Lect 5 Mathematical description of fundamental principles of quantum mechanics

1. $A|\psi_n\rangle = \lambda_n|\psi_n\rangle$

$$|\psi\rangle = \sum_n c_n|\psi_n\rangle$$

$$1 = \sum_n |\psi_n\rangle\langle\psi_n| ,$$

2° $[x, p] = i\hbar$, $p = i\hbar \frac{d}{dx}$

3° $|\psi_n^A\rangle = \sum_m |\psi_m^B\rangle\langle\psi_m^B|\psi_n^A\rangle$ $S_{mn} = \langle\psi_n^A|\psi_m^B\rangle$

$$\langle\psi_m^B|O|\psi_n^B\rangle = (S^+ O^A S)_{mn}$$

4° Postulates of QM

- Quantum states and observables
- expectation values
- time-evolution
- identical particles

§ Quantum states and Dirac symbol

physical states $|ket\rangle$. $|\psi_1\rangle, |\psi_2\rangle \cdots$, which span a linear space V. The inner product on V is defined.

For a Hermitian operator A, we define its eigenvector

$$A|\psi_n\rangle = \lambda_n |\psi_n\rangle, \qquad n=1,2,3,\cdots$$

$|\psi_n\rangle$ spans a complete normalized basis
set of

any state $|\psi\rangle \in V$, $|\psi\rangle$ can be expanded in terms of

$$\boxed{|\psi\rangle = \sum_n c_n |\psi_n\rangle}$$

1° λ_n is a real number

$$\langle\psi_n|A|\psi_n\rangle = \lambda_n\langle\psi_n|\psi_n\rangle = \lambda_n$$

$$\left.\begin{array}{l} \parallel \\ \langle A^+\psi_n|\psi_n\rangle = \langle\psi_n|A^+|\psi_n\rangle^* = \langle\psi_n|A|\psi_n\rangle^* = \lambda_n^* \end{array}\right\}$$

$$\Rightarrow \lambda_n = \lambda_n^*$$

2° if $\lambda_n \neq \lambda_m$, then $\langle\psi_n|\psi_m\rangle = 0$

$$\left.\begin{array}{l} \langle\psi_m|A|\psi_n\rangle = \langle\psi_m|\psi_n\rangle . \lambda_n \\ \parallel \\ \langle A\psi_m|\psi_n\rangle = \langle\psi_m|\psi_n\rangle \lambda_m \end{array}\right\} \Rightarrow (\lambda_n-\lambda_m)\langle\psi_m|\psi_n\rangle = 0$$

$$\Rightarrow \langle\psi_m|\psi_n\rangle = 0$$

3° If there are more than one states with the same eigenvalue λ_n. We organize them as one subspace. This situation is called degeneracy. We use another Hermitian operator B, such that $[A, B] = 0$, to decompose this subspace as different eigenstates of B.

$$B|\psi_{n,l_i}\rangle = \lambda^B_i |\psi_{n,l_i}\rangle, \quad i = 1, 2, 3, \cdots.$$

Theorem of linear algebra: "two commutable Hermitian matrices (operators) share the same sets of eigenvectors"

$$A|\psi_{n,l}\rangle = \lambda^A_n |\psi_{n,l}\rangle$$

$$B|\psi_{n,l}\rangle = \lambda^B_n |\psi_{n,l}\rangle.$$

Example: Hydrogen atom:

$$\begin{cases} H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r} \\ L^2 = l_x^2 + l_y^2 + l_z^2 \\ l_z = -i\hbar\frac{\partial}{\partial\varphi} = xP_y - yP_x \end{cases}$$

$$[H, L^2] = [H, L_z] = [L^2, L_z] = 0$$

$$\begin{cases} H\psi_{nlm} = E_n \psi_{n,l,m} \\ L^2\psi_{nlm} = l(l+1)\hbar^2 \psi_{n,l,m} \\ L_z\psi_{nlm} = m\hbar\,\psi_{nlm} \end{cases}$$

4° Completeness

$$|\psi\rangle = \sum_n C_n |\psi_n\rangle \quad \Rightarrow \quad \langle \psi_n | \psi \rangle = C_n$$

$$|\psi\rangle = \left(\sum_n |\psi_n\rangle\langle\psi_n|\right)|\psi\rangle$$ this is valid for any state vector

$$\Rightarrow \boxed{1 = \sum_n |\psi_n\rangle\langle\psi_n|}$$

5° generalization to continuous spectra

$$\hat{x}\,|x\rangle = x\,|x\rangle \qquad \int |x\rangle\langle x|\,dx = 1$$

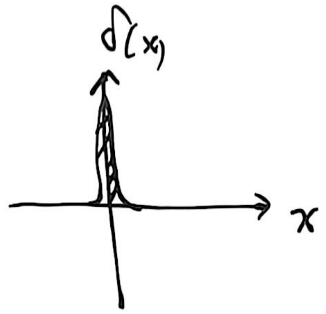
$$\langle x|x'\rangle = \delta(x-x')$$

coordinate representation

$$|\psi\rangle = \int dx\ |x\rangle\ \psi(x)$$ ← definition of wavefunction

$$\langle x|\psi\rangle = \int dx'\ \langle x'|x\rangle\ \psi(x') = \int dx'\ \delta(x-x')\,\psi(x') = \psi(x)$$

