsto P(\Lambda)$, and define H as above in equation (6.1.10) endowed with domain (6.1.7). Reading some of the above arguments involving the domain in reverse, we deduce that $H : \mathcal{D}(H) \longrightarrow \mathcal{H}$ is well-defined. Moreover, approximating H by simple functions from below as above also yields that H is symmetric.

The only thing that remains is selfadjointness, and in view of the Fundamental Criterion 5.2.4 it suffices to show $\operatorname{ran}(H \pm \mathrm{i}) = \mathcal{H}$. But this follows from observing that $H + \mathrm{i}$ is injective, because

$$\big\|(H \pm \mathrm{i})\varphi\big\|^2 \ge \|\varphi\|^2$$

holds on $\mathcal{D}(H)$, meaning $H \pm \mathrm{i}$ is invertible on $\operatorname{ran}(H \pm \mathrm{i}) \subseteq \mathcal{H}$. Moreover, $H \pm \mathrm{i}$ is also surjective since the inverse is defined as a *bounded* operator via

$$(H \pm \mathrm{i})^{-1} = \int_{\mathbb{R}} \mathrm{d}P(\lambda)\, (\lambda \pm \mathrm{i})^{-1} : \mathcal{H} \longrightarrow \mathcal{D}(H).$$

That finishes the proof. □ 2014.11.14

With the help of the Spectral Theorem, we can prove all parts of Theorem 6.1.8 but the last one. We will postpone a proof to Theorem 6.2.4 below.

Proof (Theorem 6.1.8) The operators $f(H)$ is well-defined and bounded by Lemma 6.1.7.

(i) With the exception of $(f\, g)(H) = f(H)\, g(H)$, all of the other equalities follow directly from the definition. To see the remaining equality, we note that $(f\, g)(H) = f(H)\, g(H)$ holds for simple functions since $P(\Lambda_1)\, P(\Lambda_2) = P\big(\Lambda_1 \cap \Lambda_2\big)$. To show this equality for arbitrary bounded, measurable functions, one approximates f and g by simple functions and then takes the limit. This gives meaning to the following formal manipulation:

$$\begin{aligned} f(H)\, g(H) &= \left(\int_{\mathbb{R}} \mathrm{d}P(\lambda)\, f(\lambda) \right) \left(\int_{\mathbb{R}} \mathrm{d}P(\lambda')\, g(\lambda') \right) \\ &= \int_{\mathbb{R}} \int_{\mathbb{R}} \underbrace{\mathrm{d}P(\lambda)\, \mathrm{d}P(\lambda')}_{= \mathrm{d}P(\lambda)\, \delta(\lambda - \lambda')}\, f(\lambda)\, g(\lambda') \\ &= \int_{\mathbb{R}} \mathrm{d}P(\lambda)\, f(\lambda)\, g(\lambda) \end{aligned}$$

(ii) That follows from the fact that $P(\Lambda) = 1_\Lambda(H)$ is a projection-valued measure, and defining property (iii) of projection-valued measures.

(iii) For any Borel set Λ which contains E, we have $P(\Lambda)\psi = \psi$. Consequently, $P(\{E\})\psi = \psi$ and the Spectral Theorem yields

$$f(H)\psi = \int_{\mathbb{R}} f(\lambda)\, \mathrm{d}P(\lambda)\psi = f(E)\, \psi.$$

(iv) The proof is immediate.

(v) In case f is real-valued, this is a consequence of Theorem 6.2.4 below which states

$$\overline{f\big(\sigma(H)\big)} = \sigma\big(f(H)\big).$$

The upper bound, $\|f(H)\| \leq \left\|f|_{\sigma(H)}\right\|_{L^\infty}$, is obtained from Lemma 6.1.7 and Corollary 6.2.2: the latter implies that

$$f(H) = \int_{\mathbb{R}} \mathrm{d}P(\lambda)\, f(\lambda) = \int_{\sigma(H)} \mathrm{d}P(\lambda)\, f(\lambda),$$

meaning that only the values of f on $\sigma(H)$ matter.

