Chapter 3. Quantum Mechanics Postulates, Principles, and Mathematic Formalism

§3.1. Postulates of Quantum Mechanics

1. QM State of a system is defined as the undisturbed motion of the system. The state is about the status of a motion of the physical system. Each undisturbed motion with information about energy, momentum, coordinates, angular momentum etc forms a state of the physical system at an instant time. The change of the state with time, the change of motion, or the disturbed motion belongs to the problem of time evolution of the state.

* In QM mathematical formalism, the state of any physical system at an instant time is represented by a state vector $|\psi(t)\rangle$ in an abstract state space that is formed by all possible states of the physical system.

2. QM Physical quantities / dynamic variables / observables are the physical quantities that can be measured or observed. These observables are represented by abstract linear operators $\hat{A}$.

3. QM measurements are represented by a linear operator $\hat{A}$ acting on a state vector $|\psi\rangle$, i.e., $\hat{A}|\psi\rangle$. The only possible result of the measurement is one of the eigenvalues of the corresponding observable A.

4. QM Eigenvalue Equation of a linear operator $\hat{A}$ is defined as

$$\hat{A}|\psi\rangle = \lambda|\psi\rangle$$

where $|\psi\rangle$ is the eigenstate vector of the operator $\hat{A}$,

λ is a complex number, the eigenvalue of $\hat{A}$.

5. QM state vectors and linear operators obey the followig rules:

(1) Ket vector $| \rangle$ and Bra vector $\langle |$ are "Hermitian Conjugate" with each other: $\langle | = | \rangle^*$ $\quad (|\psi\rangle = \langle \psi|^*)$

(2) The scalar product of two ket vectors $|\psi_1\rangle$ and $|\psi_2\rangle$ is given by the product of one ket vector and the conjugate of the other ket vector: $|\psi_1\rangle^* \cdot |\psi_2\rangle = \langle \psi_1 | \psi_2 \rangle$
i.e., the bra vector correspondig to one ket vector, times the other ket vector.

(3) When takig conjugate of state vector, operator, and constant, we take the conjugate of each and then reverse the order, e.g., $(\lambda \hat{A} |\psi\rangle)^* = (\langle \psi | \hat{A}^* \lambda^*)$

(4) If $\hat{A} = A^*$, then $\hat{A}$ is a Hermitian operator.

(5) Other linear operation rules: $\hat{A}|\psi\rangle = |\psi'\rangle$,

$$(\hat{A}\hat{B})|\psi\rangle = \hat{A}(\hat{B}|\psi\rangle)$$

$$\langle \psi_1 | (\hat{A}|\psi_2\rangle) = (\langle \psi_1 | \hat{A}) |\psi_2\rangle$$

$$\hat{A}(\lambda_1|\psi_1\rangle + \lambda_2|\psi_2\rangle) = \lambda_1 \hat{A}|\psi_1\rangle + \lambda_2 \hat{A}|\psi_2\rangle$$

(6) In general, $\hat{A}\hat{B} \neq \hat{B}\hat{A}$.
The commutator is $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$.

§3.2. Principle of Superposition of States

6. QM principle of superposition of states requires that
   1). Any state of a system can be considered as a superposition of two or more other states of the same system, and indeed in an infinite number of ways.
   2). The superposition of two or more states of a system forms a new state of the same system.

In QM, if a physical system has a complete orthonormal set of eigenstates $\{|u_n\rangle\}$ with discrete eigenvalues $\{a_n\}$ of a linear operator $\hat{A}$: $\hat{A}\,|u_n\rangle = a_n\,|u_n\rangle$, $\langle u_m|u_n\rangle = \delta_{mn}$, then any state of the system $|\psi\rangle$ can be expressed in terms of the complete set $\{|u_n\rangle\}$:

$$|\psi\rangle = \sum_n \left(c_n\,|u_n\rangle\right), \quad \text{where } c_n = \langle u_n|\psi\rangle.$$

If a system has a complete orthonormal set of eigenstates $\{|W_\alpha\rangle\}$ with continuous eigenvalues $\{\alpha\}$ of a linear operator $\hat{A}$: $\hat{A}\,|W_\alpha\rangle = \alpha\,|W_\alpha\rangle$, $\langle W_{\alpha'}|W_\alpha\rangle = \delta(\alpha-\alpha')$, then any state of this system $|\psi\rangle$ can be expressed in terms of the complete set $\{|W_\alpha\rangle\}$:

$$|\psi\rangle = \int C(\alpha)\,|W_\alpha\rangle\, d\alpha, \quad \text{where } C(\alpha) = \langle W_\alpha|\psi\rangle.$$

These are the mathematical expression of QM principle of superposition of states.

