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 following rules.

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

(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 corresponding to one ket vector, times the other ket vector.

(3) When taking 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 $\{|u_n\rangle\}$:

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

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 eigen value 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 eigen values $\{\alpha\}$ 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 $|A\rangle$ 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 $|\psi\rangle$: $P_\psi|\varphi\rangle = |\psi\rangle\langle\psi|\varphi\rangle$.

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 obtaing 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

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

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

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, $|\psi\rangle^* = \sum_n c_n^* \langle u_n|$

$$\begin{aligned}
\langle\psi|\hat{A}|\psi\rangle &= \left(\sum_n c_n^*\langle u_n|\right)\hat{A}\left(\sum_m c_m|u_m\rangle\right) \\
&= \sum_n\sum_m\left(c_n^* c_m \langle u_n|\hat{A}|u_m\rangle\right) \\
&= \sum_n\sum_m\left(c_n^* c_m a_m \langle u_n|u_m\rangle\right) \\
&= \sum_n\sum_m\left(c_n^* c_m a_m \delta_{nm}\right) \\
&= \sum_n c_n^* c_n a_n \\
&= \sum_n |c_n|^2 a_n \\
&= \sum_n |\langle u_n|\psi\rangle|^2 a_n \quad \text{— Equivalent !}
\end{aligned}$$

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

$$\begin{aligned}
\langle\psi|\hat{A}|\psi\rangle &= \left(\int c^*(\alpha)\langle w_\alpha|\,d\alpha\right)\hat{A}\left(\int c(\alpha')|w_{\alpha'}\rangle d\alpha'\right) \\
&= \iint c^*(\alpha)\,c(\alpha')\langle w_\alpha|\hat{A}|w_{\alpha'}\rangle\,d\alpha\,d\alpha' \\
&= \iint c^*(\alpha)c(\alpha')\,\alpha'\langle w_\alpha|w_{\alpha'}\rangle\,d\alpha\,d\alpha' \\
&= \iint c^*(\alpha)\,c(\alpha')\,\alpha'\,\delta(\alpha-\alpha')\,d\alpha\,d\alpha' \\
&= \int c^*(\alpha)\,c(\alpha)\,\alpha\,d\alpha \\
&= \int |c(\alpha)|^2\,\alpha\,d\alpha \\
&= \int |\langle w_\alpha|\psi\rangle|^2\,\alpha\,d\alpha \quad \text{— Equivalent !}
\end{aligned}$$

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 $\{|u_n^i\rangle\}$.

§3.3 Equation of Motion — Schrödinger Equation

11. QM principle of motion describes the time evolution of the state of a system, which is governed by the Schrödinger Equation.

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle,$$

where $|\psi(t)\rangle$ is the state vector, $\hat{H}(t)$ is the observable associated with the total energy of the system (called the Hamiltonian operator of the system), $\hbar$ is Planck constant divided by 2π, and $\frac{d}{dt}$ is to take derivative of time.

(1) The Schrödinger equation is a fundamental equation for the Quantum Mechanics, just like the Newtonian equation in the classical mechanics. In principle, it cannot be derived or proven from more fundamental principles, but it can only be verified by experiments. The Schrödinger equation describes the change of state with time, the time evolution of motion, or the change of motion.

(2) The Hamiltonian operator $\hat{H}$ comes from the classical Hamiltonian: $H(t) = \frac{\vec{p}^2(t)}{2m} + V(t)$,

where $\vec{p}(t)$ is the momentum, m is the mass, and $V(t)$ is the potential energy of the system. $\frac{\vec{p}^2}{2m}$ represents the kinetic energy of the system. In QM, the Hamiltonian operator is given by $\hat{H}(t) = \frac{\hat{\vec{p}}^2(t)}{2m} + \hat{V}(t)$.

(3) Note that the Schrödinger equation is expressed in the abstract state space with an abstract operator $\hat{H}$, abstract state vector $|\psi(t)\rangle$, and a full derivative $\frac{d}{dt}$

When express the Schrödinger Equation in any representation, it will become a partial derivative $\frac{\partial}{\partial t}$, and $\hat{H}(t)$ and $|\psi(t)\rangle$ will also be projected to this representation. The equation may not be such simple format, depending on what representation is chosen.

(4) The Schrödinger equation is of first order in t. From this it follows that, given the initial state $|\psi(t_0)\rangle$, the state $|\psi(t)\rangle$ at any subsequent time t is determined. There is no indeterminacy in the time evolution of a quantum system. Indeterminacy appears only when a physical quantity is measured, the state vector then undergoing an unpredictable modification (i.e., the reduction of the state to an eigenstate). However, between two measurements, the state vector evolves in a perfectly deterministic way, in accordance with the Schrödinger equation.

(5) The Schrödinger Equation is linear and homogeneous. It follows that its solution is linearly superposable.

Let $|\psi_1(t)\rangle$ and $|\psi_2(t)\rangle$ be two solutions of the Schrödinger equation: $i\hbar \frac{d}{dt}|\psi_1\rangle = \hat{H}|\psi_1\rangle$

$i\hbar \frac{d}{dt}|\psi_2\rangle = \hat{H}|\psi_2\rangle$.

Then the linear superposition of $|\psi_1(t)\rangle$ and $|\psi_2(t)\rangle$: $|\psi(t)\rangle = \lambda_1|\psi_1(t)\rangle + \lambda_2|\psi_2(t)\rangle$ (λ_1 and λ_2 are two complex constants) is also a solution to the Schrödinger Equation: $i\hbar \frac{d}{dt}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$.

The statement can be verified as below:

$$i\hbar\frac{d}{dt}|\psi\rangle = \lambda_1 i\hbar\frac{d}{dt}|\psi_1\rangle + \lambda_2 i\hbar\frac{d}{dt}|\psi_2\rangle$$
$$= \lambda_1 \hat{H}|\psi_1\rangle + \lambda_2 \hat{H}|\psi_2\rangle$$
$$= \hat{H}(\lambda_1|\psi_1\rangle + \lambda_2|\psi_2\rangle)$$
$$= \hat{H}|\psi\rangle$$

Thus, the superposition $|\psi\rangle$ is a solution to the Schrödinger equation.

(6) The norm of the state vector $|\psi(t)\rangle$ is defined as $\sqrt{\langle\psi(t)|\psi(t)\rangle}$. Since the Hamiltonian operator $\hat{H}(t)$ is a Hermitian, i.e., $\hat{H}(t) = \hat{H}^*(t)$, the square of the norm of the state vector, $\langle\psi(t)|\psi(t)\rangle$, does not depend on t as we can see below:

$$\frac{d}{dt}\langle\psi(t)|\psi(t)\rangle = \left[\frac{d}{dt}\langle\psi(t)|\right]|\psi(t)\rangle + \langle\psi(t)|\left[\frac{d}{dt}|\psi(t)\rangle\right].$$

From the Schrödinger equation, we have $\frac{d}{dt}|\psi(t)\rangle = \frac{1}{i\hbar}\hat{H}|\psi(t)\rangle$, and $\frac{d}{dt}\langle\psi(t)| = -\frac{1}{i\hbar}\langle\psi(t)|\hat{H}^* = -\frac{1}{i\hbar}\langle\psi(t)|\hat{H}$.

