

3.5. Observables, states and C^* -algebras

Recall the probabilistic interpretation of wavefunctions $\psi \in L^2(\mathbb{R}^3)$ discussed in Sect. 1.2: $|\psi(x)|^2$ yields the probability density for the random variable $x \in \mathbb{R}^3$, the position of the particle.

* Suppose F is a continuous bounded function $\mathbb{R}^3 \rightarrow \mathbb{C}$, and $x_n \in \mathbb{R}^3$ are "independent samples" of the position, $n=1, 2, \dots$, then by the (strong) law of large numbers

$$\frac{1}{N} \sum_{n=1}^N F(x_n) \rightarrow \int_{\mathbb{R}^3} dx |\psi(x)|^2 F(x) \quad \text{almost surely.}$$

For this reason, $\int dx |\psi(x)|^2 F(x) =: \langle F \rangle_\psi$ is called the expectation of $F(x)$ for the wavefunction ψ .

* We can also write $\langle F \rangle_\psi = \int dx \psi(x)^* \underbrace{(F(x)\psi(x))}_{=: (M_F \psi)(x)}$
 $= (\psi, M_F \psi)$ where $M_F \in \mathcal{B}(\mathcal{H})$ is the multiplication operator corresponding to the bounded function F . (More about multiplication operators later.)

* Example: \mathbb{P}_ψ ("particle is in the region $\Omega \subset \mathbb{R}^3$ ") = $\langle F \rangle_\psi$ for $F(x) = \mathbb{1}(x \in \Omega)$.

3.5.1. Analogically, we use here the following terminology:

Definition: The expectation of an observable

$A \in \mathcal{B}(\mathcal{H})$ for a wavefunction $\psi \in \mathcal{H}$ is defined as $\langle A \rangle_\psi := (\psi, A\psi)$.

3.5.2. Motivation & connection to measurements:

Suppose the measurement apparatus has $N (< \infty)$ possible "outcomes": after the measurement, the apparatus shows one of the values $\alpha_n \in \mathbb{C}$, $n=1, \dots, N$,
 "..."

... and we know that for each outcome α_n the particle will have a state $\phi_n \in \mathcal{H}$. Assume, in addition, that if the particle is initially in state $\psi \in \mathcal{H}$, then the outcome " α_n " appears with probability $|\langle \phi_n, \psi \rangle|^2$. Then there is a probability $p_0 := 1 - \sum_{n=1}^N |\langle \phi_n, \psi \rangle|^2$ such that the particle is not detected at all. Set $\alpha_0 := 0$.

Then for a wavefunction ψ , the expectation value for the outcome of the measurement is given by $\sum_{n=1}^N \alpha_n |\langle \phi_n, \psi \rangle|^2$. This coincides with

$\langle A \rangle_\psi$ for the following observable:

Define $P_n \in \mathcal{B}(\mathcal{H})$ by $P_n \psi := \frac{\langle \phi_n, \psi \rangle}{\langle \phi_n, \psi \rangle} \phi_n$.

(In physics, this is denoted by $P_n := |\phi_n\rangle\langle \phi_n|$)

Set $A := \sum_{n=1}^N \alpha_n P_n \Rightarrow A \in \mathcal{B}(\mathcal{H})$ and

$$\langle A \rangle_\psi = \sum_{n=1}^N \alpha_n \langle \phi_n, \psi \rangle \langle \psi, \phi_n \rangle = \sum_{n=1}^N \alpha_n |\langle \phi_n, \psi \rangle|^2.$$

* Note that any such "measurement apparatus" also fulfills the standard "measurement axiom" of quantum mechanics.

* We will discuss measurements with a continuous outcome possibilities ($N = \infty$ above) later. Note that " x ", the particle position, falls into this category.

* Example: Stern-Gerlach experiment for spin- $\frac{1}{2}$ particles. (1927, hydrogen atoms; see the Wikipedia page.)
1922, silver atoms

3.5.3, C^* -algebraic formulation of quantum mechanics

* Basic idea: instead of $\psi_t \in \mathcal{H}$ as the basic dynamical variable, look at the evolution of $A_t \in \mathcal{B}(\mathcal{H})$ as defined by the rule

$$\forall \psi_0 \in \mathcal{H} : (\psi_0, A_t \psi_0) := (\psi_t, A \psi_t)$$

(If $\psi_t = e^{-itH} \psi_0$, then $A_t = e^{itH} A e^{-itH}$.)

