Introduction to Quantum Mechanics

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DISCLAIMER

- The purpose of this talk is to give a very brief introduction to the mathematical aspects of Quantum Mechanics making special emphasis on those points that are relevant for Fernando Barbero's mini-course on *Quantum Geometry and Quantum Gravity*. I will left untouched many interesting mathematical results and *all* the physical ones!

- I will follow an approach that, although standard in certain mathematical literature, it is not the standard in the physical one
  - The starting point in (most of the) physics books is the definition of physical observables as self-adjoint operators on a certain Hilbert space $\mathfrak{H}$ and (pure) states of the system as vectors on $\mathfrak{H}$. The emphasis there is on vector states
  - Here the starting point will be the C^*-algebra generated by the (bounded) physical observables. In this approach the states of a system are secondary (derived) objects

PLAN OF THE TALK

1. General considerations about physical systems: Observables and states
2. Classical kinematics: Observables and states in Classical Mechanics
3. The crisis of Classical Physics (very very brief!)
4. Quantum kinematics: Observables and states in Quantum Mechanics (Segal approach)
5. The simplest quantum system:

   The quantum point particle $\equiv$ Weyl C^*-algebra
6. Quantum dynamics: Schrödinger and Heisenberg equations

Systems The 'things' of the physical world in which we will be interested will be called physical systems (or systems)

- A free point particle in Euclidean space
- A point particle constrained to move on a smooth surface in Euclidean space
- Electric and magnetic fields without sources in Euclidean space

But if we try to give a more precise definition, we need to specify what is a 'thing'?

Operational point of view: A system is defined by the physical properties –observables $\mathcal{O}$– that can be measured on it (by concrete physical devices) and the relations between them

- **Observables:** A system is defined by a set $\mathcal{O}$ of observables endowed with certain algebraic and metrical properties

- **States:** The set $\mathcal{S}$ of states is characterized by the results of the measurements of all the observables in the following sense:
  Given a state $\omega \in \mathcal{S}$, for any $A \in \mathcal{O}$, the expectation value $\omega(A)$ is the average over the results of measurements of the observable A.
  Thus, a state of a system is a functional $\omega : \mathcal{O} \rightarrow \mathbb{R}$ (that satisfies some properties that we will specify later)

A typical system in classical mechanics is described in the cotangent bundle $T^*\mathcal{C}$ of a configuration space $\mathcal{C}$

- The configuration space $\mathcal{C}$ of the system is the space of all possible positions $q \in \mathcal{C}$ that it can attain (possibly subject to external constraints)
  - A single particle moving in ordinary Euclidean 3-space: $\mathcal{C} = \mathbb{R}^3$
  - A double planar pendulum: $\mathcal{C} = \mathbb{T}^2 = \mathbb{S}^1 \times \mathbb{S}^1$
  - A rigid body: $\mathcal{C} = \mathbb{R}^3 \times SO(3)$
- The phase space of the system $T^*\mathcal{C}$ consists of all possible values of position and momentum variables (q, p_a). $T^*\mathcal{C}$ has a canonical symplectic form $\Omega_{\alpha\beta}$

Classical observables belong to some class of functions on $T^*\mathcal{C}$, say

$$\mathcal{O} = C^\infty(T^*\mathcal{C}; \mathbb{R}) \subset C^\infty(T^*\mathcal{C}; \mathbb{C})$$

In this case $\mathcal{O}$ is a commutative and associative $*$-algebra (the elements of $\mathcal{O}$ satisfy $A = A^*$)

The symplectic structure of $T^*\mathcal{C}$ endows $\mathcal{O}$ with the structure of a Poisson $*$-algebra with Poisson bracket

$$\{A, B\} := \Omega^{\alpha\beta}(\mathrm{d}A)_\alpha(\mathrm{d}B)_\beta\,, \quad \forall A, B \in \mathcal{O}\,.$$

This Poisson structure is relevant in many respects

- The dynamical evolution of the system is defined through $\{\cdot,\cdot\}$ once a special observable –the classical Hamiltonian of the system $H \in \mathcal{O}$– is given:
$$\frac{dA}{dt} = \{A, H\}$$
- As we will see, the Poisson bracket is the classical analogue of the quantum commutator (quantum observables will define a non abelian algebra)

- **Configuration observables $Q(f)$:** For any $f \in C^\infty(\mathcal{C})$ let

$$Q(f)(q, p_a) := f(q)$$

- **Momentum observables $P(v)$:** For any $v \in \mathfrak{X}^\infty(\mathcal{C})$ let

$$P(v)(q, p_a) := v^a(q) p_a$$

This family of observables is closed under Poisson brackets

$$\{Q(f_1), Q(f_2)\} = 0,\ \{Q(f), P(v)\} = Q(\mathcal{L}_v f),\ \{P(v_1), P(v_2)\} = -P(\mathcal{L}_{v_1} v_2)$$

If $\mathcal{C}$ is the Euclidean 3-space we can choose Euclidean coordinates x, y, $z : \mathcal{C} \to \mathbb{R}$ and consider the 6 Killing vector fields of the Euclidean metric:

- the configuration observables $X = Q(x)$, $Y = Q(y)$, and $Z = Q(z)$ are the usual position observables
- the momentum observables $P_X = P(\partial_x)$, $P_Y = P(\partial_y)$, $P_Z = P(\partial_z)$ are the components of the usual linear momenta, and $L_X = P(y\partial_z - z\partial_y)$, $L_Y = P(z\partial_x - x\partial_z)$, $L_Z = P(x\partial_y - y\partial_x)$ are the components of the familiar angular momenta.

