

$\hat{H} \Psi(\vec{x}, t) = i\hbar \frac{\partial}{\partial t} \Psi(\vec{x}, t)$  "TDSE"

If  $\int d^3x \Psi^*(\vec{x}, t) \Psi(\vec{x}, t) = 1$

$\Psi(\vec{x}, t) = \sum_n c_n e^{-i/\hbar E_n t} \psi_n(\vec{x})$

$\Rightarrow \sum_n |c_n|^2 = 1$  "Completeness Relation"

only true if  $\hat{H} \neq \hat{H}(t)$

$\hat{H} \psi_n(\vec{x}) = E_n \psi_n(\vec{x})$  "TISE"

$\langle \hat{H} \rangle = \int d^3x \Psi(\vec{x}, t) \hat{H} \Psi(\vec{x}, t) = \sum_n |c_n|^2 E_n$  "Conservation of Energy"

$|c_n|^2$ : prob. that if we measure the energy on a system represented by  $\Psi(\vec{x}, t)$  we will obtain the value  $E_n$

The possible result of measuring the energy is restricted to the set of values  $\{E_1, E_2, E_3, \dots, E_n\}$

The set of values  $c_n$  is determined by the initial conditions of the system.

$c_n = \int d^3x' \psi_n^*(\vec{x}') \tilde{\Psi}(\vec{x}', 0)$

In Linear Algebra, in a basis  $\{\hat{e}_1, \hat{e}_2, \hat{e}_3\}$

$\vec{v} = v_1 \hat{e}_1 + v_2 \hat{e}_2 + v_3 \hat{e}_3 = v_i \hat{e}_i$

$v_i = \hat{e}_i \cdot \vec{v}$

$\hat{e}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}; \hat{e}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}; \hat{e}_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$

$\vec{v} = (\hat{e}_i \hat{e}_i) \cdot \vec{v}$

(Outer Product)

$\hat{e}_1 \hat{e}_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$

$\hat{e}_3 \hat{e}_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

$\hat{e}_2 \hat{e}_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$

$\hat{e}_i \hat{e}_i = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \mathbb{1}$

$(1 \ 0 \ 0) \otimes \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \mathbb{1}$  \*

$\sum_i |v_i|^2 = |\vec{v}|^2 = 1$

in component form:

$(\sum_i |\hat{e}_i|^2)_{lm} = \delta_{lm}$  \*

"Closure Relation"

Closure Relation In Q.M.

$\Psi(\vec{x}, t) \Big|_{t=0} = \sum_n c_n e^{-i/\hbar E_n t} \psi_n(\vec{x}) \Big|_{t=0}$

$\vec{A} \cdot \vec{B} = A_i B_i$

$\vec{A} \cdot \vec{B} \vec{C} \cdot \vec{D} = A_i B_j C_j D_i$

$\Psi(\vec{x}, 0) = \sum_n \int d^3x' \psi_n^*(\vec{x}') \Psi(\vec{x}', 0) \psi_n(\vec{x})$

$$\underbrace{\Psi(\vec{x}, 0)}_{*} = \sum_n \int d^3x' \psi_n^*(\vec{x}') \Psi(\vec{x}', 0) \psi_n(\vec{x})$$

$$= \int d^3x' \left( \sum_n \psi_n^*(\vec{x}') \psi_n(\vec{x}) \right) \Psi(\vec{x}', 0)$$

$$\Rightarrow \sum_n \psi_n^*(\vec{x}') \psi_n(\vec{x}) = \delta^3(\vec{x} - \vec{x}') \quad * \quad \text{"Closure Relation"}$$

$\begin{pmatrix} 1 \\ e_i \end{pmatrix}$   
↑  
↑

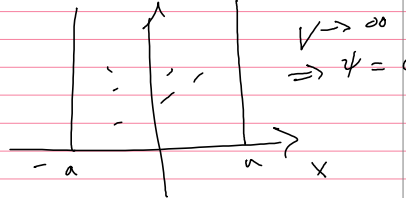
$\psi_n(\vec{x})$   
↑ ↑

$$\delta^3(\vec{x} - \vec{x}') = \delta(x - x') \delta(y - y') \delta(z - z')$$

$$\vec{x} = (x, y, z)$$

for Example for a Particle in a Box

$$V(x) = \begin{cases} 0 & |x| < a \\ \infty & \text{forall other } x \end{cases}$$



