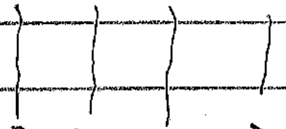
MATSCI 201 10/03/23.

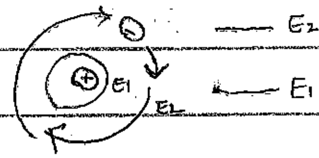
Myung Chul Jeon

- Classical wave eq: $\nabla^2\phi - \frac{1}{v^2}\frac{\partial^2}{\partial t^2}\phi = 0$.
  - $\Rightarrow$ General sol : $\phi(r,t) = f(-\vec{k}\cdot\vec{r} \pm \omega t)$ (for monochromatic wave)
  - $\Rightarrow$ Standing waves : $\phi(x,t) = X(x)\,T(t)$
  - $\Rightarrow$ ① $\partial^2/\partial x^2\, X + k^2 X = 0$ → Helmholtz equation.
    - ② $\partial^2/\partial t^2\, T + \omega^2 T = 0$

- Intro, to Q.M. ① Bohr model → ② Bohr's postulate.



discrete!



Angular momentum = Quantized

$\vec{L} = \underbrace{\cancel{mvr}}_{\vec{r}\times\vec{p}} = n\hbar$

② continued.

Kepler's law : r^2/T^3 = constant.

① $\Delta E = hf = h\,1/T \propto r^{-3/2} \propto E^{3/2}$

② $L \propto \sqrt{r} \rightarrow E \propto 1/r \propto 1/L^2 \Rightarrow \Delta E = E_2 - E_1 = \frac{1}{(L+\hbar)^2} - \frac{1}{L^2} \propto \frac{2\hbar}{L^2} \sim E^{3/2}$

→ Thus we can come up with intuition of L quantized.

③ de Broglie model. (electron = wave)

$2\pi r = n\lambda$

$mvr = n\hbar$ (②)

$\Rightarrow 2\pi r = n\,(h/mv)$ → $\lambda = h/p$ → $p = \frac{h}{\lambda}$ (Wave particle duality)

④ Schrödinger equation.

$\nabla^2\psi(\vec{r}) + k^2\psi(r) = 0$ → Helmholtz equation.

$$\frac{2\pi}{\lambda}$$
$$\parallel$$

Relations : $k = (\omega/v) = \frac{h}{\lambda} = p$

$\Rightarrow \nabla^2\psi + (p/\hbar)^2\psi = 0 \quad \Rightarrow \hbar^2 \cdot \nabla^2 \psi(r) + p^2\psi(r) = 0$

$\Rightarrow -\hbar^2/2m \nabla^2\psi(\vec{r}) = p^2/2m \, \psi(r)$ $\left(\text{note that } E = \underbrace{p^2/2m}_{=E-V} + V\right)$

$$\Rightarrow -\frac{\hbar^2}{2m}\nabla^2\psi = (E - V(\vec{r}))\psi \Rightarrow$$

(Let $\hat{p} = -j\hbar\vec{\nabla}$ where $\hat{p}\cdot\hat{p} = \hat{p}^2 = -\hbar^2\nabla^2$)

$$\Big(\underbrace{-\frac{\hat{p}^2}{2m} + V(\vec{r})}_{= \text{Hamiltonian} : \hat{H}}\Big)\psi = E\psi \Rightarrow \boxed{\hat{H}\psi = E\psi}$$

$\Rightarrow \nabla^2\psi = -\frac{2m(E-V)}{\hbar^2}\psi$ where $k = \sqrt{\frac{2m(E-V)}{\hbar^2}}$

$\Rightarrow \nabla^2\psi = -k^2\psi$

⑤ Max Born

$|\psi(r)|^2 = P(r)$: probability of finding electron at $\vec{r}$.

⑥ EM vs QM

		Intensity
EM	$\vec{\nabla}^2 E(\vec{r}) + k^2 E(\vec{r}) = 0.$	$I(t) \propto \lvert\vec{E}(t)\rvert^2$
QM	$\nabla^2 \psi(\vec{r}) + k^2\psi(\vec{r}) = 0$	$P(\vec{r}) \propto \lvert\psi(\vec{r})\rvert^2$

(linear equation.

⑦ Normalization.

$\int P(\vec{r})\, d^3\vec{r} = 1$

Since $\tilde{\psi} = c\psi$ also solution,

$|c|^2 \int |\psi|^2 d^3r = 1$

$\Rightarrow |c| = \frac{1}{\sqrt{\int |\psi|^2 d^3\vec{r}}}$ Normalization factor

$\tilde{\psi} = \frac{\psi}{|c|}$ for probability.

10/05/23.

MATSCI - 201

• Example : possible soln.

Born's scale $\rightarrow P(\vec{r}) = |\psi(\vec{r})|^2$ where $\int |\psi(\vec{r})|^2 = 1$. $\rightarrow$ normalization.

$\nabla^2 \psi + k^2 \psi = 0$ $\rightarrow$ Helmholtz.

deBroglie : $\lambda = h/p \Rightarrow k = \frac{2\pi}{\lambda} = p/\hbar$

$\rightarrow \nabla^2 \psi + (p/\hbar)^2 \psi = 0$ where $E = \frac{p^2}{2m} + V$

• Eigenvalues / eigenfunctions — $H\psi = E\psi$ (!)

• Degeneracy. = More than 1 eigenvalue! — states (multiple)

$\hookrightarrow$

• Parity operators. $\hat{Q}$

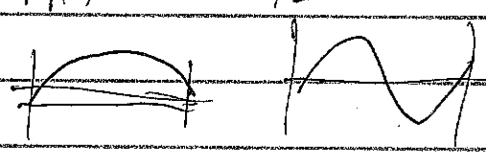
$\hat{Q} f(x) = f(-x)$.

$\hat{Q} \psi_1(x) = \psi_1(-x) = \psi(x)$. $\rightarrow$ Eigen value $= 1$

$\hat{Q} \psi_2(x) = \psi_2(-x) = -\psi_2(x)$ $\rightarrow$ Eigenvalue $= -1$.

$q = +1$; even parity
$= -1$; odd parity.

$\psi_1(x)$ ψ_2



Note. $f(x) = a_0 + \sum_{n=1}^{\infty} a_n \cos\left(2\pi \frac{nx}{L}\right) + b_n \sin\left(2\pi \frac{nx}{L}\right)$

$a_0 = \int_a^b f(x)\,dx \cdot \frac{1}{L}$

$a_n = \frac{2}{L} \cdot \int_a^b f(x) \cos\left(2\pi \frac{nx}{L}\right) dx$

$b_n = \frac{2}{L} \int_a^b f(x) \sin\left(2\pi \frac{nx}{L}\right) dx$

• $E_n = \frac{\hbar^2 \pi^2}{2mL^2} n^2$, $1\,eV = 1.6 \cdot 10^{-19}$ J

electron charge unit.

• In a box

$-\frac{\hbar^2}{2m} \nabla^2 \psi = E\psi \rightarrow \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) XYZ = -\frac{2mE}{\hbar^2} \cdot XYZ \Rightarrow \frac{X''}{X} + \frac{Y''}{Y} + \frac{Z''}{Z} = -\frac{2mE}{\hbar^2}$

$\Rightarrow X'' = \left(-\frac{2mE_x}{\hbar^2}\right) X$ for x, y, z (E_x, E_y, E_z).

MATSCI 201 : Appl. Quant. Mech 10/10/23.

Particle in Wells

$f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x)$ $\left\{ \int_{-\infty}^{\infty} dx\, \psi_n^* \psi_m = \delta_{nm} \right\}$ Orthogonality

$k(6,7) < 0.5$

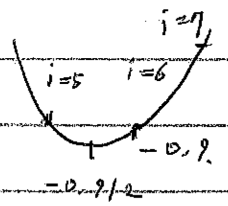
$x = -1.5 + 6 \cdot 0.1 = -0.9$

$\Rightarrow c_n = \int_{-L/2}^{L/2} dx\, f(x) \psi_n^*(x)$.

$x + dx = -0.8$

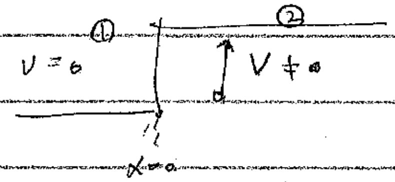
$(6,1)\ 2x + -1.5 = 0.9$

$$\Rightarrow \boxed{f(x) = \sum_{n=1}^{\infty} \left[\int_{-L/2}^{L/2} dx'\, f(x') \psi_n^*(x') \right] \psi_n(x)}$$



- A set of functions $[\psi_n(x),\ n=1,2,\ldots]$
  1. normalized $\int |\psi|^2 = 1$
  2. mutually orthogonal

  → The set is called Basis



$$\begin{cases} ① & -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi = E\psi \\ ② & -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi + V_0 \psi = E\psi \end{cases}$$

(otherwise diverges).

① : $\psi = A e^{jkx} + B e^{-jkx}$ ② : $\psi = \cancel{C e^{bx}} + D e^{-bx}$ $b > 0$

~~1) $\psi_1(x=0) = \psi_2(x=0) \rightarrow A + B = D$.~~

2) $\partial \psi_1 / \partial x \big|_{x=0} = \partial \psi_2 / dx \big|_{x=0} \Rightarrow A - B = \frac{jb}{k} D$.

$k(24, j) = ?$

$\Rightarrow$ Find out relationship ÷ $\frac{1}{2}$

Update ...

Time dependence : $e^{-j(E/\hbar) t}$

6 5 4 5 6 7 ...

must be terminated ...

$\psi = A e^{j(kx - \omega t)} + B e^{-j(kx - \omega t)}$

plane wave → plane wave ←

forward reflected

10/12/23

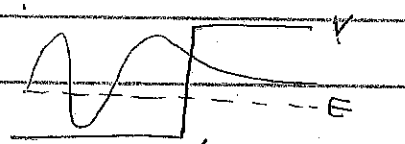
EE 222 - Appl. Quant. Mech.

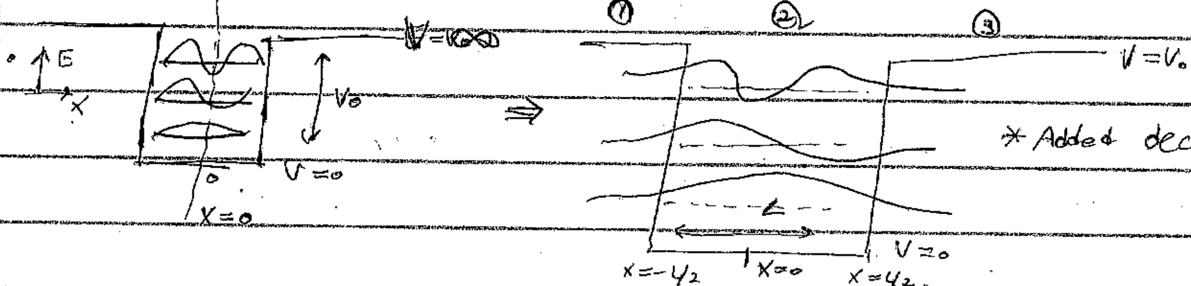
- $\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial \vec{r}^2} + V(\vec{r})\right]\psi(\vec{r}) = E\cdot\psi(\vec{r})$; Time independent S.E.

$\psi \propto e^{+jk\vec{x}}$

$\Rightarrow \frac{\partial^2}{\partial r^2}\psi = -\frac{2m(E-V)}{\hbar^2}\psi = -k^2\psi \Rightarrow k = \sqrt{\frac{2m(E-V)}{\hbar^2}}$ (constant V) ~~(1 Dimension)~~

(If $E < V$) $\psi = e^{jkx} = e^{j(jb)x} = e^{-bx}$ (decaying).
↳ $k = jb$





* Added decaying term

$k = \sqrt{\frac{2mE}{\hbar^2}}$ (region ②), $b = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$ (region ① and ③)

① : $\psi_1(x) = D_L\cdot e^{bx} + \cancel{E_L}\cdot e^{-bx}$ ($\because \lim_{x\to-\infty} e^{-bx} = \infty$). $x < -L/2$

② : $\psi_2(x) = Ae^{jkx} + Be^{-jkx}$ $\quad -L/2 \le x \le L/2$

③ $\psi_3(x) = \cancel{D_R}e^{bx} + E_R e^{-bx}$ ($\because \lim_{x\to\infty} e^{bx} = \infty$). $x > L/2$

B.C.s) $\psi_1(-L/2) = \psi_2(L/2)$, $\psi_2(L/2) = \psi_3(L/2)$, $\psi_1'(-L/2) = \psi_2'(-L/2)$, $\psi_2'(L/2) = \psi_3'(L/2)$

Unknown var : D_L, A, B, E_R (4) $\Leftrightarrow$ Equations : (4) $\rightarrow$ solvable!

