SHORT DESCRIPTION OF THE MATHEMATICAL FORMALISM OF QUANTUM MECHANICS

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1. States

Let $\mathcal{H}$ be a complex Hilbert space. The *projectivization* of $\mathcal{H}$ is the quotient:

$$(\mathcal{H} \setminus \{0\})/\sim \tag{1}$$

where the equivalence relation $\sim$ is defined by:

$$\psi_1 \sim \psi_2 \Longleftrightarrow \text{there exists } c \in \mathbb{C} \text{ with } \psi_2 = c\psi_1,$$

for all $\psi_1, \psi_2 \in \mathcal{H} \setminus \{0\}$. The projectivization of $\mathcal{H}$ plays in the formalism of Quantum Mechanics the role that the phase space (the symplectic manifold) plays in Classical Mechanics. An element of the projectivization of $\mathcal{H}$ will be called a *state*. In practice, to avoid dealing with equivalence classes, we will simply call any nonzero element of $\mathcal{H}$ a state and if $\psi_2 = c\psi_1$ we say that ψ_1 and ψ_2 define the same state. We will usually assume, without loss of generality, that states ψ are *normalized*, i.e., $\|\psi\| = 1$ (notice that ψ is identified with $\frac{\psi}{\|\psi\|}$ in (1)).

2. Dynamics

In Classical Mechanics the dynamics is governed by the *Hamiltonian* which is a smooth real-valued function on phase space. In Quantum Mechanics the dynamics is governed by a (possibly unbounded) self-adjoint operador H on $\mathcal{H}$ which we also call the *Hamiltonian* (or *Hamiltonian operator*). The dynamics is given by *Schrödinger's equation*:

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\,\psi_t = H\psi_t, \quad t \in \mathbb{R},$$

where $\hbar = \frac{h}{2\pi}$ is Dirac's constant, h is Planck's constant and $t \mapsto \psi_t$ is a curve in $\mathcal{H}$. More precisely, the dynamics is given by:

$$\psi_t = U_t\psi_0, \quad t \in \mathbb{R},$$

where $t \mapsto U_t$ is a (strongly continuous) one-parameter group of unitary operators given by:

$$U_t = \exp(-\tfrac{i}{\hbar}tH), \quad t \in \mathbb{R}.$$

Observe that if ψ_0 is normalized then ψ_t is also normalized, for all t.

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3. Observables

In Classical Mechanics, a *observable* is normally regarded as a real-valued function on phase space[1]. In Quantum Mechanics, observables are associated to (possibly unbounded) self-adjoint operators on the Hilbert space $\mathcal{H}$. Assume that the state of the system is given by a unit vector $\psi \in \mathcal{H}$. Let A be a self-adjoint operator corresponding to some observable[2]. First, let us assume that the spectrum:

$$\sigma(A) = \big\{\lambda \in \mathbb{C} : \lambda - A \text{ is not invertible}\big\}$$

is discrete. Observe that, since A is self-adjoint, $\sigma(A)$ is a subset of $\mathbb{R}$. Since $\sigma(A)$ is discrete, every $\lambda \in \sigma(A)$ is an eigenvalue of A and $\mathcal{H}$ is the closure of the orthogonal direct sum of the eigenspaces $\mathrm{Ker}(A-\lambda)$, $\lambda \in \sigma(A)$. Denote by P_λ the orthogonal projection onto $\mathrm{Ker}(A-\lambda)$. If we measure the observable A, the result is always an eigenvalue λ of A; the probability that the result of the measurement is λ is equal to[3]:

$$\langle P_\lambda \psi, \psi\rangle = \|P_\lambda \psi\|^2. \tag{2}$$

The equality is justified by the fact that P_λ is idempotent and self-adjoint. Notice that:

$$\sum_{\lambda\in\sigma(A)} \|P_\lambda \psi\|^2 = \|\psi\|^2 = 1.$$

The *expected value* of A is obtained by averaging the eigenvalues $\lambda \in \sigma(A)$ by the corresponding probabilities:

$$\sum_{\lambda\in\sigma(A)} \lambda\, \langle P_\lambda \psi, \psi\rangle = \langle A\psi, \psi\rangle,$$

since:

$$A\psi = \sum_{\lambda\in\sigma(A)} \lambda\, P_\lambda \psi.$$

More generally, given any function $f : \mathbb{R} \to \mathbb{R}$, the expected value of $f(A)$ is given by:

$$\sum_{\lambda\in\sigma(A)} f(\lambda)\langle P_\lambda \psi, \psi\rangle = \langle f(A)\psi, \psi\rangle,$$

where:

$$f(A)\psi = \sum_{\lambda\in\sigma(A)} f(\lambda) P_\lambda \psi,$$

[1] Typical examples are: some coordinate of the position of some particle, some coordinate of the momentum of some particle, some coordinate of the angular momentum of some particle, some coordinate of the total momentum of the system, the total energy of the system (which is just the Hamiltonian), etc.

[2] We will deal later with the problem of figuring out what operator corresponds to what observable.