The lower bound is deduced from a Weyl sequence argument: let us define

$$E = \sup\left|\sigma\big(f(H)\big)\right| = \sup\left|f\big(\sigma(H)\big)\right|.$$

Consequently, for all $\varepsilon > 0$ there exists a $\lambda \in \mathbb{R}$ so that $|f(\lambda)| \in (E-\varepsilon, E]$. While the sign of $f(\lambda)$ could be positive or negative, let us assume without loss of generality that in fact $f(\lambda) = |f(\lambda)|$ (the case where $-f(\lambda) = |f(\lambda)|$ is analogous). Then by the Weyl criterion there exists a Weyl sequence $\{\psi_n\}_{n\in\mathbb{N}}$ to $f(\lambda)$,

$$\big\|f(H)\psi_n - (E-\varepsilon)\psi_n\big\| \xrightarrow{n\to\infty} 0,$$

for which evidently

$$E - \varepsilon \leq \lim_{n\to\infty} \big\|f(H)\psi_n\big\| = f(\lambda) \leq \|f(H)\|$$

holds. Given that ε can be chosen to be arbitrarily small, we have also shown the lower bound.

For complex-valued functions the proof is slightly more elaborate, and relies on an extension of functional calculus to bounded normal operators. (An operator T is normal if and only if T and its adjoint T^* commute.) □

6.2 Fundamental properties

The Spectral Theorem 6.1.11 links selfadjoint operators to (projection-valued) measures. This suggests to transfer notions from measure theory to selfadjoint operators. Moreover, we will discuss where projection-valued measures appear in the physics literature.

6.2.1 Relation between spectrum and projection-valued measure

First of all, the spectrum as a set has a characterization in terms of the projection-valued measure:

Proposition 6.2.1 *For a selfadjoint operator H its spectrum is characterized by*

$$\sigma(H) = \Big\{\lambda \in \mathbb{R} \;\Big|\; P\big((\lambda-\varepsilon, \lambda+\varepsilon)\big) \neq 0 \;\forall \varepsilon > 0\Big\}.$$

A simple consequence is that selfadjoint operators H are uniquely determined by their PVM on their spectrum:

Corollary 6.2.2 *For any selfadjoint operator H, the projection-valued measure $P(\Lambda) = 1_\Lambda(H)$ is completely determined on $\sigma(H)$, i. e. we have $P\big(\mathbb{R} \cap \rho(H)\big) = 0$ and $P\big(\sigma(H)\big) = \mathrm{id}_{\mathcal{H}}$.*

The proof needs a weak version of the Weyl criterion: while we do not get an if and only if statement, the existence of a Weyl sequence for some $\lambda \in \mathbb{R}$ implies $\lambda \in \sigma(H)$. On the plus side, the proof only relies on a simple estimate and does not involve the projection-valued measure.

Lemma 6.2.3 (Weak Weyl Criterion) *Let A be a densely defined, closed operator with domain $\mathcal{D}(A)$. We have $z \in \sigma(A)$ if there exists a sequence $\psi_n \in \mathcal{D}(A)$ such that $\|\psi_n\| = 1$ and $\lim_{n\to\infty} \big\|(A - z)\psi_n\big\| = 0$. Such a sequence is called a* Weyl sequence*.*

Proof Let $\{\psi_n\}_{n\in\mathbb{N}}$ be a Weyl sequence to $z \in \mathbb{C}$. If $z \in \rho(A)$, then $(A - z)^{-1}$ exists as a bounded operator, and consequently, we can deduce this contradiction:

$$\begin{aligned} 1 = \|\psi_n\| &= \big\|(A - z)^{-1}\,(A - z)\psi_n\big\| \\ &\leq \big\|(A - z)^{-1}\big\|\,\big\|(A - z)\psi_n\big\| \xrightarrow{n\to\infty} 0 \end{aligned}$$

Hence, z is in the spectrum, $z \in \sigma(A)$. □

Proof (Proposition 6.2.1) Take $\Lambda_n := \big(\lambda_0 - 1/n, \lambda_0 + 1/n\big)$ and suppose $P(\Lambda_n) \neq 0$ for all $n \in \mathbb{N}$. For each $n \in \mathbb{N}$ we can find a normalized vector $\psi_n \in P(\Lambda_n)\mathcal{H}$. Then in view of the estimate

$$\big\|(H - \lambda_0)\psi_n\big\|^2 = \Big\|(H - \lambda_0)\,P(\Lambda_n)\psi_n\Big\|^2 = \int_{\mathbb{R}} \mathrm{d}\mu_{\psi_n}(\lambda)\,1_{\Lambda_n}(\lambda)\,(\lambda - \lambda_0)^2 \leq \frac{1}{n^2},$$

we arrive at the conclusion that $\{\psi_n\}$ is a Weyl sequence, and thus, $\lambda \in \sigma(H)$ by the weak Weyl criterion Lemma 6.2.3.