$\Rightarrow$ Solution. $\begin{cases} 1)\ D_L = E_R \rightarrow \tan(kL/2) = b/k \\ 2)\ D_L = -E_R \rightarrow \cancel{\tan}(kL/2) = -b/k \end{cases}$

$\boxed{\text{Taking shortcut.}}$

Consider parity op. $\hat{Q} : x \rightarrow -x$ $\hat{Q}f(x) = f(-x)$

S.E. : $\hat{H}\psi = E\psi$, $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V \rightarrow \hat{Q}[\hat{H}\psi(x)] = \hat{Q}\left[\left(-\frac{\hbar^2}{2m}\partial^2/\partial x^2 + V\right)\psi\right]$

$\Rightarrow \hat{Q}[H\psi] = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial(-x)}\cdot\psi(-x) + V(-x)\psi(-x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(-x) + V(x)\psi(x)$ $\left(\because V(-x) = V(x)\right)$

$\Rightarrow = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(-x) = \hat{H}\psi(-x) = \hat{H}[Q\psi(x)]$

Solve for. . . .

$\hat{Q}, \hat{H}$ · Commute.

$\hat{Q}\hat{H}\psi(x) = \hat{H}\hat{Q}\psi(x) \Rightarrow \hat{Q}\hat{H} = \hat{H}\hat{Q}$ (Interchange.) – order matter X

$\Rightarrow \hat{H}\psi = E\psi \Rightarrow \underbrace{\hat{H}\psi_n(x) = E_n\psi_n(x)}_{\text{Eigen value (n)}} \Rightarrow \hat{H}[\hat{Q}\psi_n(x)] = \hat{Q}\hat{H}\psi_n(x) = \hat{Q}E_n\psi_n(x)$

$= E_n\hat{Q}\psi_n(x)$.

$\Rightarrow \hat{H}[\hat{Q}\psi_n(x)] = E_n[\hat{Q}\psi_n(x)] \rightarrow \hat{Q}\psi_n(x)$ also satisfies S.E.

$\Rightarrow \boxed{\hat{Q}\psi_n(x) = C\cdot\psi_n(x)}$, Eigenvalue problem.

Here, $C = \pm 1$ (∵ magnitude shouldn't change)

$\Rightarrow \underbrace{\psi_n(x) = \psi_n(-x)}_{C=1}$ or $\underbrace{\psi_n(x) = -\psi_n(-x)}_{C=-1}$.

↓ symmetric (even) ↳ anti-symmetric (odd),

③ $\psi_2(x) = A\sin(kx) + B\cos(kx)$

[Even]

$\psi_n(x) = \psi_n(-x)$

① $D_n = E_R$

② $A = 0$ (∵ even)

$\Rightarrow \psi_1 = D_L e^{bx}$

$\psi_2 = B\cos kx$

$\psi_3 = D_L\cdot e^{-bx}$

1) At $x = -L/2$

$D_L e^{-b\cdot L/2} = B\cos(kL/2)$ and $bD_L e^{-bL/2} = +Bk\sin(kL/2)$

2) At $x = +L/2$

~~$D_L e^b$~~ symmetric → not necessary.

$1/b = 1/k$ ① $\Rightarrow \tan(kL/2) = b/k$

[odd]

$\psi_n(x) = -\psi_n(-x)$

① $D_n = -E_R$

③ $B = 0$. (odd)

$\psi_1 = D_L\cdot e^{bx}$

$\psi_2 = A\sin kx$

1) At $x = -L/2$

$\Rightarrow D_L\cdot e^{-bL/2} = A\sin(k(-L/2))$

and

$-b\cdot D_L\cdot e^{-bL/2} = Ak\cos(kL/2)$

Ratio

$\Rightarrow -\cot(kL/2) = b/k$

→ How to solve

$b/k = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)} \Big/ \sqrt{\frac{2m}{\hbar^2}E} = \sqrt{\frac{V_0 - E}{E}} = \sqrt{\frac{N_0 - \epsilon}{\epsilon}}$

$kL/2 = \frac{L}{2}\sqrt{\frac{2m}{\hbar^2}E} = \frac{\pi}{2}\sqrt{\underbrace{\frac{2mL^2}{\pi^2\hbar^2}}_{=E_1}E} = \frac{\pi}{2}\sqrt{E/E_1^\infty} = \pi/2\sqrt{\epsilon}$.

$\epsilon = \frac{E}{E_1^\infty}$

$N_0 = \frac{V_0}{E_1^\infty}$

~~$\Rightarrow$ Even: $\tan\left(\frac{\pi}{2}\sqrt{\epsilon}\right) = \sqrt{\frac{N_0-\epsilon}{\epsilon}}$~~

odd: $-\cot\left(\frac{\pi}{2}\sqrt{\epsilon}\right) = \sqrt{\frac{N_0-\epsilon}{\epsilon}}$ → solve!

① Most imp. in PhD.

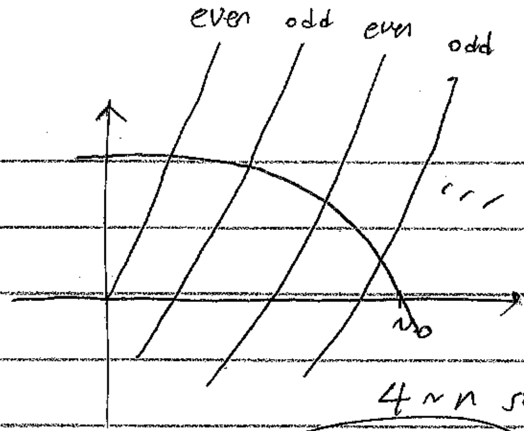
② courses – how

③ scholarships.

④ Statistical mechanics? – where is it?

Solving equations graphically,

$$\left.\begin{aligned} \tan\left(\frac{\pi}{2}\sqrt{\varepsilon}\right) &= \sqrt{\frac{\nu_0-\varepsilon}{\varepsilon}} \\ -\cot\left(\frac{\pi}{2}\sqrt{\varepsilon}\right) &= \sqrt{\frac{\nu_0-\varepsilon}{\varepsilon}} \end{aligned}\right\}$$



4 ~ n solutions

Note. as V_0 gets larger → ν_0 larger → more solutions

⇒ $V_0 \to \infty$ (infinite potential well) → Infinite energy states.

10/16/23.

ME300A — Bases, Dimension, Rank.

- Showing it is a (non-empty) subset of a known V.S. ~~$\Rightarrow$ S = Vector space.~~
  and ensuring ① $\phi \in S$ ② $x, y \in S \Rightarrow \alpha x + \beta y \in S$

Eg.. $N(A) = \{x \mid Ax = 0\}$ is V.S (pf)

① $N(A) \subseteq \mathbb{R}^n$ ③ $x \in N(A)$, $y \in N(A)$ $\rightarrow \alpha x + \beta y \in N(A)$

② $\phi \in N(A)$ $\rightarrow A(\alpha x + \beta y) = \alpha A x + \beta A y = 0$.

$\Rightarrow$ $N(A)$ is a vector-space

Thus, $x = x_0 \rightarrow x = t x_0$ is also solution.

- $\text{span}\{v_1, \dots, v_m\} = \{\alpha_1 v_1 + \cdots + \alpha_m v_m \mid \alpha_1, \dots, \alpha_m \in \mathbb{R}\}$.
  = set of all linear combination $(v_1 \sim v_m)$.

Eg.) $\text{row}(A) = \text{span}(r_1, \dots r_m)$ $\text{col}(A) = \text{span}(c_1, \dots, c_n)$

$\rightarrow$ $\text{span}(v_1, \dots, v_m)$ is always a V.S.

pf) ① $\alpha_1 \sim \alpha_m = 0 \rightarrow 0 \in \text{span}\{v_1, \dots, v_m\}$

② $\alpha x + \beta y \in \text{span}(v_1 \sim v_m)$ for any $x, y \in \text{span}(v_1, \dots, v_m)$.

Fact): $\text{span}(v_1 \sim v_m)$ is smallest V.S. containing $v_1 \sim v_m$

~~For any V~~, Given any V.S. V $\rightarrow$ we can find list $v_1 \sim v_m$ that $V = \text{span}(v_1 \sim v_m)$

- Every V.S has spanning list, any $v \in$ V.S. $\Rightarrow$ v = linear comb. span (V.S.)
  $= a_1 v_1 + \cdots + a_m v_m$.

$\Rightarrow$ Q) only one way to describe V? $V = c_1 v_1 + \cdots + c_m v_m$

A) Not always!

Suppose you have $d_1 \sim d_m \rightarrow V = d_1 v_1 + \cdots + d_m v_m$. $\Rightarrow (c_1 - d_1) v_1 + \cdots + (c_m - d_m) v_m = 0$

if $c_1 - d_1 = \cdots c_m - d_m = 0 \rightarrow$ unique way of description.

$\boxed{\text{(Def) } v_1 \sim v_m \text{ is lin. indep. if linear comb is unique}}$ $\equiv (c_1 - d_1) v_1 + \cdots + (c_m - d_m) v_m = 0$.

10/17/23.

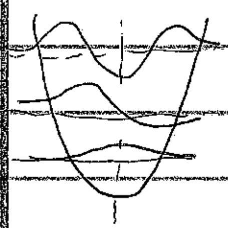
A.Q.M.

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

$\Rightarrow \hat{Q}\psi(x) = \pm\psi(x)$ $\quad P.E. = \frac{1}{2}k x^2 - \frac{1}{2}m\omega^2 x_0^2 = \frac{1}{2}\hbar\omega$

$x_0 = \sqrt{\hbar/(m\omega)}$, $\xi = x/x_0$

< Harmonic Potential > $\quad$ ↳ zero-point fluctuation $\quad$ ↳ normalized length.

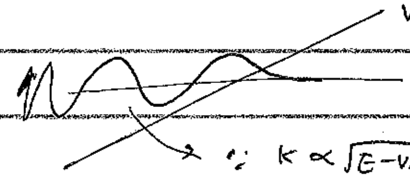


$V(x) = \frac{1}{2}k_s x^2$ $\quad \Rightarrow \left(\partial^2/\partial\xi^2 - \xi^2\right)\psi(\xi) = -\left(\frac{2E}{\hbar\omega}\right)\psi(\xi)$

$\psi_n(\xi) = \underbrace{A_n e^{-\xi^2/2}}_{\text{envelope}} \cdot \underbrace{H_n(\xi)}_{\text{Hermit polynomials}}$ & $E_n = (n+1/2)\hbar\omega$. $(n = 0, 1, 2 \ldots)$

- Hermit polynomials
  - $H_0(\xi) = 1$
  - $H_1(\xi) = 2\xi$
  - $H_2(\xi) = 4\xi^2 - 1$

< Linear varying potential >



$V = e\mathcal{E}x$

$\therefore k \propto \sqrt{E - V(x)} = \frac{2\pi}{\lambda}$ $\quad \lambda\uparrow$

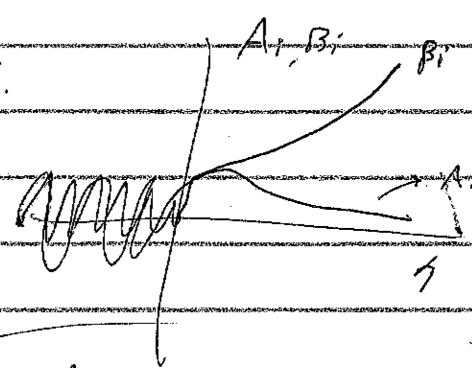
$\rightarrow \partial^2/\partial x^2\,\psi = -\frac{2m}{\hbar^2}\{E - e\mathcal{E}x\}\psi(x) = \frac{2me\mathcal{E}}{\hbar^2}\left\{x - \frac{E}{e\mathcal{E}}\right\}\psi(x)$

$\frac{1}{x_0^3} = \frac{2me\mathcal{E}}{\hbar^2} \Rightarrow x_0 = \left(\frac{\hbar^2}{2me\mathcal{E}}\right)^{1/3}$, $\eta = x/x_0$ or $\left(x - E/e\mathcal{E}\right)/x_0$

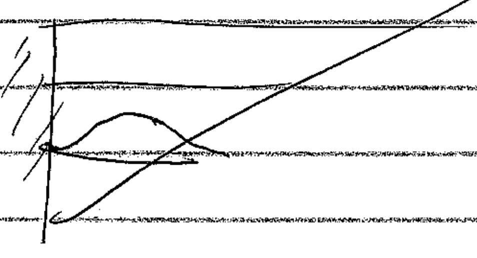
$\Rightarrow \partial^2/\partial x^2\,\psi - \eta\cdot\psi(x) = 0$ $\quad \left(\eta = \frac{x - \frac{E}{e\mathcal{E}}}{x_0} = k^2\right)$

① $\eta > 0 \rightarrow e\mathcal{E}x > E \Rightarrow e^{\pm kx}$ $\quad k = \sqrt{\eta}$.