This rule defines A_t uniquely, once A_0 and the unitary evolution of ψ have been given, (Exercise)
 \Rightarrow evolution equation on the C^* -algebra $\mathcal{B}(\mathcal{H})$.

- * Benefits: a) Easy to handle more general states (for instance thermal equilibrium ensembles) than the "pure state" defined by $\psi \in \mathcal{H}$.
- b) Can easily focus attention to "subsystems": consider only the evolution induced on some subalgebra of C^* -algebra $\mathcal{B}(\mathcal{H})$.

Example: Consider the subalgebra generated by $f(H)$, $f \in C_b(\mathbb{R})$, i.e. the collection of observables which are formed by the continuous bounded functions of the Hamiltonian operator. Since H is "conserved" \Rightarrow the evolution is always trivial. (= nothing changes).

* More generally, instead of wavevectors, one has the evolution of states: Suppose \mathcal{A} is a C^* -algebra. Then a map $\rho: \mathcal{A} \rightarrow \mathbb{C}$ is called a state if it is

- (i) linear
- (ii) positive: $\rho(A^*A) \geq 0 \quad \forall A \in \mathcal{A}$
- (iii) normalized: $\|\rho\| = 1$,
 $(\|\rho\| := \sup \{ |\rho(A)| \mid A \in \mathcal{A}, \|A\| = 1 \})$

* Examples of states over $\mathcal{B}(\mathcal{X})$:

a) If $\psi_0 \in \mathcal{X}$, then $\rho(A) := (\psi_0, A\psi_0)$ defines a state.

(Check: obviously linear, $\rho(A^*A) = \|A\psi_0\|^2 \geq 0$ and $|\rho(A)| \leq \|A\| \Rightarrow \|\rho\| \leq 1$. Since also $\rho(1) = (\psi_0, \psi_0) = 1 \Rightarrow \rho$ is a state.)

b) If ν is a Borel probability measure on $S := \{\psi \in \mathcal{X} \mid \|\psi\| = 1\}$ (= unit ball of \mathcal{X}) then

$$\rho(A) := \int_S \nu(d\psi) (\psi, A\psi)$$

defines a state. (Proof: as in "a".)

c) If $\mathcal{X} = \mathbb{C}^N$ and $H \in \mathbb{C}^{N \times N}$ is a self-adjoint matrix, then $\forall \beta > 0$

$$\rho_\beta(A) := \frac{\text{tr}(e^{-\beta H} A)}{\text{tr}(e^{-\beta H})} \text{ defines a state on } \mathcal{B}(\mathcal{X}) = \mathbb{C}^{N \times N}$$

(Proof: H self-adjoint \Leftrightarrow it has an eigensystem (E_n, ϕ_n) , $n=1, \dots, N$, where $E_n \in \mathbb{R}$ are the eigenvalues and $\phi_n \in \mathcal{X}$ are normalized eigenvectors forming an ONB for \mathcal{X} . Write the trace in this ONB

$$\Rightarrow Z_\beta := \text{tr}(e^{-\beta H}) = \sum_{n=1}^N (\phi_n, e^{-\beta H} \phi_n) = \sum_{n=1}^N e^{-\beta E_n} > 0,$$

$$\Rightarrow \rho_\beta(A) = \sum_{n=1}^N p_n (\phi_n, A\phi_n) \text{ with } p_n := \frac{1}{Z_\beta} e^{-\beta E_n}.$$

Since $\sum_{n=1}^N p_n = 1$, ρ_β is of the same form as

in "b)", for the measure $\nu(d\psi) := \sum_{n=1}^N p_n \delta(\psi - \phi_n) d\psi$

= mixture of "Dirac measures".)

* With a proper physical interpretation, it is mainly a matter of choice if one starts defining QM starting from \mathcal{H} (as here) or from an observable algebra \mathcal{A} .