Substituting these two items into above derivative equation, we have

$$\frac{d}{dt}\langle\psi(t)|\psi(t)\rangle = -\frac{1}{i\hbar}\langle\psi(t)|\hat{H}|\psi(t)\rangle + \frac{1}{i\hbar}\langle\psi(t)|\hat{H}|\psi(t)\rangle$$
$$= 0$$

Therefore, $\langle\psi(t)|\psi(t)\rangle = \langle\psi(t_0)|\psi(t_0)\rangle = 1$.

The last equality comes if the state vector $|\psi_0(t)\rangle$ is normalized at time t_0.

The property of the norm conservation is very useful in quantum mechanics. For example, it becomes indispensable when we interpret the square of the modulus $|\psi(\vec{r},t)|^2 = |\langle\vec{r}|\psi\rangle|^2$ of the wave function of a spinless particle as being the position probability density. Time evolution does not modify the global probability of finding the particle in all space, which alway remains equal to 1. Therefore,

$$\langle\psi(t)|\psi(t)\rangle = \int d^3r\,|\psi(\vec{r},t)|^2 = 1.$$

12. QM Commutation Relation.

Consider coordinate $\hat{x}$ and momentum $\hat{P}_x$; $\hat{P}_x = -i\hbar\frac{\partial}{\partial x}$ in the $\{|x\rangle\}$ representation. For any arbitrary state $|\psi\rangle$ in the $\{|x\rangle\}$ representation $\psi(x)$,

$$\hat{P}_x \hat{x}\,\psi(x) = \hat{P}_x[\hat{x}\,\psi(x)]$$

$$= -i\hbar\frac{\partial}{\partial x}[x\,\psi(x)]$$

$$= -i\hbar\left(\frac{\partial}{\partial x}x\right)\psi(x) - i\hbar\, x\frac{\partial}{\partial x}\psi(x)$$

$$= -i\hbar\,\psi(x) - x\cdot i\hbar\frac{\partial}{\partial x}\psi(x)$$

$$= \left(-i\hbar + \hat{x}\hat{P}_x\right)\psi(x).$$

$$\therefore \left(\hat{x}\hat{P}_x - \hat{P}_x\hat{x}\right)\psi(x) = i\hbar\,\psi(x)$$

since $\psi(x)$ is arbitrary, we conclude that

$$\hat{x}\hat{P}_x - \hat{P}_x\hat{x} = i\hbar$$

Define $[\hat{x}, \hat{P}_x] = \hat{x}\hat{P}_x - \hat{P}_x\hat{x}$,

$\therefore\ [\hat{x}, \hat{P}_x] = i\hbar$. But $[\hat{x}, \hat{P}_y] = 0$

Similarly, $[\hat{y}, \hat{P}_y] = i\hbar$ ... ...

$[\hat{z}, \hat{P}_z] = i\hbar$

$$\therefore [\hat{r}_i, \hat{P}_j] = i\hbar\,\delta_{ij} \quad (i, j = x, y, z)$$

Most operators are not commutej with each other. So you are NOT supposed to switch their orders when doing calculation. $[\hat{r}_i, \hat{P}_j] = i\hbar\,\delta_{ij}$, or $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ is called the commutation relation.

§3.4 Principle of Uncertainty – Indeterminacy

13. QM Principle of Uncertainty is a fundamental principle in Quantum Mechanics. It puts a fundamental limit on the accuracy of simultaneously determining the numerical values of two non-commuting observables. When these two non-commuting observables are a canonical coordinate and momentum of a particle, the product of the uncertainties of the coordinate and momentum is given by

$$\Delta Q \cdot \Delta P \geq \frac{\hbar}{2},$$ where Q is coordinate and P is momentum.

This relation is called the Heisenberg's Principle of Uncertainty or Heisenberg's uncertainty relation.

(1) The interpretation of this uncertainty relation is as follows: it is impossible to define at a given time both the position of the particle and its momentum to an arbitrary degree of accuracy When the lower limit imposed by above relation is reached, increasing the accuracy in the position (decreasing ΔQ) implies that the accuracy in the momentum diminishes (increasing ΔP), and vice versa.

The limitation expressed by this uncertainty relation arises from the fact that the Planck constant h is not zero. It is the very small value of h ($= 6.626 \times 10^{-34}$ J·s) on the macroscopic scale that renders this limitation totally negligible in classical mechanics, but has considerable effect in microscopic world.

For example, let us consider a dust particle with a diameter on the order of $1\,\mu m$ and mass $m \approx 10^{-15}\,kg$, having a speed $v = 10^{-3}\,m/s$. Its momentum is then equal to

$$p = mv = 10^{-8}\ kg\cdot m/s.$$

If its position is measured to within $0.01\,\mu m$, then the uncertainty Δp in the momentum must satisfy

$$\Delta p \geq \frac{\hbar/2}{\Delta Q} \cong \frac{10^{-34}}{10^{-8}} = 10^{-26}\,kg\cdot m/s, \text{ i.e., } \frac{\Delta p}{p} \geq 10^{-8}.$$

Such a small uncertainty is totally negligible in the macroscopic world, as in practice, a momentum measurement device is incapable of attaining the required relative accuracy of 10^{-8}. In the macro world, we can regard $h \to 0$, so a particle can still have accurate position and momentum simultaneously, i.e., a certain motion orbit.

Now let us consider the microscopic world, for example, the hydrogen atom. Assume the electron is moving along the n_1 orbit, and position uncertainty $\Delta x \sim a_1 = 0.53\times10^{-10}\,m$. The momentum uncertainty is given by

$$\Delta p \geq \frac{\hbar/2}{\Delta x} = \frac{6.626\times10^{-34}/2}{0.53\times10^{-10}} = 6.25\times10^{-24}\,kg\cdot m/s.$$

However, the momentum of the electron itself is given by

$$p = m_e v_1 = m_e\sqrt{\frac{e^2}{4\pi\varepsilon_0 m_e a_1}} = e\sqrt{\frac{m_e}{4\pi\varepsilon_0 a_1}}$$

$$= 1.6\times10^{-19}\times\sqrt{\frac{9.1\times10^{-31}}{4\pi\times8.85\times10^{-12}\times0.53\times10^{-10}}}$$

$$= 2.0\times10^{-24}\,kg\cdot m/s.$$

Thus, $\frac{\Delta p}{p} \geq \frac{6.25\times10^{-24}}{2.0\times10^{-24}} \cong 3$, i.e., $\frac{\Delta p}{p} \geq 300\%$!

The relative uncertainty is so large that we cannot tell how much the electron momentum is !!!

(2) Derivation of Uncertainty Relation from commutation relation:

First, we need a precise definition of the uncertainties of the coordinate Q and momentum P. The uncertainties ΔQ and ΔP are defined as the root-mean-square deviation given by

$$\Delta Q = \sqrt{\langle (\hat{Q} - \langle \hat{Q} \rangle)^2 \rangle}$$

$$\Delta P = \sqrt{\langle (\hat{P} - \langle \hat{P} \rangle)^2 \rangle}$$

where, "$\langle\ \rangle$" means taking mean, e.g., $\langle \hat{Q} \rangle = \langle \psi | \hat{Q} | \psi \rangle$, $|\psi\rangle$ is an arbitrary state vector.