Pure states: Classical Physics assumes that canonical variables can be simultaneously measured with infinite precision. This leads us to identify the points of the phase space with the (pure) states of the system. If $\gamma = (q, p_a) \in T^*\mathcal{C}$ is determined with total precision, the expectation value of any observable is given by

$$\omega_\gamma(A) = A(q, p_a)\,.$$

Pure states play a fundamental role in non-statistical mechanic: An experiment performed on a system described by a pure state will attain maximal theoretical accuracy

Mixed states: In many situations it is not possible to determine the pure state of the system. If a system is in a state ω_1 with probability α and in a state ω_2 with probability $1-\alpha$ the effective state of the system w is

$$\omega(A) = \alpha\,\omega_1(A) + (1-\alpha)\,\omega_2(A)\,.$$

The state ω is the *mixture* of the states ω_1 and ω_2.

States: In dealing with a system of a very large (say 10^{23}) number of particles it is impossible in practice to determine all the positions and all the velocities of the particles. *Classically we always assume that the system is in a pure state* but we may be unable to determine it. This is the usual situation in Classical Statistical Mechanics.

Classical states $\mathcal{S}$ are probability measures μ on $T^*\mathcal{C}$

$$\omega_\mu(A) = \int_{T^*\mathcal{C}} A \, \mathrm{d}\mu$$

Pure states corresponds to Dirac measures

Variance: The variance of an observable A relative to the state ω

$$\Delta^2_\omega(A) := \omega(A^2) - \omega(A)^2$$

In classical physics, ω is a pure state iff $\Delta_\omega(A) = 0$ for all $A \in \mathcal{O}$

A proposition in Classical Mechanics is of the form

$$\mathfrak{p}(S) := \text{"the pure state } (q, p_a) \text{ of the systems lies in } S \subset T^*\mathcal{C}\text{"}$$

Typically $S = \{A \in \Delta \subset \mathbb{R}\}$ for some $A \in \mathcal{O}$
Classically, these propositions are either true or false and can be evaluated if the pure state of the system is known. In general, if we are given a state $\omega_\mu \in \mathcal{S}$, we can only measure the plausibility of a proposition to be true:

$$\mathrm{Prob}(\mathfrak{p}(\{A \in \Delta\}) \,|\, \omega_\mu) = \mu(\{A \in \Delta\}) = \int_{\{A\in\Delta\}\subset T^*\mathcal{C}} \mathrm{d}\mu$$

By associating propositions with subsets of $T^*\mathcal{C}$ it is clear that the logical structure of Classical Physics is the standard Boolean logic

$$\mathfrak{p}(S_1) \vee \mathfrak{p}(S_2) = \mathfrak{p}(S_1 \cup S_2)\,,\ \mathfrak{p}(S_1) \wedge \mathfrak{p}(S_2) = \mathfrak{p}(S_1 \cap S_2)\,,\ \neg\mathfrak{p}(S) = \mathfrak{p}(T^*\mathcal{C} \setminus S)\,,$$
$$\mathfrak{p}_1 \wedge (\mathfrak{p}_2 \vee \mathfrak{p}_3) = (\mathfrak{p}_1 \wedge \mathfrak{p}_2) \vee (\mathfrak{p}_1 \wedge \mathfrak{p}_3)\,, \quad \mathfrak{p}_1 \vee (\mathfrak{p}_2 \wedge \mathfrak{p}_3) = (\mathfrak{p}_1 \vee \mathfrak{p}_2) \wedge (\mathfrak{p}_1 \vee \mathfrak{p}_3)$$

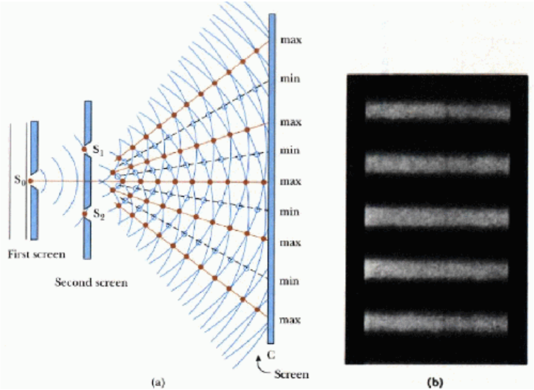
Classical Mechanics is a beautiful and natural way to model physical systems. However it suffers from one serious problem: Nature is not classical...

