
Mathematical Aspects of Quantum Mechanics
held by Prof. Dr. Speicher in Winter 2020

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General Information

This write-up is created by a student of the course, it is an *unauthorised write-up*. Typesetting is no warrant for accuracy. If you find mistakes in the write-up, a hint via E-Mail would be appreciated:

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Chapter I.

Introduction

This course on mathematical aspects of quantum mechanics centers around the *canonical commutator relations*. In one degree of freedom for the momentum operator p and the position operator q , those read

$$pq - qp = [p, q] = -i\hbar 1.$$

For several degrees of freedom and operators p_i and q_j the canonical commutation relations read $[p_i, q_j] = -i\hbar\delta_{ij}$. In the following, especially the case where we have an infinite family of operators will be of central interest.

In the usual setting of quantum mechanics, observables, that is experimentally measurable quantities, correspond to selfadjoint operators on a Hilbert space. Unfortunately it turns out that there is no realisation of the canonical commutation relations by bounded operators. Thus there is a need for the introduction of unbounded operators, especially of selfadjoint unbounded operators.

An unbounded operator A on an Hilbert space \mathcal{H} is a linear operator that is defined on some subset $D(A) \subseteq \mathcal{H}$, usually $D(A)$ is dense in \mathcal{H} , and which has no finite operator norm. As opposed to bounded operators, where the property “hermitian” (or “symmetric”) is equivalent to the property “selfadjoint”, this is not true for unbounded operators.¹ For an unbounded operator, the natural analogon “For all $x, y \in D(A)$ it holds $\langle Ax, y \rangle = \langle x, Ay \rangle$ ” is a weaker condition than “ $A = A^*$ ”, which also includes $D(A) = D(A^*)$.

The hermitian property is easily checked, most formal operators in physics are of this form. Sadly, mathematically speaking, not much can be said about unbounded operators that are merely hermitian. The selfadjointness of an unbounded operator is hard to check, but there are strong mathematical results for those operators (e.g. the Spectral Theorem and the Theorem of Stone).

¹Recall that a bounded operator $A: \mathcal{H} \rightarrow \mathcal{H}$ is called hermitian, if for all $x, y \in \mathcal{H}$ it holds $\langle Ax, y \rangle = \langle x, Ay \rangle$.

The Spectral Theorem for unbounded operators is some kind of continuous analogon of the Spectral Theorem known from linear algebra, which states that symmetrical matrices can be diagonalised. More precisely, an unbounded operator A can be written in the form

$$A = \int \lambda dE(\lambda),$$

where λ are the elements of the spectrum of A that have a certain meaning in the correspondence between observables and selfadjoint operators. The λ are the possible values of the observable A in measurement.

The Theorem of Stone characterises unitary semigroups. Given a family of unitary operators $(U(t))_{t \in I}$ such that it holds $U(t)U(s) = U(t+s)$ and some sort of continuity on this family, the Theorem of Stone states that the members of the family are of the form $U(t) = e^{itH}$, where H is selfadjoint and the nature of the operator H depends on the “strength” of the continuity. In physics, this operator is usually the Hamilton operator. Given the Hamilton operator of some system, we can pass to the semigroup generated by H and interpret it as the Schrödinger picture $\psi_t = U(t)\psi$. Taking the derivative of $U(t)$ gives us the Schrödinger equation:

$$\frac{d}{dt}U(t) = iHU(t).$$

A central question for this lecture will be: Given a symmetric operator, can we extend it to a selfadjoint operator? This extension corresponds to prescribing boundary conditions. Usually, such an extension (if it even exists) is not unique. There is a general theory due to von Neumann of “defect indices”, which characterise possible selfadjoint extensions.

In the second part of the lecture, we ask for realisations of the canonical commutation relations for finitely many degrees of freedom. Instead of treating the problem

$$pq - qp = -i\hbar 1,$$

which due to the nature of the operators p and q inherently enforces dealing with cumbersome technical details like the possibly different domains of p and q , we pass, using the Theorem of Stone, over to operators $U(t) = e^{itp}$, $V(t) = e^{isq}$ such that

$$U(t)V(s) = e^{its}V(s)U(t).$$

Those relations are called the *Weyl relations*. The Uniqueness Theorem of von Neumann states that each representation of the Weyl relations is equivalent to a direct sum of the Schrödinger representation of the canonical commutation relations.

In the third part of the lecture, we will concern ourselves with infinitely many degrees of freedom which leads us straight into quantum field theory. In this framework, different physical theories correspond to non-equivalent representations of the canonical commutation relations.

Because the sensible choice of representation depends on the physical framework, it is not really the operators themselves which are important, but the algebraic relations between them. We thus consider a universal C^* -algebra generated by the canonical commutation relations. This C^* -algebra then encodes the algebraic properties of the canonical commutation relations. A concrete physical situation corresponds to a state on this C^* -algebra and by a Gelfand-Neumark-Segal type construction we obtain a realisation on a concrete Hilbert space.

Chapter II.

Prerequisites

1. Hilbert Spaces

Definition II.1 (Hilbert Space): Let \mathcal{H} be a complex vector space, i.e. an abelian group $(\mathcal{H}, +)$ together with a scalar multiplication $\cdot: \mathbb{C} \times \mathcal{H} \rightarrow \mathcal{H}$ such that for all $x, y \in \mathcal{H}$ and $\lambda, \mu \in \mathbb{C}$ it holds $1x = x$, $(\lambda + \mu)x = \lambda x + \mu x$, $\lambda(\mu x) = (\lambda\mu x)$. If there is a map $\langle \cdot, \cdot \rangle: \mathcal{H} \times \mathcal{H} \rightarrow \mathbb{C}$ which satisfies for all $x, y, z \in \mathcal{H}$ and $\lambda \in \mathbb{C}$ that

- (i) $\langle x, y + z \rangle = \langle x, y \rangle + \langle x, z \rangle$,
- (ii) $\langle x, \lambda y \rangle = \lambda \langle x, y \rangle$,
- (iii) $\langle x, y \rangle = \langle y, x \rangle^*$,
- (iv) $\langle x, x \rangle \geq 0$ and $\langle x, x \rangle = 0$ if and only if $x = 0$,

and if \mathcal{H} is complete¹ with respect to the norm $\|x\| := \langle x, x \rangle^{1/2}$, then \mathcal{H} is called a *Hilbert space*.

Example II.2: (i) The vector space $\mathcal{H} = \mathbb{C}^n$ turns into a Hilbert space with the inner product

$$\langle x, y \rangle = \sum_{j=1}^n (x^j)^* y^j,$$

where $x = (x^1, \dots, x^n)^t$ and $y = (y^1, \dots, y^n)^t$.

(ii) The vector space $\mathcal{H} = \ell_2 = \{(x_n)_{n \in \mathbb{N}} \in \mathbb{C}^{\mathbb{N}} \mid \sum_{n=1}^{\infty} |x_n|^2 < \infty\}$ turns into a Hilbert space with the inner product

$$\langle (x_n)_{n \in \mathbb{N}}, (y_n)_{n \in \mathbb{N}} \rangle := \sum_{n=1}^{\infty} (x_n)^* y_n.$$

¹Recall that a metric space is called complete, if every Cauchy sequence in said metric space converges therein.

(iii) Given a σ -algebra \mathfrak{F} on \mathbb{R} and a measure μ on \mathfrak{F} , then $\mathcal{H} = L^2(\mathbb{R}, \mathfrak{F}, \mu)$ is a complex vector space with the pointwise operations. A vector x is just a square integrable function f on \mathbb{R} , i.e. f is measurable with respect to μ such that $\int |f(t)|^2 d\mu(t) < \infty$. It turns into a Hilbert space together with the inner product declared via

$$\langle f, g \rangle := \int f(t)^* g(t) d\mu(t).$$

Theorem II.3 (Cauchy-Schwarz Inequality): *Let \mathcal{H} be a Hilbert space. Then for all $x, y \in \mathcal{H}$ we have the estimate*

$$|\langle x, y \rangle| \leq \|x\| \|y\|.$$

In the above estimate it holds equality if and only if $\{x, y\}$ linearly dependent.

Notation II.4: Let \mathcal{M} be a closed linear subspace of \mathcal{H} (i.e. \mathcal{M} is itself a Hilbert space). Then

$$\mathcal{M}^\perp := \{x \in \mathcal{H} \mid \text{For all } y \in \mathcal{M} \text{ it holds } \langle x, y \rangle = 0\}$$

is called the *orthogonal complement of \mathcal{M}* . Any element x of \mathcal{H} can be uniquely decomposed in a sum $x = z + w$, where z belongs to \mathcal{M} and w belongs to \mathcal{M}^\perp .

Theorem II.5: *Let \mathcal{H} be a Hilbert space and let \mathcal{M} be a sub-Hilbert space. Then any $x \in \mathcal{H}$ can be uniquely written as $x = z + w$ with $z \in \mathcal{M}$ and $w \in \mathcal{M}^\perp$. We then write $\mathcal{H} = \mathcal{M} \oplus \mathcal{M}^\perp$.*

Notation II.6: Let \mathcal{H} be a Hilbert space. We denote by

$$\mathcal{H}' = \{\xi: \mathcal{H} \rightarrow \mathbb{C} \mid \xi \text{ is linear and continuous}\}$$

the *topological dual space of \mathcal{H}* .

Theorem II.7 (Riesz Representation Theorem): *Let \mathcal{H} be a Hilbert space. For each $\xi \in \mathcal{H}'$ there is a unique vector $y \in \mathcal{H}$ such that for all $x \in \mathcal{H}$ it holds $\xi(x) = \langle y, x \rangle$.*

Denote $\Theta: \mathcal{H} \rightarrow \mathcal{H}'$, $x \mapsto \Theta_x$, where $\Theta_x: \mathcal{H} \rightarrow \mathbb{C}$, $y \mapsto \langle x, y \rangle$. The Riesz Representation Theorem tells us that \mathcal{H} is canonically isomorphic to its topological dual space via Θ , when the topological dual space is equipped with the dual inner product $\langle \xi, \eta \rangle_* := \langle \Theta^{-1}\eta, \Theta^{-1}\xi \rangle$.

2. Bounded Operators on Hilbert Spaces

Proof: Let $\xi \in \mathcal{H}' - \{0\}$ be given. Denote by $\mathcal{N} := \ker \xi = \{z \in \mathcal{H} \mid \xi(z) = 0\}$. Then $\text{codim } \mathcal{N} = \dim \mathcal{N}^\perp = 1$. Taking any $x_0 \in \mathcal{N}^\perp - \{0\}$ and normalising it allows to declare the vector y for which it holds $\xi = \Theta_y$, namely

$$y = \frac{\xi(x_0)^*}{\|x_0\|^2} x_0. \quad \square$$

Remark II.8: The Riesz Representation Theorem justifies Dirac's bra-ket notation in physics. A vector $x \in \mathcal{H}$ is written $|x\rangle$ and called a *ket*. A functional $\xi \in \mathcal{H}'$ is written $\langle y|$, where $y = \Theta^{-1}\xi$, and called a *bra*. Now the action of ξ on x is just $\langle y|x\rangle$.

Definition II.9: Let \mathcal{H} be a Hilbert space. If \mathcal{H} has a countable dense subset, then \mathcal{H} is called *separable*.

In this lecture we will only deal with separable Hilbert spaces. Most natural Hilbert spaces are separable, thus this is no real restriction for our purposes.

Theorem II.10: *Each separable Hilbert space \mathcal{H} has an orthonormal basis, i.e. there is a family $(x_i)_{i \in I}$ with an index set I which is at most countable such that for all $i, j \in I$ it holds $\langle x_i, x_j \rangle = \delta_{ij}$ and such that for all $x \in \mathcal{H}$ it holds*

$$x = \sum_{i \in I} \langle x, x_i \rangle x_i.$$

For any $x \in \mathcal{H}$ it holds $\|x\|^2 = \sum_{i \in I} |\langle x_i, x \rangle|^2$, the so-called Identity of Parseval, which can be understood as a generalisation of Pythagoras Theorem.

Such an orthonormal basis can be produced by the Gram-Schmidt process. Orthonormal bases are not unique, but their cardinality is. The cardinality N of an orthonormal basis of \mathcal{H} is called its Hilbert space dimension, in signs $\dim \mathcal{H} = N$.

Theorem II.11: *Hilbert spaces with the same dimension are isomorphic, i.e. each separable Hilbert space \mathcal{H} is either isomorphic to \mathbb{C}^n , if $\dim \mathcal{H} = n < \infty$, or ℓ_2 , if $\dim \mathcal{H} = \infty$.*

2. Bounded Operators on Hilbert Spaces

In the following, let \mathcal{H} always be a separable Hilbert space.

Definition II.12: Let $T: \mathcal{H} \rightarrow \mathcal{H}$ be a function. If T is linear, i.e. if for all $x, y \in \mathcal{H}$ and $\lambda \in \mathbb{C}$ it holds

$$T(x + y) = T(x) + T(y), \quad T(\lambda x) = \lambda T(x),$$

then T is called a *linear operator*, or briefly an *operator*.

Remark II.13: In finite dimensions (i.e. if $\dim \mathcal{H} < \infty$), any linear operator $T: \mathcal{H} \rightarrow \mathcal{H}$ is automatically continuous. This is false for infinite-dimensional Hilbert spaces.

Lemma II.14: For a linear operator $T: \mathcal{H} \rightarrow \mathcal{H}$, the following statements are equivalent:

- (i) T is continuous,
- (ii) T is continuous in zero,
- (iii) There is a positive real number C such that

$$\|T\| := \sup\{\|Tx\| : x \in \mathcal{H}, \|x\| = 1\} < C.$$

In this case, T is called *bounded*.² The number $\|T\|$ is then the smallest constant such that for all $x \in \mathcal{H}$ it holds $\|Tx\| \leq \|T\|\|x\|$.

Proof: The implication “(i) \Rightarrow (ii)” is tautological.

For “(ii) \Rightarrow (iii)” let T be continuous in zero. For $\delta = 1$ there is $\varepsilon > 0$ such that whenever $\|y\| \leq \varepsilon$, then $\|Ty\| \leq \delta = 1$. Let now x be an element of \mathcal{H} with $\|x\| = 1$. Then $y := \varepsilon x$ has norm $\|y\| = \varepsilon$ and thus $\|Ty\| = \|T(\varepsilon x)\| = \varepsilon\|Tx\| \leq 1$. Hence $\|Tx\| \leq 1/\varepsilon$ for all $x \in \mathcal{H}$ with $\|x\| = 1$.

For “(iii) \Rightarrow (i)” let $(x_n)_{n \in \mathbb{N}}$ be a sequence in \mathcal{H} that converges to $x \in \mathcal{H}$, i.e. $\|x_n - x\| \rightarrow 0$. Then

$$\|Tx_n - Tx\| = \|T(x_n - x)\| \leq \|T\|\|x_n - x\| \rightarrow 0,$$

hence $(Tx_n)_{n \in \mathbb{N}}$ converges to Tx which shows that T is sequentially continuous. □

Notation II.15: We call $\|T\|$ the *operator norm of T* and put

$$B(\mathcal{H}) := \{T: \mathcal{H} \rightarrow \mathcal{H} \mid T \text{ is linear and bounded}\}.$$

²Note that T is not really bounded in the sense that its image is bounded, but T is bounded on bounded sets. This naming convention survived due to historical reasons.

Theorem II.16: *The set of bounded operators on \mathcal{H} is a Banach algebra, i.e. as a vector space (with the pointwise operations) it is complete with respect to the operator norm and for all $T, S \in B(\mathcal{H})$ it holds*

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

Remark II.17: For $\dim \mathcal{H} = n < \infty$, the bounded operators $B(\mathcal{H})$ can (via choice of an orthonormal basis) be identified with $M_n(\mathbb{C})$, the algebra of complex $n \times n$ -matrices.

If $\dim \mathcal{H} = \infty$, then the bounded operators $B(\mathcal{H})$ can be identified with a subset of formal infinite arrays of complex numbers, but this is not useful; in particular, for an operator $T: \mathcal{H} \rightarrow \mathcal{H}$ that corresponds to the array $(t_{ij})_{i,j \in \mathbb{N}}$, there is no useful criterion in terms of the t_{ij} to decide whether $\|T\| < \infty$.