Conversely, if $P\big((\lambda_0 - \varepsilon, \lambda_0 + \varepsilon)\big) = 0$, we define the function

$$f_\varepsilon(\lambda) = 1_{\mathbb{R}\setminus(\lambda_0-\varepsilon,\lambda_0+\varepsilon)}(\lambda)\,(\lambda - \lambda_0)^{-1}.$$

Then using Functional Calculus 6.1.8 combined with the assumption $P\big((\lambda_0-\varepsilon, \lambda_0+\varepsilon)\big) = 0$ yields

$$(H - \lambda_0)\,f_\varepsilon(H) = \big((\lambda - \lambda_0)\,f_\varepsilon\big)(H) = 1_{\mathbb{R}\setminus(\lambda_0-\varepsilon,\lambda_0+\varepsilon)}(H) = \mathrm{id}_{\mathcal{H}}.$$

Analogously, we obtain $f_\varepsilon(H)\,(H - \lambda_0) = \mathrm{id}_{\mathcal{D}(H)}$ which means $\lambda_0 \in \rho(H)$. □

The characterization of the spectrum in terms of the projection-valued measure also yields a relationship between the spectrum of H and $f(H)$ assuming that f is continuous on the spectrum. There are weaker versions of this statement (cf. e. g. [Tes09, Lemma 3.12]) which work also for functions which are just measurable.

Theorem 6.2.4 *Let H be a selfadjoint operator and f be a measurable, real-valued function that is continuous on $\sigma(H)$. Then $\sigma\big(f(H)\big) = \overline{f\big(\sigma(H)\big)}$ where the closure can be dropped if $\sigma(H)$ is bounded.*

This Theorem also yields the proof of Theorem 6.1.8 (v) for the special case of real-valued functions: the upper bound, $\|f(H)\| \leq \|f\|_{L^\infty}$, is obtained from Lemma 6.1.7 while the lower bound is deduced from an argument involving Weyl sequences.

Proof Because f is real-valued, not only H but also $f(H)$ is selfadjoint. Hence, the Spectral Theorem 6.1.11 applies to both of them, and we can write $f(H)$ in two ways,

$$f(H) = \int_{\sigma(H)} 1_{\mathrm{d}\lambda}(H)\, f(\lambda) = \int_{\sigma(f(H))} 1_{\mathrm{d}\mu}\big(f(H)\big)\, \mu,$$

once, in terms of the PVM of H and also in terms of the PVM of $f(H)$. In both cases, the support of the PVM is the spectrum (Theorem 6.2.1), and thus writing the spectrum of $f(H)$ can be characterized in two ways, namely

$$\begin{aligned}\sigma\big(f(H)\big) &= \Big\{\lambda \in \mathbb{R} \;\Big|\; 1_{(\lambda-\varepsilon,\lambda+\varepsilon)}\big(f(H)\big) \neq 0 \;\; \forall \varepsilon > 0\Big\} \\ &= \Big\{\lambda \in \mathbb{R} \;\Big|\; 1_{f^{-1}((\lambda-\varepsilon,\lambda+\varepsilon))}(H) \neq 0 \;\; \forall \varepsilon > 0\Big\}. \qquad (6.2.1)\end{aligned}$$

At this point we only get the inclusion $\sigma\big(f(H)\big) \subseteq \overline{f\big(\sigma(H)\big)}$ rather than equality, because the set $\Lambda_\varepsilon = f^{-1}\big((\lambda-\varepsilon, \lambda+\varepsilon)\big)$ could have measure 0 according to the projection-valued measure, i. e. $1_{\Lambda_\varepsilon}(H) = 0$ where Λ_ε is as above.

To show the opposite inclusion, we need to make use of the continuity: $f \in \mathcal{C}\big(\sigma(H)\big)$ means the preimage

$$f^{-1}\big(\big(f(\lambda)-\varepsilon, f(\lambda)+\varepsilon\big)\big) \supseteq \big(\lambda-\delta, \lambda+\delta\big), \qquad \delta \ll 1,$$

of an ε-neighborhood of $f(\lambda)$ contains an open interval around λ. Combining this with equation (6.2.1) yields that if $\lambda \in \sigma(H)$ then also $f(\lambda) \in \sigma\big(f(H)\big)$. Hence, we have also shown $\sigma\big(f(H)\big) \supseteq \overline{f\big(\sigma(H)\big)}$. □

6.2.2 Distinction between spectral types

The Lebesgue decomposition of measures (Theorem 6.1.4) also yields a natural distinction between different spectral types:

Definition 6.2.5 *Let H be a selfadjoint operator on a Hilbert space $\mathcal{H}$. Then we define* pure point, absolutely continuous *and* singularly continuous *subspaces as*

$$\begin{aligned}\mathcal{H}_{\text{pp}} &= \big\{\psi \in \mathcal{H} \;\big|\; \mu_\psi \text{ is a point measure}\big\},\\ \mathcal{H}_{\text{ac}} &= \big\{\psi \in \mathcal{H} \;\big|\; \mu_\psi \text{ is an absolutely continuous measure}\big\},\\ \mathcal{H}_{\text{sc}} &= \big\{\psi \in \mathcal{H} \;\big|\; \mu_\psi \text{ is a singularly continuous measure}\big\},\end{aligned}$$

where μ_ψ is the measure from (6.1.2)*.*

Given that any Borel measure on $\mathbb{R}$ splits into these three contributions, the Hilbert space $\mathcal{H}$ splits into the direct sum of these three subspaces. For a proof, we refer to [RS72, Theorem VII.4].

Theorem 6.2.6 *Let H be a selfadjoint operator on a Hilbert space $\mathcal{H}$. Then the Hilbert space*

$$\mathcal{H} = \mathcal{H}_{\text{pp}} \oplus \mathcal{H}_{\text{ac}} \oplus \mathcal{H}_{\text{sc}}$$

decomposes into pure point, absolutely continuous and singularly continuous subspaces.

This decomposition of the Hilbert space yields a *third* decomposition of the spectrum $\sigma(H)$.

Definition 6.2.7 (Pure point, ac and sc spectrum) *For a selfadjoint operator H on a Hilbert space $\mathcal{H}$, we define* pure point, absolutely continuous *and* singularly continuous *spectrum as*

$$\begin{aligned}\sigma_{\text{pp}}(H) &= \sigma\big(H|_{\mathcal{H}_{\text{pp}}}\big),\\ \sigma_{\text{ac}}(H) &= \sigma\big(H|_{\mathcal{H}_{\text{pp}}}\big),\\ \sigma_{\text{sc}}(H) &= \sigma\big(H|_{\mathcal{H}_{\text{pp}}}\big).\end{aligned}$$

These three sets need not be disjoint. To understand this decomposition better, we recap the other two spectral decompositions that have been introduced in Definition 4.1.6 and Theorems 5.2.8–5.2.9:

$$\begin{aligned}\sigma(H) &= \sigma_{\text{p}}(H) \cup \sigma_{\text{c}}(H) \cup \sigma_{\text{r}}(H) = \sigma_{\text{p}}(H) \cup \sigma_{\text{c}}(H)\\ &= \sigma_{\text{disc}}(H) \cup \sigma_{\text{ess}}(H)\\ &= \sigma_{\text{pp}}(H) \cup \sigma_{\text{ac}}(H) \cup \sigma_{\text{sc}}(H)\end{aligned}$$

First of all, for selfadjoint operators the residual spectrum is empty, so only the point and the continuous spectrum remain. The second decomposition consists of discrete spectrum (eigenvalues of finite multiplicity) and the remainder, the essential spectrum. These spectral components are related: the discrete, point and pure point spectrum are all nested,

$$\sigma_{\text{disc}}(H) \subseteq \sigma_{\text{p}}(H) \subseteq \sigma_{\text{pp}}(H) = \overline{\sigma_{\text{p}}(H)},$$

but they need not be equal: $\sigma_{\mathrm{p}}(H)$ may contain eigenvalues of infinite multiplicity, and by definitions these are part of the *essential* spectrum. The energy levels of the Landau hamiltonian are infinitely degenerate and contribute to the essential rather than the discrete spectrum. Moreover, accumulation points in $\sigma_{\mathrm{p}}(H)$ need not be contained in it (the point spectrum need not be closed). One physical example where this occurs is the point 0 for the spectrum of the hydrogen hamiltonian H: while 0 is not an eigenvalue, $0 \notin \sigma_{\mathrm{p}}(H)$, it is nevertheless the accumulation point of the energy levels below 0, and thus, $0 \in \sigma_{\mathrm{pp}}(H)$. States associated to $\sigma_{\mathrm{pp}}(H)$, i. e. linear combinations of eigenfunctions, are *bound states*, because they remain localized under time evolution.

Similarly, one obtains an inclusion of continuous, absolutely continuous (ac), singularly continuous (sc) and essential spectrum:

$$\sigma_{\mathrm{c}}(H) = \sigma_{\mathrm{ac}}(H) \cup \sigma_{\mathrm{sc}}(H) \subseteq \sigma_{\mathrm{ess}}(H)$$

Wave functions associated to $\sigma_{\mathrm{ac}}(H)$ are *scattering states*, because in case of $\mathcal{H} = L^2(\mathbb{R}^d)$ over time such states leave any bounded subset $\Lambda \subseteq \mathbb{R}^d$. While this is false for states associated to $\sigma_{\mathrm{sc}}(H)$, in most physical situations one can prove that $\mathcal{H}_{\mathrm{sc}} = \{0\}$, and thus, any state is either a bound state or a scattering state.

