# Summary of Quantum Mechanics



1 author:

Gennaro Auletta
Università degli studi di Cassino e del Lazio Meridionale

# Summary of Quantum Mechanics

*Gennaro Auletta*

Quantum mechanics is based on three fundamental theoretical entities:

- **States**: they are conventionally symbolized as $|\psi\rangle, |\phi\rangle, \ldots$ and called *kets*. The scalar product between $|\psi\rangle$ and $|\phi\rangle$ is indicated by

$$\langle \psi \,|\, \phi \rangle = \langle \phi \,|\, \psi \rangle^* \ . \tag{1}$$

The dual $\langle \psi | = |\psi\rangle^\dagger$ is its transposed complex conjugated vector called a *bra*. Kets and bras constitute what is know as the Dirac's algebra. States are taken as normal (their norm is =1). Any quantized state $|\psi\rangle$ can be expanded thanks to an orthonormal basis $\{|b_j\rangle\}$ in a Hilbert space with a certain dimension $n$:

$$\begin{aligned} |\psi\rangle &= \sum_{j=1}^{n} c_j \,|b_j\rangle \\ &= \sum_{j=1}^{n} \langle b_j \,|\, \psi\rangle \,|b_j\rangle \ , \end{aligned} \tag{2}$$

where the $c_j$'s are (in general complex) coefficients called *probability amplitudes*. A basis is orthonormal if

$$\forall j, \langle b_j \,|\, b_j \rangle = 1 \text{ and } \forall\, j \neq k, \langle b_j \,|\, b_k \rangle = 0.$$

It is said that the state $|\psi\rangle$ above represents a *superposition* of kets $|b_j\rangle$. The vectors constituting the basis can be written:

$$|b_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \ldots \\ 0 \end{pmatrix} , \ |b_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \ldots \\ 0 \end{pmatrix} , \ |b_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ \ldots \\ 0 \end{pmatrix} , \ \ldots, \ |b_n\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \ldots \\ 1 \end{pmatrix} ,$$

so that we can write

$$|\psi\rangle = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \ldots \\ c_n \end{pmatrix} \tag{3}$$

The explicit vectorial forms of the bras are written in terms of row vectors instead of columnar ones. The square modulus of any of the coefficients, e.g.

$$|c_j|^2 = |\langle b_j \,|\, \psi\rangle|^2 = \langle b_j \,|\, \psi\rangle \langle \psi \,|\, b_j\rangle = \wp_j \tag{4}$$

gives the probability $\wp_j$ to get the component $|b_j\rangle$ when a system in the state $|\psi\rangle$ is measured. I recall that probabilities are normalized.

In the case in which the expansion of the state is continuous (paramountly a free particle), we need to substitute the sum with an integral:

$$|\psi\rangle = \int c(j)\,|j\rangle\, dj. \tag{5}$$

In such a case we have to replace the notion of probability with that of probability density.

States can be operationally understood as equivalence classes of *preparations* (representing the first stage of a measurement process). For instance, a photon can be prepared in a state of linear polarization by either (i) symmetrically superposing two photons, the one in a vertical polarization state and the other in a horizontal polarization state, or (ii) letting a photon in an arbitrary polarization state pass a polarization filter at 45° (in such a case a part of the photons will be eliminated).

- **Observables**: The observables $\hat{O}$ are the degrees of freedom of a system. They are represented by matrices and are therefore called q-numbers for differentiating them from ordinary scalar numbers. Moreover, any observable needs to be represented by a Hermitian operator, i.e. $\hat{O} = \hat{O}^\dagger$, where $\hat{O}^\dagger$ is the conjugate transposed matrix of $\hat{O}$ (we take the complex conjugate of each element $o_{jk}$ and interchange columns and rows). The reason is that the eigenvalues of a Hermitian operator are real and not complex numbers. In the $n$–dimensional space, an observable $\hat{O}$ can be written as:

$$\hat{O} = \begin{bmatrix} o_1 & 0 & \dots & 0 \\ 0 & o_2 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & o_n \end{bmatrix}, \tag{6}$$