Theorem II.18: *Let T be a bounded operator on \mathcal{H} . Then there is one and only one bounded operator T^* on \mathcal{H} such that for all $x, y \in \mathcal{H}$ it holds*

$$\langle x, Ty \rangle = \langle T^*x, y \rangle.$$

Proof: Let x be an element of \mathcal{H} . How do we define T^*x ? Consider the linear map

$$\xi: \mathcal{H} \longrightarrow \mathbb{C}, \quad y \longmapsto \langle x, Ty \rangle.$$

This map ξ is continuous; to see this let $(y_n)_{n \in \mathbb{N}}$ be a sequence in \mathcal{H} such that $y_n \rightarrow y$, i.e. $\|y_n - y\| \rightarrow 0$. Then

$$|\xi(y_n) - \xi(y)| = |\xi(y_n - y)| = |\langle x, T(y_n - y) \rangle| \leq \|T\| \|x\| \|y_n - y\| \rightarrow 0,$$

thus ξ is sequentially continuous and hence $\xi \in \mathcal{H}'$. Due to the Riesz Representation Theorem we know that there is one and only one element z of \mathcal{H} such that $\langle z, y \rangle = \xi(y) = \langle x, Ty \rangle$ for all $y \in \mathcal{H}$, hence we put $T^*x := z$. Now it remains to show that the assignment $x \mapsto T^*x$ is linear and that T^* is indeed bounded. \square

Example II.19: In the finite-dimensional setting, passing from T to T^* corresponds to taking the hermitian transpose of the transformation matrix of T with respect to an orthonormal basis of the Hilbert space.

Theorem II.20: *For all $T \in B(\mathcal{H})$ the following hold:*

- (i) $(T^*)^* = T$,
- (ii) $\|T^*\| = \|T\|$,

$$(iii) \|TT^*\| = \|T\|^2$$

Definition II.21: Let T, P, U, V and N be bounded operators on \mathcal{H} .

- (i) If $T = T^*$, then T is called *selfadjoint*.
- (ii) If $P = P^2 = P^*$, then P is called an *orthogonal projection*.
- (iii) If $U^*U = UU^* = 1$, then U is called *unitary*.
- (iv) If $V^*V = 1$, then V is called an *isometry*.
- (v) If $NN^* = N^*N$, then N is called *normal*.

Remark II.22: (i) An orthogonal projection P really is an algebraic projection from \mathcal{H} down to its range $P\mathcal{H}$. Because $P\mathcal{H}$ is closed, we have the decomposition $\mathcal{H} = P\mathcal{H} \oplus (P\mathcal{H})^\perp$.

(ii) A unitary operator U corresponds to a “rotation of the coordinate system”, i.e. it maps an orthonormal basis to another orthonormal basis.

(iii) An isometry V preserves lengths and angles, because for $x \in \mathcal{H}$ it holds

$$\|Vx\|^2 = \langle Vx, Vx \rangle = \langle x, V^*Vx \rangle = \langle x, x \rangle = \|x\|^2$$

and because of the Polarisation Identity. The difference between a unitary and an isometry is that isometries are not necessarily surjective. In the finite-dimensional setting, an isometry automatically is unitary because of the dimension formula. However, a standard-counterexample for the infinite-dimensional setting is the following: Let $(e_n)_{n \in \mathbb{N}}$ be an orthonormal basis of \mathcal{H} . Then, the operator declared by linear extension of

$$V: \mathcal{H} \longrightarrow \mathcal{H}, \quad e_i \longmapsto e_{i+1}$$

is an isometry, the so-called the one-sided shift. The adjoint V^* is uniquely determined via $V^*e_i = e_{i-1}$ for $i \geq 1$ and $V^*(e_0) = 0$. The adjoint cannot be an isometry, because it is not injective. Thus V is not unitary.

Chapter III.

Unbounded Operators

Motivation III.1: We want to understand possible realisations of the canonical commutation relation $QP - PQ = i1$.¹

Immediate realisations are given on $L^2(\mathbb{R}) := L^2(\mathbb{R}, \mathfrak{B}, \lambda)$ by the multiplication operator Q and the differentiation operator P , which are declared for a suitable function f via $(Qf)(t) := tf(t)$ and $(Pf)(t) := -if'(t)$. For those operators, we formally have

$$(QP - PQ)f(t) = -i[tf'(t) - (tf(t))'] = -i[tf'(t) - f(t) - tf'(t)] = if(t).$$

However, those operators P and Q are not bounded, and it can be shown that there are no bounded operators on $L^2(\mathbb{R})$ satisfying the canonical commutation relations.

Theorem III.2: *Let \mathcal{H} be any Hilbert space. There are no bounded operators P and Q on \mathcal{H} which satisfy $QP - PQ = i1$.*

Proof: Assume there were $P, Q \in B(\mathcal{H})$ such that $QP - PQ = i1$. Then for any natural number n we had $Q^n P - PQ^n = inQ^{n-1} \neq 0$. The initial step is clear and assuming the claim holds for the natural number n , it holds

$$Q^{n+1}P - PQ^{n+1} = Q^n(QP - PQ) + (Q^n P - PQ^n)Q = i(n+1)Q^n,$$

and inductively $Q^n \neq 0$, which establishes the claim.

From the equality $Q^n P - PQ^n = inQ^{n-1} \neq 0$ we obtained

$$n\|Q^{n-1}\| = \|Q^n P - PQ^n\| \leq \|Q^n P\| + \|PQ^n\| \leq 2\|Q^{n-1}\|\|Q\|\|P\|.$$

Because for any natural number n we knew that $\|Q^{n-1}\| \neq 0$, we were able to cancel $\|Q^{n-1}\|$ and got

$$n \leq 2\|Q\|\|P\|.$$

This had to hold for any natural number, which is absurd. □

¹Compared to the canonical commutation relations in Chapter I, we set \hbar to 1.

Definition III.3: Let \mathcal{H} be a Hilbert space. If there are a linear subspace $D(T) \subseteq \mathcal{H}$ and a linear map $T: D(T) \rightarrow \mathcal{H}$, then T is called an *unbounded operator on \mathcal{H}* . The subspace $D(T)$ is called the *domain*. Usually, we assume $D(T)$ to be dense in \mathcal{H} (i.e. $\text{cl}(D(T)) = \mathcal{H}$).

Note that we understand a bounded operator T on \mathcal{H} as an unbounded operator on \mathcal{H} with $D(T) = \mathcal{H}$.

Example III.4 (The Position Operator): Let $\mathcal{H} = L^2(\mathbb{R})$. Recall that a function $f: \mathbb{R} \rightarrow \mathbb{C}$ belongs to $L^2(\mathbb{R})$, if f is measurable with respect to the Lebesgue measure and if $\int_{\mathbb{R}} |f(t)|^2 d\lambda(t) < \infty$. The subspace

$$D(Q) := \left\{ f \in L^2(\mathbb{R}) : \int_{\mathbb{R}} t^2 |f(t)|^2 d\lambda(t) < \infty \right\}$$

together with the linear map $Q: D(Q) \rightarrow L^2(\mathbb{R})$, $Q(f)(t) = tf(t)$ constitutes an unbounded operator on $L^2(\mathbb{R})$ and indeed, $D(Q)$ is dense in $L^2(\mathbb{R})$.

Note that Q is really unbounded on its domain. To see this, consider a function f with $\int_{\mathbb{R}} |f(t)|^2 d\lambda(t) = 1$, whose support is contained in a small open interval around a large real number t_0 . Then $\int_{\mathbb{R}} t^2 |f(t)|^2 d\lambda(t)$ is roughly equal to t_0^2 , thus $\|Qf\|/\|f\|$ can become arbitrarily large, i.e. $\|Q\| = \infty$.

Remark III.5: We should choose the domain $D(T)$ of an unbounded operator T as large as possible.

(i) If the operator T is continuous on its domain, then we can extend T from the dense subset to the entire Hilbert space \mathcal{H} . Given a sequence $(x_n)_{n \in \mathbb{N}}$ in $D(T)$ that converges to x in \mathcal{H} , then also $(Tx_n)_{n \in \mathbb{N}}$ converges in \mathcal{H} , say to y . This y does not depend on the sequence converging to x , hence we can define $Tx := y$.

(ii) If T is not bounded, we can still make the above extension, if we require the convergence of all sequences $Tx_n \rightarrow y$ to the same y .

This is a weaker kind of continuity property on T , called “closeable”, and extension of T gives a “closed” operator.

Definition III.6 (Extension): Let \mathcal{H} be a Hilbert space and let $T_1: D(T_1) \rightarrow \mathcal{H}$, $T_2: D(T_2) \rightarrow \mathcal{H}$ be unbounded operators on \mathcal{H} . If $D(T_1) \subseteq D(T_2)$ and if for all $x \in D(T_1)$ it holds $T_1x = T_2x$, then T_2 is called an *extension of T_1* and in this case, we write $T_1 \subseteq T_2$.

Definition III.7 (Graph): Let \mathcal{H} be a Hilbert space and let $T: D(T) \rightarrow \mathcal{H}$ be an unbounded operator. Then

$$\Gamma(T) := \{(x, Tx) \mid x \in D(T)\} \subseteq \mathcal{H} \times \mathcal{H}$$

is called the *graph of T* . If $\Gamma(T)$ is closed in $\mathcal{H} \times \mathcal{H}$, then T is called a *closed operator*. If T has a closed extension, then T is called *closeable*. It then has a smallest closed extension, called the *closure of T* , denoted by $\text{cl}(T)$.

Note that $\Gamma(T) \subseteq \mathcal{H} \times \mathcal{H}$ is closed, if for any sequence $(x_n, y_n)_{n \in \mathbb{N}}$ in $\Gamma(T)$ converging to $(x, y) \in \mathcal{H} \times \mathcal{H}$, also (x, y) belongs to $\Gamma(T)$. Because the x_n belong to $D(T)$ by definition and the y_n are precisely Tx_n , we can understand this requirement as described before.

If an unbounded operator T on the Hilbert space \mathcal{H} is closeable, then the graph of its closure $\Gamma(\text{cl}(T))$ is indeed just $\text{cl}(\Gamma(T))$, i.e. the closure of the graph of T .

Definition III.8 (Adjoint of Unbounded Operator): Let \mathcal{H} be a Hilbert space and let $T: D(T) \rightarrow \mathcal{H}$ be a densely defined unbounded operator. Let furthermore

$$D(T^*) := \{x \in \mathcal{H} \mid \text{There is } y \in \mathcal{H} \text{ such that} \\ \text{for all } z \in D(T) \text{ it holds } \langle x, Tz \rangle = \langle y, z \rangle\}.$$

Then $T^*: D(T^*) \rightarrow \mathcal{H}$, $x \mapsto T^*y$ is called the *adjoint of T* .

Remark III.9: (i) We defined T^* in such a way that for all $z \in D(T)$ and $x \in D(T^*)$ it holds $\langle Tz, x \rangle = \langle z, T^*x \rangle$.

(ii) By Riesz Representation Theorem, some element x of \mathcal{H} belongs to $D(T^*)$ if and only if $D(T) \rightarrow \mathbb{C}$, $z \mapsto \langle x, Tz \rangle$ is a continuous mapping, which by the denseness of $D(T)$ in \mathcal{H} indeed does belong to \mathcal{H}' .

(iii) If T_1 and T_2 are unbounded operators and T_2 is an extension of T_1 , then T_1^* is an extension of T_2^* .

(iv) The domain $D(T^*)$ of T^* is clearly a linear subspace of \mathcal{H} , but in general it will not be dense in \mathcal{H} . However, it is densely defined if and only if T is closeable.

Theorem III.10: Let \mathcal{H} be a Hilbert space and let $T: D(T) \rightarrow \mathcal{H}$ be an unbounded operator on \mathcal{H} .

- (i) *The operator T is closeable if and only if $D(T^*)$ is dense in \mathcal{H} . In this case we have $\text{cl}(T) = T^{**}$.*
- (ii) *If T is closeable, then $\text{cl}(T^*) = T^*$. In particular, adjoints of closeable operators are always closed.*

Proof: Why is being closeable related to the domain of the adjoint $D(T^*)$? Assume T was not closeable, i.e. there were sequences $(x_n)_{n \in \mathbb{N}}$ and $(\bar{x}_n)_{n \in \mathbb{N}}$ in $D(T)$ such that $\lim_{n \rightarrow \infty} x_n = x = \lim_{n \rightarrow \infty} \bar{x}_n$, but there were y and \bar{y} in \mathcal{H} such that $y \neq \bar{y}$ and $\lim_{n \rightarrow \infty} Tx_n = y$ and $\bar{y} = \lim_{n \rightarrow \infty} T\bar{x}_n$. For all $w \in D(T^*)$ we then had

$$\langle y - \bar{y}, w \rangle = \lim_{n \rightarrow \infty} \langle T(x_n - \bar{x}_n), w \rangle = \lim_{n \rightarrow \infty} \langle x_n - \bar{x}_n, T^*w \rangle = 0,$$

i.e. $0 \neq y - \bar{y}$ belonged to $D(T^*)^\perp$ and thus $D(T^*)$ couldn't be dense in \mathcal{H} . Formally, the proof goes via graphs. The map

$$V: \mathcal{H} \times \mathcal{H} \longrightarrow \mathcal{H} \times \mathcal{H}, \quad (x, y) \longmapsto (-y, x)$$

is unitary with $\Gamma(T^*) = V(\Gamma(T)^\perp)$ and now everything can be deduced using general facts for orthogonal complements of linear subspaces in a Hilbert space. For example, given a linear subspace $\mathcal{M} \subseteq \mathcal{H}$, the orthogonal complement \mathcal{M}^\perp is always closed and $\mathcal{M} \subseteq \mathcal{M}^{\perp\perp}$. In fact, for a linear subspace $\mathcal{M} \subseteq \mathcal{H}$ it holds $\text{cl}(\mathcal{M}) = \mathcal{M}^{\perp\perp}$. \square

Proposition III.11: *Let \mathcal{H} be a Hilbert space and let T be an unbounded operator on \mathcal{H} . Then we have $\text{ran } T^\perp = \ker T^*$.*

The kernel of a closed operator is always closed, however this is generally not true for the range of a closed operator.

Proof: An element x of \mathcal{H} belongs to $\text{ran } T^\perp$ if and only if for all $y \in D(T)$ it holds $\langle x, Ty \rangle = 0$. This in turn holds if and only if x belongs to $D(T^*)$ and $T^*x = 0$, i.e. $x \in \ker T^*$. \square

Chapter IV.

Symmetric and Selfadjoint Operators

Definition IV.1: Let \mathcal{H} be a Hilbert space and let $T: D(T) \rightarrow \mathcal{H}$ be an unbounded operator.

- (i) If for all x and y in $D(T)$ it holds $\langle Tx, y \rangle = \langle x, Ty \rangle$, then T is called *symmetric* or *Hermitean*. Note that this means that T^* is an extension of T .
- (ii) If $T = T^*$, then T is called *selfadjoint*. In this case, T is symmetric and $D(T) = D(T^*)$.
- (iii) If T is closeable and $\text{cl}(T)$ is selfadjoint, then T is called *essentially selfadjoint*.

Remark IV.2: (i) Note that a densely defined symmetric operator T is closeable, since $D(T) \subseteq D(T^*)$ and $D(T)$ already is dense in \mathcal{H} .

(ii) The operator T is essentially selfadjoint if and only if T has precisely one selfadjoint extension (namely its closure $\text{cl}(T)$).

Assume S and T were operators, T was an extension of S and both S and T were selfadjoint. Then we had $T = T^* \subseteq S^* = S$, i.e. S had to be equal to T .

(iii) The essentially selfadjoint operators form a proper subset of the symmetric operators.

(iv) All the good things (like the Spectral Theorem or the Theorem of Stone) are only true for essentially selfadjoint operators, but not for symmetric operators in general.

Theorem IV.3 (Basic Criterion for Selfadjointness): Let \mathcal{H} be a Hilbert space and let $T: D(T) \rightarrow \mathcal{H}$ be a symmetric unbounded operator on \mathcal{H} . Then the following are equivalent:

- (i) *The operator T is selfadjoint.*
- (ii) *The operator T is closed, $\ker(T^* + i) = \{0\}$ and $\ker(T^* - i) = \{0\}$.*
- (iii) *It holds $\text{ran}(T - i) = \mathcal{H}$ and $\text{ran}(T + i) = \mathcal{H}$.*

Of course, here $T + i$ stands for $T + i \text{id}$ and $D(T + i) = D(T)$.

Proof: “(i) \implies (ii)”: We assume that $T = T^*$, i.e. T is a closed operator. Let $\lambda \in \mathbb{C} - \mathbb{R}$ be given and let $x \in D(T^* - \lambda) = D(T^*) = D(T)$ such that $(T^* - \lambda)x = 0 = (T - \lambda)x$, i.e. $Tx = T^*x = \lambda x$. But then

$$\lambda^* \langle x, x \rangle = \langle \lambda x, x \rangle = \langle Tx, x \rangle = \langle x, Tx \rangle = \lambda \langle x, x \rangle.$$

Since we assumed that $0 \neq \lambda^* \neq \lambda$, this can only be true if $\langle x, x \rangle = 0$. Thus x must be zero and $\ker(T^* - \lambda) = \{0\}$.