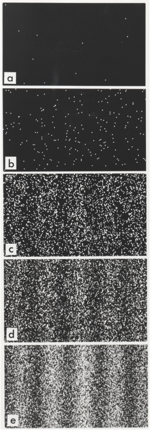
Atoms (10^{-8}cm) are made of a nucleus (neutrons and protons) and electrons. Electrons and protons are charged particles. The electrons are bound to the nucleus thought the Coulomb interaction

- Atoms are obviously stable (we are here!). However, the stability of electron orbits is incompatible with the laws of EM (accelerated charges emits EM radiation $\Rightarrow$ energy loss)
- Experimental results show that the radiation absorbed or emitted by an atom can have only a discrete set of sharply defined wavelengths (only a discrete set of 'orbits' –energy levels– seem to be allowed)

A beam of photons (electrons, or atoms) produces interference patterns

The interference pattern still results even if only one electron traverses the apparatus at a time (right figure)





QUANTUM LOGIC IS NOT CLASSICAL LOGIC

Consider the following propositions

$\mathfrak{p} :=$ "interference pattern is produced by the particle on the screen"

$\mathfrak{s}_1 :=$ "the particle has passed through the slit 1"

$\mathfrak{s}_2 := \neg\mathfrak{s}_1 =$ "the particle has passed through the slit 2"

Experimentally, the interference pattern does not appear if we close one of the slits so that we known for sure that the particle passes through the other

$$\mathfrak{p} \wedge \mathfrak{s}_1 = \mathfrak{p} \wedge \mathfrak{s}_2 = \emptyset \Rightarrow (\mathfrak{p} \wedge \mathfrak{s}_1) \vee (\mathfrak{p} \wedge \mathfrak{s}_1) = \emptyset$$

On the other hand the particle has passed through one of the slits so

$$\mathfrak{s}_1 \vee \mathfrak{s}_2 = 1 \Rightarrow \mathfrak{p} \wedge (\mathfrak{s}_1 \vee \mathfrak{s}_2) = \mathfrak{p}$$

Then $\mathfrak{p} \wedge (\mathfrak{s}_1 \vee \mathfrak{s}_2) \neq (\mathfrak{p} \wedge \mathfrak{s}_1) \vee (\mathfrak{p} \wedge \mathfrak{s}_1)$ so we cannot use the classical Boolean logic to deal with these microscopic systems

Heisenberg uncertainty 'principle'

When dealing with systems at atomic scales (atoms 10^{-8}cm; nucleus 10^{-23}cm) any attempt to measure the position of a particle with sharper and sharper precision will produce a larger and larger variance in the momentum

In more mathematical terms: Let $\mathcal{C}$ the Euclidean 3-space and $X = Q(x)$, $P_X = P(\partial_x)$ the canonical position and linear momenta in the x direction

$$\Delta_\omega(P_X) \cdot \Delta_\omega(X) \geq \frac{\hbar}{2} \qquad (\hbar \sim 10^{-34}\mathrm{J}\cdot\mathrm{s})$$

In general, for the configuration and momentum observables

$$\Delta_\omega(P(v)) \cdot \Delta_\omega(Q(f)) \geq \frac{\hbar}{2}|\omega(Q(L_v f))|$$

This implies that no states exist with the properties of the pure states of Classical Physics ($\nexists \omega$ such that $\Delta_\omega(A) = 0$, $\forall A$)

If we accept the Heisenberg principle, we need to reconsider the mathematical structure of $\mathcal{O}$ and $\mathcal{S}$. **This required the development of a new mathematical framework for Mechanics –Quantum Mechanics– in which $\mathcal{O}$ no longer is an abelian algebra**

By the early 1930s the mathematical theory of quantum mechanics was firmly founded by von Neumann (and Stone). The basic rules could be summarized as follows:

(1) an observable is a self-adjoint operator $\hat{A}$ on a Hilbert space $\mathfrak{H}$;
(2) a (pure) state is a unit vector in $\psi \in \mathfrak{H}$;
(3) the expected value of $\hat{A}$ in the state ψ is given by $\langle \psi \,|\, \hat{A}\psi \rangle$;
(4) the dynamical evolution of the system is determined by the specification of a self-adjoint operator $\hat{H}$ through one of the following rules: $\psi \mapsto \psi_t = \exp(it\hat{H})\psi$ or $\hat{A} \mapsto \hat{A}_t = \exp(it\hat{H})A\exp(-it\hat{H})$

In this talk we will follow the Segal approach to Quantum Mechanics because it is an operational formalism that can be generalized to QFT in a straightforward way

Segal's postulates (kinematics)

Segal's postulates try to encode the minimal set of properties that the class of observables for any physical theory should satisfy

Definition: Segal system

1. $\mathcal{O}$ is a linear space over $\mathbb{R}$
2. $(\mathcal{O}, ||\cdot||)$ is a real Banach space
3. $\mathcal{O} \ni A \mapsto A^2 \in \mathcal{O}$ is a continuous function on $(\mathcal{O}, ||\cdot||)$
4. $||A^2|| = ||A||^2$, and $||A^2 - B^2|| \leq \max(||A^2||, ||B^2||)$