where the $o_1, o_2, \dots, o_n$ are the *eigenvalues* of $\hat{O}$, so that they satisfy the eigenvalues equation

$$\hat{O}\,|o_j\rangle = o_j\,|o_j\rangle \ . \tag{7}$$

The eigenvalue $o_j$ is that (real or rational) number that we get on a graduate scale of an apparatus when measuring the observable $\hat{O}$ and having $|o_j\rangle$ as an outcome. The $|o_j\rangle$ are called eigenvectors of $\hat{O}$ and constitute another orthonormal basis, i.e. $\forall\,|\psi\rangle$ of dimension $n$ we can write

$$\begin{aligned} |\psi\rangle &= \sum_{j=1}^{n} \eta_j\,|o_j\rangle \\ &= \sum_{j=1}^{n} \langle o_j\,|\,\psi\rangle\,|o_j\rangle\ , \end{aligned} \tag{8}$$

where the $\eta_j = \langle o_j\,|\,\psi\rangle$ are again probability amplitudes. We can pass to one basis to another thanks to the following transformations:

$$\langle o_1\,|\,\psi\rangle = (\langle o_1\,|\,b_1\rangle\,\langle b_1| + \langle o_1\,|\,b_2\rangle\,\langle b_2| + \ldots + \langle o_1\,|\,b_n\rangle\,\langle b_n|)\,|\psi\rangle\ , \tag{9a}$$
$$\langle o_2\,|\,\psi\rangle = (\langle o_2\,|\,b_1\rangle\,\langle b_1| + \langle o_2\,|\,b_2\rangle\,\langle b_2| + \ldots + \langle o_2\,|\,b_n\rangle\,\langle b_n|)\,|\psi\rangle\ , \tag{9b}$$
$$\ldots = \ldots$$
$$\langle o_n\,|\,\psi\rangle = (\langle o_n\,|\,b_1\rangle\,\langle b1| + \langle o_n\,|\,b_2\rangle\,\langle b_2| + \ldots + \langle o_n\,|\,b_n\rangle\,\langle b_n|)\,|\psi\rangle\ . \tag{9c}$$

These transformations can be written in a compact form as:

$$\begin{pmatrix} \langle o_1\,|\,\psi\rangle \\ \langle o_2\,|\,\psi\rangle \\ \ldots \\ \langle o_n\,|\,\psi\rangle \end{pmatrix} = \begin{bmatrix} \langle o_1\,|\,b_1\rangle & \langle o_1\,|\,b_2\rangle & \ldots & \langle o_1\,|\,b_n\rangle \\ \langle o_2\,|\,b_1\rangle & \langle o_2\,|\,b_2\rangle & \ldots & \langle o_2\,|\,b_n\rangle \\ \ldots & \ldots & \ldots & \ldots \\ \langle o_n\,|\,b_1\rangle & \langle o_n\,|\,b_2\rangle & \ldots & \langle o_n\,|\,b_n\rangle \end{bmatrix} \begin{pmatrix} \langle b_1\,|\,\psi\rangle \\ \langle b_2\,|\,\psi\rangle \\ \ldots \\ \langle b_n\,|\,\psi\rangle \end{pmatrix} \tag{10}$$

where the matrix

$$\hat{U} = \begin{bmatrix} \langle o_1\,|\,b_1\rangle & \langle o_1\,|\,b_2\rangle & \ldots & \langle o_1\,|\,b_n\rangle \\ \langle o_2\,|\,b_1\rangle & \langle o_2\,|\,b_2\rangle & \ldots & \langle o_2\,|\,b_n\rangle \\ \ldots & \ldots & \ldots & \ldots \\ \langle o_n\,|\,b_1\rangle & \langle o_n\,|\,b_2\rangle & \ldots & \langle o_n\,|\,b_n\rangle \end{bmatrix} \tag{11}$$

represents a *unitary* operator. Unitary operators express in quantum mechanics the concept of reversible transformations. They owe their name to the property

$$\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = \hat{I}\ , \tag{12}$$

where $\hat{U}^\dagger$ is the conjugate transposed matrix of $\hat{U}$ and $\hat{I}$ is the identity matrix, i.e. the matrix that induces no transformation of the vectors and is the diagonal sum of all 1s (all other elements are 0):

$$\hat{I} = \begin{bmatrix} 1 & 0 & \ldots & 0 \\ 0 & 1 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & \ldots & 1 \end{bmatrix}\ . \tag{13}$$