“(ii) \implies (iii)”: Assume that $\ker(T^* + i) = \{0\}$. By Proposition III.11 we obtain that $\text{ran}(T - i)^\perp = \ker(T - i)^* = \{0\}$, hence $\text{ran}(T - i) \subseteq \mathcal{H}$ must be dense. It remains to show that $\text{ran}(T - i)$ is closed. Assume that $(y_n)_{n \in \mathbb{N}}$ were a sequence in $\text{ran}(T - i)$ which converged to some $y \in \mathcal{H}$. For the index n there were an element $x_n \in \mathcal{H}$ such that $y_n = (T - i)x_n$. Note that for any $z \in D(T - i) = D(T)$ it holds

$$\begin{aligned} \|(T - i)z\|^2 &= \langle (T - i)z, (T - i)z \rangle \\ &= \langle Tz, Tz \rangle + i \langle z, Tz \rangle - i \langle Tz, z \rangle + \langle z, z \rangle = \|Tz\|^2 + \|z\|^2. \end{aligned}$$

For our problem at hand we use it as follows: Because $(y_n)_{n \in \mathbb{N}}$ converged to y , it were a Cauchy sequence and we had

$$\|y_n - y_m\|^2 = \|(T - i)(x_n - x_m)\|^2 = \|T(x_n - x_m)\|^2 + \|x_n - x_m\|^2,$$

which forced both the sequence $(x_n)_{n \in \mathbb{N}}$ and $(Tx_n)_{n \in \mathbb{N}}$ to be Cauchy sequences in \mathcal{H} . Hence we had $z \in \mathcal{H}$ such that Tx_n converged to z and we had $x \in \mathcal{H}$ such that x_n converged to x . As T is closed, this meant that x belonged to $D(T)$ and that $Tx = z$. But then $y = \lim_{n \rightarrow \infty} (T - i)x_n = Tx - ix = (T - i)x$ and thus y belonged to $\text{ran}(T - i)$ and $\text{ran}(T - i)$ is closed.

The proof of “(iii) \implies (i)” is similar in nature to the proofs of the other implications and thus omitted. \square

Theorem IV.4: *Let \mathcal{H} be Hilbert space and let $T: D(T) \rightarrow \mathcal{H}$ be a symmetric operator. Then the following are equivalent:*

- (i) *The operator T is essentially selfadjoint.*

- (ii) It holds $\ker(T^* + i) = \{0\}$ and $\ker(T^* - i) = \{0\}$.
- (iii) The spaces $\text{ran}(T - i)$ and $\text{ran}(T + i)$ are dense in \mathcal{H} .

Remark IV.5: (i) For a closed symmetric operator T and $\lambda = \pm i$ we have the situation

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and T is selfadjoint if and only if $\dim \ker(T^* + \lambda^*) = 0$ both for $\lambda = i$ and $\lambda = -i$.

Note that $\lambda \mapsto \dim(T^* - \lambda)$ is constant both on the upper halfplane and the lower halfplane.

(ii) The possible selfadjoint extensions of a symmetric operator T are completely characterised by its *defect indices* $m := \dim \ker(T^* - i) = \dim \text{ran}(T + i)^\perp$ and $n := \dim \ker(T^* + i) = \dim \text{ran}(T - i)^\perp$. In particular, T is essentially selfadjoint if and only if $(m, n) = (0, 0)$. The operator T has selfadjoint extensions if and only if $(m, n) = (k, k)$ for some natural number k .

Example IV.6 (The Position Operator): Let $\mathcal{H} = L^2(I)$, where $I = [a, b]$, $[a, \infty)$, $(-\infty, b]$ or $(-\infty, \infty)$ and let $T = Q$ be the position operator defined via

$$T: D(T) \longrightarrow \mathcal{H}, \quad (Tf)(t) = tf(t).$$

Then $D(T) = \{f \in L^2(I) \mid tf(t) \in L^2(I)\}$ is the domain of T . What is the adjoint T^* of T ? As stated before, the domain of the adjoint is

$$D(T^*) = \{g \in \mathcal{H} \mid \text{There is } h \in \mathcal{H} \text{ such that} \\ \text{for all } f \in D(T) \text{ it holds } \langle Tf, g \rangle = \langle f, h \rangle\}.$$

That is, in our case,

$$\int_I t^* f(t)^* dt = \langle Tf, g \rangle = \langle f, h \rangle = \int_I f(t)^* h(t) dt,$$

thus we get the following determining equation for g : “For all $f \in D(T)$ it holds $\int_I f(t)^* [tg(t) - h(t)] dt = 0$ ”. Hence, $tg(t) - h(t)$ has to be zero almost everywhere (with respect to the Lebesgue measure), i.e. $h(t) = tg(t) \in L^2(I)$, which requires g to belong to $D(T)$. Finally, because of $(T^*g)(t) = h(t) = tg(t)$, the operator T is really selfadjoint. Note that the condition $(m, n) = (0, 0)$ is obvious in this case.

Example IV.7 (The Momentum Operator): The momentum operator T was formally given by $i \frac{d}{dt}$, i.e. $Tf = if'$. In the following, we want to make this rigorous. Let \mathcal{H} be the Hilbert space $L^2([0, 1])$ and let

$$D(T) := \{f \in L^2([0, 1]) \mid f \text{ is continuously differentiable, } f(0) = 0 = f(1)\}.$$

The operator T is symmetric, since for f and g in $D(T)$ we have

$$\begin{aligned} \langle Tf, g \rangle &= \int_0^1 i^* f'(t)^* g(t) dt \\ &= -i \int_0^1 f'(t)^* g(t) dt \\ &= i \int_0^1 f(t)^* g'(t) dt - i[f^*g]_0^1 = \int_0^1 f(t)^* i g(t) dt = \langle f, Tg \rangle \end{aligned}$$

and in particular $T \subseteq T^*$. Now for the adjoint of T . Let g be an element of $D(T^*)$, i.e. there is $h = T^*g$ such that for all $f \in D(T)$ it holds

$$\int_0^1 g(t)^* i f'(t) dt = \langle g, Tf \rangle = \langle h, f \rangle = \int_0^1 h(t)^* f(t) dt.$$

Without proof we make use of the fact that there is a function H such that $H' = h$ almost everywhere, i.e. $H(t) = \int_0^1 h(s) ds$, and thus

$$\begin{aligned} \int_0^1 h(t)^* f(t) dt &= \int_0^1 H'(t)^* f(t) dt \\ &= - \int_0^1 H(t)^* f'(t) dt + H(1)^* f(1) + H(0)^* f(0) \\ &= - \int_0^1 H(t)^* f'(t) dt. \end{aligned}$$

Hence for all $f \in D(T)$ it holds $\int_0^1 f'(t)[ig(t)^* + H(t)^*] dt = 0$. Consequently $ig^* + H^* \in \{f' \mid f \in D(T)\}^\perp = \mathbb{C}1$. For g we thus get $g^* = iH^* + c$, where c is some constant. The function $iH^* + c$ is absolutely continuous. Note that no boundary conditions on g are imposed by our calculation and note that we have $T^*g = h = H' = ig'$, which makes sense because absolutely continuous functions are almost every differentiable. Our calculation thus shows that $D(T^*)$ is contained in the set

$$\{g \in L^2([0, 1]) \mid g \text{ is absolutely continuous and } g' \in L^2([0, 1])\}.$$

By directly checking we also get the other inclusion. In particular, we obtain that T is not selfadjoint.

As T is symmetric, it is closeable, but not closed. We get its closure as $\text{cl}(T) = T^{**}$ with domain

$$D(\text{cl}(T)) = \{f \in L^2([0, 1]) \mid f \text{ is absolutely continuous,} \\ f' \in L^2([0, 1]) \text{ and } f(0) = 0 = f(1)\}$$

and $\text{cl}(T)f = if'$. In particular we see that T^* is not symmetric anymore, because $T^{**} \subsetneq T^*$. Because of the chain of inclusions $\text{cl}(T) = T^{**} \subsetneq T^* = \text{cl}(T)^*$, the closure $\text{cl}(T)$ is not selfadjoint and T is not essentially selfadjoint.

To answer the question whether we can find a more well-behaved selfadjoint extension of T is answered by the defect indices.

We have $m = \dim \ker(T^* - i) = 1$, as the solutions of $T^*f = if$ are precisely the functions ce^t , where c is some constant. The other defect index is one, too, thus we have the defect indices $(m, n) = (1, 1)$.

What do we make of this? How can we find a selfadjoint extension S ? We want to have that

$$\begin{aligned} i \int_0^1 f(t)^* g'(t) dt &= \langle f, Sg \rangle \\ &= \langle Sf, g \rangle \\ &= -i \int_0^1 f'(t)^* g(t) dt \\ &= i \int_0^1 f(t)^* g'(t) dt - i[f(1)^* g(1) - f(0)^* g(0)] \end{aligned}$$

and we need some condition that is in a sense weaker than $f(0) = 0 = f(1)$. If we impose the condition $f(0) = 0 = f(1)$, then we do not need any conditions for g . If instead we ask $f(1) = \alpha f(0)$, then we also need that $g(1) = \alpha g(0)$ for some $\alpha \in \mathbb{T} = \{z \in \mathbb{C} \mid |z| = 1\}$ and we get that

$$f(1)^* g(1) - f(0)^* g(0) = \alpha^* f(0)^* \alpha g(0) - f(0)^* g(0) = 0.$$

For each $\alpha \in \mathbb{T}$ we define an operator T_α with domain

$$D(T_\alpha) := \{f \in L^2([0, 1]) \mid f \text{ is absolutely continuous,} \\ f' \in L^2([0, 1]) \text{ and } f(1) = \alpha f(0)\}$$

and action $T_\alpha f := if'$. All those operators T_α are (different) selfadjoint extensions of T . It can be shown that those are precisely all selfadjoint extensions of T .

Chapter V.

Spectrum and Spectral Theorem

Let \mathcal{H} be a finite-dimensional Hilbert space and let A be a (bounded) linear operator on \mathcal{H} . Then A can be identified with a matrix and the spectrum of A , denoted $\sigma(A)$, is given by the eigenvalues of A .

The Spectral Theorem for selfadjoint operators ensures that selfadjoint operators (respectively their associated transformation matrices) may be diagonalised.

In the following, we aim to generalise results of this shape and form to infinite-dimensional Hilbert spaces \mathcal{H} and unbounded operators on said Hilbert space.

Lets start with the spectrum. In the finite-dimensional setting, a complex number λ belongs to $\sigma(A)$ if and only if it is an eigenvalue of A , i.e. if there is $x \in \mathcal{H} - \{0\}$ such that $Ax = \lambda x$. This is equivalent to saying that $(A - \lambda \text{id})x = 0$. Because of the dimension formula, this happens if and only if $A - \lambda \text{id}$ is not invertible.

Note that if \mathcal{H} is finite-dimensional, injectivity of an operator $A \in B(\mathcal{H})$ is the same as surjectivity and thus even bijectivity.

The “correct” generalisation of the notion of eigenvalues to infinite dimension is asking the question, if $(A - \lambda \text{id})^{-1}$ exists.

Definition V.1: Let \mathcal{H} be Hilbert space and let $T: D(T) \rightarrow \mathcal{H}$ be a closed unbounded operator on \mathcal{H} .

(i) The set

$$\rho(T) := \{\lambda \in \mathbb{C} \mid T - \lambda \text{id}: D(T) \rightarrow \mathcal{H} \text{ is a bijection} \\ \text{and } (T - \lambda \text{id})^{-1} \in B(\mathcal{H})\}$$

is called the *resolvent set of T* and $\sigma(T) := \mathbb{C} - \rho(T)$ is called the *spectrum of T*.

(ii) Denote

$$\begin{aligned}\sigma_p(T) &:= \{\lambda \in \mathbb{C} \mid \text{There is } x \in \mathcal{H} - \{0\} \text{ such that } Tx = \lambda x\} \\ \sigma_c(T) &:= \{\lambda \in \mathbb{C} - \sigma_p(T) \mid \text{ran}(T - \lambda \text{id}) \text{ is dense in } \mathcal{H}, \\ &\quad \text{but } (T - \lambda \text{id})^{-1}: \text{ran}(T - \lambda \text{id}) \rightarrow D(T) \text{ is not bounded}\} \\ \sigma_r(T) &:= \{\lambda \in \mathbb{C} - \sigma_p(T) \mid \text{ran}(T - \lambda \text{id}) \text{ is not dense in } \mathcal{H}\}\end{aligned}$$

The set $\sigma_p(T)$ is called *point spectrum of T* , $\sigma_c(T)$ is called the *continuous spectrum of T* and $\sigma_r(T)$ is called the *residual spectrum of T* .

It can be shown that $\sigma(T)$ decomposes as $\sigma(T) = \sigma_p(T) \cup \sigma_c(T) \cup \sigma_r(T)$ and additionally that this union is in fact disjoint.

Remark V.2: (i) The point spectrum consists of eigenvalues, for which there are eigenvectors, i.e. for $\lambda \in \sigma_p(T)$ we have non-zero solutions for the equation $Tx = \lambda x$.

(ii) The continuous spectrum consists of complex numbers λ , for which we have *approximate eigenvectors*. More precisely, let $\lambda \in \sigma_c(T)$. Then $T - \lambda \text{id}: D(T) \rightarrow \text{ran}(T - \lambda \text{id})$ is a bijective mapping and $\text{ran}(T - \lambda \text{id})$ is dense, but $(T - \lambda \text{id})^{-1}: \text{ran}(T - \lambda \text{id}) \rightarrow D(T)$ is, by assumption, not bounded. That is, we find a sequence $(x_n)_{n \in \mathbb{N}}$ in $\text{ran}(D - \lambda \text{id})$ such that for all $n \in \mathbb{N}$ it holds $\|x_n\| = 1$, but the sequence defined via $\alpha_n := \|(T - \lambda \text{id})^{-1}x_n\|$ tends to infinity when n gets large.

If we put $y_n := \alpha_n^{-1}(T - \lambda \text{id})^{-1}x_n$ (those are normalised), then we obtain $\|(T - \lambda \text{id})y_n\| = \alpha_n^{-1}\|x_n\| \rightarrow 0$. The vectors y_n are called approximate eigenvectors and $Ty_n \approx \lambda y_n$.

(iii) In many cases the residual spectrum is absent, in particular: If T is selfadjoint, then $\sigma_r(T) = \emptyset$.

(iv) For the spectrum of a closed symmetric operator there are the following possibilities:

- (1) $\sigma(T) = \mathbb{C}_0^+ := \text{cl}(\mathbb{H})$,
- (2) $\sigma(T) = \mathbb{C}_0^- := \text{cl}(-\mathbb{H})$,
- (3) $\sigma(T) = \mathbb{C}$,
- (4) $\sigma(T) \subseteq \mathbb{R}$,

and it holds $\sigma(T) \subseteq \mathbb{R}$ if and only if T is selfadjoint.

Example V.3 (Position Operator): Let \mathcal{H} be the Hilbert space $L^2(I)$ for some interval $I \subseteq \mathbb{R}$ and consider the operator $T: D(T) \rightarrow \mathcal{H}$, which is defined via $(Tf)(t) = tf(t)$ on $D(T) = \{f \in L^2(I) \mid Tf \in L^2(I)\}$.

By Example IV.6 we know that $T = T^*$. Thus, $\sigma(T) \subseteq \mathbb{R}$. First, we look for eigenvalues $\lambda \in \mathbb{R}$ of T . The eigenvalue equation $Tf = \lambda f$ reads $tf(t) = \lambda f(t)$ almost everywhere and it has no non-trivial solution in \mathcal{H} . That means $\sigma_p(T) = \emptyset$.

Intuitively speaking, the eigenvalue equation can only be fulfilled by a non-zero function that vanishes everywhere but in one point, where it “takes the value infinity”, thus we should focus attention on the δ -distribution. For $\lambda \in I$, we can approximate the δ -distribution at λ with actual elements of \mathcal{H} , e.g. by the functions declared via

$$\delta_n: I \longrightarrow \mathbb{R}, \quad x \longmapsto \sqrt{n}\chi_{[-1/2n, 1/2n]}(x).$$

For those we have $\|\delta_n\| = 1$ and $T\delta_n \approx \lambda\delta_n$. Hence any $\lambda \in I$ belongs to $\sigma_c(T)$. For $\lambda \in \mathbb{R} - I$, then λ belongs to $\rho(T)$, since we can just write down the inverse

$$(T - \lambda)^{-1}f(t) = \frac{1}{t - \lambda}f(t),$$

which is again square-integrable on I . This means $\sigma_p(T) = \emptyset = \sigma_r(T)$ and $\sigma(T) = \sigma_c(T) = I \subseteq \mathbb{R}$.