② $\eta < 0 \rightarrow e\mathcal{E}x < E \Rightarrow e^{\pm j|k|x}$



G.S.: $\psi(\eta) = aA_i(\eta) + bB_i(\eta)$.



$\eta < 0 \rightarrow A_i, B_i$ acts like sin/cos

10/19/23.

EE 201 - Appl. Qun. Mech.

< Time dependent S.E.>

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

$$(\text{if } V=0)\quad \psi(\vec{r},t) = \exp\{-j(\omega t - \vec{k}\cdot\vec{r})\}$$

Independent of Time! (eigenstates). ~~Stationary~~ States

$$\Rightarrow \underbrace{\psi_n(\vec{r},t)}_{T.D.S.E} = \underbrace{\psi_n(\vec{r})}_{T.I.S.E} \cdot \exp(-jE_n t/\hbar)$$

Eigenstates — Corresponding. Eigenfunctions.

- Born's rule. : $|\psi_n(\vec{r},t)|^2 = \psi_n(\vec{r},t)\cdot\psi_n^*(\vec{r},t) = \psi_n(\vec{r})e^{-j\omega t}\psi_n^*(\vec{r})e^{j\omega t} = |\psi_n(\vec{r})|^2$
- Predict along time : $\psi(\vec{r},t_0) \rightarrow \psi(\vec{r},t_0+\delta t) \approx \psi(\vec{r},t_0) + (\delta t)\cdot\left.\frac{\partial\psi}{\partial t}\right|_{t_0}$

since we already know $\frac{\partial\psi}{\partial t} = \frac{1}{j\hbar}\left[\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r},t)\right)\psi(\vec{r},t)\right].$

10 3

- linearity of T.D.S.E

$\Rightarrow \{\psi_n(\vec{r},t) \mid S.E(\psi)=0\}$ is a vector space $\Leftrightarrow c_1\psi_1 + c_2\psi_2 = \psi_3$ is also solution.

- linear superposition of every eigenstates.

$\tilde{\psi}(\vec{r},t) = \sum_n c_n\psi_n(\vec{r},t)$ at $t=0 \rightarrow$

Normalization $\Rightarrow \int_{-\infty}^{\infty} dr^3\, |\psi(\vec{r},0)|^2 = 1 = \int_{-\infty}^{\infty} d\vec{r}^3 (c_n c_m^*)\psi_n(\vec{r})\psi_m^*(\vec{r})$

$$= \sum_n\sum_m c_n c_m \delta_{n,m} \checkmark$$

superposition of plane waves. = wave packets

$\rightarrow \psi = e^{jk(x - \omega/k\, t)}$ $\rightarrow$ phase velocity $V_p = \omega/k$,

$\rightarrow \psi_1 = e^{j(k_1 x - \omega t)} + e^{+j(k_2 x - \omega t)} = \underline{e^{j(kx-\omega t)}\cdot 2\cos(\delta k x - \delta\omega t)}$ $(k_1 = k+\delta k \quad k_2 = k-\delta k)$

$\rightarrow$ Depends on differences in frequencies.

$\rightarrow d\omega/dk = V_g$ (group velocity) $\rightarrow$ $V_g(k) = \partial\omega/\partial k$ $\quad \omega(k)$

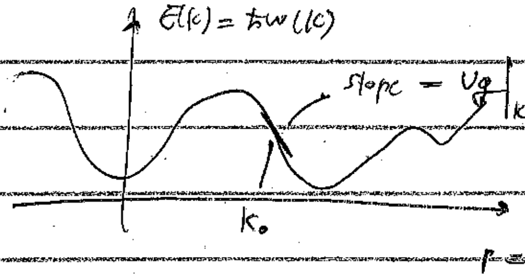
$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} \rightarrow \omega = E/\hbar \rightarrow V_g = p/m \quad v_p = p/2m$

↳ Classical ↳ non-classical

- Dispersion.

$E = \hbar\omega.$

$E(k) = \hbar\omega(k).$



slope $= v_g\big|_{k=k_0} = \partial\omega/\partial k\big|_{k_0} = \partial E/\partial k\big|_{k_0} \frac{1}{\hbar}$

10/24/23

Appl. Quant. Mech. (EE 222)

- Quantum Measurement / operators.

<operators>

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V.$$

$$\langle E \rangle = \sum E_n p_n = \int_{-\infty}^{\infty} d^3\vec{r}\, \psi^* \hat{H} \psi$$

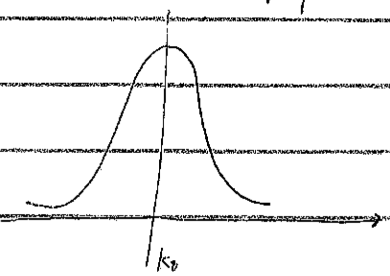
$$\sum E_n |c_n|^2 \text{ where } \boxed{\psi = \sum_n c_n e^{-j\frac{E_n}{\hbar}t}\psi_n}$$

$$\psi(\vec{r},t) = \sum_n c_n \cdot \psi_n(\vec{r}) \cdot e^{-jE_n t/\hbar} = \sum_n d_n(t)\cdot \phi_n(\vec{r}).$$

$\rightarrow$ superposition : $\psi(x,t) = \sum_k C_k \cdot e^{j(kx-\omega t)} \rightarrow \int_{-\infty}^{\infty} dk\, C(k)\cdot e^{j(kx-\omega t)}$.

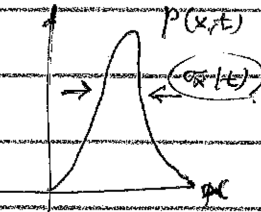
Background

e.g.) Assume $C(k) = \exp\left\{-\frac{(k-k_0)^2}{\sigma_k^2}\right\}$.



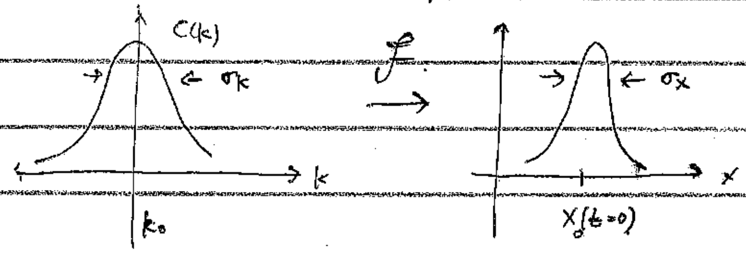
$$\Rightarrow \quad \psi(x,t) = \int_{-\infty}^{\infty} dk \cdot \exp\left\{-\frac{(k-k_0)^2}{\sigma_k^2}\right\} e^{j(kx-\omega t)}$$

$$\Rightarrow p(x,t) = \|\psi(x,t)\|^2 \quad \Rightarrow$$



$p(x,t)$ is dependent on time.

Note : At $t=0$ $\quad \psi(x,0) = \int_{-\infty}^{\infty} dk\, C(k)\, e^{jkx} \Rightarrow \boxed{\text{Fourier Transform}}$



$(\sigma_x(t=0) = 1/\sigma_k)$ —— ①

$$\left(\begin{array}{l} p = \hbar k \rightarrow \sigma_p = \hbar\sigma_k \\ \text{Note that } \sigma_x = \frac{\hbar}{\sigma_p} \\ \sim \text{Heisenberg's p...} \end{array}\right)$$

$$x_0(t) = x_0(0) + v_0 \cdot t \quad \text{where } v_0 = \frac{\hbar k_0}{m} = \left.\frac{\partial\omega}{\partial k}\right|_{k=k_0}$$

$$\sigma_x(t) = \underbrace{\sigma_x(t=0)}_{\text{at } t=0.} \sqrt{1+\left(\frac{\hbar^2}{2m}\frac{t^2}{\sigma_x^2}\right)}$$

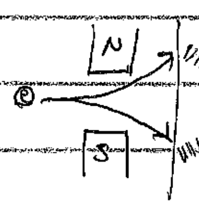
- Quantum Measurement. = Random collapse into eigenstate associated with the measurement of interest.

$$\psi \qquad \langle E \rangle = \sum_n E_n p_n$$

E.g. Stern – Gerlach experiment.

$$\underbrace{\langle A(t) \rangle}_{\text{observables}} = \sum_n A_n p_n(t) = \sum_n A_n |c_n(t)|^2$$

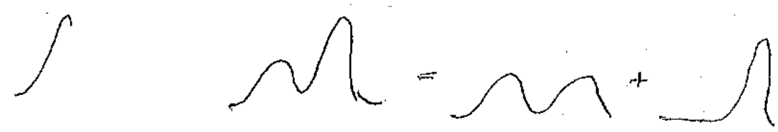
$$\psi(t) = \sum_n c_n(t)\, \underbrace{\phi(A_n)}_{\text{eigenstate that outputs } A_n \text{ under measurement of } A.}$$



$S = \pm\frac{1}{2}\hbar$ (spin up & down)

$S_\mu = m_\mu \hbar$

$(\mu = x, y, z)$



10/26/23.

< Operators & Framework for QM ⟺ Lin. Alg. >

- Operators = Action!

→ $\hat{H}$: Energy → Energy op. ⇒ $\hat{H}\psi = E\psi$

$$\psi = \sum_n c_n \cdot e^{-j E_n/\hbar \cdot t}\, \psi_n(\vec{r})$$

→ Measurement = Random Collapse → $P_n = \|c_n\|^2$

→ $\langle E\rangle = \sum E_n P_n = \sum E_n \|c_n\|^2 = \int_{-\infty}^{\infty} d^3\vec{r} \cdot \psi^*(r,t)\, \hat{H}\, \psi(r,t)$ ✓

Exponential of operator

$$\exp\left(-j\frac{t}{\hbar}\hat{H}\right) = \sum_{k=0}^{\infty} \frac{1}{k!}\left(-\frac{jt}{\hbar}\right)^k \hat{H}^k$$

Note that $\hat{H}\psi_n = E_n\psi_n$, $\hat{H}^2\psi_n = \hat{H}E_n\psi_n = E_n\hat{H}\psi_n = E_n^2\psi_n$

⇒ $\hat{H}^k\psi_n = E_n^k\psi_n$

$$\Rightarrow \exp\left(-j\, t/\hbar\, \hat{H}\right)\psi_n = \sum_{k=0}^{\infty}\frac{1}{k!}\left(-\frac{jt}{\hbar}\right)^k \hat{H}^k\psi_n$$

$$= \sum_{k=0}^{\infty}\frac{1}{k!}\left(-jt/\hbar\, E_n\right)^k\psi_n = \exp\left(-j\,t/\hbar\, E_n\right)\psi_n \quad \text{— ①}$$

Only for Eigen states

From ①, $\psi(\vec{r},t) = \sum_n c_n \cdot e^{-j E_n/\hbar \cdot t}\, \psi_n(\vec{r})$

$$= \sum_n c_n\, e^{-j\hat{H}t/\hbar}\cdot\psi_n(\vec{r}) = e^{-j\hat{H}t/\hbar}\left(\sum_n c_n\cdot\psi_n(\vec{r})\right)$$

$$= e^{-j\hat{H}/\hbar\cdot t}\cdot\psi(r,0)$$ → We can take out the exponential operator!

