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An Institute of NET-JRF, IIT-JAM, GATE, JEST,
TIFR & CUET in Physics & Physical Sciences

Quantum Mechanics

(NET/JRF, GATE, JEST, TIFR)

CONTENT: QUANTUM MECHANICS

2. POSTULATES OF QUANTUM MECHANICS

The quantum mechanical postulates enable us to understand.

- how a quantum state is described mathematically at a given time *t*.
- how to calculate the various physical quantities from this quantum state.
- Knowing the system's state at a time *t*, how to find the state at any later time *t*. i.e., how to describe the time evolution of a system.

2.1 Postulates of Quantum Mechanics

2.1.1 Postulate 1- State of a Quantum Mechanical System

The state of any physical system is specified, at each time *t*, by a state vector $|\psi(t)\rangle$ in the Hilbert space. $|\psi(t)\rangle$ contains all the needed information about the system. Any superposition of state vectors is also a state vector.

2.1.2 Postulate 2- Physical Measurement of State: To every measurable quantity A to be called an observable or dynamical variable. There corresponds a linear Hermitian $\hat{A}$ whose eigen vectors form a complete basis. $A|\phi_n\rangle = a_n|\phi_n\rangle$

2.1.3 Postulate 3 (a) Probabilistic Measurement of Eigen Value on State: When the physical quantity A is measured on a system in the state $|\psi\rangle$ the probability P(a_n) of obtaining the non-degenerate eigen value an of the corresponding observable A is

$$P(a_n) = \frac{|\langle\phi_n|\psi\rangle|^2}{\langle\psi|\psi\rangle} \quad \text{where } A|\phi_n\rangle = a_n|\phi_n\rangle$$

Postulate 3 (b): When the physical quantity A is measured on a system in the state $|\psi\rangle$. The probability P(a_n) of the obtaining the eigen value an of the corresponding observable A is

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

Where g_n is the degree of degeneracy of an and $|\phi_n^i\rangle$ (i = 1, 2, 3, &, g_n) is orthonormal set of vector which forms a basis in the eigen subspace en associated with eigen value an of A.

2.1.4 Postulate 4: State Just after Measurement

The measurement of an observable A many be represented formally by an action of $\hat{A}$ on a state vector $|\psi(t)\rangle$.

The state of the system immediately after the measurement is the normalized projection $\frac{P_n|\psi\rangle}{\sqrt{\langle\psi|P_n|\psi\rangle}}$ of $|\psi\rangle$ onto the eigen subspace associate with an.

2.1.5 Postulate 5: Time Evolution of State

The time evaluation of the state vector $|\psi(t)\rangle$ is governed by Schrodinger equation

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

Where H is Hamiltonion of the system.

The solution of Schodinger equation must be

(a) single valued and value must be finite

(b) continuous

(c) differentiable

(d) square integrable.

2.2 Expectation Value of Measurement

The expectation value of operator A is given $\langle A\rangle = \dfrac{\langle\psi|A|\psi\rangle}{\langle\psi|\psi\rangle}$ $\Rightarrow \langle A\rangle = \sum_n \dfrac{a_n|\langle\phi_n|\psi\rangle|^2}{\langle\psi|\psi\rangle}$

Where $\langle\psi_m|A|\psi_n\rangle = a_n\delta_{mn} \Rightarrow \langle A\rangle = \sum_n a_n P_n(a_n)$

For continuous variable

- $\langle A\rangle = \dfrac{\int_{-\infty}^{\infty} a|\psi(a)|^2\, da}{\int_{-\infty}^{\infty}|\psi(a)|^2\, da}$

2.3 The momentum and position representation of wave function.

- The ket $|r\rangle$ is eigen ket at X, Y, Z. which is given as
  $X|r\rangle = x|r\rangle \quad Y|r\rangle = y|r\rangle \quad Z|r\rangle = z|r\rangle$
- The ket $|p\rangle$ is the eigen ket of p_x, p_y, p_z which is defined as
  $P_x|p\rangle = p_x|p\rangle \quad P_y|p\rangle = p_y|p\rangle \quad P_z|p\rangle = p_z|p\rangle$

It is given that $\langle r|X|\psi\rangle = x\langle r|\psi\rangle \quad \langle r|Y|\psi\rangle = y\langle r|\psi\rangle \quad \langle r|Z|\psi\rangle = z\langle r|\psi\rangle$

and $\langle r|\psi\rangle = \psi(r)$ and $\langle\psi|r\rangle = \psi^*(r)$.