Motivation V.4: (i) Let \mathcal{H} be a finite-dimensional Hilbert space of dimension n and let $A \in B(\mathcal{H})$ be a selfadjoint operator. Since the spectrum $\sigma(A)$ consists only of real numbers, we may write $\sigma(A) = \{\lambda_1 < \lambda_2 < \dots < \lambda_k\}$. For $\lambda \in \sigma(A)$, denote by

$$\mathcal{H}_\lambda := \{x \in \mathcal{H} \mid Ax = \lambda x\}$$

the eigenspace to the eigenvalue λ . The Spectral Theorem for selfadjoint matrices can be stated in the following way: The Hilbert space \mathcal{H} decomposes into the orthogonal direct sum $H = \bigoplus_{\lambda \in \sigma(A)} H_\lambda$, i.e. eigenspaces to different eigenvalues are orthogonal and for any element $x \in \mathcal{H}$ there are eigenvectors $x_i \in \mathcal{H}_{\lambda_i}$, $1 \leq i \leq k$, such that $x = \sum_{i=1}^k x_i$.

Denote by $P_\lambda: \mathcal{H} \rightarrow \mathcal{H}_\lambda$ the orthogonal projection onto the eigenspace \mathcal{H}_λ . Then the eigenvectors x_i in the representation of x from above are precisely the $P_{\lambda_i}(x)$. Finally, we may write

$$Ax = \sum_{i=1}^k Ax_i = \sum_{i=1}^k \lambda_i x_i = \sum_{i=1}^k \lambda_i P_{\lambda_i}(x),$$

thus $A = \sum_{i=1}^k \lambda_i P_{\lambda_i} = \sum_{\lambda \in \sigma(A)} \lambda P_\lambda$.

(ii) We'd like to generalise this to infinite dimensions. Thus, consider an infinite-dimensional Hilbert space \mathcal{H} and an selfadjoint operator T on \mathcal{H} . We know that its spectrum may be written as $\sigma(T) = \sigma_p(T) \cup \sigma_c(T)$, and while for $\sigma_p(T)$ the Spectral Theorem works as above, for $\lambda \in \sigma_c(T)$, it holds $\mathcal{H}_\lambda = \{0\}$ and $P_\lambda = 0$, hence the approach described above fails.

Consider the multiplication operator Q on $L^2(\mathbb{R})$, defined via $(Qf)(t) = tf(t)$. For a real number λ , let Δ be a small interval with $\lambda \in \Delta$ and let

$$\mathcal{H}_\Delta := \{f \in L^2(\mathbb{R}) \mid f|_{\mathbb{R}-\Delta} \equiv 0\}$$

and $E_\Delta: \mathcal{H} \rightarrow \mathcal{H}_\Delta$ be the orthogonal projection onto \mathcal{H}_Δ .

Using this notation, for $\Delta_1 \cap \Delta_2$, the corresponding spaces \mathcal{H}_{Δ_1} and \mathcal{H}_{Δ_2} are orthogonal.

If $\Delta = \Delta_1 \cup \Delta_2$, then for the corresponding orthogonal projections it holds $E_\Delta = E_{\Delta_1} + E_{\Delta_2}$; in particular $\mathcal{H}_\Delta = \mathcal{H}_{\Delta_1} \oplus \mathcal{H}_{\Delta_2}$.

If $\mathbb{R} = \cup_i \Delta_i$, then $\mathcal{H} = \bigoplus_i \mathcal{H}_i$.

How can we now represent Q using this data? If $|\Delta|$ is small and x belongs to \mathcal{H}_Δ , then $Qx \approx \lambda x$ for some fixed $\lambda \in \Delta$. Hence we may write

$$Qx = \sum_i Q E_{\Delta_i} x \approx \sum_i \lambda_i E_{\Delta_i} x \quad (\lambda_i \in \Delta_i).$$

We might hope that Q corresponds to the limit

$$\lim_{|\Delta_i| \rightarrow 0} \sum_i \lambda_i E_{\Delta_i} = \int \lambda dE(\lambda),$$

where $E(\lambda) := E_{(-\infty, \lambda]}$. Indeed, any selfadjoint operator T may be written as an operator-valued Stieltjes integral $T = \int \lambda dE(\lambda)$ for a corresponding so-called *resolution of identity* $\lambda \mapsto E(\lambda) =: E_\lambda$.

Definition V.5: Let \mathcal{H} be a Hilbert space and let $(E(\lambda))_{\lambda \in \mathbb{R}}$ be a family of bounded operators on \mathcal{H} . If for each $\lambda \in \mathbb{R}$ the operator E_λ is an orthogonal projection, i.e. $E_\lambda = E_\lambda^2 = E_\lambda^*$; if for any real numbers λ, μ with $\lambda \leq \mu$ it holds $E_\lambda E_\mu = E_\mu E_\lambda = E_\lambda$; if for all $x \in \mathcal{H}$ it holds

$$\lim_{\lambda \rightarrow -\infty} E_\lambda x = 0, \quad \lim_{\lambda \rightarrow +\infty} E_\lambda x = x$$

and if $\lambda \mapsto E_\lambda$ is right-continuous, i.e. for all $x \in \mathcal{H}$ it holds $\lim_{\varepsilon \downarrow 0} E_{\lambda+\varepsilon} x = E_\lambda x$, then this family is called a *resolution of identity* or *projection-valued measure*.

Remark V.6: (i) Note that the properties of a resolution of identity enforce that for each $x \in \mathcal{H}$ the function

$$\mathbb{R} \longrightarrow [0, \infty), \quad \lambda \longmapsto \langle x, E_\lambda x \rangle = \langle x, E_\lambda^* E_\lambda x \rangle = \|E_\lambda x\|^2$$

has precisely the properties of a distribution function (see Definition A.1), i.e. we can define Lebesgue-Stieltjes integrals of the form $\int f(\lambda) d\langle x, E_\lambda x \rangle$.

(ii) In order to define our operator-valued Stieltjes integral $\int f(\lambda) dE(\lambda)$ as operator, we need to define the inner products $\langle x, \int f(\lambda) dE(\lambda) y \rangle$ for suitable elements x and y in \mathcal{H} .

By polarisation it suffices to define this for the special case $x = y$, but then we can define $\langle x, \int f(\lambda) dE(\lambda) x \rangle = \int f(\lambda) d\langle x, E_\lambda x \rangle$. For each x , the integral $\int f(\lambda) d\langle x, E_\lambda x \rangle$ is nothing but an ordinary Stieltjes integral.

Proposition V.7: *Let $(E_\lambda)_{\lambda \in \mathbb{R}}$ be a projection valued measure and let $f: \mathbb{R} \rightarrow \mathbb{C}$ be measurable. Then there is a densely defined operator $T_f = \int f(\lambda) dE(\lambda)$ with domain $D(T_f) = \{x \in \mathcal{H} : \int |f(\lambda)|^2 d\langle x, E_\lambda x \rangle < \infty\}$ that, for $x \in D(T_f)$, is uniquely determined via*

$$\langle x, T_f x \rangle = \int f(\lambda) d\langle x, E_\lambda x \rangle.$$

Furthermore, for any $x \in D(T_f)$ it holds $\|T_f x\|^2 = \int |f(\lambda)|^2 d\langle x, E_\lambda x \rangle$.

Theorem V.8 (Spectral Theorem):

- (i) *Let $(E_\lambda)_{\lambda \in \mathbb{R}}$ be a projection valued measure. Then $T := \int \lambda dE_\lambda$ is a selfadjoint operator with domain $D(T) = \{x \in \mathcal{H} \mid \int \lambda^2 d\langle x, E_\lambda x \rangle < \infty\}$.*
- (ii) *Let T be an unbounded selfadjoint operator. Then there is a uniquely determined resolution of identity $(E_\lambda)_{\lambda \in \mathbb{R}}$ such that $T = \int \lambda dE_\lambda$.*

Example V.9: (i) Let \mathcal{H} be a finite-dimensional Hilbert space of dimension n , let A be a selfadjoint operator and let $\sigma(A) = \{\lambda_1 < \dots < \lambda_k\}$. Furthermore, denote by \mathcal{H}_λ the eigenspace with respect to λ and by P_λ the orthogonal projection onto \mathcal{H}_λ . Then $E_\lambda = \sum_{\lambda_i \leq \lambda} P_{\lambda_i}$ and $A = \int \lambda dE_\lambda = \sum_{i=1}^k \lambda_i P_{\lambda_i}$.

(ii) Let Q be the multiplication operator on $L^2(\mathbb{R})$, i.e. $(Qf)(t) = tf(t)$. Then the resolution of identity $(E_\lambda)_{\lambda \in \mathbb{R}}$ is given by

$$(E_\lambda f)(t) = \begin{cases} f(t), & \text{if } t \leq \lambda, \\ 0, & \text{if } t > \lambda \end{cases}$$

and Q may be written as $Q = \int \lambda dE(\lambda)$.

Theorem V.10 (Functional Calculus): Let \mathcal{H} be a Hilbert space and let T be a selfadjoint operator on \mathcal{H} with spectral decomposition $T = \int \lambda dE(\lambda)$.

(i) For each measurable function $f: \mathbb{R} \rightarrow \mathbb{C}$ there is an operator

$$f(T) := \int f(\lambda) dE(\lambda),$$

with $D(f(T)) = \{x \in \mathcal{H} \mid \int |f(\lambda)|^2 d\langle x, E_\lambda x \rangle < \infty\}$ that is uniquely determined by $\langle x, f(T)x \rangle = \int f(\lambda) d\langle x, E_\lambda x \rangle$ for all $x \in D(f(T))$.

(ii) Let $f, g: \mathbb{R} \rightarrow \mathbb{C}$ be measurable functions. Then $f(T)g(T) \subseteq (fg)(T)$ and $D(f(T)g(T)) = D(g(T)) \cap D((fg)(T))$.

(iii) For a measurable function $f: \mathbb{R} \rightarrow \mathbb{C}$ it holds

$$f(T)^* = \int f(\lambda)^* dE(\lambda) = f^*(T).$$

In particular we obtain that by applying a real-valued function f to our operator, we end up with a selfadjoint operator $f(T)$.

Remark V.11: (i) Note that this gives a very general functional calculus for selfadjoint operators. For unbounded operators not even polynomials are a priori well-defined. Thinking a bit about the equation $T^2x = T(Tx)$ makes clear that T^2 might not have a dense domain.

(ii) For Borel sets $B \subseteq \mathbb{R}$ and $f = \chi_B$ we get our “projection valued measure” μ_T defined via

$$B \longmapsto \mu_T(B) = \chi_B(T) = \int_B dE(\lambda) =: E(B)$$

with the following properties:

- For each Borel set B the operator $E(B)$ is an orthogonal projection,
- It holds $E(\emptyset) = 0$ and $E(\mathbb{R}) = 1$,
- For Borel sets B_1 and B_2 we have $E(B_1)E(B_2) = E(B_1 \cap B_2)$,
- If $(B_n)_{n \in \mathbb{N}}$ is a sequence of pairwise disjoint Borel sets and $B = \bigcup_{n \in \mathbb{N}} B_n$, then for all $x \in \mathcal{H}$ it holds $E(B)x = \sum_{n \in \mathbb{N}} E(B_n)x$.

(iii) Let $(B_i)_{1 \leq i \leq n}$ be a family of pairwise disjoint Borel sets. Then

$$\sum_{i=1}^n \alpha_i E(B_i) = \int \left(\sum_{i=1}^n \alpha_i \chi_{B_i} \right) dE(\lambda)$$

and $\|\sum_{i=1}^n \alpha_i E(B_i)\| = \max\{|\alpha_i| \mid E(B_i) \neq 0\}$. In the same way we see that

$$\left\| \int f(\lambda) dE(\lambda) \right\| = \text{ess sup}\{|f(\lambda)| \mid \lambda \in \text{supp}(E)\},$$

where $\text{supp}(E)$ is the smallest subset $C \subseteq \mathbb{R}$ such that $E(C^c) = 0$. Let λ_0 be some fixed real number. If $f(\lambda) = (\lambda - \lambda_0)^{-1}$, then $(T - \lambda_0)^{-1} = \int \frac{1}{\lambda - \lambda_0} dE(\lambda)$ and

$$\text{ess sup}_{\lambda \in \text{supp}(E)} \left| \frac{1}{\lambda - \lambda_0} \right| = \|(T - \lambda_0)^{-1}\| = \begin{cases} \Gamma < \infty, & \text{if } \lambda_0 \in \rho(T), \\ \infty, & \text{if } \lambda_0 \in \sigma(T) \end{cases}$$

which yields that $\text{supp}(E) = \sigma(T)$ and thus $\int f dE(\lambda) = \int_{\sigma(T)} f dE(\lambda)$. Thus the function f only needs to be defined on the spectrum $\sigma(T)$.

Axiomatic V.12 (von Neumann Axiomatic of Quantum Mechanics):

(i) A quantum mechanical system corresponds to a complex separable Hilbert space \mathcal{H} .

(ii) A pure state corresponds to a unit vector $x \in \mathcal{H}$, i.e. $\|x\| = 1$. If we take $\alpha \in \mathbb{T}$, then αx describes the same state as x .

(iii) Observables correspond to selfadjoint operators on \mathcal{H} .

(iv) The measurement of an observable corresponding to a selfadjoint operator $T = \int \lambda dE(\lambda)$ on a system corresponding to $x \in \mathcal{H}$ has as possible outcomes values λ in $\sigma(T)$ with probability distribution given by $d\langle x, E(\lambda)x \rangle$, i.e. for a real number λ_0 it holds $P(\{\lambda \in (-\infty, \lambda_0]\}) = \langle x, E(\lambda_0)x \rangle$. More generally for any Borel set $B \subseteq \mathbb{R}$ it holds $P(\{\lambda \in B\}) = \langle x, E(B)x \rangle$.

(v) In the setting of (iv) and for a measurable function $f: \sigma(T) \rightarrow \mathbb{R}$ the selfadjoint operator $f(T)$ corresponds to the composition of the observable followed by f .

Remark V.13: (i) Let λ be an element of $\sigma_p(T)$. Then $E(\{\lambda\})$ is the projection onto vectors which give value λ with probability one.

(ii) If λ belongs to $\sigma_c(T)$, then $E(\{\lambda\}) = 0$, so the probability of measuring exactly λ is zero. However, for any $\varepsilon > 0$ and the interval $\Delta_\varepsilon := (\lambda - \varepsilon, \lambda + \varepsilon)$, it holds $E(\Delta_\varepsilon) \neq 0$, thus we have states $x_\varepsilon \in \mathcal{H}$ such that the measurement in such a case gives with probability one a result in Δ_ε .

Chapter VI.

Theorem of Stone

The time evolution of a quantum mechanical system is given by time evolution operators $(U_t)_{t \geq 0}$. If we denote by ψ_0 the unit vector that describes our system at time $T = 0$ and by ψ_t the system at time $T = t$, then it is given by $\psi_t = U_t \psi_0$.

Standing to reason we demand that the operators U_t are isometries, i.e. $\|\psi_t\| = \|\psi_0\|$. If those U_t are also invertible, then they are in fact unitaries. Furthermore, we demand that $U_0 = 1$ and that $U_t U_s = U_{t+s}$.

For a given quantum mechanical system, we want to see how do these time evolution operators come about. It will turn out that there is a selfadjoint operator H such that $U_t = e^{-itH}$ and that the unitarity of the U_t corresponds to the property of H being selfadjoint. Given $U_t = e^{-itH}$ it holds $\frac{d}{dt} U_t = -iH U_t$ respectively

$$i \frac{dU_t}{dt} \psi = H U_t \psi, \quad i \frac{\partial \psi_t}{\partial t} = H \psi_t. \quad (\text{VI.1})$$

The equation above is the famous *Schrödinger Equation*. The operator H is called *Hamilton operator of the system* and it governs the time evolution.

In the following, we will thus address the following mathematical problem: Given a unitary group $(U_t)_{t \in \mathbb{R}}$, is there a generator A for this group, i.e. is there an operator A such that $U_t = e^{-itA}$?

Theorem VI.1: *Let \mathcal{H} be a Hilbert space and let $A \in B(\mathcal{H})$ be a selfadjoint operator. For a real number t , denote*

$$U_t := e^{itA} = \sum_{n=0}^{\infty} \frac{(it)^n}{n!} A^n.$$

Then we have the following:

- (i) *For all real numbers t , U_t is unitary with $U_t^* = U_{-t}$.*
- (ii) *For $t = 0$, we obtain $U_0 = 1$.*

- (iii) For all $t, s \in \mathbb{R}$ it holds $U_t U_s = U_{s+t}$.
- (iv) For $t \rightarrow 0$ we have $\|U_t - 1\| \rightarrow 0$.