[3] Notice that if we replace ψ with $c\psi$, where $c \in \mathbb{C}$, $|c| = 1$, then $\langle P_\lambda \psi, \psi\rangle$ does not change. So, the probability actually depends only on the equivalence class of ψ in (1).

for all $\psi \in \mathcal{H}$ for which:

$$\sum_{\lambda\in\sigma(A)} |f(\lambda)|^2 \|P_\lambda\psi\|^2 < +\infty.$$

If ψ is the state of the system before the measurement and if the result of the measurement of A is an eigenvalue λ then, after the measurement, the state *collapses* to:

$$\frac{P_\lambda\psi}{\|P_\lambda\psi\|}.$$

Now, let us deal with an arbitrary self-adjoint operator A. Given a normalized state $\psi \in \mathcal{H}$ (the state of the system before measurement), we have a Borel probability measure $\mathbb{P}_A^\psi$ in $\mathbb{R}$ defined by:

$$\mathbb{P}_A^\psi(B) = \langle \chi_B(A)\psi, \psi\rangle = \|\chi_B(A)\psi\|^2, \tag{3}$$

for every Borel subset B of $\mathbb{R}$, where $\chi_B : \mathbb{R} \to \{0, 1\}$ denotes the characteristic function of B. We are using here the *Borel functional calculus* that associates a bounded operator $f(A)$ to every bounded Borel measurable function $f : \mathbb{R} \to \mathbb{C}$. Notice that if A has discrete spectrum and $\lambda \in \sigma(A)$ then $\chi_{\{\lambda\}}(A)$ equals the orthogonal projection onto $\mathrm{Ker}(A - \lambda)$ and (3) agrees with (2). We have:

$$\mathbb{P}_A^\psi\big(\sigma(A)\big) = 1,$$

since $\chi_{\sigma(A)}(A)$ is the identity map. The expected value of A is given by the integral:

$$\int_{\mathbb{R}} \lambda \,\mathrm{d}\mathbb{P}_A^\psi(\lambda) = \langle A\psi, \psi\rangle.$$

More generally, if $f : \mathbb{R} \to \mathbb{R}$ is a Borel measurable function then the expected value of $f(A)$ is given by:

$$\int_{\mathbb{R}} f(\lambda) \,\mathrm{d}\mathbb{P}_A^\psi(\lambda) = \langle f(A)\psi, \psi\rangle.$$

We can also consider a more general notion of observable: observables whose values are not real numbers (in Classical Mechanics, they would correspond to not necessarily real-valued maps defined on phase space). The formal definition is as follows: let $(S, \mathcal{A})$ be a measurable space, i.e., S is a set and $\mathcal{A}$ is a σ-algebra of subsets of S. We call the elements of $\mathcal{A}$ the *measurable* subsets of S. Recall that a *projection valued measure* (PVM) on $(S, \mathcal{A})$ is a map:

$$\mathbb{P} : S \longrightarrow \mathcal{B}(\mathcal{H}),$$

where $\mathcal{B}(\mathcal{H})$ is the space of bounded operators on $\mathcal{H}$, satisfying the following conditions:

(a) for every $B \in \mathcal{A}$, $\mathbb{P}(B)$ is an orthogonal projection of $\mathcal{H}$ (i.e., an idempotent bounded self-adjoint operator);
(b) $\mathbb{P}(S)$ is the identity map;

(c) $\mathbb{P}$ is σ-additive with respect to the strong operator topology, i.e., given a sequence $(B_n)_{n\geq 1}$ of pairwise disjoint measurable subsets of S then:

$$\mathbb{P}(B)\psi = \sum_{n=1}^{\infty} \mathbb{P}(B_n)\psi,$$

for all $\psi \in \mathcal{H}$, where $B = \bigcup_{n=1}^{\infty} B_n$.

A PVM on $(S, \mathcal{A})$ will be called an *S-valued observable*. Given a normalized state $\psi \in \mathcal{H}$, we therefore get a probability measure:

$$\mathbb{P}^{\psi} : \mathcal{A} \longrightarrow [0, 1]$$

on $(S, \mathcal{A})$ given by:

$$\mathbb{P}^{\psi}(B) = \langle \mathbb{P}(B)\psi, \psi \rangle = \|\mathbb{P}(B)\psi\|^2,$$

for all $B \in \mathcal{A}$.

Notice that if A is a self-adjoint operator on $\mathcal{H}$ then $\mathbb{P}_A(B) = \chi_B(A)$ defines a PVM on $\mathbb{R}$ (endowed with the Borel σ-algebra) and that $A \mapsto \mathbb{P}_A$ is actually a bijection between self-adjoint operators on $\mathcal{H}$ and PVMs on $\mathbb{R}$. Therefore, observables with values in $\mathbb{R}$ are identified with self-adjoint operators. There is also a natural bijection between $\mathbb{R}^n$-valued observables and n-tuples of mutually commuting self-adjoint operators on $\mathcal{H}$.

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