6.2.3 Physical interpretation

To link these notions back to physics, let us start with the Spectral Theorem 6.1.11 which states that a selfadjoint operator can be thought of as

$$H = \int_{\sigma(H)} \mathrm{d}P(\lambda)\, \lambda$$

where the projection-valued measure $P(\Lambda)$ has a concise physical interpretation. In fact H is *uniquely determined by its projection-valued measure* (that is the content of the Spectral Theorem 6.1.11), and consequently, on the level of mathematics it is a matter of taste whether to speak of projection-valued measures or selfadjoint operators.

On the level of physics, selfadjoint operators H can be seen *bookkeeping devices* for *idealized experiments* which keep track of outcomes of measurements and statistics. Not only energy, but also other observables such as position, momentum and angular momentum are important.

(i) The spectrum $\sigma(H)$ is the set of possible outcomes of measurements.

(ii) The projection-valued measure contains the *statistics* of the experiment, meaning that given a pure state φ, the probability to measure an outcome λ in a "window" $\Lambda \subseteq \mathbb{R}$ is given by

$$\mathbb{P}(\lambda \in \Lambda | \varphi) = \mu_\varphi(\Lambda) = \int_\Lambda \mathrm{d}\mu_\varphi(\lambda) = \int_\Lambda \big\langle \varphi, 1_{\mathrm{d}\lambda}(H)\varphi \big\rangle = \big\langle \varphi, P(\Lambda)\varphi \big\rangle$$

where μ_φ is the Borel measure from equation (6.1.2).

(iii) Expectation values, i. e. the statistical average of the outcome of an experiment if it is repeated often enough, is computed via the expectation value,

$$\mathbb{E}_\varphi(H) = \langle \varphi, H\varphi \rangle = \int_{\mathbb{R}} \langle \varphi, 1_{\mathrm{d}\lambda}(H)\varphi \rangle \, \lambda = \Big\langle \varphi, \int_{\mathbb{R}} \lambda \, 1_{\mathrm{d}\lambda}(H)\varphi \Big\rangle.$$

Physicists use projection-valued measures when they speak of *resolutions of the identity*, and to keep things simple, let us consider the case $\mathcal{H} = L^2(\mathbb{R})$. Observables such as position $Q = \hat{x}$ and momentum $P = -\mathrm{i}\partial_x$ define selfadjoint operators, and these operators have purely absolutely continuous spectrum,

$$\begin{aligned} \sigma(Q) = \sigma_{\mathrm{ac}}(Q) = \mathbb{R} = \sigma_{\mathrm{ac}}(P) = \sigma(P), \\ \sigma_{\mathrm{pp}}(Q) = \emptyset = \sigma_{\mathrm{pp}}(P). \end{aligned}$$

Hence, Q and P do not have eigenfunctions in $L^2(\mathbb{R})$, and a discrete resolution of the identity

$$\mathrm{id}_{L^2(\mathbb{R})} = \sum_{n=1}^{\infty} |\varphi_n\rangle\langle\varphi_n|$$

composed of eigenfunctions *does not exist*. Nevertheless, physicists write (see e. g. [Sak94, pp. 41–46])

$$\mathrm{id}_{L^2(\mathbb{R})} = \int_{\mathbb{R}} \mathrm{d}x \, |x\rangle\langle x|$$

where $|x\rangle$ is a "pseudoeigenfunction". Comparing this to equation (6.1.10), we see that $\mathrm{d}x\,|x\rangle\langle x|$ is just the projection-valued measure $\mathrm{d}P(x) = 1_{\mathrm{d}x}(\hat{x})$! 2014.11.21

6.3 Stone's theorem and the quantum time evolution

One important application of functional calculus is the rigorous definition of the unitary time evolution $\mathrm{e}^{-\mathrm{i}tH}$ and other unitary one-parameter groups generated by selfadjoint operators such as translations in real or momentum space. As indicated already in Chapter 4.3.2, especially Theorem 4.3.5, there exists a one-to-one relationship between selfadjoint operators and unitary evolution groups:

Theorem 6.3.1 (Stone) *To every strongly continuous one-parameter unitary group $t \mapsto U(t)$ on a Hilbert space $\mathcal{H}$, there exists a selfadjoint operator $H = H^*$ which generates $U(t) = \mathrm{e}^{-\mathrm{i}tH}$. Conversely, every selfadjoint operator H generates the unitary evolution group $U(t) = \mathrm{e}^{-\mathrm{i}tH}$.*

While a complete proof is easily within our means, we skip the details to one directions because spelling out these ideas is a tad technical.