From an operational point of view, only bounded observables play a fundamental role. The norm of an observable is to be thought as its maximum numerical value. If A_1 and A_2 are bounded observables, it is possible to justify that $\lambda_1 A_1 + \lambda_2 A_2$ is also an observable

It is possible to characterize the mathematical systems satisfying these postulates

- **Special Segal systems:** there exists an asociative C^*-algebra $\mathcal{A}$ with identity, $\mathbf{1} \in \mathcal{A}$, such that
  - $\mathcal{O} = \{A \in \mathcal{A} \,|\, A = A^* \quad \text{(i.e. } A \text{ is self-adjoint)}\}$
  - $\mathcal{A}$ is generated by $\mathcal{O}$
- **Exceptional Segal systems** if this is not the case. Exceptional Segal systems are difficult to construct and, so far, no one has been able to give an interesting physical application of these systems

Summarizing, for special Segal's systems:

- A physical system is defined by its C^*-algebra $\mathcal{A}$ with identity $\mathbf{1}$
- The states $\mathcal{S}$ are normalized positive linear functionals that separate the observables
- A state is call *pure* if it cannot be written as a nontrivial convex combination of other states

- *Positive:* ω positive in $\mathcal{A}$ if $\omega(A^*A) \geq 0\,, \forall A \in \mathcal{A}$. All positive functionals are continuous on $(\mathcal{A}, ||\cdot||)$
- *Normalized:* ω is normalized if $\omega(\mathbf{1}) = 1$
- Notice that the set of states over $\mathcal{A}$ is a convex subset of $\mathcal{A}^*$ (the topological dual of $\mathcal{A}$)
- *Functional separates the observables:* If $A_1 \neq A_2$ then $\exists \omega$ such that $\omega(A_1) \neq \omega(A_2)$ (*full* set of states)

An observable A is said to have a definite value in a state ω if $\Delta^2_\omega(A) := \omega(A^2) - \omega(A)^2 = 0$

A class of observables are called simultaneously observable if there exists a sufficient large number of states in which they simultaneously have definite values

A collection $\mathfrak{C}$ of observables is simultaneously observable if the system generated by $\mathfrak{C}$, $\mathcal{A}(\mathfrak{C})$ has a full set of states in each of which every observable in $\mathcal{A}(\mathfrak{C})$ has a definite value

Theorem

$\mathfrak{C}$ is simultaneously observable if and only if it is commutative

Gelfand-Naimark characterization of abelian C^*-algebras

An abelian C^*-algebra $\mathcal{A}$ with identity is isometrically isomorphic to the C^*-algebra of continuous functions on a compact Hausdorff topological space (which is the Gelfand spectrum of $\mathcal{A}$, $sp(\mathcal{A})$, with the topology induced by the weak $*$ topology)

If $\mathcal{A}$ is abelian with identity there exists an isomorphism $\mathcal{A} \to C(sp(\mathcal{A}))$, $A \mapsto f_A$. The Riesz-Markov theorem tells us that there is a measure μ on $sp(\mathcal{A})$ associated to every sate ω

$$\omega(A) = \int_{sp(\mathcal{A})} f_A d\mu$$

If $\mathfrak{C}$ is simultaneously observable class then it is isomorphic to the system of all real valued continuous functions on a compact Hausdorff space $sp(\mathcal{A}(\mathfrak{C}))$. In this case

$$\omega(A) = \int_{sp(\mathcal{A}(\mathfrak{C}))} f_A(s) d\mu(s)\,, \quad \forall A \in sp(\mathcal{A}(\mathfrak{C}))$$

The situation for $\mathfrak{C}$ is exactly the same as in Classical Mechanics. **In order to incorporate de Heisenberg uncertainty principle $\mathcal{A}$ is required to be a non-abelian C^*-algebra**

If $A \in \mathcal{A}$ is normal ($AA^* = A^*A$) the C^*-algebra $\mathcal{A}(A)$ generated by $\mathbf{1}$, A, and A^* is abelian and it is possible to show that

$$sp(\mathcal{A}(A)) = \sigma(A) = \{\lambda \in \mathbb{C} \,|\, \lambda\mathbf{1} - A \text{ does not have a two-sided inverse}\}$$

Then, given any state ω, we can applying the GN-theorem

$$\omega(B) = \int_{\sigma(A)} f_B(\lambda) \mathrm{d}\mu_{\omega,A}(\lambda)\,, \quad \forall B \in \mathcal{A}(A)\,.$$

In particular $\omega(A) = \int_{\sigma(A)} \lambda \mathrm{d}\mu_{\omega,A}(\lambda)$. If we remember that $\omega(A)$ is the expectation value of A on ω, the interpretation is clear. If A is an observable ($A = A^*$)

- The possible values that A can take in any experiment belong to $\sigma(A)$
- When the state is ω, the probability that A takes values on some subset of $\sigma(A)$ is defined in terms of $\mu_{\omega,A}$
- For pure states $\mu_{\omega,A}$ is not, in general, a Dirac measure. Pure states in Quantum Mechanics have statistical interpretation!