7. QM principle of spectral decomposition is to describe the probability of obtaining a specific eigenvalue of an observable operator when making measurements of a system in certain state.

(1) If an observable $\hat{A}$ has eigenvalues $\{a_n\}$ (discrete) associated with its eigenstates $\{|u_n\rangle\}$, i.e., $\hat{A}|u_n\rangle = a_n|u_n\rangle$.

When the physical quantity $\hat{A}$ is measured on the system in the state $|\psi\rangle$, the probability of obtaining a non-degenerate eigenvalue a_n of $\hat{A}$ is given by

$$P(a_n) = \frac{|\langle u_n|\psi\rangle|^2}{\langle\psi|\psi\rangle} = \frac{|C_n|^2}{\langle\psi|\psi\rangle},$$

where $|\psi\rangle = \sum_n C_n|u_n\rangle$, and $C_n = \underline{\langle u_n|\psi\rangle}$ is called the probability amplitude.

(2) In general, if a_n is degenerate, the probability is given by

$$P(a_n) = \frac{\sum_{i=1}^{g_n}|\langle u_n^i|\psi\rangle|^2}{\langle\psi|\psi\rangle} = \frac{\sum_{i=1}^{g_n}|C_n^i|^2}{\langle\psi|\psi\rangle}$$

(3) If an observable $\hat{A}$ has continuous eigenvalues $\{\alpha\}$ associated with eigenstates $\{|W_\alpha\rangle\}$, i.e., $\hat{A}|W_\alpha\rangle = \alpha|W_\alpha\rangle$.

When the physical quantity $\hat{A}$ is measured on the system in the state $|\psi\rangle$, the probability of obtaining a non-degenerate eigenvalue between α and $\alpha+d\alpha$ is given by

$$dP(\alpha) = \frac{|\langle W_\alpha|\psi\rangle|^2}{\langle\psi|\psi\rangle}d\alpha = \frac{|C(\alpha)|^2}{\langle\psi|\psi\rangle}d\alpha$$

where $|\psi\rangle = \int C(\alpha)|W_\alpha\rangle d\alpha$, and $\underline{|C(\alpha)|^2 = \frac{|\langle W_\alpha|\psi\rangle|^2}{\langle\psi|\psi\rangle}}$ is probability density.

8. Projector operator and two useful relations :

(1) $|\psi\rangle\langle\varphi|$ becomes an operator, because when it applies to an arbitrary ket vector, it gives another ket vector. Take an arbitrary ket vector and apply "$|\psi\rangle\langle\varphi|$" to it:

$$(|\psi\rangle\langle\varphi|)\,|A\rangle = |\psi\rangle\langle\varphi|A\rangle$$

Since $\langle\varphi|A\rangle$ is the scalar product so a complex number, thus, above equation gives another ket vector. Therefore, $|\psi\rangle\langle\varphi|$ is an operator.

(2) Let $|\psi\rangle$ be a normalized ket vector, i.e., $\langle\psi|\psi\rangle = 1$. The operator $P_\psi = |\psi\rangle\langle\psi|$ is a projector operator that projects any arbitrary ket vector $|\varphi\rangle$ onto the ket vector $|\psi\rangle$: $\quad P_\psi|\varphi\rangle = |\psi\rangle\langle\psi|\varphi\rangle$.

This is further confirmed by the fact $P_\psi^2 = P_\psi$, i.e., projecting twice in succession onto a given vector is equivalent to projecting a single time.

$$P_\psi^2 = P_\psi P_\psi = |\psi\rangle\langle\psi|\psi\rangle\langle\psi| = |\psi\rangle\langle\psi| = P_\psi.$$

(3) For a complete orthonormal set of eigenstates $\{|u_n\rangle\}$, we have the projector operator $P = \sum_n |u_n\rangle\langle u_n| = 1$.