Thus we get: If A is a selfadjoint bounded operator on \mathcal{H} , then we obtain a norm continuous unitary group $(U_t)_{t \in \mathbb{R}}$.

Theorem VI.2: Let $(U_t)_{t \in \mathbb{R}}$ be a norm continuous unitary group on a Hilbert space \mathcal{H} , that is all operators are unitary, the operator U_0 is the identity, for all $t, s \in \mathbb{R}$ it holds $U_t U_s = U_{t+s}$ and it holds $\lim_{t \rightarrow 0} \|U_t - 1\| = 0$. Then there exists a uniquely determined selfadjoint bounded operator A such that $U_t = e^{itA}$.

Proof: Intuitively, A should be given as $A = \frac{d}{dt} U_t|_{t=0}$. However, a priori we do not know that this limit exists. Maybe a better way for obtaining A is trying to make sense of

$$\int_0^t U_\tau d\tau = \frac{1}{iA} [U_\tau]_0^t = \frac{1}{iA} [U_t - 1],$$

which would give that

$$iA = \frac{1}{t} (U_t - 1) \left[\frac{1}{t} \int_0^t U_\tau d\tau \right]^{-1}.$$

In the following, we denote $X_t := \frac{1}{t} \int_0^t U_\tau d\tau$. If we can show the above, then we should have for times t and s that $iA = \frac{1}{t} (U_t - 1) X_t^{-1} = \frac{1}{s} (U_s - 1) X_s^{-1}$ and thus

$$\frac{1}{t} (U_t - 1) X_s = \frac{1}{s} (U_s - 1) X_t. \quad (\text{VI.2})$$

We will now proceed showing the above equation. By the norm continuity of our family we get that $\|X_t - 1\| \rightarrow 0$ as $t \rightarrow 0$ and the inverse X_t^{-1} exists in $B(\mathcal{H})$ for t small enough, say for $t < t_0$. For $0 < s < t$ we have

$$\begin{aligned} \frac{1}{t} (U_t - 1) X_s &= \frac{1}{t} (U_t - 1) \frac{1}{s} \int_0^s U_\tau d\tau \\ &= \frac{1}{st} \int_0^s (U_t U_\tau - U_\tau) d\tau \\ &= \frac{1}{st} \int_0^s (U_{t+\tau} - U_\tau) d\tau = \frac{1}{st} \int_0^t (U_{s+\tau} - U_\tau) d\tau = \frac{1}{s} (U_s - 1) X_t \end{aligned}$$

If we now fix t in Eq. (VI.2) and send s to zero, then we get

$$\frac{1}{t} (U_t - 1) = \lim_{s \rightarrow 0} \frac{1}{t} (U_t - 1) X_s = \lim_{s \rightarrow 0} \frac{1}{s} (U_s - 1) X_t.$$

Denoting $iA := \lim_{s \rightarrow 0} \frac{1}{s}(U_s - 1)$ we get from the above that $iAX_t = \frac{1}{t}U_t - 1$, and thus

$$\begin{aligned} U_t &= 1 + iAtX_t \\ &= 1 + iA \int_0^t U_\tau d\tau \\ &= 1 + iA \int_0^t \left(1 + iA \int_0^\tau U_\sigma d\sigma \right) d\tau = 1 + itA + (iA)^2 \iint U_\tau d\sigma d\tau \dots \end{aligned}$$

By iteration and checking details, $U_t = \sum_{n=0}^{\infty} [(it)^n/n!]A^n = e^{itA}$ follows as claimed. \square

The theorem just proven establishes a correspondence between bounded selfadjoint operators A on a Hilbert space and norm continuous unitary groups $(U_t)_{t \in \mathbb{R}}$ via $U_t = e^{itA}$. Unfortunately, norm continuous time evolutions or bounded Hamiltonians are not realistic in many situations.

Theorem VI.3: *Let \mathcal{H} be a Hilbert space and let T be an unbounded selfadjoint operator on \mathcal{H} . For real numbers t , define $U_t := e^{itT}$ via functional calculus, i.e. $T = \int \lambda dE(\lambda)$ and $U_t := \int e^{it\lambda} dE(\lambda)$. Then we have:*

- (i) *All operators U_t are unitary.*
- (ii) *The operator U_0 is the identity.*
- (iii) *For real numbers r and s it holds $U_s U_t = U_{s+t}$.*
- (iv) *For $x \in \mathcal{H}$ it holds $\lim_{t \rightarrow 0} \|U_t x - x\| = 0$.*

The proof of this statement can be done as an exercise. The properties just rely on functional calculus.

A family $(U_t)_{t \in \mathbb{R}}$ with the properties from VI.3 is called *strongly continuous one parameter unitary group* or briefly a *strongly continuous unitary group*.

Theorem VI.4 (of Stone): *Let $(U_t)_{t \in \mathbb{R}}$ be a strongly continuous unitary group. Then there is a uniquely determined unbounded selfadjoint operator T such that for all real numbers t it holds $U_t = e^{itT}$.*

Proof: Again, we hope to find that $T = -i \frac{d}{dt} U_t|_{t=0}$ does the job. The domain of our unbounded operator T should be

$$D(T) := \left\{ x \in \mathcal{H} : iTx := \lim_{t \rightarrow 0} \frac{1}{t}(U_t x - x) \text{ exists} \right\}.$$

Our main problem will be showing that $D(T)$ is indeed dense in \mathcal{H} . As before, for $t \in \mathbb{R}$ we let $X_t := \frac{1}{t} \int_0^t U_\tau d\tau$. For $s \rightarrow 0$ we then obtain $\|X_s y - y\| \rightarrow 0$. Even in this more general situation, for sufficiently small s and t we still have

$$\frac{1}{t}(U_t - 1)X_s = \frac{1}{s}(U_s - 1)X_t.$$

Fixing t and sending s to zero, we obtain again that

$$\frac{1}{t}(U_t - 1)y = \lim_{s \rightarrow 0} \frac{1}{t}(U_t - 1)X_s y = \lim_{s \rightarrow 0} \frac{1}{s}(U_s(X_t y) - X_t y)$$

which shows that for vectors $y \in \mathcal{H}$ and $t > 0$, the $x = X_t y$ belong to $D(T)$. Since $\|X_t y - y\| \rightarrow 0$ when $t \rightarrow 0$, the set $\{X_t y \mid y \in \mathcal{H}, t > 0\} \subseteq D(T)$ is dense in \mathcal{H} .

Now we have to show that T is indeed selfadjoint. Let therefore $y \in D(T^*)$ be given. Then there is $z \in \mathcal{H}$ such that for all $x \in D(T)$ it holds $\langle Tx, y \rangle = \langle x, z \rangle$ (and this z will be T^*y). Now for all $x \in D(T)$ it holds

$$\begin{aligned} \langle Tx, y \rangle &= \left\langle -i \lim_{t \rightarrow 0} \frac{1}{t}(U_t x - x), y \right\rangle \\ &= i \lim_{t \rightarrow 0} \frac{1}{t} (\langle U_t x, y \rangle - \langle x, y \rangle) \\ &= i \lim_{t \rightarrow 0} \frac{1}{t} (\langle x, U_{-t} y \rangle - \langle x, y \rangle) \\ &= -i \lim_{t \rightarrow 0} \frac{1}{-t} \langle x, U_{-t} y - y \rangle = \left\langle x, -i \lim_{t \rightarrow 0} \frac{1}{-t} (U_{-t} y - y) \right\rangle = \langle x, z \rangle \end{aligned}$$

which yields that $\lim_{t \rightarrow 0} \frac{1}{t}(U_t y - y)$ exists and equals iT^*y . Hence y belongs to the domain of T and $T^*y = Ty$, which means that T is indeed a selfadjoint generator. It remains to show that indeed, for any real number t , it holds $U_t = e^{iT}$. This is more or less straight forward and thus omitted. \square

Chapter VII.

Canonical Commutation Relations and Weyl Relations

Definition VII.1: Let \mathcal{H} be a Hilbert space and let P and Q be selfadjoint operators on \mathcal{H} . If they are defined on the same dense domain $D \subseteq \mathcal{H}$ such that $P(D) \subseteq D$, $Q(D) \subseteq D$ and such that on D it holds

$$[P, Q] := PQ - QP = -i1,$$

they are said to satisfy the *canonical commutation relations* (often abbreviated CCR). In physics, one usually requires $[P, Q] = -i\hbar 1$.

Remark VII.2: (i) As we know from (3.2), there are no bounded realisations of the canonical commutation relations.

(ii) If we put $a := 2^{-1/2}(Q + iP)$ and $a^* := 2^{-1/2}(Q - iP)$, then

$$[a, a^*] = \frac{1}{2}(i[P, Q] - i[Q, P]) = 1,$$

thus the canonical commutation relations can be expressed equivalently as $[a, a^*] = aa^* - a^*a = 1$.

(iii) There also is a “fermionic analogue”, called the *canonical anticommutation relations* (often abbreviated CAR) and given by $\{b, b^*\} := bb^* + b^*b = 1$. Those however *do* have bounded realisations, like the matrices

$$b = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad b^* = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}.$$

Example VII.3 (Schrödinger Representation): Let \mathcal{H} be the Hilbert space $L^2(\mathbb{R})$ and let $D := S(\mathbb{R})$ be the functions of rapid decrease, i.e.

$$S(\mathbb{R}) = \left\{ f \in L^2(\mathbb{R}) : \text{For all } n, m \in \mathbb{N} \text{ it holds } \lim_{|t| \rightarrow \infty} t^n \frac{d^m f}{dt^m} = 0 \right\}.$$

Because the position operator $(Qf)(t) = tf(t)$ as well as the momentum operator $(Pf)(t) = -if'(t)$ map $S(\mathbb{R})$ into itself and because Q and P are essentially selfadjoint on $S(\mathbb{R})$, this domain is a suitable candidate for the canonical commutation relations. Indeed, P and Q satisfy the canonical commutation relations: For all $f \in S(\mathbb{R})$ it holds $(PQ - QP)f = -if$.

The natural question to ask is whether this is (up to unitary equivalence) the only irreducible representation of the canonical commutation relations.

Remark VII.4: (i) Note that with $a = 2^{-1/2}(Q+iP)$ and $a^* := 2^{-1/2}(Q-iP)$ we find a vector Ω in D such that $a\Omega = 0$. Such an Ω is called a *vacuum vector*. Indeed,

$$0 = a\Omega = \frac{1}{\sqrt{2}}(Q + iP)\Omega = \frac{1}{\sqrt{2}}(t\Omega(t) + \Omega'(t)),$$

which is equivalent to $\Omega'(t) = -t\Omega(t)$, i.e. Ω is given by $\Omega(t) = Ce^{-t^2/2}$ for some real constant C .

(ii) If we have an irreducible representation of the canonical commutation relations with such a vacuum vector, i.e. $[a, a^*] = 1$ and $a\Omega = 0$ with $\|\Omega\| = 1$, everything is uniquely determined. Let $e_0 := \Omega$ and for $n \in \mathbb{N}$ put $e_n := a^{*n}\Omega$. Then for any natural number n it holds $a^*e_n = e_{n+1}$ and $ae_n = ne_{n-1}$, which can be shown by induction as

$$\begin{aligned} ae_n &= aa^{*n}\Omega \\ &= aa^*a^{*n-1}\Omega \\ &= a^*ae_{n-1} + e_{n+1} = a^*(n-1)e_{n-2} + e_{n-1} = (n-1)e_{n-1} + e_{n-1} = ne_{n-1}. \end{aligned}$$

By irreducibility the collection $(e_n)_{n \in \mathbb{N}}$ span a dense subset of \mathcal{H} . Furthermore all inner products are determined, as we have

$$\langle e_n, e_m \rangle = \langle a^{*n}\Omega, a^{*m}\Omega \rangle = \langle \Omega, a^n a^{*m}\Omega \rangle = \langle \Omega, a^{n-m} a^m e_m \rangle = \langle \Omega, a^{n-m} m! \Omega \rangle$$

and the last inner product equals 0 if $n > m$ and $m!$ if $n = m$. This yields $\langle e_n, e_m \rangle = 0$ for $n \neq m$ and $\|e_n\| = (n!)^{1/2}$. Usually in this context one thus takes $f_n := (n!)^{-1/2}e_n$ which then is an orthonormal basis.

(iii) If we are looking for irreducible representations of $[a, a^*] = 1$, then the question for equivalence to the Schrödinger representation is equivalent to asking for the existence of a vacuum vector Ω with $a\Omega = 0$.

(iv) We rewrite the canonical commutation relations in terms of the unitary groups. Consider the Schrödinger representation from Example VII.3 and consider the position operator Q as well as the momentum operator P . Denote

the corresponding unitary groups by $U_t := e^{itP}$ and $V_t := e^{itQ}$. Those act as $(U_t f)(x) = f(x+t)$ and $(V_t f)(x) = e^{itx} f(x)$. Thus for some function f we have

$$\begin{aligned}(U_t V_s f)(x) &= (V_s f)(x+t) = e^{is(x+t)} f(x+t), \\ (V_s U_t f)(x) &= e^{isx} (U_t f)(x) = e^{isx} f(x+t).\end{aligned}$$

Hence we find the relation $U_t V_s = e^{ist} V_s U_t$.

Definition VII.5: Let $(U_t)_{t \in \mathbb{R}}$ and $(V_s)_{s \in \mathbb{R}}$ be strongly continuous unitary groups on the same Hilbert space \mathcal{H} . If for all $s, t \in \mathbb{R}$ it holds

$$U_t V_s = e^{its} V_s U_t,$$

then the pair $(U_t, V_s)_{t,s \in \mathbb{R}}$ is called a *representation of the Weyl relations*.

If there is no non-trivial sub-Hilbert space $\mathcal{K} \subseteq \mathcal{H}$ such that for all $s, t \in \mathbb{R}$ it holds $U_t \mathcal{K} \subseteq \mathcal{K}$ and $V_s \mathcal{K} \subseteq \mathcal{K}$, the representation is called *irreducible*.

Let $(U_t, V_s)_{t,s \in \mathbb{R}}$ and $(U'_t, V'_s)_{t,s \in \mathbb{R}}$ (living on the Hilbert space \mathcal{H} respectively \mathcal{H}') be two representations of the Weyl relations. If there is a unitary operator $W: \mathcal{H} \rightarrow \mathcal{H}'$ such that for all $s, t \in \mathbb{R}$ it holds $U_t = W^* U'_t W$ and $V_s = W^* V'_s W$, then $(U_t, V_s)_{t,s \in \mathbb{R}}$ and $(U'_t, V'_s)_{t,s \in \mathbb{R}}$ are called *unitarily equivalent*.

In other words: For two unitarily equivalent representations and real numbers t and s , we have the commutative diagram

$$\begin{array}{ccc} \mathcal{H} & \xrightarrow{W} & \mathcal{H}' \\ U_t \downarrow V_s & & U'_t \downarrow V'_s \\ \mathcal{H} & \xleftarrow{W^*} & \mathcal{H}' \end{array}$$

Proposition VII.6: *The Schrödinger representation of the Weyl relations on the Hilbert space $L^2(\mathbb{R})$ given by $(U_t f)(x) = f(x+t)$ and $(V_s f)(x) = e^{itx} f(x)$ is irreducible.*

Proof: Assume there were a non-trivial invariant sub-Hilbert space $\mathcal{K} \subseteq \mathcal{H}$ such that for all $t, s \in \mathbb{R}$ it held $U_t \mathcal{K} \subseteq \mathcal{K}$ and $V_s \mathcal{K} \subseteq \mathcal{K}$. Then we had $0 \neq f \in \mathcal{K}$ and $0 \neq g \in \mathcal{K}^\perp$, which yielded for all $s, t \in \mathbb{R}$ that $\langle g, V_t U_s f \rangle = 0$ (since $U_s f \in \mathcal{K}$ and $V_t U_s f \in \mathcal{K}$), i.e. for all $s, t \in \mathbb{R}$ it held

$$0 = \int g(x)^* e^{itx} f(x+s) dx.$$

If we fix s and define $h_s(x) := g(x)^* f(x+s)$ then the above equation reads “For all $t \in \mathbb{R}$: $\mathcal{F}(h_s)(t) = 0$ ”, where \mathcal{F} denotes the Fourier transform, and thus by injectivity of the Fourier transform $h_s = 0$ for any real number s . Hence, either f or g had to be zero in contradiction to our assumption. \square

Chapter VIII.

The Stone-von Neumann Uniqueness Theorem

Theorem VIII.1 (Uniqueness Theorem): *Any representation of the Weyl relations is unitarily equivalent to an at most countable direct sum of Schrödinger representations. In particular, any irreducible representation of the Weyl relations is unitarily equivalent to the Schrödinger representation.*

Remark VIII.2: (i) “Beweisansätze” by Stone in 1930.