Heisenberg uncertainty relations

Theorem (Heisenberg uncertainty relations)

Given two observables $A = A^*$ and $B = B^*$ and a state ω

$$\Delta_\omega(A) \cdot \Delta_\omega(B) \geq \frac{1}{2}|\omega([A,B])|$$

where

$$[A,B] := AB - BA\,.$$

Proof: For simplicity consider A and B such that $\omega(A) = \omega(B) = 0$ and let $C_\lambda := A - i\lambda B$, $\lambda \in \mathbb{R}$. Then, the positivity of ω implies

$$0 \leq \omega(C_\lambda^* C_\lambda) = \omega(A^2) + \lambda^2\omega(B^2) + i\lambda\omega([A,B])\,, \quad \forall\lambda \in \mathbb{R}$$

i.e.

$$\Delta_\omega(A) \cdot \Delta_\omega(B) \geq \frac{1}{2}|\omega([A,B])|\,.$$

Representations provide concrete realizations of C^*-algebras and also allow the implementation of the superposition principle of wave mechanics

Definition

A representation $(\mathcal{A}, \varrho, \mathfrak{H})$, or simply ϱ, of a C^*-algebra $\mathcal{A}$ in a Hilbert space $\mathfrak{H}$ is a $*$-homomorphism ϱ of $\mathcal{A}$ into the C^*-algebra $\mathcal{B}(\mathfrak{H})$ of bounded linear operators in $\mathfrak{H}$

We will be interested in faithful and irreducible representations:

- ϱ is faithful if $ker(\varrho) = \{0\}$
- ϱ is irreducible if $\{0\}$ and $\mathfrak{H}$ are the only closed subspaces invariant under $\varrho(\mathcal{A})$

Theorem (Gelfand-Naimark)

A C^*-algebra is isomorphic to an algebra of bounded operators in a Hilbert space

Theorem

(Gelfand-Naimark-Segal) *Given a C^*-algebra $\mathcal{A}$ with identity and a state ω, there is a Hilbert space $\mathfrak{H}_\omega$ and a representation*

$$\varrho_\omega : \mathcal{A} \to \mathcal{B}(\mathfrak{H})$$

such that
1. $\mathfrak{H}_\omega$ contains a cyclic vector ψ_ω (i.e. $\overline{\varrho(\mathcal{A})\psi_\omega} = \mathfrak{H}_\omega$)
2. $\omega(A) = \langle \psi_\omega \,|\, \varrho_\omega(A)\psi_\omega \rangle$ for all $A \in \mathcal{A}$
3. every other representation ϱ in a Hilbert space $\mathfrak{H}$ with a cyclic vector ψ such that

$$\omega(A) = \langle \psi \,|\, \varrho(A)\psi \rangle \quad \forall A \in \mathcal{A}$$

is unitarily equivalent to ϱ_ω, i.e. there exists an isometry $U : \mathfrak{H} \to \mathfrak{H}_\omega$ such that $U\psi = \psi_\omega \,, \quad U\varrho(A)U^{-1} = \varrho_\omega(A)$ for all $A \in \mathcal{A}$

- Given $(\mathcal{A}, \varrho, \mathfrak{H})$, the *unit* vectors $\psi \in \mathfrak{H}$ define states ω_ψ on $\mathcal{A}$:

$$\omega_\psi(A) := \langle \psi \,|\, \varrho(A)\psi \rangle \,, \quad \langle \psi \,|\psi \rangle = 1$$

  These states are called **state vectors** of the representation
- The converse is also true (GNS theorem). However, if a state is not pure, the representation $(\mathfrak{H}_\omega, \varrho_\omega, \psi_\omega)$ is reducible

Theorem. Let ω a state over the C^*-algebra $\mathcal{A}$ and $(\mathfrak{H}_\omega, \varrho_\omega, \psi_\omega)$ the associate cyclic representation. Then $(\mathfrak{H}_\omega, \varrho_\omega, \psi_\omega)$ is irreducible iff ω is pure

- Given a positive trace class operator b on $\mathfrak{H}$ with trace equal to one

$$\omega_b(A) := \mathrm{tr}(b\varrho(A))$$

  is a state over $\mathcal{A}$. These states are called **density matrices**

Notice that ω_b is of the form $\omega_b(A) = \sum_i \lambda_i \langle \psi_i \,|\, \varrho(A)\psi_i \rangle \,, \lambda_i \geq 0 \,, \sum_i \lambda_i = 1 \,,$ $\langle \psi_i \,|\, \psi_i \rangle = 1$. Then ω_b is a pure state iff b is a one dimensional projection

abstract special Segal's system:

- A physical system is defined by its C^*-algebra $\mathcal{A}$ with identity $\mathbf{1}$
- The states $\mathcal{S}$ are normalized positive linear functionals that separates the observables

For a given irreducible representation $(\mathcal{A}, \varrho, \mathfrak{H})$

representations of special Segal's system:

- Observables are bounded self-adjoint operators on $\mathfrak{H}$
- Vector states $\psi \in \mathfrak{H}$, $||\psi|| = 1$, define pure states

How can we describe specific Quantum Systems?