Dirac - δ - function



$$\begin{cases} \delta(x-x') = 0 & \text{if } x \neq x' \\ \int dx\ \delta(x-x') = 1 \end{cases}$$

$$\delta(x) = \frac{1}{\pi}\frac{a}{x^2+a^2}\Big|_{a\to 0}, \qquad \frac{1}{x \pm i\epsilon} = P\left(\frac{1}{x}\right) \mp i\pi\delta(x)$$

$$= \lim_{a\to 0} \frac{1}{a\sqrt{\pi}}\, e^{-\frac{x^2}{a^2}}$$

principle value

how to understand the diffential operators?

check $[\hat{x}, \hat{p}] = i\hbar$

$$\langle x'| [\hat{x}, \hat{p}] |x\rangle = \langle x'| \hat{x}\hat{p} - \hat{p}\hat{x} |x\rangle = (x'-x) \langle x' | \hat{p} | x\rangle = i\hbar\, \delta(x-x')$$

$$\langle x' | \hat{p} | x\rangle = i\hbar / x'-x \cdot \delta(x-x') = -i\hbar \frac{\delta(x-x')}{x-x'}$$

According to $\int_{-\infty}^{+\infty} dx \; x \frac{d}{dx} \delta(x) = - \int_{-\infty}^{+\infty} dx \; \delta(x) = -1$

$$\Rightarrow \quad x \frac{d}{dx} \delta(x) = -\delta(x) \quad \text{or} \quad \frac{d}{dx} \delta(x) = - \frac{\delta(x)}{x} \leftarrow$$

treat x as varible
x' as constant

$$\Rightarrow \langle x' | \hat{p} | x\rangle = i\hbar \frac{d}{dx} \delta(x-x') =$$

$$\langle x' | \hat{p} | \psi\rangle = \int dx \langle x' | \hat{p} | x\rangle \langle x | \psi\rangle = i\hbar \int dx \frac{d}{dx} \delta(x-x')\, \psi(x)$$

$$= -i\hbar \int dx\, \delta(x-x') \frac{d}{dx} \psi(x) = -i\hbar \frac{d}{dx} \psi(x) \Big|_{x=x'}$$

or $\langle x | \hat{p} | \psi\rangle = -i\hbar \frac{d}{dx} \psi(x)$

Calculate $\langle x | p\rangle \Rightarrow \quad \langle x | \hat{p} | p\rangle = p \langle x | p\rangle$

$\quad\quad\quad\; // \; \psi_p(x) \quad\quad -i\hbar \frac{d}{dx} \psi_p(x) = p\, \psi_p(x)$

$$\Rightarrow \psi_p(x) = A\, e^{i p \cdot x/\hbar}$$

normalization : box $\Rightarrow A = \frac{1}{\sqrt{L}} \Rightarrow \langle p | p'\rangle = \delta_{p,p'}$

continuum $A = \frac{1}{(2\pi)^{1/2}} \Rightarrow \langle p | p'\rangle = \delta(p-p')$

§ transformation

We can either use $\hat{A}$ or $\hat{B}$'s eigenstates $|\psi_i^A\rangle$ or $|\psi_j^B\rangle$ to represent quantum states and mechanical observables

$$|\psi\rangle = \sum_n A_n |\psi_n^A\rangle = \sum_m B_m |\psi_m^B\rangle$$

$$\boxed{A_n = \sum_m \langle \psi_n^A | \psi_m^{B'} \rangle B_m}$$

define $S_{nm} = \langle \psi_n^A | \psi_m^B \rangle$

$$\boxed{A = SB}$$

$$\boxed{\begin{aligned} |\psi_n^A\rangle &= \sum_m |\psi_m^B\rangle\langle\psi_m^B|\psi_n^A\rangle \\ &= \sum_m |\psi_m^B\rangle S_{mn}^\dagger \end{aligned}}$$

$$O = \sum_{mn} |\psi_m^A\rangle\langle\psi_m^A| O |\psi_n^A\rangle\langle\psi_n^A| = \sum_{mn} |\psi_m^A\rangle\langle\psi_n^A| \, O_{mn}^A$$

where $O_{mn}^A = \langle\psi_m^A| O |\psi_n^A\rangle$

Similarly $O_{mn}^B = \langle\psi_m^B| O |\psi_n^B\rangle$

$$= \sum_{m'n'} \langle\psi_m^B|\psi_{m'}^A\rangle\langle\psi_{m'}^A| O |\psi_{n'}^A\rangle\langle\psi_{n'}^A|\psi_n^B\rangle$$

$$= S_{mn'}^\dagger O_{m'n'}^A S_{n'm}$$

$$\Rightarrow O^B = S^\dagger O^A S$$

Born's intepretation

$$|\psi\rangle = \int dx\ |x\rangle\ \psi(x) \quad \rightarrow dP(x) = |\psi(x)|^2 dx$$