Operationally speaking, an observable can be defined as an equivalence class of premeasurements (the second step of the measurement process). In fact, we can perform the same kind of experiment and decide to measure the path followed by the particle by either (i) choosing an interferometer (a device for splitting e.g. light beams) or (ii) performing a so-called double-slit experiment (we let a beam of particles or photons go to both or one of two slits on a screen or wall). In this step we couple (through an unitary transformation) an apparatus with an object system and in such a way we select a specific degree of freedom. In fact, when choosing to measure $\hat{O}$, we have

$$\hat{U}\left(|\psi\rangle\,|A_0\rangle\right) \;=\; \sum_j \xi_j\,|o_j\rangle\,|a_j\rangle\ , \tag{14}$$

where the $\xi_j$'s are some coupling constants, the apparatus is assumed to be in an initial (ready) state $|A_0\rangle$ but after the coupling is expanded in the basis $\{|a_j\rangle\}$ that is correlated with the basis $\{|o_j\rangle\}$. In fact, the two systems, as the result of this unitary transformation, are said to be *entangled*, that is, they are in a state that is no longer factorable (it cannot be written as product of two separated expansions). A factorable state in the simple case of two dimensions is:

$$|o_1\rangle\,|a_1\rangle + |o_2\rangle\,|a_2\rangle + |o_1\rangle\,|a_2\rangle + |o_2\rangle\,|a_1\rangle = \left(|o_1\rangle + |o_2\rangle\right)\left(|a_1\rangle + |a_2\rangle\right)\ . \tag{15}$$

- **Properties**: Properties are assigned to quantum systems when certain detection event occur. Detections represent the third and final step of a measurement process, so that the whole process can be understood as a sequence of (i) preparing a system with a certain information variety, (ii) establish a mutual information between apparatus and a system, and finally (iii) selecting a specific output, where this output itself cannot be controlled. In other words, we get say the eigenvalue $o_j$ when the object system is collapsed into the state $|o_j\rangle$. In fact, the latter is only one of the possible components of the state (8). We represent this component (and therefore the relative property) by means of another operator called projector that has the peculiarity of having only a single 1 on the diagonal correspond into that component, otherwise we have all 0s. Supposing that e.g. this component is $|o_1\rangle$, we have

$$\begin{aligned} \hat{P}_1 = |o_1\,\rangle\,\langle o_1\,| \;&=\; \begin{pmatrix} 1 \\ 0 \\ \dots \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & \dots & 0 \end{pmatrix} \\ &=\; \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 0 \end{bmatrix}, \end{aligned} \tag{16}$$

and similarly for the other components. The algebraic form that a projector takes is

$$\hat{P}_k = |o_k\,\rangle\,\langle o_k\,| \ , \tag{17}$$

which when applied to an arbitrary state $|\psi\rangle$ immediately shows its selective effect:

$$\begin{aligned} \hat{P}_k\,|\psi\rangle &= |o_k\,\rangle\,\langle o_k\,| \left(\sum_j \eta_j\,|o_j\rangle\right) \\ &= \eta_k\,|o_k\rangle \ , \end{aligned} \tag{18}$$

thanks to the properties of the scalar product among vectors of any orthonormal basis. In other words, the projector $\hat{P}_k$ acts on a state $|\psi\rangle$ by selecting the component $|o_k\rangle$ with a reduced output $|\eta_k|^2 \leq 1$: for instance, a polarization filter prepares systems in a certain state by throwing away a part of them.