Usually one begins with a certain Classical System and follows some kind of ‘quantization procedure’

Dirac’s quantum conditions

There exists a map $\hat{}\;:\mathcal{O}_{\text{classical}} \subset C^\infty(T^*\mathcal{C};\mathbb{R}) \to \mathcal{O}_{\text{quantum}}$ such that

- $A \mapsto \hat{A}$ is linear over $\mathbb{R}$
- If A is a constant function, then $\hat{A}$ is the corresponding multiplication operator
- If $\{A_1, A_2\} = A_3$ then $[\hat{A}_1, \hat{A}_2] = -i\hbar\hat{A}_3$ (notice that $\mathcal{O}_{\text{classical}}$ must be closed under $\{\cdot, \cdot\}$). **The commutator is the quantum analogue of the classical Poisson bracket**

The quantum particle: Heisenberg algebra

The simplest example of a physical system is the quantum particle

How can one construct a C^*-algebra for the quantum particle?

Heisenberg Lie algebra: The basic 'observables' are position X and momentum $P = P_X$ so, naively, one can try to consider the algebra of observables generated by X and P which satisfy the Heisenberg commutation relations ($\hbar = 1$)

$$[P, X] = i\,, \quad [X, X] = 0\,, \quad [P, P] = 0$$

However, the Heisenberg algebra does not fall into the Segal scheme: X and P cannot be self-adjoint elements of any C^*-algebra because $||X||$ and $||P||$ cannot both be finite (X and P are not observables in the operational sense)

$$[P, X^n] = -inX^{n-1} \Rightarrow ||X||||P|| \geq n/2\,, \quad \forall n \in \mathbb{N}$$

Consider the polynomial algebra generated by

$$U(\alpha) = \exp(i\alpha X)\,, \quad V(\beta) = \exp(i\beta P)$$

Weyl algebra: The Weyl algebra is generated (trough complex linear combinations and products) by the elements $U(\alpha)$ and $V(\beta)$, where α, $\beta \in \mathbb{R}$, satisfy

- $U(\alpha_1)U(\alpha_2) = U(\alpha_1 + \alpha_2)\,, V(\beta_1)V(\beta_2) = V(\beta_1 + \beta_2)\,,$
  $U(\alpha)V(\beta) = V(\beta)U(\alpha)\exp(-i\alpha\beta)\,.$
- $U(0) = V(0) = \mathbf{1}$
- $U(\alpha)^* = U(-\alpha)\,, \quad V(\beta)^* = V(-\beta)$
- $U(\alpha)^*U(\alpha) = U(\alpha)U(\alpha)^* = \mathbf{1} = V(\beta)^*V(\beta) = V(\beta)V(\beta)^*$
- $||U(\alpha)|| = ||V(\beta)|| = ||U(\alpha)V(\beta)|| = 1$ (these fix the norm of any complex linear combinations and products of U's and $V's$)

Weyl C^*-algebra $\mathcal{A}_{\text{Weyl}}$ is the $||\cdot||$-completion of the Weyl algebra

The quantum particle is the physical system characterized by $\mathcal{A}_{\text{Weyl}}$

The classification of the representations of $\mathcal{A}_{\text{Weyl}}$ is solved by the following theorem due to von Neumann

Theorem (von Neumann)

All the regular irreducible representations of $\mathcal{A}_{\text{Weyl}}$ in separable Hilbert spaces are unitarily equivalent

Here 'regular' means that $\varrho(U(\alpha))$ and $\varrho(V(\beta))$ are strongly continuous in α and β respectively.

Scrödinger representation

Schrödinger representation $(\mathcal{A}_{\mathrm{Weyl}}, \varrho, \mathfrak{H})$ is a regular irreducible representation of $\mathcal{A}_{\mathrm{Weyl}}$ in the separable Hilbert space $\mathfrak{H} = L^2(\mathbb{R})$

Denoting $\hat{U}(\alpha) := \varrho(U(\alpha))$ and $\hat{V}(\beta) := \varrho(V(\beta))$, the representation is defined by

$$(\hat{U}(\alpha)\psi)(x) := e^{i\alpha x}\psi(x)\,, \quad (\hat{V}(\beta)\psi)(x) := \psi(x+\beta)\,, \quad \forall \psi \in \mathfrak{H}$$

By using the Stone theorem, the Schrödinger representation provides also a representation of the Heisenberg algebra

$$(\hat{X}\psi)(x) = x\psi(x)\,, \quad \mathcal{D}(\hat{X}) = \{\psi \,|\, \int_{\mathbb{R}} |x\psi(x)|^2 \,\mathrm{d}x < \infty\}$$

$$(\hat{P}\psi)(x) = i\psi'(x)\,, \quad \mathcal{D}(\hat{P}) = \{\psi \,|\, \psi \text{ is abs. cont. and } \int_{\mathbb{R}} |\psi'(x)|^2 \,\mathrm{d}x < \infty\}$$