(ii) The first rigorous proof was given by von Neumann in 1931.

(iii) The idea of the proof is finding the vacuum vectors in the representation, from which everything can be reconstructed. To find a vacuum Ω , we need to find a projection P onto Ω , which must be constructed from the U_t and V_s from our representation.

In the following, we fix a Hilbert space \mathcal{H} and a representation $(U_t, V_s)_{t,s \in \mathbb{R}}$ of Weyl relations.

Notation VIII.3: (i) For any tuple (s, t) of real numbers, we put

$$W(s, t) := e^{-\frac{1}{2}ist} U_s V_t = e^{\frac{1}{2}ist} V_t U_s.$$

(ii) For any integrable function $h: \mathbb{R}^2 \rightarrow \mathbb{C}$, i.e. $\iint |h(s, t)| ds dt < \infty$, we define a bounded operator on \mathcal{H} via $W_h := \int h(s, t) W(s, t) ds dt$. This is rigorously defined by

$$\langle f, W_h g \rangle = \int h(s, t) \langle f, W(s, t) g \rangle ds dt.$$

Proposition VIII.4:

- (i) All operators $W(s, t)$ are unitary and for all real numbers s_1, s_2, t_1 and t_2 we have $W(s_1, t_1)W(s_2, t_2) = W(s_1 + s_2, t_1 + t_2)e^{\frac{1}{2}i[s_1t_2 - s_2t_1]}$. In particular it holds $W(0, 0) = 1$ and $W(s, t)^* = W(-s, -t)$.
- (ii) The map $L^1(\mathbb{R}^2) \rightarrow B(\mathcal{H})$, $h \mapsto W_h$ is injective, i.e. for $h \neq 0$, also $W_h \neq 0$.
- (iii) For two integrable functions $h_1, h_2: \mathbb{R}^2 \rightarrow \mathbb{C}$, we define another integrable function $h: \mathbb{R}^2 \rightarrow \mathbb{C}$ by

$$h(s, t) = \iint e^{\frac{1}{2}i[st' - s't]} h_1(s - s', t - t') h_2(s', t') ds' dt'.$$

For those functions it holds $W_{h_1}W_{h_2} = W_h$.

Proof: The statements (i) and (iii) can be shown with simple calculations.

For (ii), assume $W_h = 0$. Then for all real numbers x and y we have that $W(-x, -y)W_hW(x, y) = 0$, i.e.

$$\begin{aligned} 0 &= W(-x, -y) \iint h(s, t)W(s, t) ds dt W(x, y) \\ &= \iint h(s, t)W(s - x, t - y)e^{\frac{1}{2}i[-xt + ys]}W(x, y) ds dt \\ &= \iint h(s, t)e^{\frac{1}{2}i[(s-x)y - (t-y)x]}e^{\frac{1}{2}i[-xt + ys]}W(s, t) ds dt \\ &= \iint h(s, t)e^{i[sy - tx]}W(s, t) ds dt. \end{aligned}$$

Thus for all real numbers x and y and vectors $f, g \in \mathcal{H}$, we have

$$0 = \iint h(s, t)e^{i[sy - tx]}\langle f, W(s, t)g \rangle ds dt.$$

This means the Fourier transform of $(s, t) \mapsto h(s, t)\langle f, W(s, t)g \rangle$ is zero almost everywhere and because the Fourier transform is injective this gives that $(s, t) \mapsto h(s, t)\langle f, W(s, t)g \rangle$ is zero almost everywhere for all $f, g \in \mathcal{H}$. Hence, $h(s, t)W(s, t)g = 0$ almost everywhere for all $g \in \mathcal{H}$. Because the $W(s, t)$ are unitary, for $g \in \mathcal{H} - \{0\}$ it holds $W(s, t)g \neq 0$, thus finally we can infer that h is zero almost everywhere. \square

Remark VIII.5: We claim that

$$P := \frac{1}{2\pi} \iint W(s, t) e^{-\frac{1}{4}(s^2+t^2)} ds dt$$

which is W_h for $h: (s, t) \mapsto \frac{1}{2\pi} e^{-1/4(s^2+t^2)}$, gives the projection onto the vacuum. Let us check this for the Schrödinger representation. Recall that there the vacuum is given by $\Omega(x) = (\frac{1}{\pi})^{1/4} e^{-x^2/2}$. There we have

$$(W(s, t)f)(x) = e^{\frac{1}{2}ist} e^{itx} f(x + s)$$

and thus

$$(Pf)(x) = \frac{1}{2\pi} \iint e^{\frac{1}{2}is+itx} f(x + s) e^{-\frac{1}{4}(s^2+t^2)} ds dt = \frac{1}{\sqrt{\pi}} \left(\int f(s') e^{-\frac{1}{2}s'^2} ds' \right) e^{-\frac{1}{2}x^2}$$

which shows that $Pf = \langle \Omega, f \rangle \Omega$.

Now to the proof of Theorem VIII.1.

Proof: Let $h = \frac{1}{2\pi} e^{-1/4(s^2+t^2)}$ and put

$$P := W_h = \frac{1}{2\pi} \iint W(s, t) e^{-\frac{1}{4}(s^2+t^2)} ds dt.$$

Then P is an orthogonal projection, i.e. $P^2 = P = P^*$. The selfadjointness is easy to see, since

$$P^* = \frac{1}{2\pi} \iint W(s, t)^* e^{-\frac{1}{4}(s^2+t^2)} ds dt = \frac{1}{2\pi} \iint W(-s, -t) e^{-\frac{1}{4}(s^2+t^2)} ds dt = P.$$

For the projection property, one calculates more generally that for all tuples of real numbers (x, y) it holds $PW(x, y)P = e^{-1/4(x^2+y^2)}P$. This can be checked by hand using the properties from Proposition VIII.4. This in particular implies $P^2 = P$ for $x = 0 = y$.

Since h is non-zero, the operator $P = W_h$ is not the zero operator and thus $P\mathcal{H} \neq \{0\}$. Choose an orthonormal basis $(\Omega_n)_{1 \leq n \leq N}$ of $P\mathcal{H}$ (where $N \in \mathbb{N} \cup \{\infty\}$) and for $1 \leq n \leq N$, put $\mathcal{H}_n := \text{cl}(\text{span}\{W(s, t)\Omega_n \mid s, t \in \mathbb{R}\})$. For those spaces, we have the following:

- (i) Each \mathcal{H}_n is invariant for the $W(x, y)$,
- (ii) For $n \neq m$, the spaces \mathcal{H}_n and \mathcal{H}_m are orthogonal,
- (iii) The Hilbert space \mathcal{H} decomposes into the \mathcal{H}_n , i.e. $\mathcal{H} = \bigoplus_{n=1}^N \mathcal{H}_n$.

(iv) If the representation is irreducible, then $N = 1$ and $\mathcal{H} = \mathcal{H}_1$.

Property (i) is clear, since $W(x, y)W(s, t)\Omega_n = e^{i\cdots}W(x + s, y + t)\Omega_n$. For property (ii), we check that

$$\begin{aligned}\langle W(x, y)\Omega_m, W(s, t)\Omega_m \rangle &= \langle \Omega_n, PW(-x, -y)W(s, t)P\Omega_m \rangle \\ &= \lambda \langle \Omega_n, P\Omega_m \rangle = \lambda \langle \Omega_n, \Omega_m \rangle = \lambda \delta_{n,m}.\end{aligned}$$

For (iii), let $\mathcal{K} := \bigoplus_{n=1}^N \mathcal{H}_n$ and assume $\mathcal{K} \subsetneq \mathcal{H}$. Then $\{W(s, t)\}|_{\mathcal{K}^\perp}$ gave a representation of the Weyl relations and the projection for this were $P|_{\mathcal{K}^\perp}$, which weren't zero. Thus, there were an $f \in \mathcal{K}^\perp - \{0\}$ with $Pf = f$, i.e. f belonged to \mathcal{K} and \mathcal{K}^\perp , which contradicted $\mathcal{K} \cap \mathcal{K}^\perp = \{0\}$.

Let now a natural number n be fixed and put $\Omega := \Omega_n$. For real numbers s and t , denote $f_{s,t} := W(s, t)\Omega$. Then we have

$$W(x, y)f_{s,t} = W(x, y)W(s, t)\Omega = e^{\frac{1}{2}i[xt-ys]}W(x + s, y + t) = e^{\frac{1}{2}i[xt-ys]}f_{x+s, y+t}$$

and

$$\begin{aligned}\langle f_{x,y}, f_{s,t} \rangle &= \langle W(x, y)\Omega, W(s, t)\Omega \rangle \\ &= \langle \Omega, PW(-x, -y)W(s, t)P\Omega \rangle \\ &= \langle \Omega, Pe^{\frac{1}{2}i[-xt+ys]}W(s - x, t - y)W(s, t)P\Omega \rangle \\ &= \langle \Omega, Pe^{\frac{1}{2}i[-xt+ys]}e^{-\frac{1}{4}[(s-x)^2+(t-y)^2]}P\Omega \rangle \\ &= e^{\frac{1}{2}i[-xt+ys]}e^{-\frac{1}{4}[(s-x)^2+(t-y)^2]}\langle \Omega, P\Omega \rangle = e^{\frac{1}{2}i[-xt+ys]}e^{-\frac{1}{4}[(s-x)^2+(t-y)^2]}.\end{aligned}$$

Thus all inner products and actions of the $W(x, y)$ are uniquely determined. If we have two such representations $(\Omega, W(s, t), \mathcal{H})$ and $(\Omega', W'(s, t), \mathcal{H}')$, then the mapping $f_{s,t} = W(s, t)\Omega \mapsto W'(s, t)\Omega' = f'_{s,t}$ extends to a unitary map which intertwines the action of the $W(s, t)$ and the $W'(s, t)$. Hence all irreducible representations are equivalent to each other, and to the Schrödinger representation. \square

Remark VIII.6: (i) Theorem VIII.1 and its proof can be generalised to the case of finitely many degrees n of freedom with the canonical commutation relations

$$[P_i, Q_j] = -i\delta_{ij}, \quad [Q_i, Q_j] = 0 = [P_i, P_j],$$

where $1 \leq i, j \leq n$. For this situation, we define $U_k(t) = e^{itP_k}$, $V_\ell = e^{isQ_\ell}$ and obtain the Weyl relations $U_k(t)U_\ell(s) = U_\ell(s)U_k(t)$, $V_k(t)V_\ell(s) = V_\ell(s)V_k(t)$ and $U_k(t)V_\ell(s) = e^{i\delta_{k\ell}st}V_\ell(s)U_k(t)$. The Schrödinger representation now lives on

$L^2(\mathbb{R}^n)$, where Q_k corresponds to multiplication with x_k and P_ℓ corresponds to taking the partial derivative with respect to x_ℓ .

Again, each irreducible representation of the Weyl relations is unitarily equivalent to the Schrödinger representation.

(ii) For an infinite number of freedoms, the proof of Theorem VIII.1 breaks down and even worse, the statement itself really does not hold anymore.

Chapter IX.

Symmetric Fock Space and Second Quantisation

In one degree of freedom, we had the canonical commutation relation $[P, Q] = -i1$. For a finite number of freedoms, we had the slightly more involved relations

$$[P_i, Q_j] = -i\delta_{ij}1, \quad [P_i, P_j] = 0 = [Q_i, Q_j].$$

Generalising this to an infinite number of freedoms is not straight forward. Instead of the canonical commutation relations, we consider the relations $[a_i, a_j^*] = \delta_{ij}1$ and $[a_i^*, a_j^*] = 0$ for the operator a_i as defined in (Reference).

Remark IX.1: Our new Hilbert space \mathcal{F} should contain a vacuum Ω , one particle elements $f \in \mathcal{H}$, n -particle elements $f_1 \otimes \cdots \otimes f_n \in \mathcal{H}^{\otimes n}$ and combinations of different numbers of particles that should be contained in $\bigoplus_n \mathcal{H}^{\otimes n}$, the so-called *full Fock space over \mathcal{H}* . Since $a_i^* a_j^* = a_j^* a_i^*$ we should consider the so-called *bosonic Fock space* or *symmetric Fock space*, where $f \otimes g = g \otimes f$.

Definition IX.2: Let \mathcal{H}_1 and \mathcal{H}_2 be Hilbert spaces and consider their algebraic tensor product

$$\mathcal{H}_1 \odot \mathcal{H}_2 := \left\{ \sum_{i=1}^n x_i \otimes y_i : n \in \mathbb{N}, x_1, \dots, x_n \in \mathcal{H}_1, y_1, \dots, y_n \in \mathcal{H}_2 \right\}$$

Then the linear extension of $\langle x_1 \otimes y_1, x_2 \otimes y_2 \rangle := \langle x_1, x_2 \rangle \langle y_1, y_2 \rangle$ defines an inner product on $\mathcal{H}_1 \otimes \mathcal{H}_2$ and we call $\mathcal{H}_1 \otimes \mathcal{H}_2 := \text{cl}(\mathcal{H}_1 \odot \mathcal{H}_2)$ the *Hilbert space tensor product of \mathcal{H}_1 and \mathcal{H}_2* .

We denote $\mathcal{H}^{\otimes 2} := \mathcal{H} \otimes \mathcal{H}$. By iteration, this construction extends to finite numbers of factors $\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_n$ and again, we write $\mathcal{H}^{\otimes n} := \bigotimes_{i=1}^n \mathcal{H}$.

Let now $(\mathcal{H}_i)_{i \in \mathbb{N}}$ be a sequence of Hilbert spaces. Then

$$\bigoplus_{i \in \mathbb{N}} \mathcal{H}_i := \left\{ (x_1, x_2, \dots) : x_i \in \mathcal{H}_i, \sum_{i \in \mathbb{N}} \|x_i\|^2 < \infty \right\}$$

is called *orthogonal direct sum of the Hilbert spaces \mathcal{H}_i* . Note that the inner product on $\bigoplus_{i \in \mathbb{N}} \mathcal{H}_i$ is determined by the requirement that \mathcal{H}_i is orthogonal to \mathcal{H}_j for $i \neq j$, where $x \in \mathcal{H}_j$ is identified with $(\delta_{ij}x)_{i \in \mathbb{N}}$.

Remark IX.3: (i) Let \mathcal{H} be a Hilbert space of dimension $d \in \mathbb{N} \cup \{+\infty\}$ and assume $(e_i)_{1 \leq i \leq d}$ is an orthonormal basis of \mathcal{H} . Then

$$\{e_{i(1)} \otimes \dots \otimes e_{i(n)} \mid 1 \leq i(1), \dots, i(n) \leq d\} \subseteq \mathcal{H}^{\otimes n}$$

is an orthonormal basis of the tensor power $\mathcal{H}^{\otimes n}$. In particular, the dimension of the tensor product of Hilbert spaces is multiplicative, i.e. $\dim \mathcal{H}^{\otimes n} = (\dim \mathcal{H})^n$.

(ii) Since \mathcal{H}_i has a unique zero vector, we can embed direct sums into each other. For example, we can identify $\mathcal{H}_1 \oplus \dots \oplus \mathcal{H}_n$ and $\mathcal{H}_1 \oplus \dots \oplus \mathcal{H}_n \oplus \{0\}$, which is contained in $\mathcal{H}_1 \oplus \dots \oplus \mathcal{H}_{n+1}$.

The infinite direct sum can be seen as the completion of all finite ones, i.e.

$$\bigoplus_{i \in \mathbb{N}} \mathcal{H}_i \cong \text{cl} \left(\bigcup_{n \in \mathbb{N}} \bigoplus_{i=1}^n \mathcal{H}_i \right).$$

However, there is no canonical “unit” in a Hilbert space which would allow for an canonical embedding of a tensor product of n Hilbert spaces into a tensor product of $n + 1$ Hilbert spaces, and thus there is no canonical infinite tensor product of Hilbert spaces.