Projectors have the following properties:

$$\hat{P}_j\hat{P}_k = \delta_{jk}\hat{P}_k \ , \tag{19a}$$

$$\sum_j \hat{P}_j = \hat{I} \ , \tag{19b}$$

where the sum must be understood over the whole orthonormal basis (for instance, $\{|o_j\rangle\}$ for the object system). The previous formalism allows us to write the observable $\hat{O}$ as a sum of projectors in conjunction with eigenvalues:

$$\begin{aligned} \hat{O} &= o_1\hat{P}_1 + o_2\hat{P}_2 + \ldots + o_n\hat{P}_n \\ &= o_1\begin{bmatrix} 1 & 0 & \ldots & 0 \\ 0 & 0 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & \ldots & 0 \end{bmatrix} + o_2\begin{bmatrix} 0 & 0 & \ldots & 0 \\ 0 & 1 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & \ldots & 0 \end{bmatrix} + \ldots + o_n\begin{bmatrix} 0 & 0 & \ldots & 0 \\ 0 & 0 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & \ldots & 1 \end{bmatrix} \\ &= \begin{bmatrix} o_1 & 0 & \ldots & 0 \\ 0 & o_2 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & \ldots & o_n \end{bmatrix} . \end{aligned} \tag{20}$$

We can use projectors for writing any state in the following form:

$$\begin{aligned} \hat{\rho}_\psi &= \hat{P}_\psi = |\psi\,\rangle\,\langle\psi\,| \\ &= \sum_j |c_j|^2\,|b_j\rangle\,\langle b_j\,| + \sum_{k\neq j} c_j c_k^*\,|b_j\,\rangle\,\langle b_k\,| \\ &= \begin{bmatrix} \wp_1 & c_1c_2^* & \ldots & c_1c_n^* \\ c_2c_1^* & \wp_2 & \ldots & c_2c_n^* \\ \ldots & \ldots & \ldots & \ldots \\ c_nc_1^* & c_nc_2^* & \ldots & \wp_n \end{bmatrix} . \end{aligned} \tag{21}$$

The symbol $\hat{\rho}_\psi$ is called a density matrix. Note that the density matrix presents off-diagonal terms that are also called *interference terms*. In such a case the system is said to be in a *pure state* (it is represented by a single projector). However, a density matrix can represent a (proper) mixture (for instance, a collection of particles in different states) and here it is expressed by a weighted sum of projectors:

$$\hat{\rho}'_\psi = \sum_j \wp \hat{P}_j = \begin{bmatrix} \wp_1 & 0 & \dots & 0 \\ 0 & \wp_2 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & \wp_n \end{bmatrix} . \tag{22}$$

Such a density matrix is deprived of interference terms. Those terms correspond to the interference among different components of a superposition. Both for pure states and mixtures the trace of a density matrix (i.e. the sums of diagonal elements) is =1:

$$\mathrm{Tr}\,(\hat{\rho}_\psi) = 1 . \tag{23}$$

Note that a projector expresses a property, and therefore a density matrix can be considered an observable. However, it is a peculiar case of observable, one whose measurement will give each time either 0 or 1 as a result (due to the dual nature of every projector).

It is quite obvious that we can operationally conceive a property as an equivalence class of detection events as far as different detection events and even with different detectors allows us to assign the same property to the system.

Since quantum observables are expressed by operators, they may not commute. This is in particular true for the (one–dimensional) position operator $\hat{x}$ and its conjugate momentum $\hat{p}_x$, i.e. $\hat{x}\hat{p}_x \neq \hat{p}_x\hat{x}$:

$$[\hat{x}, \hat{p}_x] = \imath\hbar\hat{I} , \tag{24}$$

which is valid for any state and where the expression

$$[\hat{x}, \hat{p}_x] = \hat{x}\hat{p}_x - \hat{p}_x\hat{x} \tag{25}$$

is called the commutator of these two observables. The constant $\hbar = h/2\pi$ is read *h-bar* and $h$ is the Planck constant (which has the dimension of action), given by:

$$h = 6.626069 \times 10^{-34}\mathrm{J} \cdot \mathrm{s} . \tag{26}$$

The commutation relation tells us that inverting the sequence of the measurements of the two conjugate observables on any state will in general affect the final result.