Notice that the position operator acts as a multiplicative operator whereas momentum operator acts as a derivative operator over the vector states of the Schrödinger representation

SCRÖDINGER REPRESENTATION ON $\mathcal{C}$

Given an orientable configuration space $\mathcal{C}$ choose a Riemannian metric g_{ab}, with conection ∇_a and canonical volume-form ϵ, and let $\mathfrak{H} = L^2(\mathcal{C}, \epsilon)$

$$\langle \psi_1 \,|\, \psi_2 \rangle := \int_{\mathcal{C}} \overline{\psi}_1 \psi_2 \, \epsilon \,, \quad \psi_1, \psi_2 \in \mathfrak{H}$$

We can define (densely) configuration and momentum operators

$$\begin{aligned} \hat{Q}(f)\psi &:= f\psi \\ \hat{P}(v)\psi &:= -i\hbar\Big(\mathcal{L}_v\psi + \frac{1}{2}(\mathrm{div}_\epsilon(v))\psi\Big) \end{aligned}$$

These operators satisfy the canonical commutation relations

$$[\hat{Q}(f_1), \hat{Q}(f_2)] = 0,\ [\hat{Q}(f), \hat{P}(v)] = i\hbar\hat{Q}(\mathcal{L}_v f),\ [\hat{P}(v_1), \hat{P}(v_2)] = -i\hbar\hat{P}(\mathcal{L}_{v_1} v_2)$$

Notice that there is a correspondence between the Poisson algebra of the classical configuration and momentum observables and the Lie algebra (under $[\cdot,\cdot]$) of these quantum operators

$$\{Q(f_1),Q(f_2)\}=0,\ \{Q(f),P(v)\}=Q(\mathcal{L}_v f),\ \{P(v_1),P(v_2)\}=-P(\mathcal{L}_{v_1}v_2)$$
$$[\hat{Q}(f_1),\hat{Q}(f_2)]=0,\ [\hat{Q}(f),\hat{P}(v)]=i\hbar\hat{Q}(\mathcal{L}_v f),\ [\hat{P}(v_1),\hat{P}(v_2)]=-i\hbar\hat{P}(\mathcal{L}_{v_1}v_2)$$

For the class of configuration and momentum observables (and only for this class) the correspondence is given by

$$[A,B]=i\hbar\widehat{\{A,B\}}$$

For a large class of classical mechanical systems on $\mathcal{C}$ the classical Hamiltonian takes the form

$$H(q,p_a)=\frac{1}{2}g^{ab}(q)p_a p_b+v^a(q)p_a+V(q)\,.$$

For this it class is natural to identify the 'quantum Hamiltonian' (up to Ricci curvature terms of g_{ab}) as

$$\hat{H}\psi=-\frac{\hbar^2}{2}g^{ab}\nabla_a\nabla_b\psi-i\Big(\mathcal{L}_v\psi+\frac{1}{2}(\mathrm{div}_\epsilon(v))\psi\Big)+V\psi$$

We are now interested in describing the relations between measurements at different times for non-dissipative systems. In this case it it plausible to demand the following

- The relations between the measurements at times t_1 and t_2 depends only on the difference $t_2 - t_1$
- If an observable A is defined by some experimental device at a given time, say $t = 0$, the same type of measurements performed at time t defines an observable A_t
- The algebra $\mathcal{A}$ generated by the observables is the same at any time
- The time translation $A \mapsto \alpha_t(A) = A_t$ is a $*$-automorphism (preserves the algebraic properties)
- For any state ω and any observable A, the real function $t \mapsto \omega(\alpha_t(A))$ is a continuous function

Algebraic Dynamical Systems

A dynamical system is a triplet

$$(\mathcal{A}, \mathbb{R}, \alpha)$$

where $\mathcal{A}$ is a C^*-algebra and, for each $t \in \mathbb{R}$, α_t is an automorphism of $\mathcal{A}$ and α satisfies

- $\alpha_0 = \mathrm{id}\,, \quad \alpha_{t_1} \circ \alpha_{t_2} = \alpha_{t_1+t_2}$
- α is weakly continuous i.e. $t \mapsto \omega(\alpha_t(A))$ is continuous $\forall \omega$ and A

Given a representation $(\mathcal{A}, \varrho, \mathcal{H})$ of the C^*-algebra of observables we will say that ϱ is **stable under the evolution** α_t if ϱ and $\varrho \circ \alpha_t$ are unitarily equivalent. In other words

$$\varrho(\alpha_t(A)) = \hat{U}^{-1}(t)\varrho(A)\hat{U}(t)\,, \quad \forall A \in \mathcal{O}$$

for some unitary operator

$$\hat{U}(t) : \mathfrak{H} \to \mathfrak{H}\,.$$

The weak continuity of α_t implies the weak continuity of $\hat{U}(t)$. Then applying Stone's theorem we have

$$\hat{U}(t) = \exp(-it\hat{H})\,, \quad \forall t \in \mathbb{R}$$

for some self-adjoint operator $\hat{H}$, with dense domain $\mathcal{D}(\hat{H}) \subset \mathfrak{H}$

- $\hat{H}$ is called the Quantum Hamiltonian (in the representation ϱ)
- The Hamiltonian *is* a representation dependent concept. In general it is also an unbounded operator and does not belong to the C^*-algebra generated by $\mathcal{O}$.