Thm. Let \mathcal{A} be a C^* -algebra. Then there is a Hilbert space \mathcal{H} and an isometric $*$ -isomorphism $\bar{\Psi}: \mathcal{A} \rightarrow \mathcal{A}' \subset \mathcal{B}(\mathcal{H})$ such that \mathcal{A}' is a closed subalgebra of $\mathcal{B}(\mathcal{H})$.

Proof: Needs more tools. See, for instance, Rudin, Functional analysis, Chapter 12. (Thm. 12.41.) \square

This means that to any \mathcal{A} , we can associate a Hilbert space \mathcal{H} s.t. \mathcal{A} is a subalgebra of $\mathcal{B}(\mathcal{H})$.

4. Quantum dynamics I

Defn. 4.1: Let for all $t \geq 0$ an operator $U_t \in \mathcal{B}(\mathcal{H})$ be given. The family $(U_t)_{t \geq 0}$ forms a strongly continuous unitary semi-group if

- a) $U_0 = 1$
- b) U_t is unitary $\forall t$
- c) $U_{t+s} = U_t U_s \quad \forall t, s$
- d) $\lim_{t \rightarrow 0^+} \|U_t \psi - \psi\| = 0 \quad \forall \psi \in \mathcal{H}$

* Remark: The semi-group can always be extended to a group by defining: $U_t = U_{-t}^*$ for $t < 0$.

* Remark: The conditions a) - d) correspond to those required in the Introduction, Sec. 1. (As shown in Ex. 3.4, unitarity implies conservation of norm.)

- ① * $V \subset S$ is a neighborhood of $p \in S$ if $V \in \mathcal{T}_S$ and $p \in V$.
- * A local base at $p \in S$ is a collection \mathcal{B}_p of neighborhoods of p s.t. any neighborhood of p contains a member of \mathcal{B}_p . In formulae: $\mathcal{B}_p \subset \mathcal{T}_S$, $U \in \mathcal{B}_p \Rightarrow p \in U$, and $V \in \mathcal{T}_S, p \in V \Rightarrow \exists U \in \mathcal{B}_p$ s.t. $U \subset V$.

4.2. Various topologies on \mathcal{X} and $\mathcal{B}(\mathcal{X})$

(These topics belong to Topology II course.)

See e.g. Väisälä, *Topologia II*, chapter 2.6. (induced topologies).

* Topology reminder: Suppose \mathcal{X} is a topological space and S is a set.

Then any non-empty collection \mathcal{K} of functions $S \rightarrow \mathcal{X}$ defines a topology on S via the following construction:

1) Consider the inverse images of open sets:

$$\mathcal{L} := \{ f^{-1}(U) \mid f \in \mathcal{K}, U \in \mathcal{X} \}$$

2) Let \mathcal{B} collect all finite intersections of elements in \mathcal{L} .

$$\mathcal{B} := \{ \bigcap_{i=1}^n V_i \mid \text{for some } n, V_i \in \mathcal{L} \}$$

3) The topology $\mathcal{T}_{\mathcal{K}}$ on S consists of all unions of elements of \mathcal{B} .

* $\mathcal{T}_{\mathcal{K}}$ is the topology generated by \mathcal{L} , and \mathcal{B} forms a base for $\mathcal{T}_{\mathcal{K}}$.

↑ ① In general, we recall that:

* $\mathcal{T}_{\mathcal{K}}$ is called the \mathcal{K} -weak topology,

since it is the weakest topology on S ,
for which all $f \in \mathcal{K}$ are continuous.