Theorem IX.4: *Let \mathcal{H} be a Hilbert space.*

(i) *Let n be a natural number and let $\sigma \in \mathfrak{S}_n$ be an permutation of $\{1, \dots, n\}$. Then we can uniquely extend*

$$U_\sigma(x_1 \otimes \dots \otimes x_n) = x_{\sigma(1)} \otimes \dots \otimes x_{\sigma(n)}$$

to a unitary operator $U: \mathcal{H}^{\otimes n} \rightarrow \mathcal{H}^{\otimes n}$. Furthermore, for all $\sigma, \tau \in \mathfrak{S}_n$ it holds $U_{\sigma\tau} = U_\sigma U_\tau$ and $U_{\text{id}} = 1$ (where id denotes the identity permutation). Finally, $U_\sigma^ = U_{\sigma^{-1}}$.*

(ii) *The operator $P_n := (n!)^{-1} \sum_{\sigma \in \mathfrak{S}_n} U_\sigma$ is an orthogonal projection on $\mathcal{H}^{\otimes n}$ and projects onto the symmetric tensors, i.e. x belongs to $P_n(\mathcal{H}^{\otimes n})$ if and only if for all $\sigma \in \mathfrak{S}_n$ it holds $U_\sigma x = x$.*

Proof: (i) Note that if $\sum_i x_1^{(i)} \otimes \cdots \otimes x_n^{(i)} = 0$, then also for all $\sigma \in \mathfrak{S}_n$ it holds $\sum_i x_{\sigma(1)}^{(i)} \otimes \cdots \otimes x_{\sigma(n)}^{(i)} = 0$. If $\{e_1, \dots, e_n\}$ is an orthonormal basis of \mathcal{H} , then $\{e_{i(1)} \otimes \cdots \otimes e_{i(n)} \mid 1 \leq i(1), \dots, i(n) \leq n\}$ is an orthonormal basis of $\mathcal{H}^{\otimes n}$ and for any $\sigma \in \mathfrak{S}_n$, the operator U_σ maps this basis onto itself, which shows the unitarity.

(ii) That P_n is an orthogonal projection is easily checked. Firstly it is selfadjoint since

$$P_n^* = \frac{1}{n!} \sum_{\sigma \in \mathfrak{S}_n} U_\sigma^* = \frac{1}{n!} \sum_{\sigma \in \mathfrak{S}_n} U_{\sigma^{-1}} = P_n,$$

and secondly it is a projection because

$$P_n^2 = \frac{1}{n!n!} \sum_{\sigma \in \mathfrak{S}_n} \sum_{\tau \in \mathfrak{S}_n} U_\sigma U_\tau = \frac{1}{n!n!} \sum_{\sigma \in \mathfrak{S}_n} \sum_{\pi \in \mathfrak{S}_n} U_\pi = \frac{1}{n!n!} n! \sum_{\pi \in \mathfrak{S}_n} U_\pi = P_n.$$

If on the one hand $x \in \mathcal{H}^{\otimes n}$ is given such that for all $\sigma \in \mathfrak{S}_n$ it holds $U_\sigma x = x$, then $P_n x = \frac{1}{n!} \sum_{\sigma \in \mathfrak{S}_n} U_\sigma x = x$.

If on the other hand $x \in \mathfrak{H}^{\otimes n}$ is given such that it holds $P_n x = x$, then for all $\sigma \in \mathfrak{S}_n$ we have $U_\sigma x = U_\sigma P_n x = P_n x = x$. \square

Definition IX.5: Let \mathcal{H} be a Hilbert space and for $n \in \mathbb{N}$ denote by P_n the projection from Theorem IX.4. The Hilbert space

$$\mathcal{F}_+(\mathcal{H}) := \mathcal{F}_{\text{sym}}(\mathcal{H}) := \bigoplus_{n=0}^{\infty} P_n \mathcal{H}^{\otimes n}$$

is called the *symmetric Fock space over \mathcal{H}* or *bosonic Fock space over \mathcal{H}* . Here we put $P_0 \mathcal{H}^{\otimes 0} = \mathcal{H}^{\otimes 0} = \mathbb{C}$. We call $\Omega := (1, 0, 0, \dots) \in \mathcal{F}_+$ the *vacuum*. We call \mathcal{H} the one-particle space and the tensor power $\mathcal{H}_+^{\otimes n} := P_n \mathcal{H}^{\otimes n}$ is called *n-particle space*.

Example IX.6: If $\mathcal{H} = L^2(\mathbb{R})$, then $\mathcal{H}^{\otimes n} \cong L^2(\mathbb{R}^n)$ and the symmetric space $\mathcal{H}_+^{\otimes n}$ can be identified with

$$\{f \in L^2(\mathbb{R}^n) \mid \text{For all } \sigma \in \mathfrak{S}_n : f(t_1, \dots, t_n) = f(t_{\sigma(1)}, \dots, t_{\sigma(n)})\}.$$

Remark IX.7: Let T be a bounded operator on the Hilbert space \mathcal{H} . Then we have a unique operator which is uniquely determined via

$$T^{\otimes n}(x_1 \otimes \dots \otimes x_n) = (Tx_1) \otimes \cdots \otimes (Tx_n).$$

Since for all $\sigma \in \mathfrak{S}_n$ it holds $U_\sigma T^{\otimes n} = T^{\otimes n} U_\sigma$ we get for all $\sigma \in \mathfrak{S}_n$ and $x \in \mathcal{H}_+^{\otimes n}$ (i.e. $P_n x = x$) that $T^{\otimes n} x = T^{\otimes n} U_\sigma x = U_\sigma T^{\otimes n} x$, which implies that $P_n T^{\otimes n} x = T^{\otimes n} x$. Hence $T^{\otimes n}(\mathcal{H}_+^{\otimes n}) \subseteq \mathcal{H}_+^{\otimes n}$ and we can put $\Gamma_+^n(T) := T^{\otimes n}|_{\mathcal{H}_+^{\otimes n}}$. We note a few properties of Γ_+^n :

- (i) For the identity operator on \mathcal{H} we obtain $\Gamma_+^n(1) = 1$.
- (ii) The assignment behaves well with adjoints, i.e. $\Gamma_+^n(T)^* = \Gamma_+^n(T^*)$.
- (iii) The assignment fits with compositions, i.e. $\Gamma_+^n(ST) = \Gamma_+^n(S)\Gamma_+^n(T)$.
- (iv) The norm is controllable, i.e. $\|\Gamma_+^n(T)\| = \|T\|^n$.

Note that in general $\Gamma_+^n(S + T) \neq \Gamma_+^n(S) + \Gamma_+^n(T)$. Due to property (iv), the norm of $\Gamma_+^n(T)$ stays bounded for all n if and only if T is a so-called contraction (which means $\|T\| \leq 1$).

Definition IX.8: Let T be a bounded operator on the Hilbert space \mathcal{H} with $\|T\| \leq 1$. Then

$$\Gamma_+(T) := \bigoplus_{n=0}^{\infty} \Gamma_+^n(T) \in B(\mathcal{F}_+(\mathcal{H}))$$

is called *the symmetric second quantisation of T* . An element (x_0, x_1, \dots) of the symmetric Fock space $\mathcal{F}_+(\mathcal{H})$ is mapped to $(\Gamma_+^0 x_0, \Gamma_+^1(x_1), \dots)$.

Note that for any bounded operator T on \mathcal{H} it holds $\Gamma_+^0(T) = 1$ as $\mathcal{H}^{\otimes 0} \cong \mathbb{C}$.

Remark IX.9: Let $(U_t)_{t \in \mathbb{R}}$ be a unitary group on a Hilbert space \mathcal{H} , where $U_t = e^{iHt}$. Then $(\Gamma_+^n(U_t))_{t \in \mathbb{R}}$ is a unitary group on $\mathcal{H}_+^{\otimes n}$ with generator

$$d\Gamma_+^n(H) = H \otimes 1 \otimes \cdots \otimes 1 + 1 \otimes H \otimes 1 \cdots \otimes 1 + \cdots + 1 \otimes \cdots \otimes 1 \otimes H$$

and thus $\Gamma_+^n(e^{iHt}) = e^{id\Gamma_+^n(H)t}$. Now $d\Gamma_+(H) = \bigoplus_{n=0}^{\infty} d\Gamma_+^n(H)$ lives on the symmetric Fock space and $\Gamma_+(e^{iHt}) = e^{id\Gamma_+(H)t}$. The operator $d\Gamma_+$ is called *differential second quantisation of H* .

Notation IX.10: For elements x_1, \dots, x_n of \mathcal{H} we put

$$x_1 \circ \cdots \circ x_n := \sqrt{n!} P_n(x_1 \otimes \cdots \otimes x_n) \in \mathcal{H}_+^{\otimes n}.$$

Remark IX.11: Note the following:

- (i) For any permutation $\sigma \in \mathfrak{S}_n$ it holds $x_1 \circ \cdots \circ x_n = x_{\sigma(1)} \circ \cdots \circ x_{\sigma(n)}$.

(ii) If $(e_i)_{i \in I}$ is an orthonormal basis of \mathcal{H} , then

$$\{e_{i(1)} \circ \cdots \circ e_{i(n)} \mid 1 \leq i(1) \leq \cdots \leq i(n) \leq n\} \subseteq \mathcal{H}_+^{\otimes n}$$

is an orthogonal basis of $\mathcal{H}_+^{\otimes n}$, but not an orthonormal basis. Indeed:

$$\begin{aligned} & \langle e_{i(1)} \circ \cdots \circ e_{i(n)}, e_{j(1)} \circ \cdots \circ e_{j(n)} \rangle \\ &= n! \left\langle \frac{1}{n!} \sum_{\sigma \in \mathfrak{S}_n} e_{\sigma(i(1))} \otimes \cdots \otimes e_{\sigma(i(n))}, \sum_{\pi \in \mathfrak{S}_n} e_{\pi(j(1))} \otimes \cdots \otimes e_{\pi(j(n))} \right\rangle \\ &= \frac{1}{n!} \sum_{\sigma, \pi \in \mathfrak{S}_n} \langle e_{\sigma(i(1))}, e_{\pi(j(1))} \rangle \cdots \langle e_{\sigma(i(n))}, e_{\pi(j(n))} \rangle. \end{aligned}$$

If $(i(1), \dots, i(n)) \neq (j(1), \dots, j(n))$ the last sum evaluates to zero and for $(i(1), \dots, i(n)) = (j(1), \dots, j(n))$ it evaluates to

$$\sum_{\tau \in \mathfrak{S}_n} \langle e_{i(1)}, e_{\tau(i(1))} \rangle \cdots \langle e_{i(n)}, e_{\tau(i(n))} \rangle,$$

e.g. $\langle e_1 \circ e_2 \circ \cdots \circ e_n, e_1 \circ e_2 \circ \cdots \circ e_n \rangle = 1$ and $\langle e_1 \circ \cdots \circ e_1, e_1 \circ \cdots \circ e_1 \rangle = n!$.

Definition IX.12: Let \mathcal{H} be a Hilbert space, let $f \in \mathcal{H}$ and let

$$D := \left\{ \bigoplus_{n=0}^{\infty} f^{(n)} \in \mathcal{F}_+(\mathcal{H}) : \sum_{n=0}^{\infty} n \|f^{(n)}\|^2 < \infty \right\}.$$

Then linear extension of

- (i) $A(f)\Omega = 0$, $A(f)f_1 \circ \cdots \circ f_n = \sum_{k=1}^n \langle f, f_k \rangle f_1 \circ \cdots \circ \widehat{f}_k \circ \cdots \circ f_n$,
- (ii) $A^+(f)\Omega = f$, $A^+(f)f_1 \circ \cdots \circ f_n = f \circ f_1 \circ \cdots \circ f_n$

defines unbounded operators $A(f), A^+f : D \rightarrow \mathcal{F}_+(\mathcal{H})$, called *annihilation operator* respectively *creation operator*.

Theorem IX.13: Let \mathcal{H} be a Hilbert space and let $f \in \mathcal{H}$.

- (i) The operators $A(f)$ and $A^+(f)$ are closeable and adjoints of each other.
- (ii) The operators $A(f)$ and $A^+(f)$ leave their domain D invariant, i.e. $A(f)(D) \subseteq D$ respectively $A^+(f)(D) \subseteq D$.
- (iii) On D there hold canonical commutation relations: For all f and g in \mathcal{H} it holds $[A(f), A(g)] = 0 = [A^+(f), A^+(g)]$ and $[A(f), A^+(g)] = \langle f, g \rangle 1$.

Remark IX.14: Let \mathcal{H} be a Hilbert space and let $(e_i)_{i \in I}$ be an orthonormal basis of \mathcal{H} . Putting $A_i := e_i$, $A_i^* := A^*(e_i)$ as well as $Q_i := 2^{-1/2}(A_i + A_i^*)$ and $P_i := -i2^{-1/2}(A_i - A_i^*)$, we obtain essentially selfadjoint operators Q_i and P_i . Then we get

$$\begin{aligned} [A_i, A_j] &= 0 = [A_i^*, A_j^*], & [A_i, A_j^*] &= \delta_{ij}1, \\ [Q_i, Q_j] &= 0 = [P_i, P_j], & [P_i, Q_j] &= -i\delta_{ij}1. \end{aligned}$$

If we consider the corresponding unitary groups $U_k(t) = e^{iP_k t}$ and $V_k(t) = e^{iQ_k t}$ then they satisfy the Weyl relations, more precisely for all natural numbers k and ℓ it holds

$$U_k(t)V_\ell(s) = V_\ell(s)U_k(t)e^{i\delta_{k\ell}st}.$$

For infinite dimensional Hilbert spaces \mathcal{H} , i.e. in the case $\#(I) = \infty$, we thus get a representation of the infinite-dimensional version of the Weyl relations.

Chapter X.

Infinite Tensor Products of Hilbert Spaces

Let n be a natural number or infinity. By $\text{CCR}(n)$ we denote the canonical commutation relations for n degrees of freedom.

We are interested in representations of $\text{CCR}(\infty)$. Let P_1, Q_1 on \mathcal{H}_1 and P_2, Q_2 on \mathcal{H}_2 be representations of $\text{CCR}(1)$. Then $P_1 \otimes 1, Q_1 \otimes 1, 1 \otimes P_2, 1 \otimes Q_2$ form a representation of $\text{CCR}(2)$ on $\mathcal{H}_1 \otimes \mathcal{H}_2$.

For example, the Schrödinger representation of $\text{CCR}(n)$ on $L^2(\mathbb{R}^n)$ is the n -fold tensor product of representations of $\text{CCR}(1)$ on $L^2(\mathbb{R})$.

We should think that $\text{CCR}(\infty)$ would be representable as an “infinite tensor product” of representations of $\text{CCR}(1)$ on \mathcal{H} .

This approach suffers from the problem that the notion of an infinite tensor product of Hilbert spaces cannot be canonically defined. Even worse: Different choices also lead to inequivalent representations.

Let $(\mathcal{H})_{i \in \mathbb{N}}$ be a sequence of Hilbert spaces. We want to obtain a Hilbert space $\otimes_{i \in \mathbb{N}} \mathcal{H}_i$, i.e. we also need an inner product on this thing. For pure tensors it is natural to require

$$\langle x_1 \otimes x_2 \otimes x_3 \otimes \dots, y_1 \otimes y_2 \otimes y_3 \otimes \dots \rangle = \prod_{i \in \mathbb{N}} \langle x_i, y_i \rangle \quad (\text{X.1})$$

and of course, questions of convergence arise. This leads to the notion of a *complete tensor product* respectively an *incomplete tensor product*. Note that “incomplete” is not meant in a topological sense. The convergence of the right hand side in Eq. (X.1) is clear, if $\langle x_i, y_i \rangle = 1$ for large i , i.e. for $x_i = y_i = e_i$ for some fixed $e_i \in \mathcal{H}_i$, where $\|e_i\| = 1$.

¹This definition is due to von Neumann. He coined it in a paper from 1939.

Definition X.1 (Infinite Tensor Product¹): For each $i \in \mathbb{N}$ let a Hilbert space \mathcal{H}_i and a fixed unit vector $e_i \in \mathcal{H}_i$ be given. Equip

$$\text{span}\{(x_1, x_2, x_3, \dots) \mid x_i \in \mathcal{H}_i \text{ for all } i \in \mathbb{N} \text{ and } x_i = e_i \text{ almost all } i \in \mathbb{N}\}$$

with the inner product defined in Eq. (X.1) and factor out the zero vectors. Then the completion of this quotient with respect to the norm induced by the inner product is denoted $\otimes(\mathcal{H}_i, e_i)$ and called the *incomplete tensor product of the (\mathcal{H}_i, e_i)* .

Remark X.2: Fixing the $(e_i)_{i \in \mathbb{N}}$ gives us a way of embedding $\mathcal{H}_1 \otimes \dots \otimes \mathcal{H}_n$ into $\mathcal{H}_1 \otimes \dots \otimes \mathcal{H}_{n+1}$ via $\mathcal{H}_1 \otimes \dots \otimes \mathcal{H}_n \cong \mathcal{H}_1 \otimes \dots \otimes \mathcal{H}_n \otimes e_{n+1} \subseteq \mathcal{H}_1 \otimes \dots \otimes \mathcal{H}_{n+1}$ and thus elements $x = x_1 \otimes x_2 \otimes \dots \in \otimes(\mathcal{H}_i, e_i)$ have to be understood as $x = \lim_{n \rightarrow \infty} x_1 \otimes \dots \otimes x_n \otimes e_{n+1} \otimes e_{n+2} \otimes \dots$.