⇒ $\boxed{\hat{U}(t_2,t_1)\,\psi(\vec{r},t_1) = \psi(\vec{r},t_2)}$

$$\hat{H} = -\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r}) = \frac{\hat{p}^2}{2m} + V(\vec{r}) \qquad \hat{p} = -j\hbar\vec{\nabla}$$

$$\vec{\nabla} = \frac{\partial}{\partial x}\vec{e_x} + \frac{\partial}{\partial y}\vec{e_y} + \frac{\partial}{\partial z}\vec{e_z}$$

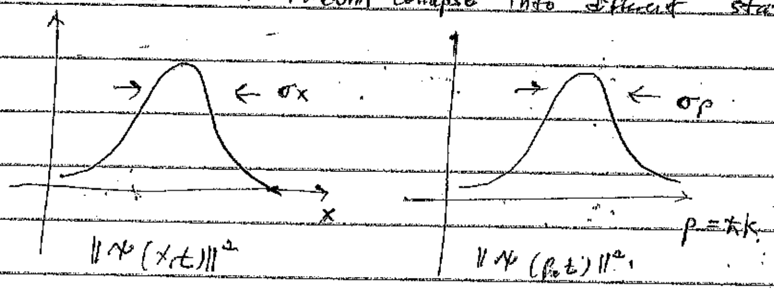
Eg.) Plane wave : $e^{j(\vec{k}\cdot\vec{r}-\omega t)} \Rightarrow \hat{p}\left[e^{j(\vec{k}\cdot\vec{r}-\omega t)}\right]$

$$= -j\hbar\cdot(j\cdot\vec{k})\left[e^{j(\vec{k}\cdot\vec{r}-\omega t)}\right] = \underbrace{\hbar\vec{k}}_{=p}\cdot\left[e^{j(\vec{k}\cdot\vec{r}-\omega t)}\right].$$

$\Rightarrow$ For operator $\hat{A}$, $\hat{A}\cdot\psi_A = A\cdot\psi_A$

- Uncertainty principle.

Measurement $\rightarrow$ Random collapse into different states.



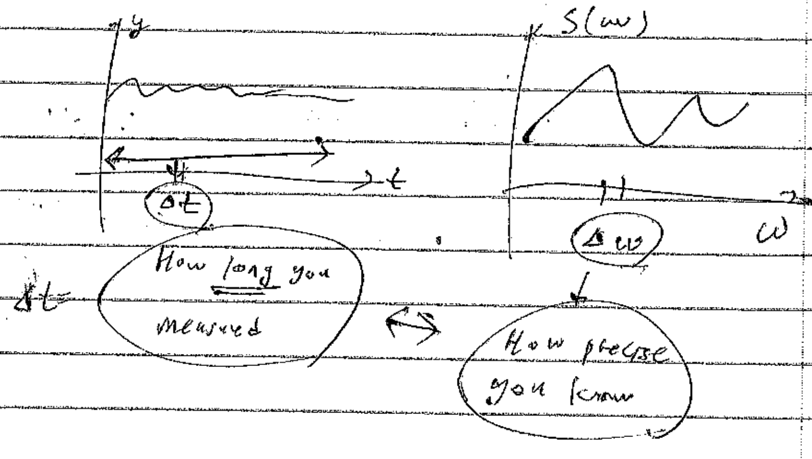
$$\psi(x,t) = \int_{-\infty}^{\infty} dp\, \psi(p,t)\, e^{-j\, p/\hbar \cdot x} \qquad p \xleftrightarrow{F.T.} x$$

(Fourier Transform)

$\rightarrow$ $\sigma_x \cdot \sigma_p \geq \hbar/2$. $\rightarrow$ $\Delta x \cdot \Delta p \geq \hbar/2$.

$\downarrow$

✓ $\Delta\omega \cdot \Delta t \geq 1/2$



11/2/23.

"Matrix" based Quantum Mechanics

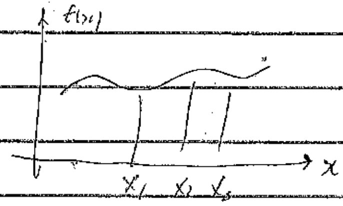
(1) Linear algebra with vectorspace (V.S.) with complex numbers.
$\equiv$ $\boxed{\text{Hilbert Space}}$

(2) Representation. $\equiv$ Choice of "basis" to describe Q.M. system & dynamics.

- Vectorization of function.

How to represent $y = f(x)$ function?

(1)



(2)

X	x_1	x_2	x_3
$f(x)$	$f(x_1)$	$f(x_2)$	$f(x_3)$

(3)

$$\vec{f}(x) = \begin{bmatrix} \vdots \\ f(x_1) \\ f(x_2) \\ \vdots \end{bmatrix} \quad \left\langle \text{Infinite dimension!} \right\rangle$$

Note that $\int_{-\infty}^{\infty} dx\, |f(x)|^2 dx = \sum_i \Delta x \cdot f^*(x_i) f(x_i) = \vec{f^*}(x)^T \cdot \vec{f}(x) \cdot \Delta x$

$$= [\cdots f(x_{i-1})\ f(x_i) \cdots] \cdot \begin{bmatrix} \vdots \\ f(x_{i-1}) \\ f(x_i) \end{bmatrix}$$

$$= \left\{\vec{f}^T(x)\right\}^* \vec{f}(x)\, \Delta x = \underbrace{\Delta x \cdot \vec{f^*}(x) \cdot \vec{f}(x)}$$

- Dirac Notation.

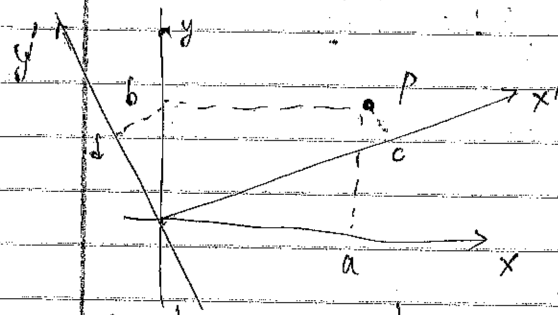
$$\vec{f}(x) \equiv \underbrace{|f\rangle}_{\text{"ket"}} = \begin{bmatrix} \vdots \\ f(x_1) \\ f(x_2) \\ \vdots \end{bmatrix} \ : \text{column vector}$$

$$\left[\vec{f}^*(x)\right]^T = \underbrace{\langle f|}_{\text{"bra"}} = [\cdots f^*(x_{i-1})\ f^*(x_i) \cdots] \ : \text{row vector.}$$

Ex. (i) $\int_{-\infty}^{\infty} dx\, |f(x)|^2 \cong \Delta x \cdot \underbrace{\langle f| \cdot |f\rangle}_{\text{dot product}} = \underbrace{\langle f|f\rangle}_{\text{"braket"}}$

(ii) $\int_{-\infty}^{\infty} dx\, f^*(x) g(x) = \langle f|g\rangle$

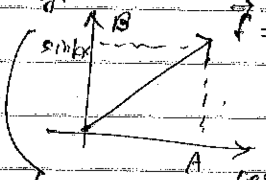
- Representation of functions (Choice of basis)



$(a,b)\Big|_{(x,y)} = (c,d)\Big|_{(x',y')}$!

$\vec{f} = |f\rangle$

- E.g.



$\vec{f} = |f\rangle$. $f(x) = A\cos kx + B\sin kx$

① $\vec{f} = |f\rangle = \begin{pmatrix} A \\ B \end{pmatrix}$

① $\cos kx = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

① $\sin kx = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$f(x) = \underset{|}{C}e^{jkx} + \underset{|}{D}e^{-jkx}$

~~different~~ coord. sys.

E.g. $\psi(x) = \sum_{n=1}^{k} c_n \psi_n(x)$

$\psi_1(x) = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$ $\psi_2(x) = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$. $\psi_3(x) = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$ $\cdots$ $\psi_k(x) = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}$

Use $\psi_1 \sim \psi_k$ as basis,

$\Rightarrow \psi(x) = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_k \end{pmatrix} = |\psi\rangle$

Recall that $\int_{-\infty}^{\infty} dx\, |\psi(x)|^2 = \int_{-\infty}^{\infty} dx \underbrace{\left(\sum_n c_n^* \psi_n^*(x)\right)}_{=\psi^*(x)} \underbrace{\left(\sum_m c_m \psi_m(x)\right)}_{=\psi(x)}$

$= \sum_n \sum_m c_n c_m \cdot \int_{-\infty}^{\infty} \psi_n^*(x)\psi_m(x)\,dx = \sum_n \sum_m c_n c_m \cdot \delta_{n,m}$

$= \sum_{n=1}^{k} |c_n|^2 = [c_1^* \; c_2^* \cdots c_k^*] \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_k \end{bmatrix} = \langle\psi|\psi\rangle$

$\Rightarrow \int_{-\infty}^{\infty} dx\, \phi^*(x)\,\psi(x) = \langle\phi|\psi\rangle$

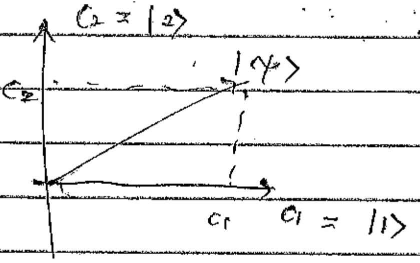
→ continued ...

→ continued ...

$\Psi(x) = \sum_n c_n \psi_n(x) = \begin{bmatrix} c_1 \\ \vdots \\ c_k \end{bmatrix}$ $\quad \langle \phi | \psi \rangle = \int_{-\infty}^{\infty} dx\, \phi^*(x) \Psi(x) dx$

$\phi(x) = \sum_n d_n \psi_n(x) = \begin{bmatrix} d_1 \\ \vdots \\ d_k \end{bmatrix}$ $\quad = [d_1^* \; d_2^* \ldots d_k^*] \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_k \end{bmatrix}$

$\Psi(x) = \sum_n c_n \psi_n(x) \Rightarrow |\Psi\rangle = \sum_n c_n |\psi_n\rangle = \sum_n c_n |n\rangle$



$\boxed{c_n = \langle n | \Psi \rangle}$ projection!

$|\psi\rangle = \sum_n \langle n | \Psi \rangle |n\rangle$

$\Rightarrow |\Psi\rangle = \sum_n c_n |n\rangle = \sum_n \langle n | \Psi \rangle |n\rangle$.

$= \sum_n |n\rangle \langle n | \psi \rangle = \sum_n (|n\rangle\langle n|) \cdot |\Psi\rangle$ — outer product.

should be I (identity matrix).

$\langle n | \lambda \rangle$: inner

$|n\rangle\langle n|$: outer. $\quad \sum$ outer $= I$ → Expand and prove yourself!

$\sum |n\rangle\langle n| = I$ has to be satisfied for all basis

(basis independent property) (E.g. $\sum |a\rangle\langle a| = I$)

- Hermitian adjoint (called "dagger") — only defined on square matrix

$(|f\rangle)^\dagger \overset{def}{=} \langle f|$. Eg. $A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1N} \\ & & & \\ a_{N1} & \cdots & & a_{NN} \end{bmatrix} = [a_{ij}]$

ket bra

$(\langle f|)^\dagger \overset{def}{=} |f\rangle$

$A^\dagger = \begin{bmatrix} a_{11}^* & \cancel{a_{12}^*} & & a_{N1}^* \\ \vdots & & & \\ a_{1N}^* & & & a_{NN}^* \end{bmatrix} \equiv [a_{ij}]^\dagger = (a_{ji})^*$

→ Hermitian adjoint continued...

T.D.S.E : $\hat{H} = -\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r})$

$$\Rightarrow \quad \hat{H}\,\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t)$$

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

↳ column vector

$$\hat{H} = \begin{bmatrix} ? \end{bmatrix}$$

11/9/23.

Dirac notation continued...

- Dirac notation.

$\Psi(x) = \sum_n c_n \psi_n(x)$

- Completeness relation. (discrete)

$\sum_\alpha |\alpha\rangle\langle\alpha| = \hat{I}$

$|\psi\rangle = \hat{I}|\psi\rangle = \left(\sum_\alpha |\alpha\rangle\langle\alpha|\right)|\psi\rangle$

$= \sum_\alpha |\alpha\rangle \cdot \underbrace{\langle\alpha||\psi\rangle}_{= c_\alpha}$

$= \sum c_\alpha |\alpha\rangle$

- Completeness relation (continuous)

$|\psi\rangle = \int_{-\infty}^{\infty} dx\, |x\rangle\langle x|\, |\psi\rangle$

$= \int_{-\infty}^{\infty} dx\, |x\rangle \underbrace{\langle x|\psi\rangle}_{= \psi(x)}$

$= \int_{-\infty}^{\infty} dx\, \psi(x) |x\rangle$

- state overlap.