Now let us assume $|\psi\rangle$ is an arbitrary state but normalized, i.e., $\langle \psi | \psi \rangle = 1$. Operators corresponding to the coordinate and momentum are $\hat{Q}$ and $\hat{P}$. Consider the ket vector

$$|\varphi\rangle = (\hat{Q} + i\lambda \hat{P}) |\psi\rangle, \quad \text{where } \lambda \text{ is an arbitrary real number.}$$

The conjugate of $|\varphi\rangle$ is $\langle \varphi | = |\varphi\rangle^* = \langle \psi | (\hat{Q}^* - i\lambda^* \hat{P}^*)$

Since $\hat{Q}$ and $\hat{P}$ are Hermitian, i.e., $\hat{Q} = \hat{Q}^*$, $\hat{P} = \hat{P}^*$, we have

$$\langle \varphi | = \langle \psi | (\hat{Q} - i\lambda \hat{P}).$$

For all λ, the square of the norm $\langle \varphi | \varphi \rangle$ is positive, i.e.,

$$\begin{aligned}
\langle \varphi | \varphi \rangle &= \langle \psi | (\hat{Q} - i\lambda \hat{P})(\hat{Q} + i\lambda \hat{P}) | \psi \rangle \\
&= \langle \psi | \hat{Q}^2 + i\lambda \hat{Q}\hat{P} - i\lambda \hat{P}\hat{Q} + \lambda^2 \hat{P}^2 | \psi \rangle \\
&= \langle \psi | \hat{Q}^2 | \psi \rangle + i\lambda \langle \psi | \hat{Q}\hat{P} - \hat{P}\hat{Q} | \psi \rangle + \lambda^2 \langle \psi | \hat{P}^2 | \psi \rangle \\
&= \langle \hat{Q}^2 \rangle + i\lambda \langle [\hat{Q}, \hat{P}] \rangle + \lambda^2 \langle \hat{P}^2 \rangle \\
&\geq \langle \hat{Q}^2 \rangle - \hbar\lambda + \langle \hat{P}^2 \rangle \lambda^2 \geq 0.
\end{aligned}$$

Recall the commutation relation $[\hat{Q}, \hat{P}] = i\hbar$.

For polynomial expression $\langle \hat{Q}^2 \rangle - \hbar\lambda + \langle \hat{P}^2 \rangle \lambda^2 \geq 0$, the discriminant of this expression must be negative or zero.

[Discriminant for quadratic $ax^2 + bx + c = 0$ is $(b^2 - 4ac)$.]

$$\hbar^2 - 4\langle\hat{P}^2\rangle\langle\hat{Q}^2\rangle \le 0.$$

Therefore, we have $\langle\hat{Q}^2\rangle\langle\hat{P}^2\rangle \ge \frac{\hbar^2}{4}$.

Now define $\hat{Q}' = \hat{Q} - \langle\hat{Q}\rangle$, $\hat{P}' = \hat{P} - \langle\hat{P}\rangle$.

Then we find $\hat{Q}'$ and $\hat{P}'$ have the same commutation relation as $\hat{Q}$ and $\hat{P}$: $[\hat{Q}', \hat{P}'] = i\hbar$

$$[\hat{Q}', \hat{P}'] = \hat{Q}'\hat{P}' - \hat{P}'\hat{Q}'$$
$$= (\hat{Q} - \langle\hat{Q}\rangle)(\hat{P} - \langle\hat{P}\rangle) - (\hat{P} - \langle\hat{P}\rangle)(\hat{Q} - \langle\hat{Q}\rangle)$$
$$= (\hat{Q}\hat{P} - \hat{Q}\langle\hat{P}\rangle - \langle\hat{Q}\rangle\hat{P} + \langle\hat{Q}\rangle\langle\hat{P}\rangle)$$
$$- (\hat{P}\hat{Q} - \hat{P}\langle\hat{Q}\rangle - \langle\hat{P}\rangle\hat{Q} + \langle\hat{P}\rangle\langle\hat{Q}\rangle)$$
$$= \hat{Q}\hat{P} - \hat{P}\hat{Q} = [\hat{Q}, \hat{P}] = i\hbar.$$

Recall $\langle\hat{Q}\rangle$ and $\langle\hat{P}\rangle$ are mean numbers, so they can switch order with each other or switch order with $\hat{Q}$ and $\hat{P}$.

Therefore, going through the same procedure as $\hat{Q} + i\lambda\hat{P}$,

$|\varphi'\rangle = (\hat{Q}' + i\lambda\hat{P}')|\psi\rangle$, the square of the norm

$$\langle\varphi'|\varphi'\rangle = \langle(\hat{Q}')^2\rangle + i\lambda\langle[\hat{Q}', \hat{P}']\rangle + \lambda^2\langle(\hat{P}')^2\rangle$$
$$= \langle(\hat{Q}')^2\rangle - \hbar\lambda + \langle(\hat{P}')^2\rangle\lambda^2 \ge 0$$

$\therefore \hbar^2 - 4\langle(\hat{Q}')^2\rangle\langle(\hat{P}')^2\rangle \le 0$

Therefore, $\langle(\hat{Q}')^2\rangle\langle(\hat{P}')^2\rangle \ge \frac{\hbar^2}{4}$.

Accordig to the definition of uncertainty :

$$\Delta Q = \sqrt{\langle(\hat{Q} - \langle\hat{Q}\rangle)^2\rangle} = \sqrt{\langle(\hat{Q}')^2\rangle}$$
$$\Delta P = \sqrt{\langle(\hat{P} - \langle\hat{P}\rangle)^2\rangle} = \sqrt{\langle(\hat{P}')^2\rangle}$$

Therefore, $\Delta Q \cdot \Delta P = \sqrt{\langle(\hat{Q}')^2\rangle\langle(\hat{P}')^2\rangle} \ge \sqrt{\frac{\hbar^2}{4}} = \frac{\hbar}{2}$.

(3) The Heisenberg Uncertainty Principle can be generalized to the following: if two observables are conjugates (like the coordinate and momentum are conjugates with each other), there exists an exact lower bound for the product of uncertainties, which is equal to $\hbar/2$.

Further generalization of uncertainty relation is that two arbitrary observables $\hat{A}$ and $\hat{B}$ have such limitation.

$$\Delta A \cdot \Delta B \geq \frac{1}{2} |\langle [\hat{A}, \hat{B}] \rangle|.$$

In other words, the mimimum bound of the product of uncertainties is determined by the commutation relation between these two observables. If $\hat{A}$ and $\hat{B}$ are commuting, i.e., $[\hat{A}, \hat{B}] = 0$, then $\Delta A \cdot \Delta B \geq 0$. This means that it is possible ~~to~~ determine simultaneously $\hat{A}$ and $\hat{B}$ precisely.

But if $[\hat{A}, \hat{B}] \neq 0$, then there is a minimum limit on the accuracy of simultaneously determining $\hat{A}$ and $\hat{B}$.

§ 3.5. Dirac Notation and Representations

14. QM Probability Amplitude and Interference Effect.

Let $|\psi_1\rangle$ and $|\psi_2\rangle$ be two orthogonal normalized states:

$$\langle\psi_1|\psi_2\rangle = 0, \quad \langle\psi_1|\psi_1\rangle = \langle\psi_2|\psi_2\rangle = 1.$$

For a given observable $\hat{A}$, $\{|u_n\rangle\}$ are complete orthonormal eigenstates corresponding to the eigenvalues $\{a_n\}$: $\hat{A}|u_n\rangle = a_n|u_n\rangle$, $\langle u_m|u_n\rangle = \delta_{mn}$.