Examples:

a) Weak topology on \mathcal{X}
 = \mathcal{K} -weak topology with $\mathcal{F} = \mathbb{C}$
 (with the standard topology) and
 $\mathcal{K} := \{ \Lambda_{\phi} : \mathcal{X} \rightarrow \mathbb{C} \mid \phi \in \mathcal{X} \}$,
 where $\Lambda_{\phi}(x) := (\phi, x)$.

b) Strong operator topology on $\mathcal{B}(\mathcal{X})$
 = \mathcal{K} -weak topology with $\mathcal{F} = \mathcal{X}$
 (with the norm-topology), and
 $\mathcal{K} := \{ E_{\phi} : \mathcal{B}(\mathcal{X}) \rightarrow \mathcal{X} \mid \phi \in \mathcal{X} \}$
 where $E_{\phi}(T) := T\phi$.

c) Weak operator topology on $\mathcal{B}(\mathcal{X})$
 = \mathcal{K} -weak topology with $\mathcal{F} = \mathbb{C}$ (stand. topol.)
 and
 $\mathcal{K} := \{ \Gamma_{\phi, \psi} : \mathcal{B}(\mathcal{X}) \rightarrow \mathbb{C} \mid \phi, \psi \in \mathcal{X} \}$
 where $\Gamma_{\phi, \psi}(T) := (\phi, T\psi)$.

Remarks: * To make matters confusing, there
 is also a weak topology on $\mathcal{B}(\mathcal{X})$,
 which is induced by
 $\mathcal{K} := \{ \Lambda : \mathcal{B}(\mathcal{X}) \rightarrow \mathbb{C} \mid \Lambda \text{ continuous} \}$.
 Since every $\Gamma_{\phi, \psi} \in \mathcal{K}$, the weak $\mathcal{B}(\mathcal{X})$ -
 topology is stronger than the weak
 operator topology.

* The above topologies are distinct from the
 norm-topologies, if $\dim \mathcal{X} = \infty$.
 (See exercises)

- Examples of convergence in norm (\rightarrow), strong (\xrightarrow{s}) and weak (\xrightarrow{w}) operator topologies are given in the exercises. The reason for introducing the zoo of convergence criteria is practical: the different notions are needed, or easier to handle, in different applications. In particular:

4.3. Why not norm-continuous U.S.G.?

Theorem: a) Let $(U_t)_{t \geq 0}$ be a norm-continuous unit. semi-group: It satisfies 4.1.a)-c) and d') $\lim_{t \rightarrow 0^+} \|U_t - 1\| = 0$.

Then there is a self-adjoint $A \in \mathcal{B}(\mathcal{H})$ s.t. $\forall t \geq 0$:

$$U_t = e^{-itA} := \lim_{N \rightarrow \infty} \sum_{n=0}^N \frac{(-itA)^n}{n!}$$

b) Conversely, if $A \in \mathcal{B}(\mathcal{H})$ is self-adjoint, then $U_t = e^{-itA}$, $t \geq 0$, defines a norm-continuous unitary semi-group.

* Remarks: (1) d') says that $U_t \rightarrow 1 = U_0$ in norm. The condition d), on the other hand, is equivalent to $U_t \xrightarrow{s} 1$, which actually implies that the mapping $t \mapsto U_t$

... is continuous in the strong operator topology, hence the name "strongly continuous".

② We will later see that Schrödinger equations lead to strongly continuous USG:s which are not norm continuous. This is the main reason why we will need to go through the trouble of unbounded operators. (Exercises 5)

③ One could imagine that requiring $U_t \xrightarrow{w} 1$ instead of $U_t \xrightarrow{s} 1$ would lead to even more general semi-group constructions. However, as shown in Exercises 5, this is not so: every weakly continuous USG is also strongly continuous.

Proof of Thm 4.3.:

a) This part cannot be proven with our results so far. For a proof see Thm. 13.36. in Rudin, F.A.

b) Let $A \in \mathcal{B}(\mathcal{X})$ be self-adjoint. Since $\|A\| < \infty$, $\forall N' \geq N \geq 0$ we have

$$\sum_{n=0}^{\infty} \left\| \frac{(-itA)^n}{n!} \right\| \leq \sum_{n=0}^{\infty} \frac{|t| \|A\|^n}{n!} = e^{|t| \|A\|} < \infty.$$

Thus the sum $\sum_{n=0}^{\infty} \frac{(-itA)^n}{n!}$ is norm-convergent;

$$\text{let } U_t := e^{-itA} := \lim_{N \rightarrow \infty} \sum_{n=0}^N \frac{(-itA)^n}{n!} \in \mathcal{B}(\mathcal{X}) \forall t \in \mathbb{R}.$$