Suppose that for all $i \in \mathbb{N}$ it holds $\|x_i\| = 1$. Then the existence of x as a limit requires that for $\varepsilon > 0$ we find an index N such that for $n, m \geq N$ it holds

$$\|x_1 \otimes \dots \otimes x_n \otimes e_{n+1} \otimes \dots - x_1 \otimes \dots \otimes x_m \otimes e_{m+1} \otimes \dots\| < \varepsilon,$$

but

$$\begin{aligned} & \|x_1 \otimes \dots \otimes x_n \otimes e_{n+1} \otimes \dots - x_1 \otimes \dots \otimes x_m \otimes e_{m+1} \otimes \dots\| \\ &= \|x_1 \otimes \dots \otimes x_n \otimes (-x_{n+1} \otimes \dots \otimes x_m + e_{n+1} \otimes \dots \otimes e_m) \otimes e_{m+1} \otimes \dots\| \\ &= \|e_{n+1} \otimes \dots \otimes e_m - x_{n+1} \otimes \dots \otimes x_m\| \\ &= 1 + 1 - \prod_{k=n+1}^m \langle e_k, x_k \rangle - \prod_{k=n+1}^m \langle x_k, e_k \rangle. \end{aligned}$$

Thus the right condition to ensure that $x_1 \otimes x_2 \otimes \dots$ (where the x_i are unit vectors) belongs to $\otimes(\mathcal{H}_i, e_i)$ is that $\sum_{k=1}^{\infty} |\langle e_k, x_k \rangle - 1| < \infty$.

Theorem X.3 (von Neumann): For each natural number i let a Hilbert space \mathcal{H}_i be given. For two sequences of unit vectors $(e_i)_{i \in \mathbb{N}}$ and $(f_i)_{i \in \mathbb{N}}$ the following are equivalent:

- (i) $\otimes_{i \in \mathbb{N}}(\mathcal{H}_i, e_i)$ can be identified with $\otimes_{i \in \mathbb{N}}(\mathcal{H}_i, f_i)$, i.e. there is a unitary $U: \otimes_{i \in \mathbb{N}}(\mathcal{H}_i, e_i) \rightarrow \otimes_{i \in \mathbb{N}}(\mathcal{H}_i, f_i)$ such that for all $n \in \mathbb{N}$ the following diagram commutes:

$$\begin{array}{ccc} & \mathcal{H}_1 \otimes \dots \otimes \mathcal{H}_n & \\ & \swarrow \quad \searrow & \\ \otimes_{i \in \mathbb{N}}(\mathcal{H}_i, e_i) & \xrightarrow{U} & \otimes_{i \in \mathbb{N}}(\mathcal{H}_i, f_i) \end{array}$$

where the vertical maps are the canonical embeddings given by

$$\begin{aligned} x_1 \otimes \cdots \otimes x_n &\longmapsto x_1 \otimes \cdots \otimes x_n \otimes e_{n+1} \otimes \cdots \\ x_1 \otimes \cdots \otimes x_n &\longmapsto x_1 \otimes \cdots \otimes x_n \otimes f_{n+1} \otimes \cdots \end{aligned}$$

(ii) The series $\sum_{i \in \mathbb{N}} |\langle e_i, f_i \rangle - 1|$ is summable.

We only give a sketch of the proof. For “(ii) \implies (i)”, we consider the following example: Let $e = e_1 \otimes e_2 \otimes \cdots \in \bigotimes_{i \in \mathbb{N}} (\mathcal{H}_i, e_i)$. This element has to appear as

$$Ue = \lim_{n \rightarrow \infty} e_1 \otimes \cdots \otimes e_n \otimes f_{n+1} \otimes \cdots \otimes f_{n+2} \otimes \cdots \in \bigotimes_{i \in \mathbb{N}} (\mathcal{H}_i, f_i).$$

That this limit exists is, by Remark X.2, ensured by $\sum_{i=1}^{\infty} |\langle e_i, f_i \rangle - 1| < \infty$.

For “(i) \implies (ii)” we work by so-called “superselection rules”.

Example X.4 (Inequivalent Representations of the $\text{CCR}(\infty)$): Consider the Schrödinger representation of $\text{CCR}(1)$ in the form $\mathcal{H} = L^2(\mathbb{R})$ with $[a, a^*] = 1$, $a\Omega = 0$ and $\psi_n := (n!)^{-1} a^{*n} \Omega$ (in the notation of 7.4 those are the f_n but we change the name to avoid confusion with the notation from above). We now want to realise $\text{CCR}(\infty)$ as an infinite tensor product of this representation of $\text{CCR}(1)$, but as stated before there are choices to be made.

For every natural number i we take $\mathcal{H}_i = \mathcal{H}$ and $e_i := \psi_n \in \mathcal{H}_i = \mathcal{H}$ for a fixed $n \in \mathbb{N}$. Then we put $\mathcal{K}_n := \bigotimes_{i \in \mathbb{N}} (\mathcal{H}_i, e_i) = \bigotimes_{i \in \mathbb{N}} (\mathcal{H}, \psi_n)$ and we can realise $\text{CCR}(\infty)$ on \mathcal{K}_n via $a_i := 1 \otimes \cdots \otimes 1 \otimes a \otimes 1 \otimes \cdots$, where a sits at the i -th position.

We claim: For $n \neq m$, the representations on \mathcal{K}_n respectively \mathcal{K}_m are not equivalent. Our Fock space representations corresponds to the representation on \mathcal{K}_0 .

Consider for $\text{CCR}(1)$ the “number operator” a^*a . Then, by definition, $a^*a\psi_n = a^*(\sqrt{n}\psi_{n-1}) = n\psi_n$.

For our representation of $\text{CCR}(\infty)$ on \mathcal{K}_n we consider the number operator $N_i := a_i^*a_i$ on \mathcal{H}_i and define

$$N = \lim_{k \rightarrow \infty} \frac{1}{k} \sum_{i=1}^k N_i,$$

which we call the averaged total number operator. Note that the limit does not exist algebraically in $\text{CCR}(\infty)$, but converges in each representation. On \mathcal{K}_n

we have for elements x of the form $x = \psi_{n_1} \otimes \psi_{n_2} \otimes \cdots \otimes \psi_{n_\ell} \otimes \psi_n \otimes \psi_n \otimes \cdots$ and for those we have

$$Nx = \lim_{k \rightarrow \infty} \frac{1}{k} (n_1 + n_2 + \cdots + n_\ell + n + n + \cdots + n) = nx$$

This goes over to sums and limits, thus for all $x \in \mathcal{K}_n$ we have $Nx = nx$. If the representations of $\text{CCR}(\infty)$ on \mathcal{K}_n and \mathcal{K}_m were unitarily equivalent, i.e. if there were a unitary $U: \mathcal{K}_n \rightarrow \mathcal{K}_m$ such that $a_i^{\mathcal{K}_n} = U^* a_i^{\mathcal{K}_m} U$, then we also had $N_i^{\mathcal{K}_n} = U^* N_i^{\mathcal{K}_m} U$ which forced $N^{\mathcal{K}_n} = U^* N^{\mathcal{K}_m} U$, but then for all $x \in \mathcal{K}_n$ it needed to hold

$$nx = N^{\mathcal{K}_n} x = U^* N^{\mathcal{K}_m} U x = U^* m U x = mx$$

and thus $n = m$.

Conclusion X.5: A physical system corresponds to an C^* -algebra of observables generated by the respective algebraic relations (e.g. Weyl relations), but different physical situations corresponds to different representations. This approach is associated to some famous names like Segal (1947) or Haag, Kastler (1964).

Appendices

Appendix A.

Lebesgue-Stieltjes Integral and Absolute Continuity

We want to integrate functions on \mathbb{R} against finite measures μ , that is we want to make sense of expressions of the form $\int f(t) d\mu(t)$.

On the real numbers, a finite measure μ can be encoded by its distribution function h , which is defined via $h(t) := \mu((-\infty, t])$, and then we write $dh(t)$ instead of $d\mu(t)$. Integrals of the form $\int f(t) dh(t)$ are called *Stieltjes integrals*.

Definition A.1 (Distribution Function): Let $h: \mathbb{R} \rightarrow \mathbb{R}$ be a function. If h is increasing, right-continuous with $\lim_{t \rightarrow -\infty} h(t) = 0$ and $\lim_{t \rightarrow +\infty} h(t) < \infty$, then h is called a *distribution function*.

In the following, by h we always denote a distribution function.

Theorem A.2: Let f be a continuous and bounded function $f: \mathbb{R} \rightarrow \mathbb{R}$. Then the limit

$$\int f(t) dh(t) := \lim_{\sup |t_{i+1} - t_i| \downarrow 0} \sum f(t_i)[h(t_{i+1}) - h(t_i)]$$

exists and is called Riemann-Stieltjes integral of f with respect to dh .

Definition A.3 (Measurable Functions): The *measurable functions* from the reals to the reals are the smallest class of functions, which contains the continuous functions, and which is closed under pointwise convergence.

Remark A.4: Any “concretely constructed” function is measurable. To obtain a non-measurable function, one has to employ the axiom of choice.

The definition of the Riemann-Stieltjes integral can be extended to measurable functions:

Definition A.5: Let $f: \mathbb{R} \rightarrow \mathbb{R}$ be a function. If f is measurable and f is non-negative almost everywhere, then $\int f(t) dh(t) \in [0, \infty]$ is always defined and is called the *Lebesgue-Stieltjes integral*.

Let $f: \mathbb{R} \rightarrow \mathbb{C}$ be a measurable function. If $\int |f(t)| dh(t)$ is finite, then f is called *integrable*. The set

$$L^1(\mathbb{R}, dh) := \{f: \mathbb{R} \rightarrow \mathbb{C} \text{ measurable} \mid f \text{ is integrable}\}$$

is called the L^1 -space of \mathbb{R} with respect to dh . More generally, for $1 \leq p \leq \infty$, the set

$$L^p(\mathbb{R}, dh) := \left\{ f: \mathbb{R} \rightarrow \mathbb{C} \text{ measurable} : \int |f(t)|^p dh(t) < \infty \right\}$$

is called L^p -space of \mathbb{R} with respect to dh .

Remark A.6: (i) For a function $f \in L^1(\mathbb{R}, dh)$, the integral $\int f(t) dh(t)$, which yields a complex number, is well-defined and one has the usual triangular inequality

$$\left| \int f(t) dh(t) \right| \leq \int |f(t)| dh(t).$$

(ii) The L^2 -space is a Hilbert space with inner product

$$\langle f, g \rangle := \int f(t)^* g(t) dh(t).$$

Theorem A.7 (Beppo-Levi-Theorem): Let $(f_n)_{n \in \mathbb{N}}$ be a sequence of real-valued, non-negative, measurable functions which is pointwise non-decreasing, i.e. for all $t \in \mathbb{R}$ it holds $0 \leq f_1(t) \leq f_2(t) \leq \dots$. Define $f: \mathbb{R} \rightarrow \mathbb{R}$ via $f(t) := \lim_{n \rightarrow \infty} f_n(t) \in [0, \infty]$. Then we have

$$\int f(t) dh(t) = \lim_{n \rightarrow \infty} \int f_n(t) dh(t)$$

with possibly $\infty = \infty$.

The Beppo-Levi-Theorem is often also called “Monotone Convergence Theorem”.

Theorem A.8 (Dominated Convergence Theorem): Let $(f_n)_{n \in \mathbb{N}}$ be a pointwise convergent sequence of measurable functions and let f be the pointwise limit, i.e. $f(t) := \lim_{n \rightarrow \infty} f_n(t)$. If there is a function $g \in L^1(\mathbb{R}, dh)$ such that for every $t \in \mathbb{R}$ and $n \in \mathbb{N}$ it holds $|f_n(t)| \leq g(t)$, then also f is integrable and we have

$$\int f(t) dh(t) = \lim_{n \rightarrow \infty} \int f_n(t) dh(t).$$

Definition A.9: Let $N \subseteq \mathbb{R}$ be a set. If for each $\varepsilon > 0$ there are countably many intervals $([s_i, t_i])_{i \in \mathbb{N}}$ such that $N \subseteq \bigcup_{i \in \mathbb{N}} [s_i, t_i]$ and $\sum_{i \in \mathbb{N}} |t_i - s_i| < \varepsilon$, then N is called a *null set* or *set of measure zero* with respect to the Lebesgue measure.

Let P be a property of real numbers. If $\{t \in \mathbb{R} \mid P \text{ does not hold for } t\}$ is a nullset, then P is said to hold *almost everywhere*.

Remark A.10: (i) In particular saying “ $f = g$ almost everywhere” means that $\{t \in \mathbb{R} \mid f(t) \neq g(t)\}$ has measure zero.

(ii) All countable sets are nullsets with respect to the Lebesgue measure, but there also are uncountable nullsets like the Cantor set.

Remark A.11: An increasing, right-continuous function $h: \mathbb{R} \rightarrow \mathbb{R}$ that also fulfils $\lim_{t \rightarrow -\infty} h(t) = 0$ and $\lim_{t \rightarrow +\infty} h(t) < \infty$ can always be uniquely decomposed as $h = h_p + h_c$, where h_p is piecewise constant, also called the atomic point measure, and h_c is continuous.

For $h_p = \sum_i \chi_{[t_i, t_{i+1})} \alpha_{i+1}$ the corresponding integral of a function f is given by

$$\int f(t) dh_p(t) = \sum_i f(t_i) [\alpha_{i+1} - \alpha_i].$$

For a continuous function h_c one might hope to have $dh_c(t) = h'_c(t) dt$ and this would reduce our integral $\int f(t) dh_c(t)$ to an “ordinary calculus integral”

$$\int f(t) h'_c(t) dt$$

with respect to the Lebesgue measure. If we want $\int f(t) dh_c(t) = \int f(t) h'_c(t) dt$, then we need that h'_c must be defined—at least almost everywhere with respect to the Lebesgue measure—and for $f = \chi_{[a,b]}$ we need

$$\begin{aligned} h_c(b) - h_c(a) &= \int_a^b dh_c(t) \\ &= \int f(t) dh_c(t) = \int f(t) h'_c(t) dt = \int_a^b h'_c(t) dt \end{aligned}$$

to be true, i.e. we needed an analogue of the Fundamental Theorem of Calculus for h_c .

That h_c is almost everywhere differentiable is ensured by a theorem of Lebesgue on increasing functions. However, we need stronger continuity conditions for h_c to have an analogue of the Fundamental Theorem of Calculus.

Definition A.12 (Absolute Continuity): Let $g: [a, b] \rightarrow \mathbb{C}$ be a function. If for any $\varepsilon > 0$ there is $\delta > 0$ such that for disjoint subintervals $[s_1, t_1], \dots, [s_n, t_n]$ of $[a, b]$ with $\sum_{i=1}^n |t_i - s_i| < \delta$ it holds $\sum_{i=1}^n |g(t_i) - g(s_i)| < \varepsilon$, then g is called *absolutely continuous*.

Remark A.13: (i) It is clear that absolute continuity implies uniform continuity, which is the same as continuity on compact sets.

(ii) There are continuous functions which are not absolutely continuous. For example the Cantor function (also called “devil’s staircase”) is such a function. It is a so-called *singular function*, i.e. it is continuous, non-constant and its derivative is zero almost everywhere (in the measure theoretic sense). Hence the Cantor function can not be recovered from its derivative by integrating, in contrast to what we are used to from the Fundamental Theorem of Calculus.

Theorem A.14 (Fundamental Theorem of Calculus):

(i) Let f be Lebesgue-integrable on the interval $[a, b]$ and declare the function $g: [a, b] \rightarrow \mathbb{R}$ via

$$g(t) := \int_a^t f(s) ds.$$

Then g is absolutely continuous and it holds $g'(t) = f(t)$ almost everywhere.

(ii) Let $g: [a, b] \rightarrow \mathbb{C}$ be absolutely continuous. Then g is differentiable almost everywhere, its derivative g' is Lebesgue-integrable on $[a, b]$ and

$$g(t) = g(a) + \int_a^t g'(s) ds.$$

Remark A.15: Now we can refine our decomposition from Remark A.11: Every function h as in Definition A.1 can be uniquely decomposed as

$$h = h_p + h_{ac} + h_s$$

where h_p is called the *atomic part*, h_{ac} is the *absolutely continuous part* and h_s is the *singular part*. This gives a decomposition of the integral

$$\int f dh = \int f dh_p + \int f dh_{ac} + \int f dh_s$$

of which we know that $\int f dh_p$ is a series and $\int f dh_{ac} = \int f h'_{ac} dt$ is an integral we can process by means of calculus.