Proof "⇒:" Suppose we are given a selfadjoint operator H with dense domain $\mathcal{D}(H) \subseteq \mathcal{H}$. Then we define the *bounded operator* $U(t) := \mathrm{e}^{-\mathrm{i}tH}$ in terms of functional calculus associated to the function $\lambda \mapsto \mathrm{e}^{-\mathrm{i}t\lambda} \in \mathcal{C}^\infty(\mathbb{R}) \cap L^\infty(\mathbb{R})$. We have to verify that $U(t)$ is a strongly continuous unitary evolution group:

(i) Clearly, $U(0) = 1_{\mathbb{R}}(H) = \mathrm{id}_{\mathcal{H}}$ and from $f(H)^* = \bar{f}(H)$ we deduce that $U(t)^* = U(-t)$.

(ii) $U(t)\,U(s) = U(t+s)$ follows immediately from $f(H)\,g(H) = (f\,g)(H)$ (functional calculus) and $\mathrm{e}^{-\mathrm{i}t\lambda}\,\mathrm{e}^{-\mathrm{i}s\lambda} = \mathrm{e}^{-\mathrm{i}(t+s)\lambda}$ on the level of functions. Hence, we deduce that $U(-t) = U(t)^{-1} = U(t)^*$ is unitary.

(iii) By (ii) it suffices to check strong continuity of $t \mapsto U(t)$ at $t = 0$ only: The spectral theorem allows us to express

$$\left\|\mathrm{e}^{-\mathrm{i}tH}\varphi - \varphi\right\|^2 = \int_{\mathbb{R}} \left\langle \varphi, \mathrm{d}P(\lambda)\varphi \right\rangle \left|\mathrm{e}^{-\mathrm{i}t\lambda} - 1\right|^2$$

in terms of $\left|\mathrm{e}^{-\mathrm{i}t\lambda} - 1\right|^2$. Evidently, $\left|\mathrm{e}^{-\mathrm{i}t\lambda} - 1\right|^2 \leq 2$ holds and

$$\left|\mathrm{e}^{-\mathrm{i}t\lambda} - 1\right|^2 \xrightarrow{t\to 0} 0$$

converges to 0 for all $\lambda \in \mathbb{R}$ pointwise, and thus, $\lim_{t\to 0}\left\|\mathrm{e}^{-\mathrm{i}tH}\varphi - \varphi\right\| = 0$ for all $\varphi \in \mathcal{H}$ follows from Dominated Convergence.

(iv) Again, it suffices to take the derivative at $t = 0$. The fact that $\psi(t) = \mathrm{e}^{-\mathrm{i}tH}\psi$ for $\psi \in \mathcal{D}(H)$ satisfies the Schrödinger equation follows $\left|\mathrm{e}^{-\mathrm{i}t\lambda} - 1\right| \leq |\lambda|$, writing out the time-derivative as a difference quotient and the observation from the Spectral
2014.11.25 Theorem that the domain of H coincides with the set

$$\left\{\varphi \in \mathcal{H} \;\middle|\; \int_{\mathbb{R}} \langle \varphi, \mathrm{d}P(\lambda)\varphi\rangle\ \lambda^2 < \infty\right\}.$$

"⇐:" Given a unitary evolution group, we can recover its generator by computing

$$H_0\varphi := \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}U(t)\varphi\Big|_{t=0}$$

on a suitable subset of "nice" vectors, i. e.

$$\varphi \in \mathcal{D}(H_0) \subseteq \left\{\varphi \in \mathcal{H} \;\middle|\; \mathrm{i}\tfrac{\mathrm{d}}{\mathrm{d}t}U(t)\varphi \in \mathcal{H}\right\}.$$

One needs to show that $\mathcal{D}(H_0)$ lies densely in $\mathcal{H}$, that H_0 is symmetric and finally use the Fundamental Criterion of Selfadjointness to prove that H_0 is indeed essentially selfadjoint. The generator is then the unique selfadjoint extension $H = \overline{H_0}$. Spelling out these ideas is not difficult, albeit a bit technical. Thus, we refer the interested reader to the proof of [RS72, Theorem VIII.8] for details. □

Now that we know how the quantum time evolution is defined, let us take a moment to compare a perturbed quantum system defined through $H_\varepsilon = H_0 + \varepsilon V$ with its unperturbed cousin. That is particularly important because almost none of the systems one encounters in "real life" have closed-form solutions, so it is immediate to study perturbations of known systems first. The physics literature usually contents itself studying approximations of *eigenvalues* of the hamiltonian, but the more fundamental question is what happens to the *dynamics*? In other words, does $H_\varepsilon \approx H_0$ imply $\mathrm{e}^{-\mathrm{i}tH_\varepsilon} \approx \mathrm{e}^{-\mathrm{i}tH_0}$. The answer is *yes* and uses a very, very nifty trick, the *Duhamel formula*.