* If the system is in the state $|\psi_1\rangle$, the probability $P_1(a_n)$ of finding a_n when $\hat{A}$ is measured on the system is given by

$$P_1(a_n) = |\langle u_n|\psi_1\rangle|^2.$$

* If the system is in the state $|\psi_2\rangle$, the probability $P_2(a_n)$ of finding a_n when $\hat{A}$ is measured on the system is given by

$$P_2(a_n) = |\langle u_n|\psi_2\rangle|^2.$$

* Now consider a normalized state $|\psi\rangle$ which is a linear superposition of $|\psi_1\rangle$ and $|\psi_2\rangle$: $|\psi\rangle = \lambda_1|\psi_1\rangle + \lambda_2|\psi_2\rangle$

$$|\lambda_1|^2 + |\lambda_2|^2 = 1.$$

The probability $P(a_n)$ of finding the eigenvalue a_n when the observable $\hat{A}$ is measured on the system in the state $|\psi\rangle$ is

$$P(a_n) = |\langle u_n|\psi\rangle|^2$$

Substituting $|\psi\rangle$ expression into $P(a_n)$ and further deriving it:

$$\begin{aligned} P(a_n) &= |\langle u_n|\psi\rangle|^2 = |\lambda_1\langle u_n|\psi_1\rangle + \lambda_2\langle u_n|\psi_2\rangle|^2 \\ &= (\lambda_1\langle u_n|\psi_1\rangle + \lambda_2\langle u_n|\psi_2\rangle)(\lambda_1^*\langle u_n|\psi_1\rangle^* + \lambda_2^*\langle u_n|\psi_2\rangle^*) \\ &= |\lambda_1|^2|\langle u_n|\psi_1\rangle|^2 + |\lambda_2|^2|\langle u_n|\psi_2\rangle|^2 \\ &\quad + \lambda_1\lambda_2^*\langle u_n|\psi_1\rangle\langle u_n|\psi_2\rangle^* + \lambda_1^*\lambda_2\langle u_n|\psi_1\rangle^*\langle u_n|\psi_2\rangle \\ &= |\lambda_1|^2 P_1(a_n) + |\lambda_2|^2 P_2(a_n) + 2\mathrm{Re}(\lambda_1\lambda_2^*\langle u_n|\psi_1\rangle\langle u_n|\psi_2\rangle) \end{aligned}$$

Thus, the cross term shows the interference effect.

Since $P(a_n)$, $P_1(a_n)$ and $P_2(a_n)$ are the probabilities, $\langle u_n|\psi\rangle$, $\langle u_n|\psi_1\rangle$, and $\langle u_n|\psi_2\rangle$ are called the probability amplitudes. The interference effect is explained by the superposition of the probality amplitudes,

$$\langle u_n|\psi\rangle = \lambda_1\langle u_n|\psi_1\rangle + \lambda_2\langle u_n|\psi_2\rangle.$$

15. Representations:

Above descriptions of QM concepts and principles have been using the abstract state vectors and the abstract linear operators in the abstract state space. They are perfect for expressing the exact meaning of QM principle of superposition of states, principle of uncertainty, principle of motion, and principle of measurements. They also give clear presentation of some derivations like projector operator, mean value, etc.

However, when facing practical problems, we need to project these abstract vectors and operators to a concrete representation in order to do some actual computation. Choosing a representation means choosing an orthonormal basis, either discrete or continuous, in the state space. We then project the state vector and linear operator onto the basis so that the state vector and linear operator are represented by numbers or functions in the actual representation. The choice of a representation is, in theory, arbitrary. In practice, it obviously depends on the particular problem being studied: in each case, one chooses the representation which leads to the simplest calculation.

Two important examples of representations and observables are the coordinate (position) $\{|\vec{r}\rangle\}$ and momentum $\{|\vec{p}\rangle\}$ representations and observables ($\hat{\vec{r}}$ and $\hat{\vec{p}}$). We will use these two as examples to show how to project state and operator to a representation, how to do actual calculation, and how to change from representation to another.

1) State vector versus wave function in $\{|\vec{r}\rangle\}$ and $\{|\vec{p}\rangle\}$ rep:

Recall the principle of superposition of states, for the complete orthonormal states $\{|\vec{r}\rangle\}$, we have $\langle\vec{r}'|\vec{r}\rangle = \delta(\vec{r}-\vec{r}')$. Similarly, for orthonormal $\{|\vec{p}\rangle\}$, we have $\langle\vec{p}'|\vec{p}\rangle = \delta(\vec{p}-\vec{p}')$.

* Any arbitrary state vector $|\psi\rangle$ can be expanded in terms of $\{|\vec{r}\rangle\}$ as: $|\psi\rangle = \int c(\vec{r}')|\vec{r}'\rangle d^3r'$, where $c(\vec{r}')$ is the probability amplitude of the system being in the state of $|\vec{r}'\rangle$, i.e., $|c(\vec{r}')|^2$ is the probability of finding the system at position $\vec{r}'$. As explained earlier,

$$\langle\vec{r}|\psi\rangle = \int c(\vec{r}')\langle\vec{r}|\vec{r}'\rangle d^3r' = \int c(\vec{r}')\delta(\vec{r}-\vec{r}')d^3r' = c(\vec{r})$$

Thus, we repeat the expression for $c(\vec{r})$ [i.e., $c(\alpha)$].

We can write $c(\vec{r}) = \langle\vec{r}|\psi\rangle \equiv \psi(\vec{r})$,

which is called the wave function in the $\{|\vec{r}\rangle\}$ representation.

* Similary, $|\psi\rangle$ can be projected onto $\{|\vec{p}\rangle\}$ representation:

$$|\psi\rangle = \int c(\vec{p}')|\vec{p}'\rangle d^3p' \Rightarrow$$

$$c(\vec{p}) = \langle\vec{p}|\psi\rangle \equiv \psi(\vec{p}),$$

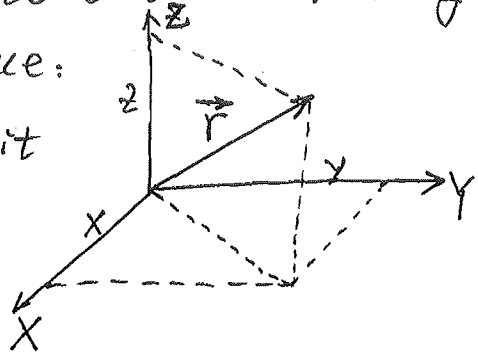
which is the wave function in the $\{|\vec{p}\rangle\}$ representation.

* Wave function $\psi(\vec{r}) = \langle\vec{r}|\psi\rangle$ has the following meaning: it is the probability amplitude of finding a particle at position $\vec{r}$. In other words, $|\psi(\vec{r})|^2 = |\langle\vec{r}|\psi\rangle|^2$ is the probability of the particle appearing at position $\vec{r}$. Similarly, $|\psi(\vec{p})|^2 = |\langle\vec{p}|\psi\rangle|^2$ is the probability of finding the particle with momentum $\vec{p}$.