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

For an arbitary representation

$$|\psi\rangle = \sum_n |\psi_n^A\rangle \langle \psi_n^A|\psi\rangle \quad \Rightarrow \quad P_n(x) = |\langle \psi_n^A|\psi\rangle|^2$$

$$\begin{aligned}\bar{A} = \sum_n P_n(x)\ \lambda_n &= \sum_n \langle \psi_n^A|\psi\rangle \langle \psi|\psi_n^A\rangle\ \lambda_n \\ &= \sum_n \langle \psi|\underbrace{\psi_n^A\rangle \lambda_n \langle \psi_n^A}|\psi\rangle \\ &= \langle \psi|A|\psi\rangle\end{aligned}$$

§ Postulates of QM

1 Quantum state and mechanical observable

One quantum state is represented by a vector in Hilbert space. An physical observable $\hat{A}$ can be described by a Hermitian operator. Momentum and coordinate satisfy the fundamental commutation relation $[\hat{x}, \hat{p}] = i\hbar$

For a classic mechanical variable $F(x, p)$, we can replace x, p by their operators and symmetrize them

2. Expectation value

$|\psi_n\rangle$ is the eigenstate of a Hermitian operater $\hat{A}$ with the eigenvalue λ_n, i.e $\hat{A}|\psi\rangle = \lambda_n |n\rangle$.

An arbitary $|\psi\rangle = \sum_n C_n |n\rangle$, if we meaure $\hat{A}$ wer $|\psi\rangle$, then the $P_n = |C_n|^2$ represent the probability to obtain λ_n.

3. time-evolution

The time evolution of a quantum state $|\psi(t=0)\rangle$ is given by $i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}\psi(t)$. The solution of $|\psi(t)\rangle$ is uniquely determined by $|\psi(0)\rangle$. $\hat{H}(x,p)$ is obtained by replace x, p by $\hat{x}, \hat{p}$ in the classic Hamiltonian.

4 identical particles

In 3+1 d space time, the many body wave funtion $\psi(x_1, \cdots x_N)$ a under exchange $x_i \leftrightarrow x_j$ is either symmetric, or antisymmetrie

8 Uncertainty principle

$$\Delta A = \hat{A} - \bar{A}, \quad \Delta B = \hat{B} - \bar{B}$$

$$\overline{(\Delta A)^2} = \overline{A^2} - (\bar{A})^2$$

Conside state $|\psi\rangle$, denote $|\alpha\rangle = \Delta A|\psi\rangle$

$|\beta\rangle = \Delta B|\psi\rangle$

$$\overline{(\Delta A)^2} = \langle\alpha|\alpha\rangle \qquad \overline{\Delta A \Delta B} = \langle\alpha|\beta\rangle$$

$$\overline{(\Delta B)^2} = \langle\beta|\beta\rangle$$

Schwartz non-equality $\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2$

$$\overline{(\Delta A)^2}\ \overline{(\Delta B)^2} \geq |\overline{\Delta A \Delta B}|^2$$

$$\Delta A \Delta B = \left[[\Delta A, \Delta B] + \{\Delta A, \Delta B\}\right]/2$$

anti-Hermitian ... Hermital

$$\overline{\Delta A \Delta B} = \frac{1}{2}\overline{[\Delta A, \Delta B]} + \frac{1}{2}\overline{\{\Delta A, \Delta B\}}$$

imagniy ... real

$$|\overline{\Delta A \Delta B}|^2 = \frac{1}{4}|\overline{[\Delta A, \Delta B]}|^2 + |\overline{\{\Delta A, \Delta B\}}|^2/4$$

$$= \frac{1}{4}\left\{|\overline{[A, B]}|^2 + |\overline{\{\Delta A, \Delta B\}}|^2\right\}$$

$$\therefore \overline{(\Delta A)^2}\ \overline{(\Delta B)^2} \geq \frac{1}{4}|\overline{[A, B]}|^2$$

$$\overline{(\Delta x)^2}\ \overline{(\Delta p)^2} \geq \frac{\hbar^2}{4} \quad \text{or} \quad \boxed{\sqrt{\overline{(\Delta x)^2}}\sqrt{\overline{(\Delta p)^2}} \geq \hbar/2}$$