$\langle\phi|\psi\rangle = \langle\phi, \hat{I}\psi\rangle = \langle\phi|\left(\sum_\alpha |\alpha\rangle\langle\alpha|\right)|\psi\rangle$

$= \sum_{\alpha=1}^{N} \langle\phi|\alpha\rangle\langle\alpha|\psi\rangle$

$= \sum_{\alpha=1}^{N} d_\alpha^* c_\alpha$

$= \begin{bmatrix} d_1^* & \cdots & d_n^* \end{bmatrix} \begin{bmatrix} c_1 \\ \vdots \\ c_n \end{bmatrix}$

$|\psi\rangle = \begin{pmatrix} c_1 \\ \vdots \\ c_n \end{pmatrix}$

$|\phi\rangle = \begin{pmatrix} d_1 \\ \vdots \\ d_n \end{pmatrix}$

→ Continuous : $\langle\phi|\psi\rangle = \langle\phi|\hat{I}|\psi\rangle = \int dx\, \langle\phi|x\rangle\langle x|\psi\rangle$.

$= \int_{-\infty}^{\infty} dx\, \phi^*(x)\psi(x)$

⇒ To calculate overlap, just calculate (represent) it based on basis.

~~Quantum state is there,~~ define basis and ~~extract property~~.

· T.D.S.E with dirac notation.

$$j\hbar \cdot \partial/\partial t \ \psi(x,t) = \hat{H} \ \psi(x,t)$$

$$\downarrow \qquad \downarrow$$

$$\underbrace{j\hbar \cdot |\Psi(t)\rangle = \hat{H} \ |\Psi(t)\rangle}$$

· Independent of basis

$$\Rightarrow \underbrace{|\Psi(t)\rangle}_{\text{Vector}} = \underbrace{\exp\left(-j\frac{\hat{H}}{\hbar}t\right)}_{\hat{U}(t,0)} \underbrace{|\Psi(0)\rangle}_{\text{vector}}$$

$$|\psi(0)\rangle = \sum_n c_n |n\rangle = \begin{pmatrix} c_1 \\ \vdots \\ c_n \end{pmatrix} \quad — ①$$

$$|\psi(t)\rangle = \begin{bmatrix} e^{-jE_1t/\hbar} & 0 & \cdots & 0 \\ 0 & e^{-jE_2t/\hbar} & & \vdots \\ \vdots & & \ddots & \\ 0 & \cdots & & e^{-jE_nt/\hbar} \end{bmatrix} \begin{bmatrix} c_1 \\ \vdots \\ c_n \end{bmatrix} = \begin{pmatrix} c_1 e^{-jE_1t/\hbar} \\ \vdots \\ c_n e^{-jE_nt/\hbar} \end{pmatrix} \quad — ②$$

we know that (in 1dimensional)

$$\hat{H} = -\frac{\hbar^2}{2m} \cdot \frac{\partial^2}{\partial x^2} + V(x)$$

Hint : $\hat{p} = -j\hbar \cdot \frac{\partial}{\partial x} \rightarrow \hat{p}\,\Psi(x) = -j\hbar\left(\frac{\partial}{\partial x}\Psi(x)\right) = -j\hbar\left(\Psi(x)\right)'$

$$\psi(x) = \begin{pmatrix} \vdots \\ \psi(x_{i-1}) \\ \psi(x_i) \\ \psi(x_{i+1}) \\ \vdots \end{pmatrix} \Rightarrow \psi'(x) = \begin{pmatrix} \vdots \\ \psi'(x_{i-1}) \\ \psi'(x_i) \\ \psi'(x_{i+1}) \\ \vdots \end{pmatrix} \begin{matrix} = \frac{1}{2\Delta x}\left(\psi_{x_i} - \psi_{x_{i-2}}\right) \\ = \frac{1}{2\Delta x}\left(\psi_{x_{i+1}} - \psi_{x_{i-1}}\right) \\ = \frac{1}{2\Delta x}\left(\psi_{x_{i+2}} - \psi_{x_i}\right) \end{matrix}$$

$$\Rightarrow \frac{d}{dx}\begin{pmatrix} \vdots \\ \Psi(x_{i-1}) \\ \Psi(x_i) \\ \Psi(x_{i+1}) \\ \vdots \end{pmatrix} = \frac{1}{2\Delta x}\begin{pmatrix} 0 & 1 & & & \\ -1 & 0 & 1 & & \\ & -1 & 0 & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & -1 & 0 \end{pmatrix}\begin{pmatrix} \vdots \\ \psi x_{i-2} \\ \psi x_{i-1} \\ \psi x_i \\ \psi x_{i+1} \\ \vdots \end{pmatrix}$$

Operator $\partial/\partial x$ can be represented in matrix!

$$\Rightarrow \hat{p}|\psi\rangle = \frac{-i\hbar}{2\Delta x}\underbrace{\begin{pmatrix} 0 & 1 & & \\ -1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ 0 & & -1 & 0 \end{pmatrix}}|\Psi\rangle$$

= Representation of $\hat{p}$ using a matrix.

- Hilbert space. — vector ~~sum~~ space with complex numbers

$|f\rangle + |g\rangle = |g\rangle + |f\rangle$ (commute)

$|f\rangle + (|g\rangle + |h\rangle) = (|f\rangle + |g\rangle) + |h\rangle$ (Associate)

$c(|f\rangle + |g\rangle) = c|f\rangle + c|g\rangle$

$\langle f|cg\rangle = c\langle f|g\rangle \qquad \langle f|(|g\rangle + |h\rangle) = \langle f|g\rangle + \langle f|h\rangle$

→ Norm = length of vector...

$\|\vec{a}\| = \sqrt{\vec{a}\cdot\vec{a}} \qquad \|f\| = \sqrt{\langle f|f\rangle}$

- Linear operators = Matrix $|\phi\rangle = \hat{A}|\psi\rangle$

if it satisfies $\hat{A}(a|\psi\rangle + b|\phi\rangle) = a\hat{A}|\psi\rangle + b\hat{A}|\phi\rangle$
then, we call $\hat{A}$ a linear operator.

- Operator algebra

① $|\psi\rangle \xrightarrow{\hat{A}} |\phi\rangle \xrightarrow{\hat{B}} |\eta\rangle = \hat{B}\hat{A}|\psi\rangle$

② $|\psi\rangle \xrightarrow{\hat{B}} |\phi'\rangle \xrightarrow{\hat{A}} |\eta'\rangle = \hat{A}\cdot\hat{B}|\psi\rangle$

In most cases, $\hat{B}\hat{A} \neq \hat{A}\hat{B} \Leftrightarrow |\eta'\rangle \neq |\eta\rangle$

we define $\boxed{\text{Commutator}}$

$[\hat{A}, \hat{B}] = \hat{A}\cdot\hat{B} - \hat{B}\hat{A}$ $= 0$ they commute!
$\neq 0$ they don't commute!

E.g. Measure A and measure B ! $\neq$ Measure B and measure A

- Suppose $\hat{A}$ = N by N matrix $= [\vec{a_1} \cdots \vec{a_n}]$

$$\hat{A}\begin{pmatrix}1\\0\\0\\\vdots\\0\end{pmatrix} = \vec{a_1} \rightarrow \hat{A}|i\rangle = \vec{a_i} \quad \left(|i\rangle = \begin{pmatrix}0\\0\\\vdots\\1\\0\\0\end{pmatrix} \rightarrow i^{th} \text{ element}\right)$$

$$\hat{A} = \left(\hat{A}|1\rangle \;\cdots\cdots\; \hat{A}|n\rangle\right)$$

columns

$\boxed{\text{operator to matrix}}$

$\hat{A} \equiv$ how basis vectors change upon $\hat{A}$ operation

$$= \begin{pmatrix}\langle 1|\hat{A}|1\rangle & & \langle 1|\hat{A}|n\rangle \\ & & \\ \langle n|A|1\rangle & & \langle n|\hat{A}|n\rangle\end{pmatrix}$$

projecting

$= A[i,j] = \langle i|\hat{A}|j\rangle$

11/14/23

- Operators

Note: $\hat{A} = \hat{I} \cdot \hat{A} \cdot \hat{I} = \left(\sum_{i=1}^{N} |i\rangle\langle i| \right) \hat{A} \left(\sum_{j=1}^{N} |j\rangle\langle j| \right)$

$$= \sum_{i=1}^{N} \sum_{j=1}^{N} \cdot \underbrace{\langle i | \hat{A} | j \rangle}_{\substack{\parallel \\ \text{constant } A_{ij}}} \underbrace{|i\rangle\langle j|}_{\parallel}$$

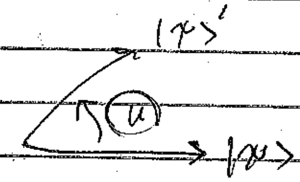
$$\begin{bmatrix} 1 & & & 0 \\ & 1 & & \\ & & \ddots & \\ 0 & & & 1 \end{bmatrix}$$

- Unitary operator

$\Rightarrow \hat{u}^{\dagger} \cdot \hat{u} = \hat{u}\, \hat{u}^{\dagger} = \hat{I}$

physically, unitary operators = rotation of vectorized quantum state

Eg.)



$|\psi'\rangle = \hat{u} \cdot |\psi\rangle$

$\Rightarrow (|\psi'\rangle)^{\dagger} = (\hat{u}\, |\psi\rangle)^{\dagger} = \langle\psi|\, \hat{u}^{\dagger}$

$\Rightarrow \langle\psi'| = \langle\psi|\, \hat{u}^{\dagger}$

$\Rightarrow \langle\psi'|\psi'\rangle = \underbrace{(\langle\psi|\, \hat{u}^{\dagger}) (\hat{u}}_{= \hat{I}} |\psi\rangle)$

$= \langle\psi|\psi\rangle \qquad \Rightarrow \underbrace{\langle\psi'|\psi'\rangle}_{\text{Norm}^2 \text{ of a vector}} = \langle\psi|\psi\rangle = |\psi|^2$

$\Rightarrow$ Norm does not change after $\hat{u}$ operation (rotation!)

$\hat{u}$

① state rotation

$|\psi\rangle = \begin{bmatrix} a \\ b \end{bmatrix} \xrightarrow{\hat{u}} |\psi'\rangle = \begin{bmatrix} c \\ d \end{bmatrix}$

② change of basis

$|\psi\rangle = \begin{bmatrix} a \\ b \end{bmatrix}_{\text{old basis}} \xrightarrow{\hat{u}} \begin{bmatrix} c \\ d \end{bmatrix}_{\text{new basis}}$

Ambiguity exists!

• Hermitian operator

Def : $\hat{M}^{+} = \hat{M}$

$$\hat{M} = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix}$$

$\downarrow$

$$\hat{M}^{+} = \begin{bmatrix} M_{11}^{*} & M_{21}^{*} \\ M_{12}^{*} & M_{22}^{*} \end{bmatrix}$$ swap + Conjugate.

< properties >

P ① Eigenvalues of $\hat{H}$ are real

$$\hat{M}|\alpha\rangle = \lambda_{\alpha}|\alpha\rangle$$

$$\langle\alpha|\hat{M}|\alpha\rangle = \lambda_{\alpha}\langle\alpha|\alpha\rangle = \lambda_{\alpha}$$

Also, $(\langle\alpha|\hat{M}^{+})^{+} = (\langle\alpha|\lambda_{\alpha}^{*})^{+}$

$\langle\alpha|\hat{M}|\alpha\rangle = \lambda_{\alpha}^{*}$ — ②

$\lambda_{\alpha} \Rightarrow \lambda_{\alpha}^{*} = \lambda_{\alpha} \rightarrow$ real!

