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 $\mathbb{R}^3 \to \mathbb{C}$, and $x_n \in \mathbb{R}^3$ are "independent samples" of the position, $n = 1, 2, \ldots$, then by the (strong) law of large numbers

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

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 $\langle F \rangle_\psi = \int dx\, \psi(x)^* \big(\underbrace{F(x)\psi(x)}_{=:(M_F\psi)(x)}\big)$

$= (\psi, M_F \psi)$ where $M_F \in \mathcal{B}(\mathcal{H})$ is the multiplication operator corresponding to the bounded function F. (More about multiplication operators later.)

* Example: $\mathbb{P}_\psi(\text{"particle is in the region } \Omega \subset \mathbb{R}^3\text{"}) = \langle F \rangle_\psi$ 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 $a_n \in \mathbb{C}$, $n = 1, \ldots, N$, ...

... 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 $|(\phi_n, \psi)|^2$. Then there is a probability $p_0 := 1 - |(\phi_n, \psi)|^2$ such that the particle is not detected at all. Set $\alpha_0 := 0$.

Then for a wave function ψ, the expectation value for the outcome of the measurement is given by $\sum_{n=1}^{N} \alpha_n |(\phi_n, \psi)|^2$. This coincides with $\langle A \rangle_\psi$ for the following observable:

Define $P_n \in \mathcal{B}(\mathcal{H})$ by $P_n \psi := \underbrace{(\phi_n, \psi)}_{\in \mathbb{C}} \underbrace{\phi_n}_{\in \mathcal{H}}$.

(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

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

* 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

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

(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 $\rho: \mathcal{A} \to \mathbb{C}$ is called a state iff. it is
  (i) linear
  (ii) positive: $\rho(A^*A) \geq 0 \quad \forall A \in \mathcal{A}$
  (iii) normalized: $\|\rho\| = 1$,
  $\left(\|\rho\| := \sup \{ |\rho(A)| \mid A \in \mathcal{A}, \|A\| = 1 \} \right)$

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

a) If $\psi_0 \in \mathcal{H}$, 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 $S := \{\psi \in \mathcal{H} \mid \|\psi\| = 1\}$ (= unit ball of $\mathcal{H}$) then

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

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

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

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

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

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

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

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 $*$-isomorfism $\Psi : \mathcal{A} \to \mathcal{A}' \subset \mathcal{B}(\mathcal{H})$ 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.). □

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) $\lim_{t \to 0^+} \| U_t \psi - \psi \| = 0 \quad \forall \psi \in \mathcal{H}$

* 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 <u>neighborhood</u> of $p \in S$ if $V \in \mathcal{T}_S$ and $p \in V$.

* A <u>local base</u> 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 $\mathcal{H}$ and $\mathcal{B}(\mathcal{H})$

* <u>Topology reminder</u>: Suppose $\mathfrak{X}$ is a topological space and S is a set. Then <u>any</u> non-empty collection $\mathcal{K}$ of functions $S \to \mathfrak{X}$ defines a topology on S via the following construction:
  1) Consider the inverse images of open sets:
  $$\mathcal{b} := \{ f^{\leftarrow}(U) \mid f \in \mathcal{K},\ U \subset \mathfrak{X} \}$$
  2) Let $\mathcal{B}$ collect all <u>finite</u> intersections of elements in $\mathcal{b}$
  $$\mathcal{B} := \{ \bigcap_{i=1}^{n} V_i \mid \text{for some } n,\ V_i \in \mathcal{b}\ \forall i \}$$
  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 <u>generated</u> by $\mathcal{b}$, and $\mathcal{B}$ forms a <u>base</u> for $\mathcal{T}_{\mathcal{K}}$.

1 In general, we recall that:

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

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

<u>Examples</u>:

a) <u>Weak topology on $\mathcal{H}$</u>
= $\mathcal{K}$-weak topology with $\mathfrak{X} = \mathbb{C}$ (with the standard topology) and
$\mathcal{K} := \{ \Lambda_\phi : \mathcal{H} \to \mathbb{C} \mid \phi \in \mathcal{H} \}$,
where $\Lambda_\phi(\psi) := (\phi, \psi)$.

b) <u>Strong operator topology on $\mathcal{B}(\mathcal{H})$</u>

= $\mathcal{K}$-weak topology with $\mathfrak{X} = \mathcal{H}$ (with the norm-topology), and
$\mathcal{K} := \{ E_\phi : \mathcal{B}(\mathcal{H}) \to \mathcal{H} \mid \phi \in \mathcal{H} \}$
where $E_\phi(T) := T\phi$.

c) <u>weak operator topology on $\mathcal{B}(\mathcal{H})$</u>

= $\mathcal{K}$-weak topology with $\mathfrak{X} = \mathbb{C}$ (stand. topol.) and

$$\mathcal{K} := \{ \Gamma_{\phi,\psi} : \mathcal{B}(\mathcal{H}) \to \mathbb{C} \mid \phi, \psi \in \mathcal{H} \}$$

where $\Gamma_{\phi,\psi}(T) := (\phi, T\psi)$.

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

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

- Examples of convergence in norm ($\to$), 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') $\lim_{t\to 0^+} \| U_t - 1 \| = 0$.

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

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

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 $U_t \to 1 = U_0$ 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 <u>not</u> 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.

<u>Proof of Thm 4.3.:</u>

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

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

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

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

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

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

$$\sum_{n=0}^{N} \frac{(-iA)^n}{n!} (t+s)^n = \sum_{n=0}^{N} \sum_{k=0}^{n} \binom{n}{k} t^{n-k} s^k \frac{(-iA)^n}{n!}$$

$$= \sum_{k=0}^{N} \underbrace{\sum_{n=0}^{N}}_{n'=n-k:\ \sum_{n'=-k}^{N-k} \mathbb{1}(n' \geq 0)} \mathbb{1}(k \leq n)\, t^{n-k} s^k \frac{1}{k!} \frac{1}{(n-k)!} (-iA)^{n-k} (-iA)^k$$

$\longrightarrow$

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

$$= \left(\sum_{k=0}^{N} \frac{(-isA)^k}{k!} \right) \cdot \left(\sum_{n=0}^{N} \frac{(-itA)^n}{n!} \right) - \underbrace{\sum_{k=1}^{N} \frac{(-isA)^k}{k!} \sum_{n=N-k+1}^{N} \frac{(-itA)^n}{n!}}$$

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

$$\xrightarrow{N \to \infty} 0 \quad \text{by dominated conv. theorem.}$$

On the hand, by Exercise 1.1.b),

$$\left(\sum_{k=0}^{N} \frac{(-isA)^k}{k!} \right) \circ \left(\sum_{n=0}^{N} \frac{(-itA)^n}{n!} \right) \xrightarrow{N \to \infty} e^{-isA} e^{-itA} \quad \text{(in norm).}$$

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

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

$\Rightarrow$

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

Also: $\forall \psi, \phi \in \mathcal{H}, s \in \mathbb{R}$: $(U_s \phi, \psi)$

$$\overset{\text{continuity}}{=} \lim_{N \to \infty} \left(\sum_{n=0}^{N} \frac{(-isA)^n}{n!} \phi, \psi \right)$$

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

$$= \lim_{N \to \infty} \left(\phi, \sum_{n=0}^{N} \frac{(isA)^n}{n!} \psi \right) = (\phi, U_{-s} \psi).$$

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')

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

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