So $\langle\phi|X|\psi\rangle = \int d^3r\langle\phi|r\rangle\langle r|X|\psi\rangle = \int d^3r\phi^*(r)x\psi(r)$

In momentum space $\langle p|P_x|\psi\rangle = p_x\langle p|\psi\rangle$, $\langle p|P_y|\psi\rangle = p_y\langle p|\psi\rangle$, $\langle p|P_z|\psi\rangle = p_z\langle p|\psi\rangle$

where $\langle p|\psi\rangle = \psi(p)$, $\langle\psi|p\rangle = \psi^*(p)$

$$\langle\phi|p_x|\psi\rangle = \int d^3p\langle\phi|p\rangle\langle p|p_x|\psi\rangle = \int d^3p\phi^*(p)p_x\psi(p)$$

2.4 Fourier transformation and Change in Basis:

Change in basis from one representation to another representation.

$|p\rangle$ is defined as $|p\rangle = \dfrac{1}{\sqrt{2\pi\hbar}}e^{i/\hbar p_x}$

The expansion of $\psi(x)$ in terms of $|p\rangle$ can be written as.

$$\psi(x) = \int_{-\infty}^{\infty} a(p)|p\rangle dp \quad \psi(x) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} a(p)e^{ipx/\hbar}dp$$

where $a(p)$ can be find $a(p) = \dfrac{1}{\sqrt{2\pi\hbar}}\displaystyle\int_{-\infty}^{\infty}\psi(x)e^{-ipx/\hbar}dx$

In 3D $a(p) = \left(\dfrac{1}{2\pi\hbar}\right)^{3/2}\displaystyle\int_{-\infty}^{\infty}\psi(r)e^{-i\vec{p}.\vec{r}/\hbar}d^3r$

Where $a(p)$ being expansion coefficient of $|p\rangle$.

- If any function $\psi(x)$ can be expressed as a linear combination of state function ϕ_n

i.e., $\psi(x) = \sum_n c_n\phi_n(x)$ then where $\int\phi_m^*\phi_n dx = \delta_{mn}$ then $c_n = \int\psi_n^*(x)f(x)dx$

which is popularly derived from fourier trick.

Delta Dirac: The notation $\langle r|r'\rangle$ defined as $\delta(r-r')$. and $\langle p|p'\rangle$ defined as $d(p-p')$

- The orthonormalisation relation in r representation and p representation respectively
  $\langle r|r'\rangle = \delta(r-r') \qquad \langle p|p'\rangle = \delta(p-p')$
- The closure relation in r representation and p representation respectively.
  $\int d^3r|r\rangle\langle r| = 1 \qquad \int d^3p|p\rangle\langle p| = 1$

2.5 Parity Operator

The parity operator Π defined by its action on the basis.

$$\Pi|r\rangle = |-r\rangle \qquad \langle r|\Pi|\psi\rangle = \psi(-r)$$

If $\psi(-r) = \psi(r)$ then state have even parity and

If $\psi(-r) = -\psi(r)$ then state have odd parity.

So parity operator have $+1$ and -1 eigen value.

Representation of postulate (4) in continuous basis.

When the physical quantity A is measured on a system state $|\psi\rangle$ the probability $dp(\alpha)$ of obtaining a result included α and $\alpha + d\alpha$ is equal to

$$dp(\alpha) = \frac{|V_\alpha|\psi\rangle|^2\, d\alpha}{\langle\psi|\psi\rangle}$$

Where $|V_\alpha\rangle$ is the eigen vector corresponding to the eigen value α of the observable A.

Example: A state function is given by

$$|\psi\rangle = |\phi_1\rangle + \frac{1}{\sqrt{2}}|\phi_2\rangle$$

It is given that $\langle\phi_i|\phi_j\rangle = \delta_{ij}$

(a) check $|\psi\rangle$ is normalized or not

(b) write down normalized wavefunction $\langle\psi|$.

(c) It is given $H|\phi_n\rangle = (n+1)\hbar\omega|\phi_n\rangle \qquad n = 0, 1, 2, 3, \ldots$

If H will measured on $|\psi\rangle$, what will be measurement with what probability.

(a) Find the expectation value at H i.e., $\langle H\rangle$

(b) Find the error in the measurement in H.