P ② If $\lambda_{\alpha} \neq \lambda_{\beta} \rightarrow \langle\alpha|\beta\rangle = 0$: "orthogonal"

$$\langle\beta|\hat{M}|\alpha\rangle = \langle\beta|\hat{M}^{+}|\alpha\rangle$$

$$\lambda_{\alpha}\langle\beta|\alpha\rangle \qquad (\hat{M}|\beta\rangle)^{+}|\alpha\rangle$$

$$= (\lambda_{\beta}|\beta\rangle)^{+}|\alpha\rangle = \langle\beta|\lambda_{\beta}^{*}|\alpha\rangle = \lambda_{\beta}^{*}\langle\beta|\alpha\rangle$$

P ③ Physically measurable quantities $\rightarrow \hat{H}$

E.g. $\hat{H}|E_n\rangle = E_n|E_n\rangle$

E.g. $\hat{P}|P_{\alpha}\rangle = P_{\alpha}|P_{\alpha}\rangle$

$$\hat{P} = \begin{pmatrix} P_1 & & 0 \\ & \ddots & \\ 0 & & P_N \end{pmatrix}$$

In general $\underbrace{\hat{A} = \sum_{\alpha} A_{\alpha}|A_{\alpha}\rangle\langle A_{\alpha}|}_{\text{"Spectral theorem"}}$

- Uncertainty principle

→ Let us introduce : Commutator between $\hat{A}$, $\hat{B}$

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

In general, $[\hat{A}, \hat{B}] \neq 0$. However if $[\hat{A}, \hat{B}] = 0$

$$\hat{A}(\hat{B}|\psi\rangle) = \hat{B}\hat{A}\cdot|\psi\rangle \quad \text{assume} \quad |\psi\rangle = |a_i\rangle$$

$$= \hat{B}\, a_i |\psi\rangle = a_i(\hat{B}|\psi\rangle) \quad \text{—— ①}$$

Thus, $\hat{B}|\psi\rangle$ must be $\underbrace{b_j}_{\text{constant}}|\psi\rangle$ from ①

$$\Rightarrow \hat{A}\hat{B}|\psi\rangle = a_i b_j |\psi\rangle$$

$$\Rightarrow |\psi\rangle = |a_i, b_j\rangle$$ simultaneous eigenvector of $\hat{A}$ and $\hat{B}$

* ∴ When $\hat{A}$, $\hat{B}$ commute, we can find eigenstate for both $\hat{A}$ and $\hat{B}$.

→ "Uncertainty"

$$|\psi\rangle = \sum_i c_i |A_i\rangle \quad p_i = |c_i|^2$$

$$\hat{A}\cdot|A_i\rangle = \underbrace{A_i}_{\text{measurement outcomes.}}|A_i\rangle$$

Expectation of $\hat{A}$ ⇒ $\bar{A} = \langle\hat{A}\rangle = \sum_i p_i A_i = \langle\psi|\hat{A}|\psi\rangle$

we are.

Adding something ...

- Variance = statistical fluctuation

$$\Rightarrow Var(\hat{A}) = \sum_i p_i (A_i - \langle \hat{A} \rangle)^2$$

$$= \langle \psi | \underbrace{(\hat{A} - \langle \hat{A} \rangle \hat{I})}_{= \Delta \hat{A}}{}^2 | \psi \rangle$$

$$\sigma_A^2 = \langle \psi | (\Delta \hat{A})^2 | \psi \rangle = \underbrace{\langle \psi | (\hat{A} - \langle \hat{A} \rangle)}_{= \langle a |} \underbrace{(\hat{A} - \langle \hat{A} \rangle) | \psi \rangle}_{= | a \rangle}$$

$$= \langle a | a \rangle$$

$$\Rightarrow \sigma_B^2 = \langle \psi | (\Delta \hat{B})^2 | \psi \rangle = \langle b | b \rangle \quad | b \rangle = (\Delta \hat{B}) | \psi \rangle$$

$$\Rightarrow \sigma_A^2 \sigma_B^2 = \langle a | a \rangle \langle b | b \rangle$$

Using Cauchy - schwartz inequality,

$$|\vec{a}|^2 |\vec{b}|^2 \geq |\vec{a} \cdot \vec{b}|^2$$

translation

$$\langle a | a \rangle \langle b | b \rangle \geq | \langle a | b \rangle |^2$$

$$\Rightarrow \sigma_A^2 \sigma_B^2 \geq | \langle a | b \rangle |^2$$ → Continued..

11/16/23

Angular momentum.

- Uncertainty principle.

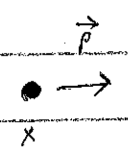
$$\sigma_A^2 = Var(\hat{A}) = \sum_i P_i^A (A_i - \langle\hat{A}\rangle)^2 = \langle\psi|(\hat{A} - \langle\hat{A}\rangle)^2|\psi\rangle \quad —— ①$$

$$\sigma_B^2 = Var(\hat{B}) = \sum_i P_i^B (B_i - \langle\hat{B}\rangle)^2 = \langle\psi|\ \hat{B} - \langle\hat{B}\rangle|\psi\rangle \quad —— ②$$

$$\rightarrow \sigma_A \cdot \sigma_B \geq \underbrace{\frac{1}{2} \left| \langle\psi| ([\hat{A}, \hat{B}]) |\psi\rangle \right|}_{\text{Lower bound.}}$$

" Order of measurement matters! "

E.g.)



$$\sigma_x \cdot \sigma_p \geq \frac{1}{2} |\langle[\hat{x}, \hat{p}_x]\rangle| = \frac{1}{2} |j\hbar| = \frac{1}{2}\hbar$$

short form of , $\langle\psi| [\hat{x}, \hat{p}_x] |\psi\rangle$

$$= \hat{x}\hat{p}_x - \hat{p}_x \cdot \hat{x} = j\hbar$$

Note: (expectation independent of $|\psi\rangle$)

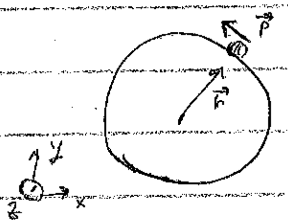
Q: why $[\hat{x}, \hat{p}_x] = j\hbar$.

$$[\hat{x}, \hat{p}_x]\psi(x) = \hat{x}\ \hat{p}_x\ \psi(x) - \hat{p}_x\ \hat{x}\ \psi(x) = \hat{x}\left(-j\hbar\, \partial/\partial x\right)\psi(x) - \left(-j\hbar\, \partial/\partial x\right) \cdot x\psi(x)$$

$$= -j\hbar \cdot x\,\psi'(x) + j\hbar\ \partial/\partial x\left(x\psi(x)\right) = j\hbar \cdot \psi(x) \quad (\text{for } |\psi(x)\rangle)$$

- Angular momentum.

※ classical mechanics



$\vec{L} = \vec{r} \times \vec{p}$

$L_x = L_y = 0$

$L_z \neq 0$

※ Quantum mechanics.

$\vec{L} \rightarrow$ 'quantized'

Recall that
$$\vec{A} \times \vec{B} = \underbrace{\begin{vmatrix} \vec{e_x} & \vec{e_y} & \vec{e_z} \\ A_x & A_y & A_z \\ B_x & B_y & B_z \end{vmatrix}}_{\text{determinant.}} = \vec{e_x}\left(A_y B_z - A_z B_y\right) - \vec{e_y}\left(A_x B_z - A_z B_x\right) + \vec{e_z}\left(A_x B_y - A_y B_x\right)$$

→ $\boxed{\text{Levi-civita symbol}}$

$$(\vec{A} \times \vec{B})_i = \varepsilon_{ijk} A_j B_k \quad \left(\text{we assume } \sum_j \sum_k \rightarrow \text{Einstein summation rule}\right)$$

$i = x, y, z$

$$L_x = \hat{y}\hat{p_z} - \hat{z}\hat{p_y}$$
$$L_y = \hat{z}\hat{p_x} - \hat{x}\hat{p_z} \rightarrow [\hat{L_x}, \hat{L_y}] = j\hbar \hat{L_z} \rightarrow [\hat{L_a}, \hat{L_b}] = j\hbar\, \varepsilon_{abc} \hat{L_c}$$
$$L_z = \hat{x}\hat{p_y} - \hat{y}\hat{p_x} \qquad [\hat{L_y}, \hat{L_z}] = j\hbar \hat{L_x}$$
$$[\hat{L_z}, \hat{L_x}] = j\hbar \hat{L_y}$$

Eigenstate of $\hat{L_x}, \hat{L_y}, \hat{L_z}$? (Note : $\hat{L_z} = -j\hbar \cdot \partial/\partial\phi$ in spherical coordinate).

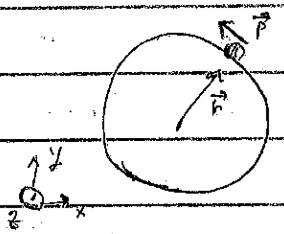
$$\hat{L_z}\, \Phi(\phi) = m\hbar\, \Phi(\phi) \Rightarrow \left(-j\hbar \cdot \partial/\partial\phi\right)\Phi(\phi) = m\hbar\, \Phi(\phi)$$

$\Rightarrow \Phi(\phi) = \exp(j \cdot m \cdot \phi)$ ✓ since $\Phi(\phi)$ is 2π periodic,

$\Phi(2\pi) = \Phi(0) = 1 \rightarrow m =$ integer $\Rightarrow \hat{L_z}\,|m\rangle = m\hbar\,|m\rangle$

- Angular momentum.

※ classical mechanics



$\vec{L} = \vec{r} \times \vec{p}$

$L_x = L_y = 0$

$L_z \neq 0$

※ Quantum mechanics.

$\vec{L} \rightarrow$ 'quantized'

Recall that $\vec{A} \times \vec{B} = \begin{vmatrix} \vec{e_x} & \vec{e_y} & \vec{e_z} \\ A_x & A_y & A_z \\ B_x & B_y & B_z \end{vmatrix} = \vec{e_x}(A_y B_z - A_z B_y) - \vec{e_y}(A_x B_z - A_z B_x) + \vec{e_z}(A_x B_y - A_y B_x)$

determinant.

$\rightarrow$ $\boxed{\text{Levi-civita symbol}}$

$(\vec{A} \times \vec{B})_i = \varepsilon_{ijk} A_j B_k$ (we assume $\sum_j \sum_k \rightarrow$ Einstein summation rule)

$i = x, y, z$

$L_x = \hat{y}\hat{p_z} - \hat{z}\hat{p_y}$

$L_y = \hat{z}\hat{p_x} - \hat{x}\hat{p_z}$ $\rightarrow [\hat{L_x}, \hat{L_y}] = j\hbar \hat{L_z} \rightarrow [\hat{L_a}, \hat{L_b}] = j\hbar\, \varepsilon_{abc} \hat{L_c}$

$L_z = \hat{x}\hat{p_y} - \hat{y}\hat{p_x}$ $\quad [\hat{L_y}, \hat{L_z}] = j\hbar \hat{L_x}$

$[\hat{L_z}, \hat{L_x}] = j\hbar \hat{L_y}$

Eigenstate of $\hat{L_x}, \hat{L_y}, \hat{L_z}$? (Note : $\hat{L_z} = -j\hbar \cdot \partial/\partial\phi$ in spherical coordinate).

$\hat{L_z}\, \Phi(\phi) = m\hbar\, \Phi(\phi) \Rightarrow (-j\hbar \cdot \partial/\partial\phi)\, \Phi(\phi) = m\hbar\, \Phi(\phi)$

$\Rightarrow \Phi(\phi) = \exp(j \cdot m \cdot \phi)$ ✓ since $\Phi(\phi)$ is 2π periodic,

$\Phi(2\pi) = \Phi(0) = 1 \rightarrow m =$ integer $\Rightarrow \hat{L_z}\,|m\rangle = m\hbar\,|m\rangle$

- $\hat{L}^2$ operator.

$\hat{L}^2 = \hat{L} \cdot \hat{L} = \hat{L_x}^2 + \hat{L_y}^2 + \hat{L_z}^2 = -\hbar^2\, \vec{\nabla}^2_{\theta\phi}$ ($\vec{r}$ not appear since we focus on the rotation only)

$\Rightarrow [\hat{L}^2, \hat{L_x}] = [\hat{L}^2, \hat{L_y}] = [\hat{L}^2, \hat{L_z}] = 0 \rightarrow$ commute!

$[\hat{L_x}, \hat{L_y}] \neq 0 \rightarrow$ not commute!

- why care $\hat{L}^2$?