A consequence of the above commutation relation is the uncertainty relation, where the uncertainty $\Delta\hat{O}$ of the observable $\hat{O}$ in the state $|\psi\rangle$ is defined by the square root of its variance in that state:

$$\Delta x \Delta p_x \geq \frac{\hbar}{2} \,. \tag{27}$$

This fundamental relation tells us that any increase in the determination of any of the two observables is payed in terms of an increase in uncertainty of the other.

A crucial observable is the energy that governs the time evolution (and therefore the dynamics) of quantum systems. The (three–dimensional) quantum–mechanical Hamiltonian, as the classical one, is the sums of a kinetic and potential component:

$$\hat{H} = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V(\hat{\mathbf{r}}) \,. \tag{28}$$

This allows us to write the fundamental Schrödinger equation:

$$\imath\hbar\frac{d}{dt}\left|\psi(t)\right\rangle = \hat{H}\left|\psi(t)\right\rangle \,. \tag{29}$$

The Schrödinger equation expresses a reversible dynamics and therefore can be written using an unitary operator:

$$\left|\psi(t)\right\rangle = \hat{U}_t(t-t_0)\left|\psi(t_0)\right\rangle \,, \tag{30}$$

where $t_0$ is some initial time. We can take advantage of the Stone's theorem and write the unitary operator in the form:

$$\hat{U}(t-t_0) = e^{-\frac{\imath}{\hbar}\hat{H}(t-t_0)} \,, \tag{31}$$

in accordance with the Schrödinger equation. Its conjugate transpose for $\tau = t - t_0$ is

$$\hat{U}_t^\dagger(\tau) = \left(e^{-\frac{\imath}{\hbar}\hat{H}\tau}\right)^\dagger = e^{+\frac{\imath}{\hbar}\hat{H}\tau}. \tag{32}$$

Multiplying both sides of Eq. (30) by

$$\hat{U}_t^\dagger(\tau) = \hat{U}_{-t}(\tau) = \hat{U}_t(-\tau) \,, \tag{33}$$

and using the unitarity property of $\hat{U}_t(\tau)$, we obtain

$$\left|\psi(t_0)\right\rangle = \hat{U}_t(-\tau)\left|\psi(t)\right\rangle , \tag{34}$$

showing, as anticipated, that time evolution in quantum mechanics is indeed reversible. The eigenvalue equation of the energy can be written as

$$\hat{H}\left|\psi_n\right\rangle = E_n\left|\psi_n\right\rangle \,. \tag{35}$$

The eigenstates of the energy are called *stationary states* since do not evolve with time.

An arbitrary initial state vector $|\psi(0)\rangle$ (where $0 = t_0$) can be expanded as a superposition of the energy eigenstates $|\psi_n\rangle$ as

$$|\psi(0)\rangle = \sum_n c_n(0)\,|\psi_n\rangle \ , \tag{36}$$

where $c_n(0) = \langle\psi_n\,|\,\psi(0)\rangle$ are the coefficients of the expansion at the initial time. An arbitrary state vector $|\psi(t)\rangle$ at a later time $t > 0$ can be found by utilizing the time evolution operator $\hat{U}_t(t)$ (since, having set $t_0 = 0$, we have $\tau = t$). From Eq. (30) we obtain

$$\begin{aligned} |\psi(t)\rangle &= \hat{U}_t(t)\,|\psi(0)\rangle \\ &= \sum_n c_n(0)\hat{U}_t(t)\,|\psi_n\rangle \\ &= \sum_n c_n(0)e^{-\frac{i}{\hbar}E_n t}\,|\psi_n\rangle \,, \end{aligned} \tag{37}$$

where used has been made of the fact that $|\psi_n\rangle$ are stationary states with energy $E_n$.