* Wave function $\psi(\vec{r})$ is the projection of the state vector $|\psi\rangle$ onto the $\{|\vec{r}\rangle\}$ representation, analogy to a vector $\vec{r}$ being projected onto a (X, Y, Z) coordinate space:

$\vec{r} = x\vec{i} + y\vec{j} + z\vec{k}$ ($\vec{i}, \vec{j}, \vec{k}$ are unit vectors along x, y, z axes)

$\therefore \vec{r} \Rightarrow (x, y, z)$.



Analogy: $|\psi\rangle = \int \psi(\vec{r})\,|\vec{r}\rangle\, d^3r$

$\therefore |\psi\rangle \Rightarrow \{\psi(\vec{r})\}$

* In 1-dimension case, $\vec{r} \to x$, so $|\psi\rangle \Rightarrow \{\psi(x)\}$. The conjugate of $|\psi\rangle$, i.e., $\langle\psi| \Rightarrow \{\psi^*(x)\}$. These are the wave functions used in HW #2, problem #2.

* Note $|\langle\vec{r}|\psi\rangle|^2 \equiv \langle\vec{r}|\psi\rangle^* \langle\vec{r}|\psi\rangle$

$|\psi(\vec{r})|^2 \equiv \psi^*(\vec{r})\,\psi(\vec{r})$.

* In priaciple, different representations are equivalent, since they represent the same state vector $|\psi\rangle$ and same operator $\hat{A}$.

(2) Operator in $\{|\vec{r}\rangle\}$ and $\{|\vec{p}\rangle\}$ representations.

In $\{|\vec{r}\rangle\}$ representation, the coordinate $\hat{\vec{r}}$ and momentum $\hat{\vec{p}}$ operators are: $\hat{x} \to x$, $\hat{\vec{r}} \to \vec{r}$

$\hat{p}_x \to -i\hbar\frac{\partial}{\partial x}$, $\hat{\vec{p}} \to -i\hbar\vec{\nabla}$, $\vec{\nabla} = \vec{e}_x\frac{\partial}{\partial x} + \vec{e}_y\frac{\partial}{\partial y} + \vec{e}_z\frac{\partial}{\partial z}$.

In $\{|\vec{p}\rangle\}$ representation, $\hat{\vec{r}}$ and $\hat{\vec{p}}$ operators are

$\vec{p}_x \to p_x$, $\hat{\vec{p}} \to \vec{p}$

$\hat{x} \to i\hbar\frac{\partial}{\partial p_x}$, $\hat{\vec{r}} \to i\hbar\vec{\nabla}_p$, $\vec{\nabla}_p = \vec{e}_{p_x}\frac{\partial}{\partial p_x} + \vec{e}_{p_y}\frac{\partial}{\partial p_y} + \vec{e}_{p_z}\frac{\partial}{\partial p_z}$

Because $\psi(\vec{r})$ and $\psi(\vec{p})$ are the Fourier transform of each other, we have $\hat{\vec{p}} = -i\hbar\vec{\nabla}$ in $\{|\vec{r}\rangle\}$ representation, while $\hat{\vec{r}} = i\hbar\vec{\nabla}_p$ in $\{|\vec{p}\rangle\}$ representation.

* $\{|\vec{r}\rangle\}$ is the most common and widely used representation, also called the Schrödinger representation, in which Schrödinger developed the Schrödinger equation. Let us write down a few other operators in the $\{|\vec{r}\rangle\}$ representation.

① Kinetic energy operator: the classical kinetic energy is given by $E_k = \frac{\vec{p}^2}{2m}$. To quantize it to derive its operator, replace $\vec{p}$ with its corresponding operator $\hat{\vec{p}}$:

$$\hat{E}_k = \frac{\hat{\vec{p}}^2}{2m} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) = -\frac{\hbar^2}{2m}\nabla^2.$$

② Hamiltonian operator $\hat{H}(t)$: the classical $H = \frac{\vec{p}^2}{2m} + V$

Then in QM, $\hat{H}(t) = \frac{\hat{\vec{p}}^2}{2m} + \hat{V}$. If $\hat{V} = V(\hat{\vec{r}})$, then $\hat{V} = V(\vec{r})$

Since $\hat{\vec{r}} = \vec{r}$ in $\{|\vec{r}\rangle\}$, $\hat{H}(t) = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V(\vec{r})$.

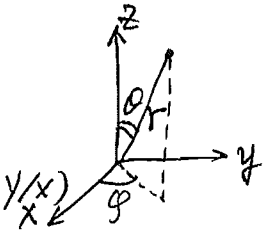
③ Angular momentum operator: the classical angular momentum is $\vec{l} = \vec{r} \times \vec{p}$, where $\vec{r}$ is position vector, $\vec{p}$ is momentum vector.

Corresponding QM operator is:

$$\hat{\vec{l}} = \hat{\vec{r}} \times \hat{\vec{p}} = -i\hbar\, \vec{r} \times \vec{\nabla}.$$

Angular momentum operator components are

$$\begin{cases} \hat{l}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) = i\hbar\left(\sin\varphi\frac{\partial}{\partial\theta} + \cot\theta\cos\varphi\frac{\partial}{\partial\varphi}\right) \\ \hat{l}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) = i\hbar\left(-\cos\varphi\frac{\partial}{\partial\theta} + \cot\theta\sin\varphi\frac{\partial}{\partial\varphi}\right) \\ \hat{l}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = -i\hbar\frac{\partial}{\partial\varphi} \end{cases}$$



The last equality is in spherical coordinates:

$$r = \sqrt{x^2+y^2+z^2},\quad \theta = \arctan\left(\sqrt{x^2+y^2}/z\right),\quad \varphi = \arctan(y/x)$$

④ The square of angular momentum:

$$\hat{\vec{l}}^2 \equiv \hat{l}_x^2 + \hat{l}_y^2 + \hat{l}_z^2$$

$$= -\hbar^2\left[\frac{1}{\sin\theta}\cdot\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right].$$

(3) Mean values in the $\{|\vec{r}\rangle\}$ and $\{|\vec{p}\rangle\}$ representations.

In the abstract state space, as we proved above, the mean value of an observable $\hat{A}$ in the state $|\psi\rangle$ of a system is given by

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

Now project state vector and operator to $\{|\vec{r}\rangle\}$ representation, recall $\int |\vec{r}\rangle\langle\vec{r}| d^3r = 1$, we have

$$\begin{aligned} \bar{A} &= \langle \psi | \hat{A} | \psi \rangle \\ &= \langle \psi | \left(\int |\vec{r}\rangle\langle\vec{r}| d^3r \right) \hat{A} | \psi \rangle \\ &= \int d^3r \langle \psi | \vec{r} \rangle \langle \vec{r} | \hat{A} | \psi \rangle . \end{aligned}$$

Recall $\langle \psi | \vec{r} \rangle = \psi^*(\vec{r})$.

If $\hat{A}$ is a function of $\hat{\vec{r}}$, i.e., $\hat{A} = A(\hat{\vec{r}})$, then since $|\vec{r}\rangle$ is an eigenstate of $\hat{\vec{r}}$, it is also an eigenstate of $A(\hat{\vec{r}})$, i.e., $A(\hat{\vec{r}})|\vec{r}\rangle = A(\vec{r})|\vec{r}\rangle$.