Solution: (a) To check normalization one should verify.

$$\langle\psi|\psi\rangle = 13$$

$$|\psi\rangle = |\phi_1\rangle + \frac{1}{\sqrt{2}}|\phi_2\rangle$$

$$\langle\psi|\psi\rangle = \langle\phi_1|\phi_1\rangle + \langle\phi_1|\phi_2\rangle\frac{1}{\sqrt{2}}\langle\phi_2|\phi_1\rangle + \frac{1}{\sqrt{2}}\langle\phi_2+\phi_2\rangle\left(\frac{1}{\sqrt{2}}\right)^2 = 1+0+0+\frac{1}{2} = \frac{3}{2}$$

The value of $\langle\psi|\psi\rangle = \frac{3}{2}$ so $|\psi\rangle$ is not normalized.

(b) Now we need to find normalized $|\psi\rangle$ let A be normalization constant.

$$|\psi\rangle = A|\phi_1\rangle + \frac{1}{\sqrt{2}}|\phi_2\rangle$$

$$\langle\psi|\psi\rangle = A^2 + \frac{A^2}{2} = 1 \quad \Rightarrow \frac{3A^2}{2} = 1 \Rightarrow A = \sqrt{\frac{2}{3}}$$

$$\text{So } |\psi\rangle = \sqrt{\frac{2}{3}}|\phi_1\rangle + \frac{1}{\sqrt{3}}|\phi_2\rangle$$

$$\langle\psi| = \langle\phi_1|\frac{2}{\sqrt{3}} + \langle\phi_2|\frac{1}{\sqrt{2}}$$

(c) It is given that

$$H|\phi_n\rangle = (n+1)\hbar\omega \qquad n = 0, 1, 2, 3\ldots$$

$$H|\phi_1\rangle = 2\hbar\omega \qquad H|\phi_2\rangle = 3\hbar\omega$$

When H will measured $|\psi\rangle$ it will measured either $2\hbar\omega$ or $3\hbar\omega$

The probability of measured $2\hbar\omega$ is $P(2\hbar\omega)$ is given by

$$P(2\hbar\omega)=\frac{|\langle\phi_1|\psi\rangle|^2}{\langle\psi|\psi\rangle}=\frac{2}{3} \qquad P(3\hbar\omega)=\frac{|\langle\phi_2|\psi\rangle|^2}{\langle\psi|\psi\rangle}=\frac{1}{3}$$

So when H will measure state $|\psi\rangle$ the following outcome will come.

Measurement of H on state	: $\lvert\phi_1\rangle$	$\lvert\phi_2\rangle$
Measurement	: $2\hbar\omega$	$3\hbar\omega$
Probability	: 2/3	1/3

(d) $$\langle H\rangle=\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}=\sum_n P_n(a_n)a_n$$

$$=2\hbar\omega\times\frac{2}{3}+3\hbar\omega\times\frac{1}{3} \qquad \langle H\rangle=\frac{7\hbar\omega}{3}$$

$$\langle H^2\rangle=\frac{\langle\psi|H^2|\psi\rangle}{\langle\psi|\psi\rangle}=\Sigma P_n(a_n)a_n^2=\frac{2}{3}\times(2\hbar\omega)^2+\frac{1}{3}\times(3\hbar\omega)^2=\frac{8\hbar^2\omega^2}{3}+\frac{9\hbar^2\omega^2}{3}=\frac{17\hbar^2\omega^2}{3}$$

(e) The error in measurement in H is given as

$$\Delta H=\sqrt{\langle H^2\rangle-\langle H\rangle^2} \qquad \langle H^2\rangle=\frac{17\hbar^2\omega^2}{3}$$

$$\langle H\rangle^2=\left(\frac{7\hbar\omega}{3}\right)^2=\frac{49\hbar^2\omega^2}{9} \qquad \Delta H=\sqrt{\frac{17}{3}-\frac{49}{9}}\hbar\omega$$

$$\Delta H=\sqrt{\frac{51-49}{9}}\hbar\omega=\frac{\sqrt{2}}{3}\hbar\omega$$

Example: (a) Plot $\psi_I(x)=A_1e^{-|x|}\quad -\infty<x<\infty$

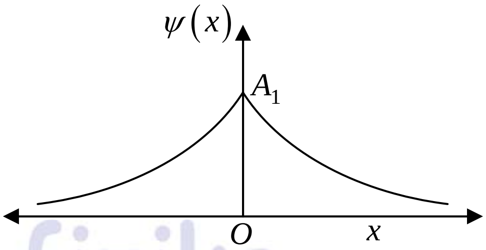
(b) Plot $\psi_{II}(x)=A_2e^{-x^2}\quad -\infty<x<\infty$

(c) discuss why ψ_I is not solution of schrodinger wave function rather ψ_{II} is solution of schrodinger wave function.