Clearly, $U_0 = 1$, so a) holds. Also, for any $t, s \in \mathbb{R}$,

$$\begin{aligned} \sum_{n=0}^N \frac{(-iA)^n}{n!} (t+s)^n &= \sum_{n=0}^N \sum_{k=0}^n \binom{n}{k} t^{n-k} s^k \frac{(-iA)^n}{n!} \\ &= \sum_{k=0}^N \sum_{n=0}^N \underbrace{\mathbb{1}(k \leq n)}_{n' = n-k \Rightarrow \sum_{n'=-k}^{N-k} \mathbb{1}(n' \geq 0)} t^{n-k} s^k \frac{1}{k!} \frac{1}{(n-k)!} (-iA)^{n-k} (-iA)^k \end{aligned} \rightarrow$$

$$= \sum_{k=0}^N \frac{(-isA)^k}{k!} \sum_{n'=0}^{N-k} \frac{(-itA)^{n'}}{n'!}$$

$$= \left(\sum_{k=0}^N \frac{(-isA)^k}{k!} \right) \cdot \left(\sum_{n=0}^N \frac{(-itA)^n}{n!} \right)$$

$$- \underbrace{\sum_{k=1}^N \frac{(-isA)^k}{k!} \sum_{n=N-k+1}^N \frac{(-itA)^n}{n!}}$$

$$\| \cdot \| \leq \sum_{k=1}^N \frac{|s|^k \|A\|^k}{k!} \sum_{n=N-k+1}^N \frac{|t|^n \|A\|^n}{n!}$$

$\xrightarrow{N \rightarrow \infty} 0$ by dominated conv. theorem.
 $(\|T\| \|U-U_n\| + \|U_n\| \|T-T_n\|)$

On the hand, using $\|TU - T_n U_n\| = \|T(U - U_n) + (T - T_n)U_n\|$

$$\left(\sum_{k=0}^N \frac{(-isA)^k}{k!} \right) \cdot \left(\sum_{n=0}^N \frac{(-itA)^n}{n!} \right) \xrightarrow{N \rightarrow \infty} e^{-isa} e^{-ita} \quad (\text{in norm})$$

This proves that $U_{s+t} = U_s U_t \quad \forall s, t \in \mathbb{R}$.

But then $U_s U_{-s} = U_0 = 1 = U_{-s} U_s \quad \forall s \in \mathbb{R}$

$$\Rightarrow \forall s \in \mathbb{R} \exists U_s^{-1} = U_{-s}$$

Also $\forall \eta, \phi \in X, s \in \mathbb{R} : (U_s \phi, \eta)$

continuity

$$= \lim_{N \rightarrow \infty} \left(\sum_{n=0}^N \frac{(-isA)^n}{n!} \phi, \eta \right)$$

$$= \lim_{N \rightarrow \infty} \sum_{n=0}^N \frac{(is)^n}{n!} \underbrace{(A^n \phi, \eta)}_{A^* = A} = (\phi, (A^*)^n \eta) = (\phi, A^n \eta)$$

$$= \lim_{N \rightarrow \infty} (\phi, \sum_{n=0}^N \frac{(isA)^n}{n!} \eta) = (\phi, U_{-s} \eta)$$

Thus $U_s^* = U_{-s} = U_s^{-1} \Rightarrow U_s^* U_s = 1 = U_s U_s^*$

$\Rightarrow U_s$ is unitary $\forall s$ (Proves b).

c) was already proven above.

d')

$$\| U_t - 1 \| = \left\| \sum_{n=1}^{\infty} \frac{(-itA)^n}{n!} \right\| \leq \sum_{n=1}^{\infty} \frac{|t|^n \|A\|^n}{n!}$$

$$\leq |t| \|A\| \sum_{n=1}^{\infty} \frac{|t|^{n-1} \|A\|^{n-1}}{(n-1)!} = |t| \|A\| e^{|t| \|A\|} \xrightarrow{t \rightarrow 0} 0 \quad \square$$