Thus, $\langle \vec{r} | \hat{A} | \psi \rangle = \langle \vec{r} | A(\hat{\vec{r}}) | \psi \rangle = A(\vec{r}) \langle \vec{r} | \psi \rangle = A(\vec{r}) \psi(\vec{r})$,

$\therefore \bar{A} = \int d^3r \, \psi^*(\vec{r}) A(\vec{r}) \psi(\vec{r})$.

Example: In HW #2, Problem #7 (1), 1-D case, $\hat{X}^2$ is a function of $\hat{X}$, i.e., $\hat{X}^2 = (\hat{X})^2$. $\because \hat{X}|x\rangle = x|x\rangle$, $\therefore \hat{X}^2|x\rangle = x^2|x\rangle$.

$\therefore \overline{X^2} = \int dx \, \psi^*(x) x^2 \psi^*(x)$.

Furthermore, since x^2 is just a polynomial term of x, it can exchange order with $\psi^*(x)$ or $\psi(x)$, so

$$\overline{X^2} = \int x^2 |\psi(x)|^2 dx .$$

For the momentum operator $\hat{\vec{p}} = -i\hbar\vec{\nabla}$ in $\{|\vec{r}\rangle\}$ representation, which is NOT a simple function of $\vec{r}$, but involves derivatives.

$$\bar{p} \equiv \langle \hat{\vec{p}} \rangle = \langle\psi|\hat{\vec{p}}|\psi\rangle$$
$$= \langle\psi|\left(\int|\vec{r}\rangle\langle\vec{r}|d^3r\right)(-i\hbar\vec{\nabla})|\psi\rangle$$
$$= \int d^3r \langle\psi|\vec{r}\rangle(-i\hbar)\langle\vec{r}|\vec{\nabla}|\psi\rangle.$$

It can be proven that $\langle\vec{r}|\vec{\nabla}|\psi\rangle = \vec{\nabla}\langle\vec{r}|\psi\rangle = \vec{\nabla}\psi(\vec{r})$

$$\therefore \bar{p} = \int d^3r\, \psi^*(\vec{r})(-i\hbar\vec{\nabla})\psi(\vec{r}).$$

If an operator is a function of $\hat{\vec{p}}$, e.g., $\hat{B} = B(\hat{\vec{p}})$,

then $\hat{B}|\vec{r}\rangle = B(-i\hbar\vec{\nabla})|\vec{r}\rangle$

$$\therefore \quad \bar{B} = \int d^3r\, \psi^*(\vec{r})B(-i\hbar\vec{\nabla})\psi(\vec{r})$$

<u>Example</u>, In HW #2, Problem #7, 1-D case, $\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$,

So $(\hat{p}_x - p_0)^2 = \left(-i\hbar\frac{\partial}{\partial x} - p_0\right)^2 = -\hbar^2\frac{\partial^2}{\partial x^2} + 2i\hbar p_0\frac{\partial}{\partial x} + p_0^2.$

$$\therefore \overline{(\hat{p}_x - p_0)^2} = \int dx\, \psi^*(x)\left[-\hbar^2\frac{\partial^2}{\partial x^2} + 2i\hbar p_0\frac{\partial}{\partial x} + p_0^2\right]\psi(x).$$

Note, since $\frac{\partial^2}{\partial x^2}$, $\frac{\partial}{\partial x}$ are derivatives, not a polynomial of x, they <u>CANNOT</u> switch order with $\psi^*(x)$ or $\psi(x)$!!!

As $\psi(x) = Ae^{-ax^2/2}e^{+ip_0x/\hbar}$, $\psi^*(x) = Ae^{-ax^2/2}e^{-ip_0x/\hbar}$,

you cannot cancel out the imaginary part <u>BEFORE</u> taking derivatives! (Of course, after taking derivatives, you only have x polynomial terms left, then you can swith these x terms with $\psi^*(x)$ or $\psi(x)$, and cancel out $e^{\pm ip_0x/\hbar}$ part !)

If you follow this procedure, Problem #2 (4) should reach a correct answer $\Delta p = \hbar\sqrt{\frac{a}{2}}$.

The same state and same operator can also be projected to different representations, e.g., $\{|\vec{P}\rangle\}$ presentation, and they are equivalent.

The momentum operator $\hat{\vec{P}} = \vec{P}$ in the $\{|\vec{P}\rangle\}$ representation,

$$\therefore \bar{P} \equiv \langle \hat{\vec{P}} \rangle = \langle \psi | \hat{\vec{P}} | \psi \rangle$$

$$= \langle \psi | \left(\int d^3p \, |\vec{P}\rangle\langle\vec{P}| \right) \vec{P} \, |\psi\rangle$$

$$= \int d^3p \, \langle \psi | \vec{P} \rangle \langle \vec{P} | \vec{P} | \psi \rangle$$

$$= \int d^3p \, \langle \psi | \vec{P} \rangle \, \vec{P} \, \langle \vec{P} | \psi \rangle$$

To distinguish $\langle \vec{P} | \psi \rangle$ from $\langle \vec{r} | \psi \rangle$, we write $\langle \vec{P} | \psi \rangle = C(\vec{P})$.

$$\therefore \bar{P} = \int d^3p \cdot C^*(p) \, \vec{P} \, C(p)$$

Similarly, if $\hat{B} = B(\hat{\vec{P}})$, then

$$\bar{B} = \int d^3p \cdot C^*(p) \, B(\vec{P}) \, C(p).$$

Example: In HW #2, Problem #7 (2), $C(P_x)$ is the Fourier transform of $\psi(x)$, and $\hat{P}_x = P_x$, $(\hat{P}_x - P_0)^2 = (P_x - P_0)^2$.

$$\therefore (\hat{P}_x - P_0)^2 = \int dP_x \, C^*(P_x) (P_x - P_0)^2 C(P_x) = \frac{\hbar}{2}\sqrt{\frac{a}{2}}$$

It gives the same result as problem #2(4). This indicates that the $\{|\vec{P}\rangle\}$ representation is equivalent to the $\{|\vec{r}\rangle\}$. With the same state $|\psi\rangle$ and same operator $\hat{p}$, you will get the same results (the root-mean-square) in the $\{|\vec{r}\rangle\}$ and $\{|\vec{P}\rangle\}$ representations. In other words, the results only depend on the state vector $|\psi\rangle$ and the observable operator $\hat{A}$, but independent of representations. But choosing different representations makes the calculation easier or complicated, just like $\hat{p}$ operator has more straightforward calculation in $\{|\vec{P}\rangle\}$.

(4) Eigenvalue Equation in $\{|\vec{r}\rangle\}$ representation.

In the abstract state space, an eigenvalue equation is

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

Where $\hat{A}$ — observable operator, $|\psi\rangle$ — state vector,

a — a complex constant (real number in reality)

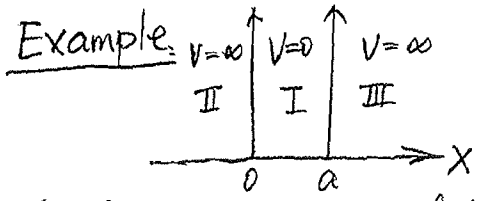
It can be proven that in the $\{|\vec{r}\rangle\}$ representation, the eigen value equation becomes

$$\hat{A}\,\psi(\vec{r}) = a\,\psi(\vec{r})$$

Where $\hat{A}$ is the representation of $\hat{A}$ operator in $\{|\vec{r}\rangle\}$.