$\hat{H}_{linear} = \hat{p}^2/2m = -\frac{\hbar^2}{2m} \cdot \vec{\nabla}^2_{x,y,z}$, $\vec{\nabla}^2_{x,y,z} = \partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2$

$\hat{H}_{rotating} = \hat{L}^2/2I = -\frac{\hbar^2}{2m} \cdot \vec{\nabla}^2_{\theta,\phi}$

$\Rightarrow \hat{H}_{rot}\, \psi(\theta,\phi) = E_{rot} \cdot \psi(\theta,\phi) \rightarrow$

$\Rightarrow \vec{\nabla}^2_{\theta,\phi}\, \underbrace{f(\theta,\phi)}_{\text{eigenstate}} = \underbrace{-2I/\hbar^2\, E_{rot}}_{\text{eigenvalue}}\, f(\theta,\phi)$

eigenvalue $=$ constant $= -\ell(\ell+1)$

$Y_{\ell,m}(\theta,\phi)$

$\Rightarrow \vec{\nabla}^2_{\theta,\phi}\, Y_{\ell m}(\theta,\phi) = -\ell(\ell+1)\, E_{rot}\, \psi(\theta,\phi)$

$\boxed{\text{Spherical harmonics}}$

• T. I. S. E of rot. particle $(V=0)$

$$\vec{\nabla}^2_{\theta,\phi} \, Y_{l,m}(\theta,\phi) = -l(l+1) \cdot Y_{l,m}(\theta,\phi)$$

$$\Rightarrow \quad Y_{lm}(\theta,\phi) = \Theta(\theta) \; \Phi(\phi)$$

$$\Rightarrow \quad ① \quad \frac{d^2}{d\phi^2} \Phi(\phi) = -m^2 \Phi(\phi) \quad \Rightarrow \quad \Phi(\phi) = \exp(jm\phi)$$

$$\underline{\hat{L_z} \, \Phi_m(\phi) = m\hbar \cdot \Phi_m(\phi)} \quad —— ①$$

$$② \quad \Theta(\theta) = P_l^m(\cos\theta)$$

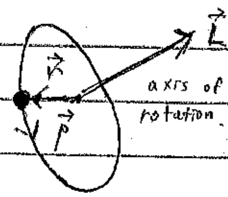
$$P_l^m(x) = \frac{1}{2^l \, l!} (1-x^2)^{m/2} \frac{d^{l+m}}{dx^{l+m}} (x^2-1)^l \quad —— ②$$

From ①. and ②, $\quad Y_{lm} = \Theta(\theta) \, \Phi(\phi) = \underline{P_l^m(\cos\theta) \cdot e^{jm\phi}}$

11/28/23.

- Hydrogen atom.

→ Recap : angular momentum operator



$\vec{L} = \vec{r} \times \vec{p}$ $\xrightarrow{\text{Q.M.}}$ $\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}}$ (operators).

$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$ $\quad (x,y,z) \to (r,\theta,\phi) = -\hbar^2 \vec{\nabla}^2_{\theta,\phi}$ — ①

$\hat{H} = \hat{P}^2/2m = \hat{L}^2/2I$

T.I.S.E. $\hat{H}|\psi\rangle = E|\psi\rangle$ → see textbook for full form.

→ $\boxed{|\psi\rangle = |l,m\rangle \ , \ E_{l,m} = \frac{\hbar^2}{2I} l(l+1).}$ —— (*)

$(l = 0,1,2,\ldots)$, $\underbrace{(-l \le m \le l)}_{2l+1 \text{ values.}}$

→ degenerate.

→ If you specify l, you have $2l+1$ degeneracy of energy eigenstates

E.g.) $l=0$, $m=0$ → $E_{00} = 0$

$l=1$, $m=-1,0,1$ → $E_{1,-1} = E_{1,0} = E_{1,1} = E_1 = \frac{\hbar^2}{2I} \cdot 2 = \hbar^2/I$

↳ Degeneracy of 3 $(= 2l+1)$

In spherical coordinate,

disregard $\vec{r}$ since operator ①

$|l,m\rangle = \hat{I}\,|l,m\rangle = \left(\int d\Omega\ |\theta,\phi\rangle\langle\theta,\phi|\right)|l,m\rangle$

spherical harmonics

$= \int d\Omega\ |\theta,\phi\rangle \cdot \underbrace{\langle\theta,\phi|l,m\rangle}_{Y_{l,m}(\theta,\phi)} = \int d\Omega\ Y_{lm}(\theta,\phi)\ |\theta,\phi\rangle$

(Y^2 is prob. density)

scalar $\quad$ Legendre function.

$$\Rightarrow Y_{lm}(\theta,\phi) = \underbrace{A_{l,m}}_{\text{scalar}} \; P_l^m(\cos\theta)\, \underbrace{e^{jm\phi}}_{\text{Base vector}}$$

E.g. $X = \cos\theta$

At $l=0, m=0 \rightarrow P_0^0(X) = 1$

$l=1, m=1 \rightarrow P_1^1(X) = \sqrt{1-X^2}$

$\vdots$

$$Prob(\theta,\phi) = |Y_{lm}(\theta,\phi)|^2$$

(similar to $|\Psi(x)|^2 = P(X)$)

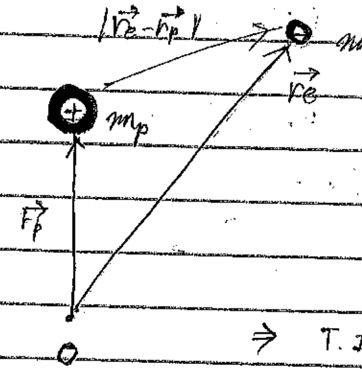
- Dirac notation.

$$\hat{L}^2 \underbrace{|l,m\rangle}_{\text{eigenstate}} = \hbar^2\, l(l+1).\, |l,m\rangle$$

$$[\hat{L}^2, \hat{L}_z] = 0 \Rightarrow \hat{L}_z\, |l,m\rangle = \hbar \cdot m\, |l,m\rangle$$

11/28/23

- Hydrogen atoms. (atom)



$$\hat{H} = \frac{\hat{P_e}^2}{2m_e} + \frac{\hat{P_p}^2}{2m_p} + \underbrace{V(|\vec{r_e}-\vec{r_p}|)}$$

(Interaction (potential) between p and e)

Note : $V(r) = -\frac{e^2}{4\pi\varepsilon_0} \cdot \frac{1}{r}$

$\Rightarrow$ T.I.S.E. $\rightarrow$ $\hat{H}|\psi\rangle = E|\psi\rangle$

$\vec{r_e} = (x_e, y_e, z_e)$, $\vec{r_p} = (x_p, y_p, z_p)$

$\Rightarrow \hat{H}\psi(\vec{r_e}, \vec{r_p}) = E\psi(\vec{r_e}, \vec{r_p})$

$\hat{p_e}^2 = -\hbar^2 \cdot \vec{\nabla_e}^2$, $\hat{p_p}^2 = -\hbar^2 \cdot \vec{\nabla_p}^2$ (6 variable equation).

$\rightarrow$ $\boxed{\text{Use change of variable. (to solve 6D!)}}$

① $M \equiv m_e + m_p \approx m_p$ ($m_p \gg m_e$) for our case.

② $\mu \equiv \frac{m_e m_p}{m_e + m_p}$ (reduced mass) $= \left(1/m_e + 1/m_p\right)^{-1}$

$\Rightarrow \hat{H} = \frac{\hat{P}_{com}^2}{2M} + \frac{\hat{P}_{rel}^2}{2\mu} + V(\vec{r_{rel}}) = \hat{H}_{com} + \hat{H}_{rel}$

(addition of seperate Hamiltonians)

where $\vec{r_{rel}} = \vec{r_e} - \vec{r_p}$ (relative)

$\vec{r_{com}} = \frac{m_e\vec{r_e} + m_p\vec{r_p}}{m_e + m_p}$ (center of mass)

$\hat{P}_{rel} = -i\hbar\vec{\nabla}_{rel}$

$\hat{P}_{com} = -i\hbar \cdot \vec{\nabla}_{com}$

$\Rightarrow \hat{H}\psi(\vec{r_e}, \vec{r_p}) = \hat{H}\psi(\vec{r_{com}}, \vec{r_{rel}})$

$= (\hat{H_{com}} + \hat{H_{rel}})\psi(\vec{r_{com}}, \vec{r_{rel}}) = E\psi(\vec{r_{com}}, \vec{r_{rel}})$

$\longrightarrow$ We can separate variables!

$$\psi(\vec{r_{com}}, \vec{r_{rel}}) = S(\vec{r_{com}})\, U(\vec{r_{rel}})$$

$$\Rightarrow \hat{H_{com}}\, S(\vec{r_{com}}) = E_{com}\, S(\vec{r_{com}})$$
$$\hat{H_{rel}}\, U(\vec{r_{rel}}) = E_{rel}\, U(\vec{r_{rel}})$$

$$\hat{H}_{com} = -\frac{\hbar^2}{2M}\vec{\nabla}_R^{\,2}$$

① $S(\vec{R}) = e^{i\vec{k}\vec{R}}$, $E_{com} = \frac{\hbar^2 k^2}{2M}$ $k = |\vec{k}|$

$$\left(-\frac{\hbar^2}{2\mu}\vec{\nabla}_r^{\,2} + V(\vec{r})\right) U(\vec{r}) = E_{rel} \cdot u(\vec{r})$$

$$\Rightarrow u(\vec{r}) = \underbrace{\frac{1}{r} A(\vec{r})}_{C(\vec{r})}\, B(\theta, \phi)$$

$$\Rightarrow U(\vec{r}) = \frac{1}{r} A(\vec{r})\, \beta(\theta, \phi)$$

$$B(\theta, \phi) = Y_{lm}(\theta, \phi) \quad -(1)$$

$$\left\{\underbrace{-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r^2}}_{K.E.} + \underbrace{\left(V(\vec{r}) + \frac{\hbar^2}{2\mu}\cdot\frac{l(l+1)}{r^2}\right)}_{V_{eff}^{(l)}(r) = P.E.}\right\} A(\vec{r}) = E_{rel} \cdot A(\vec{r})$$

Bohr radius

$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{e^2\mu} \approx 0.53\,\text{Å}$$

dimensionless

$$R_{nl}(r) = \frac{1}{r} A_{nl}(r) = C_{nl} \cdot r^l \underbrace{L_{n-l-1}^{2l+1}}\left(\frac{2r}{n a_0}\right) \exp\left(-\frac{r}{n a_0}\right)$$

Associated Laguerre function (polynomials)

11/30/23.

- Hydrogen atom - continued

$$\hat{H} = \underbrace{\frac{\hat{p}_e^2}{2m_e} + \frac{\hat{p}_p^2}{2m_p}}_{K.E.} - \underbrace{\frac{e^2}{4\pi\varepsilon_0} \cdot \frac{1}{r}}_{P.E.} \rightarrow \text{T.I.S.E} \quad \hat{H}|\psi\rangle = E|\psi\rangle$$

$\rightarrow$ Variable change ! $M = m_e + m_p$, $\mu = \frac{m_p m_e}{m_p + m_e}$

$$\Rightarrow \hat{H} = \underbrace{\frac{\hat{p}_{COM}^2}{2M}}_{\downarrow} + \underbrace{\frac{\hat{p}_{rel}^2}{2\mu} + V(\vec{r_{rel}})}$$

$$= \hat{H}_{COM} + \hat{H}_{rel}$$

$$\Rightarrow |\psi\rangle = \psi(\vec{r_{com}}, \vec{r_{rel}}) = S(\vec{r_{com}}) \cdot u(\vec{r_{rel}})$$

$$(\hat{H}_{com} + \hat{H}_{rel})\, S(\vec{r_{com}})\, u(\vec{r_{rel}}) = (E_{com} + E_{rel})\, S(\vec{r_{com}})\, u(\vec{r_{rel}})$$

$\underline{\hat{H}_{com} S = E_{com} S}$ and $\underline{\hat{H}_{rel}\, u = E_{rel} \cdot u}$

① $u(\vec{r}) = R_{nl}(r) \cdot Y_{lm}(\theta, \phi)$ (Note: $\hat{L}^2 Y_{l,m}(\theta,\phi) = \hbar^2 l(l+1) Y_{l,m}(\theta,\phi)$
$\hat{L}_z Y_{l,m}(\theta,\phi) = \hbar \cdot m \cdot Y_{l,m}(\theta,\phi)$)

$E_{rel} = -E_1/n^2$ $(n = 1, 2, \dots)$

$\hookrightarrow$ Hydrogen has huge degeneracy ✱

$0 \leq l \leq n-1$
$-l \leq m \leq l$ $\Big\}$ $\longrightarrow \uparrow$

n^{th} - orbital, $E_n = -E_1/n^2$

Degeneracy : $\sum_{l=0}^{n-1} (2l+1) = n^2 \rightarrow$ ~~wow~~ A lot!