Solution: (a) $\psi_I(x)=A_1e^{+x}\, x<0$

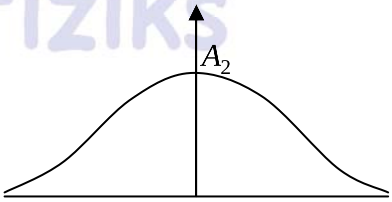
$\psi_{II}(x)=A_1e^{-x}\, x>0$

The plot is given by



(b) $\psi_{II}(x)=A_2e^{-x^2}\quad -\infty<x<\infty$

The plot is given by



(c) Both the function ψ_I and ψ_{II} are single value, continuous, square integrable by ψ_I is not differentiable of $x = 0$ rather ψ_{II} is differentiable at $x=0$

So ψ_{II} can be solution of schrodinger wave function but ψ_I is not solution of schrodinger wave function.

Example: A time $t = 0$ the state vector $|\psi(0)\rangle$

$$|\psi(0)\rangle=\frac{1}{\sqrt{2}}\left(|\phi_1\rangle+|\phi_2\rangle\right)$$

It is given as Hamiltonion is defined as $H|\phi_n\rangle=n^2\in_0|\phi_n\rangle$

(a) What is wave function $|\psi(t)\rangle$ at later time t.

(b) Write down expression of evolution of $|\psi(x,t)|^2$

(c) Find ΔH

(d) Find the value of ΔH · Δt

Solution: (a) $|\psi(t)\rangle = \frac{1}{\sqrt{2}}\left[e^{\frac{-i\in_0 t}{\hbar}}|\phi_1\rangle + e^{\frac{-i4\in_0 t}{\hbar}}|\phi_2\rangle\right]$

$$|\psi(t)\rangle \propto \left[|\phi_1\rangle + e^{-\omega_{21}t}|\phi_2\rangle\right]$$

Where $\omega_{21} = \frac{E_2 - E_1}{\hbar} = \frac{3\in_0}{\hbar}$

(b) Evolution of shape of the wave packet

$$|\psi(x,t)|^2 = \frac{1}{2}|\phi_1(x)|^2 + \frac{1}{2}|\phi_2(x)|^2 + \phi_1\phi_2\cos\omega_{21}t$$

(c) $\Delta H = \left(\langle H^2\rangle - \langle H\rangle^2\right)^{1/2}$

$$\langle H\rangle = \frac{1}{2}E_1 + \frac{1}{2}E_2 = \frac{5}{2}E_1 \qquad \langle H^2\rangle = \frac{1}{2}E_1^2 + \frac{1}{2}E_2^2 = \frac{17}{2}E_1^2$$

$$\Delta H = \frac{3}{2}E_1 \qquad \Delta H = \frac{3}{2}\times\in_0$$

(d) $\Delta H = \frac{3}{2}\in_0 \qquad \Delta t = \frac{1}{\Delta\omega_{21}} \qquad \Delta t = \frac{\hbar}{3\in_0} \qquad \Delta H\cdot\Delta t = \frac{3}{2}\in_0\times\frac{\hbar}{3\in_0} = \frac{\hbar}{2}$

$$\Delta H\cdot\Delta t = \frac{\hbar}{2}$$

Example: Consider a one-dimensional particle which is confined within the region $0 \le x \le a$ and whose wave function is $\psi(x,t) = \sin\left(\frac{\pi x}{a}\right)e^{i\omega t}$. Find the potential $V(x)$.