Theorem 6.3.2 (Duhamel) *Let H_0 and $H_\varepsilon = H_0 + \varepsilon V$ be two selfadjoint operators defined on a common domain, and suppose that V defines a bounded operator on $\mathcal{H}$. Then the two evolutions are ε-close in norm,*

$$\left\| \mathrm{e}^{-\mathrm{i}tH_\varepsilon} - \mathrm{e}^{-\mathrm{i}tH_0} \right\|_{\mathcal{B}(\mathcal{H})} = \mathcal{O}\big(\varepsilon\,|t|\big). \tag{6.3.1}$$

Note that this error estimate holds for *all* times, because quantum mechanics is a *linear* theory (as opposed to, say, classical mechanics).

Proof The idea is to write the difference

$$\begin{aligned}
\Big(\mathrm{e}^{-\mathrm{i}tH_\varepsilon} - \mathrm{e}^{-\mathrm{i}tH_0}\Big)\varphi &= \int_0^t \mathrm{d}s\, \frac{\mathrm{d}}{\mathrm{d}s}\Big(\mathrm{e}^{-\mathrm{i}sH_\varepsilon}\, \mathrm{e}^{-\mathrm{i}(t-s)H_0}\Big)\varphi \\
&= -\mathrm{i} \int_0^t \mathrm{d}s\, \mathrm{e}^{-\mathrm{i}sH_\varepsilon} \left(H_\varepsilon - H_0\right) \mathrm{e}^{-\mathrm{i}(t-s)H_0}\varphi \\
&= -\varepsilon\,\mathrm{i} \int_0^t \mathrm{d}s\, \mathrm{e}^{-\mathrm{i}sH_\varepsilon}\, V\, \mathrm{e}^{-\mathrm{i}(t-s)H_0}\varphi
\end{aligned}$$

as the integral of a total derivative for some $\varphi \in \mathcal{D}(H_\varepsilon) = \mathcal{D}(H_0)$. We have proven in Theorem 4.3.5 (i) that the domain is left invariant by $\mathrm{e}^{-\mathrm{i}(t-s)H_0}$ so that the derivative with respect to s exists in the strong sense. Consequently, the integrand is bounded in norm by $\varepsilon\, \|V\|_{\mathcal{B}(\mathcal{H})}\, \|\varphi\|_{\mathcal{H}}$ for all $s \in [0,t]$, and by density of $\mathcal{D}(H_\varepsilon) = \mathcal{D}(H_0) \subseteq \mathcal{H}$ we obtain equation (6.3.1). □

6.4 Other approaches to functional calculus

The approach to functional calculus presented here is by no means the only one, three other popular ones are *holomorphic functional calculus* [Dav95], functional calculus via the

heat semigroup of selfadjoint operators which are bounded from below [Dav95], and the "multiplication operator form" of the spectral theorem (which as shown in Chapter 6.1.3 implies the functional calculus) [RS72, Theorem VII.3]. There are at times subtle differences between them in the classes of functions and the types operators for which they hold. However, if more than one method can be used, the resulting operators necessarily need to agree.

For instance, suppose we are interested in a relevant part of the spectrum $\sigma_{\text{rel}} \subset \sigma(H)$ of some selfadjoint operator H, and that the relevant part of the spectrum is separated from the remainder by a *spectral gap*,

$$\operatorname{dist}\bigl(\sigma_{\text{rel}}, \sigma(H) \setminus \sigma_{\text{rel}}\bigr) > 0.$$

Then we can express $1_{\sigma_{\text{rel}}}(H)$ as a contour integral with respect to the resolvent,

$$P := \frac{\mathrm{i}}{2\pi} \int_\Gamma \mathrm{d}z \, (H - z)^{-1},$$

where Γ is a contour which encloses only σ_{rel}. P is called *Riesz projection*. There is a lot of freedom in the choice of contour, because just like in complex analysis the shape of the contour is immaterial as long as the same poles are enclosed in them. And since poles of the resolvent are the spectrum, and these poles are of "first order", we already suspect $P = 1_{\sigma_{\text{rel}}}(H)$.