$\psi(\vec{r})$ called the eigen wave function, is the projection of the eigen state $|\psi\rangle$ on the $\{|\vec{r}\rangle\}$ representation.

Example:



(1-D) Infinite High Potential Well

A particle moves within a potential well between $x=0$ and $x=a$. The normalized wave function is given by

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right), & 0<x<a \\ 0, & \text{elsewhere.} \end{cases}$$

① Try to derive the mean of the particle's momentum and kinetic energy

② Verify whether this wave function is an eigen-function of momentum, whether an eigen wave function of kinetic energy.

Solution: In $\{|x\rangle\}$ representation, $\hat{\vec{p}} = -i\hbar\frac{\partial}{\partial x}$, $\frac{\hat{\vec{p}}^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$.

$$\overline{p} = \int_{-\infty}^{+\infty} dx\, \psi_n^*(x)\left(-i\hbar\frac{\partial}{\partial x}\right)\psi_n(x) = -\frac{2i\hbar}{a}\int_0^a dx \sin\left(\frac{n\pi x}{a}\right)\left(-i\hbar\frac{\partial}{\partial x}\right)\sin\left(\frac{n\pi x}{a}\right)$$

$$= -i\hbar\frac{2}{a}\cdot\frac{n\pi}{a}\int_0^a \sin\left(\frac{n\pi x}{a}\right)\cos\left(\frac{n\pi}{a}\right)dx$$

$$= -i\hbar\frac{2}{a}\cdot\frac{1}{2}\sin^2\left(\frac{n\pi x}{a}\right)\Big|_0^a = 0-0 = 0.$$

Kinetic energy mean:

$$\overline{\frac{p^2}{2m}} = \int_{-\infty}^{+\infty} \psi_n^*(x)\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\psi_n(x)\,dx$$

$$= -\frac{\hbar^2}{ma}\int_0^a \sin\left(\frac{n\pi x}{a}\right)\frac{\partial^2}{\partial x^2}\sin\left(\frac{n\pi x}{a}\right)dx$$

$$= \frac{\hbar^2}{ma}\left(\frac{n\pi}{a}\right)^2\int_0^a \sin^2\left(\frac{n\pi x}{a}\right)dx$$

$$= \frac{\hbar^2\pi^2n^2}{2ma^2}$$

$$\boxed{\sin^2\theta = \frac{1-\cos 2\theta}{2}}$$

Verifying eigen wave function:

"Apply the operator to the wave function to see whether you can obtain a number times the same wave function!"

(1) $\hat{p}\psi_n(x) = -i\hbar\frac{\partial}{\partial x}\psi_n(x) = -i\hbar\sqrt{\frac{2}{a}}\frac{\partial}{\partial x}\sin\left(\frac{n\pi x}{a}\right) = i\sqrt{\frac{2}{a}}\frac{\hbar n\pi}{a}\cos\left(\frac{n\pi x}{a}\right)$

— $\psi_n(x)$ is NOT $\hat{p}$'s eigen function.

(2) $\frac{\hat{p}^2}{2m}\psi_n(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_n(x) = -\frac{\hbar^2}{2m}\sqrt{\frac{2}{a}}\frac{\partial^2}{\partial x^2}\sin\left(\frac{n\pi x}{a}\right)$

$$= \frac{\hbar^2}{2m}\sqrt{\frac{2}{a}}\left(\frac{n\pi}{a}\right)^2\sin\left(\frac{n\pi x}{a}\right) = \frac{\hbar^2\pi^2n^2}{2ma^2}\psi_n(x)$$

$\therefore \psi_n(x)$ is the eigen function of kinetic energy.

The eigen value is $\frac{\hbar^2\pi^2n^2}{2ma^2}$, the same as the mean we derived above — of course, the mean of the kinetic energy in its own eigenstate is equal to the eigenvalue.

Thus, we solved the HW#3, Problem #3. You may practice it yourself. Then apply similar technique to HW#3, Problem#2.

(5) Schrödinger Equation in $\{|\vec{r}\rangle\}$ and $\{|\vec{p}\rangle\}$ representations.

In the abstract state space, the Schrödinger equation is

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = \hat{H}(t)\,|\psi(t)\rangle.$$

For a (spinless) particle in a scalar potential $V(\vec{r})$, the operator $\hat{H} = \frac{\hat{\vec{p}}^2}{2m} + V(\hat{\vec{r}})$.

It can be proven that in the $\{|\vec{r}\rangle\}$ representation, the Schrödinger equation becomes:

$$i\hbar \frac{\partial}{\partial t}\psi(\vec{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\psi(\vec{r},t).$$

In the $\{|\vec{p}\rangle\}$ representation, the Schrödinger equation is

$$i\hbar \frac{\partial}{\partial t}\bar{\psi}(\vec{p},t) = \frac{\vec{p}^2}{2m}\bar{\psi}(\vec{p},t) + (2\pi\hbar)^{-3/2}\int d^3p'\, \bar{V}(\vec{p}-\vec{p}')\,\bar{\psi}(\vec{p}',t).$$

Here, $\psi(\vec{r},t) \equiv \langle \vec{r}\,|\psi\rangle$

$\bar{\psi}(\vec{p},t) \equiv \langle \vec{p}\,|\psi\rangle$.

$\bar{V}(\vec{p}) = (2\pi\hbar)^{-3/2}\int d^3r\, e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{r}}\, V(\vec{r})$.

§3.6 Solutions to Eigenvalue Equation and Schrödinger Equation

16. Solution to Eigenvalue Equation and Schrödinger Equation.

Schrödinger equation: $i\hbar \frac{\partial}{\partial t}\psi(\vec{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\psi(\vec{r},t)$.

If $V(\vec{r})$ is not explicitly dependent on time t, then we have

$$\psi(\vec{r},t) = \psi(\vec{r})\,T(t).$$

Substituting this into the Schrödinger equation:

$$\frac{i\hbar}{T}\frac{dT}{dt} = \frac{1}{\psi(\vec{r})}\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\psi(\vec{r}) = E$$

(E: total energy)

$$\therefore \frac{i\hbar}{T}\frac{dT}{dt} = E \quad \Rightarrow T = T_0 e^{-iEt/\hbar}$$

$$\begin{cases} \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\psi(\vec{r}) = E\,\psi(\vec{r}) \\ \therefore \psi(\vec{r},t) = \psi(\vec{r})\,e^{-iEt/\hbar}. \end{cases}$$

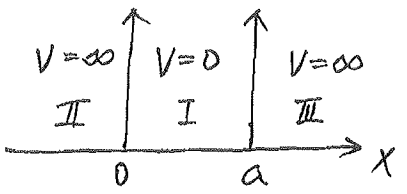
Probability density $= |\psi(\vec{r},t)|^2 = |\psi(\vec{r})|^2$ is independent of t.

i.e., the probability of the particle appearing at position $\vec{r}$ does not change with time!