Solution: From the fifth postulate.

$$H\psi = i\hbar\frac{\partial\psi}{\partial t} \qquad H = \frac{P^2}{2m} + V(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi = i\hbar\frac{\partial\psi}{\partial t}$$

$$\frac{\pi^2\hbar^2}{2ma^2}\sin\frac{\pi x}{a}e^{i\omega t} + V(x)\frac{\sin\pi x}{a}e^{i\omega t} = i\hbar\sin\frac{\pi x}{a}(-i\omega)e^{i\omega a}$$

$$\frac{\pi^2\hbar^2}{2ma^2} + V(x) = -\hbar\omega \qquad V(x) = -\hbar\omega - \frac{\pi^2\hbar^2}{2ma^2} \qquad V(x) = -\left(\hbar\omega + \frac{\pi^2\hbar^2}{2ma^2}\right)$$

Example: If eigen value of operator A is 0, $2a_0$, $2a_0$ and corresponding normalized eigen vector is $\frac{1}{\sqrt{2}}\begin{pmatrix}0\\-i\\1\end{pmatrix}, \frac{1}{\sqrt{2}}\begin{pmatrix}0\\i\\1\end{pmatrix}$ and $\begin{pmatrix}1\\0\\0\end{pmatrix}$ respectively *t* system is in state $\frac{1}{6}\begin{pmatrix}1\\0\\4\end{pmatrix}$ then

(a) When A is measured on system in state $\frac{1}{6}\begin{pmatrix}1\\0\\4\end{pmatrix}$ then what is probability to getting value $0,\ 2a_0$, respectively.

(b) What is expectation value of A?

Solution: Let $|\phi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\-i\\1\end{pmatrix}$ $\quad\lambda_1 = 0$ $\quad ,|\phi_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\i\\1\end{pmatrix}$ $\lambda_2 = 2a_0$

$\lambda_2 = \lambda_3 = 2a_0$ i.e., $\lambda = 2a_0$ is doubly degenerate.

$$P(0) = \frac{|\langle\phi_1|\psi(t)\rangle|^2}{\langle\psi|\psi\rangle} = \frac{8}{17}$$

$$P(2a_0) = \frac{|\langle\phi_2|\psi(t)\rangle|^2}{\langle\psi|\psi\rangle} + \frac{|\langle\phi_3|\psi(t)\rangle|^2}{\langle\psi|\psi\rangle} = \frac{\left[\left(\frac{1}{\sqrt{2}}(0\ \ -i\ \ 1)\right)\frac{1}{6}\begin{pmatrix}1\\0\\4\end{pmatrix}\right]^2}{\frac{1}{6}(1\ \ 0\ \ 4)\frac{1}{6}\begin{pmatrix}1\\0\\4\end{pmatrix}} + \frac{\left[(1\ \ 0\ \ 0)\frac{1}{6}\begin{pmatrix}1\\0\\4\end{pmatrix}\right]^2}{\frac{1}{6}(1\ \ 0\ \ 4)\frac{1}{6}\begin{pmatrix}1\\0\\4\end{pmatrix}}$$

$$= \frac{\frac{1}{2}\times\frac{1}{36}\times 16}{\frac{1}{36}\cdot(1+16)} + \frac{\frac{1}{36}}{\frac{17}{36}}$$

$$= \frac{\frac{2}{9}}{\frac{17}{36}} + \frac{1}{17} = \frac{9}{17} \Rightarrow \langle A\rangle = 0\times\frac{8}{17} + 2a_0\times\frac{9}{17} \Rightarrow \langle A\rangle = \frac{18a_0}{17}\text{ average value.}$$

Example: A free particle which is initially localized in the range $-a < x < a$ is released at time $t = 0$.

$$\psi(x) = \begin{cases} A & \text{if } -a < x < a \\ 0 & \text{otherwise} \end{cases}$$

Find (a) A such that $\psi(x)$ is normalized.

(b) Find $\phi(x)$ i.e., wave function in momentum space.

(c) Find $\psi(x,t)$ i.e., wave function after t time.

Solution: (a) $\int_{-\infty}^{\infty}|\psi(x,t)|^2\,dx = A^2\int_{-a}^{a}dx = 1 \Rightarrow A = \frac{1}{\sqrt{2a}}$

(b) $\phi(x) = \frac{1}{\sqrt{2\pi}}\int_{-a}^{a}e^{-ikx}\psi(x)dx = \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2a}}\int_{-a}^{a}e^{-ikx} = \frac{1}{\sqrt{2\pi}}\frac{\sin ka}{k}$

(c) $\psi(x,t) = \frac{1}{\pi\sqrt{2a}}\int_{-\infty}^{\infty}\frac{\sin ka}{k}e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)}dk$