However, one can show using only the resolvent identity and suitable choices of contours that P defined as above is an orthogonal projection $P^2 = P = P^*$: To show the first equality, let Γ' be another contour contained in the interior of Γ. Then using the resolvent identity,

$$-(z - z') \, (H - z)^{-1} \, (H - z')^{-1} = (H - z)^{-1} - (H - z')^{-1},$$

we obtain

$$\begin{aligned} P^2 &= \left(\frac{\mathrm{i}}{2\pi}\right)^2 \int_\Gamma \mathrm{d}z \int_{\Gamma'} \mathrm{d}z' \, (H - z)^{-1} \, (H - z')^{-1} \\ &= +\frac{1}{(2\pi)^2} \int_\Gamma \mathrm{d}z \int_{\Gamma'} \mathrm{d}z' \, (z - z')^{-1} \, (H - z)^{-1} + \\ &\quad - \frac{1}{(2\pi)^2} \int_\Gamma \mathrm{d}z \int_{\Gamma'} \mathrm{d}z' \, (z - z')^{-1} \, (H - z')^{-1}. \end{aligned}$$

Since $z \in \Gamma$ and Γ' is contained in the interior of Γ, the function $z' \mapsto (z - z')^{-1}$ is actually holomorphic on a domain which includes Γ' and its interior. That means $\int_{\Gamma'} \mathrm{d}z' \, (z - z')^{-1} = 0$ and the first term vanishes.

To treat the second term, we reverse the order of integration and use that $z \mapsto (z-z')^{-1}$ has a pole at z', and hence, the residue theorem yields

$$\begin{aligned} P^2 &= 0 - \frac{1}{(2\pi)^2} \int_{\Gamma'} \mathrm{d}z' \underbrace{\left(\int_{\Gamma} \mathrm{d}z \, (z-z')^{-1} \right)}_{=-\mathrm{i}2\pi} (H-z')^{-1} \\ &= \frac{\mathrm{i}}{2\pi} \int_{\Gamma'} \mathrm{d}z' \, (H-z)^{-1} = P. \end{aligned}$$

To show selfadjointness, we pick a contour which is symmetric with respect to reflections around the real axis, i. e. $\overline{\Gamma} = \Gamma$. With this contour, we obtain

$$\begin{aligned} P^* &= \left(\frac{\mathrm{i}}{2\pi} \int_{\Gamma} \mathrm{d}z \, (H-z)^{-1} \right)^* = -\frac{\mathrm{i}}{2\pi} \int_{\Gamma} \mathrm{d}\bar{z} \left((H-z)^{-1} \right)^* \\ &= -\frac{\mathrm{i}}{2\pi} \int_{\Gamma} \mathrm{d}\bar{z} \, (H-\bar{z})^{-1} = +\frac{\mathrm{i}}{2\pi} \int_{\overline{\Gamma}} \mathrm{d}z \, (H-z)^{-1} = P. \end{aligned}$$

Note that one sign change stems from the flip of orientation of the curve which traces Γ.

As $H = H^*$ is selfadjoint, we can use functional calculus. For instance, we can express

$$(H-z)^{-1} = \int_{\sigma(H)} (\lambda - z)^{-1} \, \mathrm{d}P(\lambda)$$

in terms of the function $\lambda \mapsto (\lambda - z)^{-1}$ and the projection-valued measure $\mathrm{d}P(\lambda)$ associated to H. Once we plug this into the definition of P, we obtain

$$\begin{aligned} P &= \frac{\mathrm{i}}{2\pi} \int_{\Gamma} \mathrm{d}z \, (H-z)^{-1} = \frac{\mathrm{i}}{2\pi} \int_{\Gamma} \mathrm{d}z \int_{\sigma(H)} (\lambda - z)^{-1} \, \mathrm{d}P(\lambda) \\ &= \frac{\mathrm{i}}{2\pi} \int_{\sigma(H)} \underbrace{\left(\int_{\Gamma} \mathrm{d}z \, (\lambda - z)^{-1} \right)}_{=\mathrm{i}2\pi \, 1_{\sigma_{\mathrm{rel}}}(\lambda)} \mathrm{d}P(\lambda) = \int_{\sigma(H)} 1_{\sigma_{\mathrm{rel}}}(\lambda) \, \mathrm{d}P(\lambda) \\ &= 1_{\sigma_{\mathrm{rel}}}(H). \end{aligned}$$

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