In the Region  $x \in \{-a, a\}$   $V(x) = 0 \Rightarrow H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$

$$\Rightarrow \text{In } \{-a, a\} \Rightarrow H\psi(x) = E\psi(x)$$

$$\psi(x) = A e^{\pm ikx} ; \quad E = \frac{\hbar^2 k^2}{2m}$$

B.C.  $\psi(a) = \psi(-a) = 0$

$$\Rightarrow k \text{ is quantized } \left. \begin{matrix} k_n = \frac{n\pi}{a} \\ n = 1, 2, \dots \end{matrix} \right\}$$

$$\psi(x) = \frac{e^{ikx} \pm e^{-ikx}}{\sqrt{2}} \quad \begin{matrix} \cos kx \\ \sin kx \end{matrix}$$

Normalization:  $\int_{-a}^a \psi^*(x) \psi(x) dx = 1 \Rightarrow A = \sqrt{\frac{2}{a}}$

$$\psi_n^{(e)}(x) = \sqrt{\frac{2}{a}} \cos k_n x \quad \psi_n^{(o)}(x) = \sqrt{\frac{2}{a}} \sin k_n x$$

$n: \text{ odd} \quad \left( k_n = \frac{n\pi}{2a} \right) \quad n: \text{ even}$

$$\frac{2}{a} \sum_n \cos k_n x \cos k_n x' = \delta(x - x')$$

Commutability, Compatibility & the Uncertainty Relations

Recall,  $\hat{P}_j = i\hbar \frac{\partial}{\partial x_j}$  "operator"

$$\hat{X}_j = X_j$$

Defn: commutator of two operators  $\hat{A}$  &  $\hat{B}$ :  $[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$

$$[\hat{X}_1, \hat{P}_m] \Psi(\vec{x}, t) = (\hat{X}_1 \hat{P}_m - \hat{P}_m \hat{X}_1) \Psi(\vec{x}, t)$$

$$= -i\hbar \left( X_1 \frac{\partial}{\partial x_m} - \frac{\partial}{\partial x_m} X_1 \right) \Psi(\vec{x}, t)$$

$$\begin{aligned}
 [X_1, P_m] \psi(x, t) &= (X_1 P_m - P_m X_1) \psi(x, t) \\
 &= -i\hbar \left( X_1 \frac{\partial}{\partial x_m} - \frac{\partial}{\partial x_m} X_1 \right) \psi(x, t) \\
 &= +i\hbar \left( \frac{\partial}{\partial x_m} X_1 \right) \psi(x, t) = +i\hbar \delta_{m1}
 \end{aligned}$$

$$\underline{[X_1, P_m] = i\hbar \delta_{m1}}$$

Thm: If two operators commute then we can find (Hermitian) simultaneous eigenfunctions.

$$\hat{B} (\hat{A} \phi(\vec{x})) = a \phi(\vec{x})$$

In general,

$$\hat{A} \psi(\vec{x}, t) = \psi'(\vec{x}, t)$$

$$\hat{A} (\hat{B} \phi(\vec{x})) = b \phi(\vec{x})$$

$$\hat{B} \hat{A} \phi(\vec{x}) = a \hat{B} \phi(\vec{x}) = a b \phi(\vec{x})$$

$$(\hat{B} \hat{A} - \hat{A} \hat{B}) \phi(\vec{x}) = 0$$

$$\hat{B} \hat{A} - \hat{A} \hat{B} = 0 \Rightarrow [\hat{A}, \hat{B}] = 0$$

If  $[\hat{A}, \hat{B}] = 0$  and  $\hat{A}^\dagger = \hat{A}$ ,  $\hat{B}^\dagger = \hat{B} \Rightarrow (\hat{A} \hat{B})^\dagger = \hat{A} \hat{B}$

$$\hat{A} \hat{B} \phi(x) = a b \phi(x)$$

The converse is true if  $[\hat{A}, \hat{B}] = 0 \Rightarrow$  we can find simultaneous eigenfunction

$$[\hat{A}, \hat{B}] \psi(x) = 0 \quad \hat{A} \hat{B} \psi(x) = \hat{B} \hat{A} \psi(x)$$

$$\text{SPS } \hat{B} \psi(x) = b \psi(x)$$

$$\hat{A} b \psi(x) = \hat{B} \hat{A} \psi(x)$$

$$\hat{B} (\hat{A} \psi(x)) = b (\hat{A} \psi(x))$$

$\Rightarrow \hat{A} \psi(x)$  is an eigenfunction of  $\hat{B}$  w/ eigenvalue  $b$ .

$$\Rightarrow \hat{A} \psi(x) = a \psi(x)$$

The expression  $\hat{A} \psi(\vec{x}, t)$  is representative of the measurement of  $\hat{A}$  in  $\psi$  state by  $\psi(\vec{x}, t)$