In a continuous eigenvalue case $\{|W_\alpha\rangle\}$,

$$P = \int |W_\alpha\rangle\langle W_\alpha|\, d\alpha = 1.$$

This can be derived as below.

(4) For a complete orthornormal set of eigenstates $\{|u_n\rangle\}$, $\boxed{\langle u_m|u_n\rangle = \delta_{mn}}$

any state $|\psi\rangle$ can be expressed as:

$$|\psi\rangle = \sum_n C_n |u_n\rangle.$$

where $C_n = \langle u_n|\psi\rangle$. - Substitute C_n into above equation.

Then, $|\psi\rangle = \sum_n C_n |u_n\rangle$

$$= \sum_n \langle u_n|\psi\rangle |u_n\rangle$$

As $\langle u_n|\psi\rangle$ is a scalar product, i.e., a complex number, It can switch order with $|u_n\rangle$. Thus,

$$|\psi\rangle = \sum_n |u_n\rangle\langle u_n|\psi\rangle = \left(\sum_n |u_n\rangle\langle u_n|\right)|\psi\rangle.$$

Because this equation is true for any arbitrary $|\psi\rangle$, the only conclusion is $\sum_n |u_n\rangle\langle u_n| = 1$.

(5) Similarly, for a continuous case: $\{|W_\alpha\rangle\}$ and $\langle W_{\alpha'}|W_\alpha\rangle = \delta(\alpha-\alpha')$. Any state $|\psi\rangle$ is expressed

as $|\psi\rangle = \int C(\alpha)|W_\alpha\rangle d\alpha$.

where $C(\alpha) = \langle W_\alpha|\psi\rangle$. Substitute $C(\alpha)$ into above equation:

$$|\psi\rangle = \int \langle W_\alpha|\psi\rangle |W_\alpha\rangle d\alpha$$

$$= \left(\int |W_\alpha\rangle\langle W_\alpha| d\alpha\right)|\psi\rangle.$$

Since this is true for any $|\psi\rangle$, we conclude

$$\int |W_\alpha\rangle\langle W_\alpha| d\alpha = 1$$

9. Mean value of an observable $\hat{A}$ from many times of measurements on a system in the state $|\psi\rangle$ is given by

$$\bar{A} = \langle\psi|\hat{A}|\psi\rangle.$$

To understand this, $\langle\psi| = |\psi\rangle^*$, i.e., $\langle\psi|$ is the conjugate of $|\psi\rangle$. $\hat{A}|\psi\rangle$ becomes another ket vector. So above equation implicates that the mean of $\hat{A}$ should be calculated by using $|\psi\rangle^*$ to take a scalar product with $(\hat{A}|\psi\rangle)$ ket vector.

This mean-value equation is true for all possible cases, regardless discrete or continuous eigenvalues. It is a natural conclusion from the principle of spectral decomposition. $\hat{A}$ has a complete orthonormal eigenstate set $\{|u_n\rangle\}$ or $\{|w_\alpha\rangle\}$. $\hat{A}|u_n\rangle = a_n|u_n\rangle$, $\hat{A}|w_\alpha\rangle = \alpha|w_\alpha\rangle$.

Any state $|\psi\rangle$ can be expressed as

$$|\psi\rangle = \sum_n c_n|u_n\rangle \quad \text{or} \quad |\psi\rangle = \int c(\alpha)|w_\alpha\rangle d\alpha.$$

where $c_n = \langle u_n|\psi\rangle$, or $c(\alpha) = \langle w_\alpha|\psi\rangle$.

The probability of obtaining a_n result is $P(a_n) = |\langle u_n|\psi\rangle|^2$, and for α and $\alpha + d\alpha$, $dP(\alpha) = |\langle w_\alpha|\psi\rangle|^2 d\alpha$.

Thus, the mean of $\hat{A}$ should be calculated as

$$\bar{A} = \sum_n \left[P(a_n)\, a_n\right] \quad \text{or} \quad \bar{A} = \int \alpha\, dP(\alpha)$$

$$= \sum_n \left[|\langle u_n|\psi\rangle|^2 a_n\right] \quad\quad = \int |\langle w_\alpha|\psi\rangle|^2 \alpha\, d\alpha.$$

Now let us verify whether $\langle\psi|\hat{A}|\psi\rangle$ is equivalent to the above two means of $\hat{A}$.