Equation $\left[-\frac{\hbar^2}{2m}\nabla^2 + \vec{V}(\vec{r})\right]\psi(\vec{r}) = E\,\psi(\vec{r})$ is called the stationary state Schrödinger equation. Essentially, it is the energy eigenvalue equation.

Here, we show a few examples of how to solve the stationary state Schrödinger equation, i.e., the energy eigenvalue equation, to derive the system states and eigenvalues.

(1) 1-Dimension Infinite potential Well



$$V(x) = \begin{cases} \infty, & x<0 \\ 0, & 0<x<a \\ \infty, & x>a \end{cases}$$

The stationary-state Schrödinger equation is: $\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V\right]\psi(x)=E\psi(x)$.

Since a particle cannot be in an infinite potential, $\therefore \psi=0$ in regions II and III. (Physics)

In region I, $V=0$, the equation is simplified to

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) = E\psi(x)$$

Let $k \equiv \sqrt{\frac{2mE}{\hbar^2}}$, then: $\frac{d^2\psi}{dx} + k^2\psi = 0$

The general solution to this equation is

$$\psi = A\sin(kx+\delta),$$

where A and δ are constants to be determined from boundary conditions and normalization requirements.

Considering from physics aspects, since the particle cannot be in the $V=\infty$ region, i.e., the probability to be in regions II and III is zero. Therefore, $\psi(x=0)=0$, $\psi(x=a)=0$.

At $x=0$, $0 = A\sin\delta$.

Since $A\neq 0$ (otherwise, the solution is no meaning),

$\therefore \delta = 0$

At $x=a$, $0 = A\sin ka$.

Since $A\neq 0$, $\therefore \sin ka = 0 \Rightarrow ka = n\pi$ $(n = 1,2,3,\cdots)$

$\therefore k = \frac{n\pi}{a}$.

Here, we kick out $n=0$ and $n<0$ solutions, as they have no meaning in reality. Now: $\psi_n = A\sin\left(\frac{n\pi}{a}x\right)$.

$\because k = \frac{n\pi}{a} = \sqrt{\frac{2mE}{\hbar^2}} \Rightarrow E_n = \frac{\hbar^2\pi^2n^2}{2ma^2}$, $n=1,2,3,\cdots$

$E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2}$ indicates that the particle energy is quantized in the infinit high potential well.

$|\psi(x)|^2$ is the probability density of finding the particle at position x. Since the probability of finding the particle in all space is 1 (i.e., normalization requirement), we have

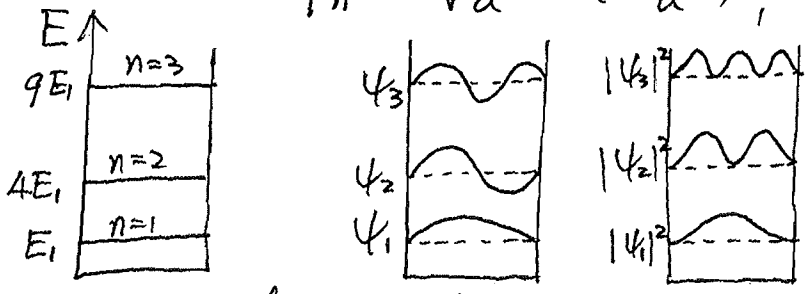
$$\int |\psi(x)|^2 dx = 1$$

$$\therefore \int_0^a A^2 \sin^2 kx\, dx = \int_0^a A^2 \sin^2 \frac{n\pi}{a} x\, dx = A^2 \cdot \frac{a}{2} = 1$$

$$\Rightarrow A = \sqrt{\frac{2}{a}}.$$

$\therefore$ the normalized wave function (eigen wave function) is

$$\psi_n = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right), \quad n = 1, 2, 3, \cdots$$



(a) energy level E_n (b) ψ_n (c) $|\psi_n|^2$

Particle's motion in a potential well is a common phenomenon, e.g., the electron in hydrogen atom does 3-D motion in the Coulomb potential, just the wall is not a square, but distributes along $-\frac{1}{r}$.

* Note: the lowest energy $E_1 \neq 0$, which is completely different from classical mechanics. This is due to the wave nature of particle — "a wave at rest" does not exist!

* Note: the full wave function $\psi_n(x,t) \propto \sin\left(\frac{n\pi x}{a}\right) e^{-iE_n t/\hbar}$, which is a standing wave.

(2) Harmonic Oscillator (1-D):

The force that a particle experiences $F = -kx$, where x is the displacement of particle relative to its balance point 0. $\therefore E_{potential} = \frac{1}{2}kx^2 = V$.

The stationary-state Schrödinger equation is

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x} + \frac{1}{2}kx^2\right)\psi = E\psi.$$

Let $\beta = \alpha x$, where $\alpha = (mk/\hbar^2)^{1/4}$.

$$\therefore \frac{d^2\psi}{d\beta^2} + (\lambda - \beta^2)\psi = 0$$

where $\lambda = \frac{2mE}{\hbar^2\alpha^2} = \frac{2E}{\hbar}\sqrt{\frac{m}{k}} = \frac{2E}{\hbar\omega}$. $\omega = \sqrt{k/m}$.

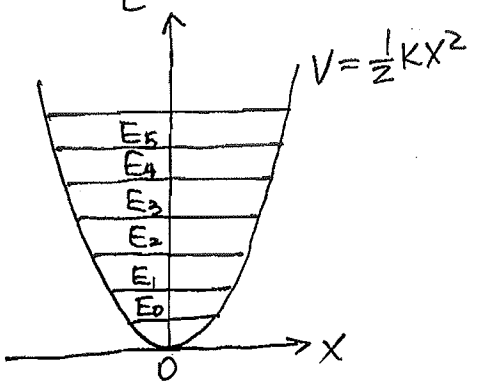
The solution to the equation is:

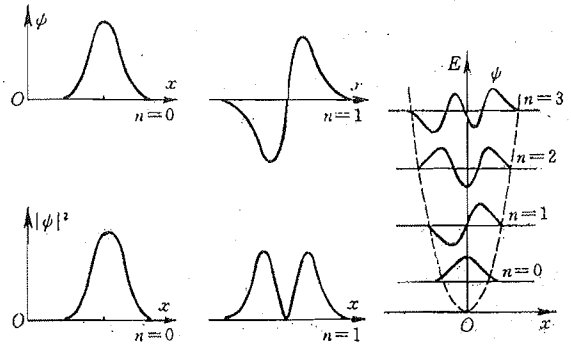
$$E_n = (n + \tfrac{1}{2})\hbar\omega, \quad n = 0, 1, 2, \cdots$$

$$\psi_n = \left(\frac{\alpha}{\sqrt{\pi}\,2^n \cdot n!}\right)^{1/2} e^{-\frac{1}{2}\alpha^2x^2} H_n(\alpha x),$$

where $H_n(\alpha x)$ is Hermitian polynomial

$H_0(\alpha x) = 1$, $H_1(\alpha x) = 2\alpha x$, $H_2(\alpha x) = 4(\alpha x)^2 - 2, \cdots$





① Plot energy levels within the potential energy curve. The length of horizontal lines shows the oscillator motion range.

② When $n = 0$, $E_0 = \frac{1}{2}\hbar\omega \neq 0$. ⇒ no oscillator at rest!

③ E_n are equally separated — similar to Planck's hypothesis — quanta of oscillator energy!