Let ψ_0 a vector state of a stable representation. Then

$$\omega_0(\alpha_t(A)) = \langle \psi_0 \,|\, \hat{U}(t)^{-1} \varrho(A) \hat{U}(t) \psi_0 \rangle = \langle \hat{U}(t)\psi_0 \,|\, \varrho(A) \hat{U}(t) \psi_0 \rangle = \omega_t(A)$$

where ω_t is the pure state defined by

$$\psi(t) := \hat{U}(t)\psi_0 \in \mathfrak{H}$$

By choosing $\psi_0 \in \mathcal{D}(\hat{H})$, we can differentiate $\psi(t)$ with respect to t to get the Schrödinger equation

Schrödinger equation

The Scrödinger equation is the time evolution equation for pure states

$$i\frac{\mathrm{d}\psi}{\mathrm{d}t} = \hat{H}\psi\,, \quad \psi(0) = \psi_0 \in \mathcal{D}(\hat{H})\,.$$

where $\hat{H}$ is the (self-adjoint) quantum Hamiltonian of the system

Heisenberg equation

The evolution can be equivalently formulated in terms of observables. Given an observable represented by

$$\hat{A}_0 := \varrho(A_0)$$

and defining

$$\hat{A}(t) := U(t)^{-1}\hat{A}_0 U(t)\,,$$

we get the Heisenberg equation:

Heisenberg equation

The evolution equation for an observable (in a certain representation) is

$$\frac{\mathrm{d}\hat{A}}{\mathrm{d}t} = i[\hat{H},\hat{A}]\,, \quad A(0) = A_0 \in \mathcal{B}(\mathfrak{H})$$

For the Scrhödinger representation, given a Hamiltonian $\hat{H}$, the Heisenberg equations are the analog of the classical Hamilton equations:

$$\dot{\hat{X}} = i[\hat{H}, \hat{X}]\,, \quad \dot{\hat{P}} = i[\hat{H}, \hat{P}]$$

In particular, for the class of Hamiltonians

$$\hat{H} = H(\hat{X}, \hat{P})\,, \text{ where } H(X, P) = \frac{P^2}{2} + V(X)$$

these are (formally)

Heisenberg equations for a particle in a potential

$$\begin{aligned} \dot{\hat{X}} &= \frac{\partial H}{\partial P}(\hat{X}, \hat{P}) = \hat{P}\,, \\ \dot{\hat{P}} &= -\frac{\partial H}{\partial X}(\hat{X}, \hat{P}) = V'(\hat{X}) \end{aligned}$$

Is the ‘quantum Hamiltonian’

$$\hat{H} = \frac{\hat{P}^2}{2} + V(\hat{X})$$

well defined in the Schrödinger representation?

It is easy to show that $\frac{1}{2}\hat{P}^2 + V(\hat{X})$ defines a symmetric operator… but symmetric operators have several or none self-adjoint extensions!!

The taste of Kato’s theorems: For a potential V in a Kato class, the Cauchy problem for the Scrödinger equation

$$i\frac{\partial \psi}{\partial t}(x,t) = -\frac{1}{2}\frac{\partial^2 \psi}{\partial x^2}(x,t) + V(x)\psi(x,t)$$
$$\psi(x,0) = \psi_0(x) \in \mathcal{D}(\hat{P}^2)$$

is well possed and the corresponding Cauchy problem has a unique solution global in time.

SUMMARY

We have provided a description of Quantum Mechanics in which, for systems whose classical configuration space $\mathcal{C}$ is finite dimensional

- Physical observables can be represented as bounded self-adjoint operators $\hat{A}$ in the Schrödinger representation on $L^2(\mathcal{C}, \epsilon)$
- Canonical variables do not commute. They cannot be simultaneously measured
- Pure states are vector states $\psi \in L^2(\mathcal{C}, \epsilon)$, $||\psi|| = 1$
- In contrast with classical mechanics, the observables do not have well-defined values on pure states

When $\mathcal{C}$ is infinite dimensional there are important differences

- The Schrödinger representation cannot be defined on $\mathcal{C}$ but on a more general space $L^2(\overline{\mathcal{C}}, \mathrm{d}\mu)$
- The von Neumann uniqueness theorem cannot be applied. In fact, one usually finds an infinite number of inequivalent representations of the C^*-algebra of elementary variables. In this case, some additional input is needed to fix a representation (symmetries can be used for this)

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