In discrete eigenvalue case, $|\psi\rangle^* = \sum_n C_n^* \langle u_n|$

$$\langle\psi|\hat{A}|\psi\rangle = \left(\sum_n C_n^* \langle u_n|\right)\hat{A}\left(\sum_m C_m |u_m\rangle\right)$$
$$= \sum_n\sum_m\left(C_n^* C_m \langle u_n|\hat{A}|u_m\rangle\right)$$
$$= \sum_n\sum_m\left(C_n^* C_m a_m \langle u_n|u_m\rangle\right)$$
$$= \sum_n\sum_m\left(C_n^* C_m a_m \delta_{nm}\right)$$
$$= \sum_n C_n^* C_n a_n$$
$$= \sum_n |C_n|^2 a_n$$
$$= \sum_n |\langle u_n|\psi\rangle|^2 a_n .$$ — Equivalent !

In continuous eigenvalue case, $|\psi\rangle^* = \int c^*(\alpha)\langle W_\alpha|\,d\alpha$

$$\langle\psi|\hat{A}|\psi\rangle = \left(\int c^*(\alpha)\langle W_\alpha|\,d\alpha\right)\hat{A}\left(\int c(\alpha')|W_{\alpha'}\rangle\,d\alpha'\right)$$
$$= \iint c^*(\alpha)\,c(\alpha')\,\langle W_\alpha|\hat{A}|W_{\alpha'}\rangle\,d\alpha\,d\alpha'$$
$$= \iint c^*(\alpha)\,c(\alpha')\,\alpha'\,\langle W_\alpha|W_{\alpha'}\rangle\,d\alpha\,d\alpha'$$
$$= \iint c^*(\alpha)\,c(\alpha')\,\alpha'\,\delta(\alpha-\alpha')\,d\alpha\,d\alpha'$$
$$= \int c^*(\alpha)\,c(\alpha)\,\alpha\,d\alpha$$
$$= \int |c(\alpha)|^2\alpha\,d\alpha$$
$$= \int |\langle W_\alpha|\psi\rangle|^2\alpha\,d\alpha .$$ — Equivalent !

10. QM reduction of the state: assume that we make measurement of $\hat{A}$ on a system in the state $|\psi\rangle$. Let us first consider the case where the measurement of $\hat{A}$ yields a simple eigenvalue a_n of the observable $\hat{A}$. QM postulates the state of the system immediately after the measurement is the eigenstate $|u_n\rangle$ associated with a_n: $(\hat{A}|u_n\rangle = a_n|u_n\rangle)$

$$|\psi\rangle \xRightarrow{(a_n)} |u_n\rangle.$$

If we perform a second measurement of $\hat{A}$ immediately after the first one (that is, before the system has had time to evolve), we shall always find the same result a_n, since the state of the system immediately before the second measurement is $|u_n\rangle$ (the eigenstate), and no longer $|\psi\rangle$.

When the eigenvalue a_n given by the measurement is degenerate, the reduction of the state can be generalized as follows. If the expansion of the state $|\psi\rangle$ immediately before the measurement is written as $|\psi\rangle = \sum_n \left(\sum_{i=1}^{g_n} c_n^i |u_n^i\rangle \right)$, where g_n is the degeneracy factor of eigenvalue a_n, the reduction of the state becomes $|\psi\rangle \xRightarrow{(a_n)} \frac{1}{\sqrt{\sum_{i=1}^{g_n} |c_n^i|^2}} \sum_{i=1}^{g_n} c_n^i |u_n^i\rangle$.

Let $\hat{P}_n$ be the projector operator, then we have the above reduction of state written as: $|\psi\rangle \xRightarrow{(a_n)} \frac{\hat{P}_n|\psi\rangle}{\sqrt{\langle\psi|P_n|\psi\rangle}}$, i.e.,

the state of the system immediately after the measurement is the normalized projection of $|\psi\rangle$ onto the eigen-subspace $\{|u_n^i\rangle\}$.