$\uparrow$
$-l \leq m \leq l$

2008 . B.S

2019 Ph.D ?

Recall $u(\vec{r}) = R_{nl}(\vec{r}) \cdot Y_{lm}(\theta, \phi)$ $S=1$ (static hydrogen)

$\rightarrow \langle \vec{r} | \psi \rangle = \langle r, \theta, \phi | \psi \rangle$

$\hat{H} | \psi_{n,l,m} \rangle = E_n | \psi_{n,l,m} \rangle$

$= | n, l, m \rangle$

$|S| \, |U_{n,l,m}(r, \theta, \phi)|^2$ = Prob. of finding the electron.

at (r, θ, ϕ)

we denote $|\psi_{n,l,m}\rangle = |n, l, m\rangle$

$l=0 \rightarrow$ s - orbital

$l=1 \rightarrow$ p - orbital

$l=2 \rightarrow$ d - orbital

$\vdots$

Perturbation theory

- Q.S. interacts with external E.M. fields (lasers, etc.)

$$\hat{H} = \underbrace{\hat{H}_0}_{\text{original Ham.}} + \underbrace{\hat{H}_p}_{\text{perturbing Ham.}}$$

T.I.S.E for $\hat{H}|\psi\rangle = E|\psi\rangle$, $\hat{H} = \hat{H}_0 + \hat{H}_p$

Assuming $\hat{H}_0 \gg \hat{H}_p$ (weak perturbation)

$$(\hat{H}_0 + \gamma \hat{H}_p)|\psi_n\rangle = E_n|\psi_n\rangle$$

" γ = perturbation strength "

$$E_n = E_n^{(0)} + \gamma E_n^{(1)} + \gamma^2 E_n^{(2)} + \cdots$$

$$\hat{H}_0 |\psi_n^{(0)}\rangle = E_n^{(0)} \cdot |\psi_n^{(0)}\rangle$$

$$|E_n\rangle = |E_n^{(0)}\rangle + \gamma |E_n^{(1)}\rangle + \cdots$$

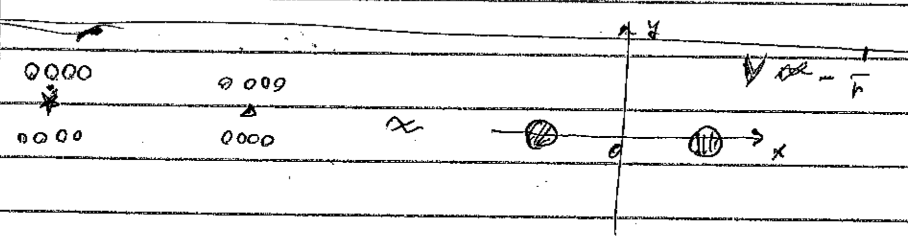
$$(\hat{H}_0 + \gamma \hat{H}_p)|E_n\rangle = E_n |E_n\rangle$$

$$\Rightarrow (\hat{H}_0 + \gamma \hat{H}_p)\left[\sum_{k=0}^{\infty} \gamma^k \cdot |E_n^{(k)}\rangle\right] = \left[\sum_{m=0}^{\infty} \gamma^m E_n^{(m)}\right]\left[\sum_{k=0}^{\infty} \gamma^k |E_n^{(k)}\rangle\right]$$

γ of 0^{th} order $\rightarrow \hat{H}_0 |E_n^{(0)}\rangle = E_n^{(0)} |E_n^{(0)}\rangle$

γ of 1^{st} order $\rightarrow \cancel{\hat{H}_0 |E_n^{(1)}\rangle + \hat{H}_p |E_n^{(1)}\rangle} = E_n^{(0)} |E_n^{(1)}\rangle + E_n^{(1)} |E_n^{(0)}\rangle$

γ of 2^{nd} order $\rightarrow \hat{H}_0 |E_n^{(2)}\rangle + \hat{H}_p |E_n^{(1)}\rangle = E_n^{(0)} |E_n^{(2)}\rangle + E_n^{(1)} |E_n^{(1)}\rangle + E_n^{(2)} |E_n^{(0)}\rangle$



- 1st order correction.

$$\hat{H}_0 | E_n^{(1)} \rangle + \hat{H}_p | E_n^{(1)} \rangle = E_n^{(0)} | E_n^{(1)} \rangle + E_n^{(1)} | E_n^{(0)} \rangle$$

$$\Rightarrow \{ \hat{H}_0 - E_n^{(0)} \} \cdot | E_n^{(1)} \rangle = \{ E_n^{(1)} - \hat{H}_p \} \cdot | E_n^{(0)} \rangle$$

$$\langle E_n^{(0)} | \cdot \underbrace{\{ \hat{H}_0 - E_n^{(0)} \}}_{\to 0} | E_n^{(1)} \rangle = \langle E_n^{(0)} | E_n^{(1)} - \hat{H}_p | E_n^{(0)} \rangle$$

$$\Rightarrow 0 = E_n^{(1)} \langle E_n^{(0)} | E_n^{(0)} \rangle - \langle E_n^{(0)} | \hat{H}_p | E_n^{(0)} \rangle$$

$$\Rightarrow \boxed{E_n^{(1)} = \langle E_n^{(0)} | \hat{H}_p | E_n^{(0)} \rangle}$$

1st order correction of energy

$$E_n^{(0)} + \gamma E_n^{(1)} + \cdots$$

What about

$| E_n^{(1)} \rangle$?

$$\Rightarrow \langle E_i^{(0)} | \hat{H}_0 - E_n^{(0)} | E_n^{(1)} \rangle = \langle E_i^{(0)} | E_n^{(1)} - \hat{H}_p | E_n^{(0)} \rangle$$

assume $i \neq N$

$$\Rightarrow | E_n^{(1)} \rangle = \sum_i^N a_i^{(1)} | E_i^{(0)} \rangle$$ (express in already known $| E_i^{(0)} \rangle$)

$\Rightarrow$ all the math — plug in.

$$\Rightarrow a_i^{(1)} = - \frac{\langle E_i^{(0)} | \hat{H}_p | E_n^{(0)} \rangle}{E_i^{(0)} - E_n^{(0)}}$$

$|\psi\rangle = |n, l, m\rangle$ $\qquad l = 0, 1, 2, \ldots$

$\psi(x)$ $\qquad\qquad\qquad \downarrow$

$\qquad\qquad\qquad -l \leq m \leq l$

$$\hat{H} = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \cancel{V} \right)$$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \right) \psi(x) = E\,\psi(x)$$

$$\langle x|\psi\rangle \qquad \hat{H} = \frac{\hat{L}^2}{2I} = \frac{p^2}{2m} + \cancel{V}$$

$$|\psi\rangle \longrightarrow \langle x|\psi\rangle = \psi(x)$$

$$\langle x, y, z|\psi\rangle = \psi(x, y, z)$$

$$\langle r, \theta, \phi|\psi\rangle = \psi(r, \theta, \phi)$$

$$\hat{L}^2 = \left(-\hbar^2 \hat{\nabla}^2_{(\theta, \phi)} \right) \psi(r, \theta, \phi)$$

$$\boxed{\hat{L}^2 |\psi\rangle = \hat{L}^2 |l, m\rangle = \hbar^2 l(l+1) |l, m\rangle}$$

$$\langle r, \theta, \phi|l, m\rangle = \langle \theta, \phi|l, m\rangle = Y_{lm}(\theta, \phi)$$

$$\langle r, \theta, \phi | n l m \rangle = R_{nl}(r)\, Y_{lm}(\theta, \phi)$$

$$\hat{H} | n l m \rangle = -\frac{E_1}{n^2} | n l m \rangle$$

$$\hat{L}^2 | l m \rangle = \hbar^2 l(l+1) | l m \rangle$$

$$\hat{L}_z | l m \rangle = m\hbar | l m \rangle$$

$$\hat{O} | l m \rangle = \lambda\omega | l m \rangle$$

$$\cancel{\langle \theta, \phi | l m \rangle}$$

$$E_i^{(0)} - E_n^{(0)}$$

12/5/23

- Perturbations.

T.I.S.E : $\hat{H}_0 |E^0\rangle = E^0 |E^0\rangle$

'perturbed' T.I.S.E. $\equiv (\hat{H}_0 + \hat{H}_p)|E\rangle = E|E\rangle$ (find E and $|E\rangle$)

perturbation strength. $\|\hat{H}_p\| / \|\hat{H}_0\| = \gamma \ll 1$ (assumption)

① Method 1 $\Rightarrow$ $\hat{H} = \hat{H}_0 + \hat{H}_p = \sum_i \sum_j \langle i | \hat{H}_0 + \hat{H}_p | j\rangle \, |i\rangle\langle j|$

$|i\rangle = |E_i^{(0)}\rangle$

② Method 2 : Perturbation theory.

(1) $|E_n\rangle = |E_n^{(0)}\rangle + \underbrace{\delta |E_n\rangle}_{\text{correction}}$ where (2) $E_n = E_n^{(0)} + \delta E_n \rightarrow$ correction.

change eigenstate — change eigenvalue.

- Energy eigenvalues. · Energy eigenstate

$\delta E_n = \underbrace{E_n^{(1)}}_{\propto \gamma^1} + \underbrace{E_n^{(2)}}_{\propto \gamma^2} + \cdots$ $\qquad \delta|E_n\rangle = \underbrace{|E_n^{(1)}\rangle}_{\propto \gamma^1} + \underbrace{|E_n^{(2)}\rangle}_{\propto \gamma^2} + \cdots$

correction — correction.

<Value corrections>

works as basis.

$(E_n^{(1)}) = \langle E_n^{(0)} | \hat{H}_p | E_n^{(0)}\rangle$

$$* E_n^{(2)} = -\sum_{i \neq n} \frac{|\langle E_i^{(0)} | \hat{H}_p | E_n^{(0)}\rangle|^2}{E_i^{(0)} - E_n^{(0)}}$$

<State corrections>

use same basis (∵ already complete!)

$|E_n^{(1)}\rangle = \sum_i a_i^{(1)} |E_i^{(0)}\rangle$

$|E_n^{(2)}\rangle = \sum_i a_i^{(2)} |E_i^{(0)}\rangle \quad \rightarrow \quad |E_n^{(k)}\rangle = \sum_i a_i^{(k)} |E_i^{(0)}\rangle$

so, for states $|E_n^{(k)}\rangle = \sum_i a_i^{(k)} |E_i^{(0)}\rangle$

where $a_i^{(1)} = -\dfrac{\langle E_i^{(0)}| H_p | E_n^{(0)}\rangle}{E_i^{(0)} - E_n^{(0)}}$ (1st correction)

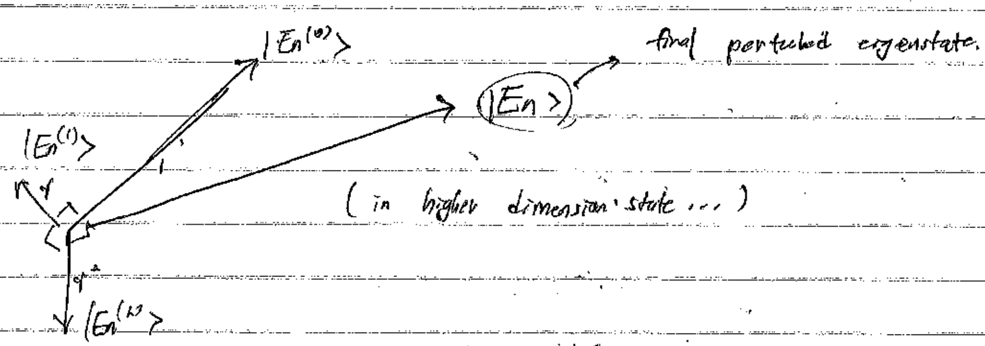
$$a_i^{(2)} = \frac{E_n^{(1)} a_i^{(1)} - \langle E_i^{(0)} | H_p | E_n^{(1)}\rangle}{E_i^{(0)} - E_n^{(0)}}$$ (2nd correction)

$$a_i^{(1)} = f(\hat{H_p}, |E^{(0)}\rangle)$$
$$a_i^{(2)} = g(\hat{H_p}, \{|E^{(0)}\rangle\}, \{E^{(0)}\}, \{|E^{(1)}\rangle\}, \{E^{(1)}\})$$

Compute higher order correction using lower order results.

→ In summary,

$$|E_n\rangle = |E_n^{(0)}\rangle + \underbrace{|E_n^{(1)}\rangle}_{\propto q} + \underbrace{|E_n^{(2)}\rangle}_{\propto q^2} + \cdots$$



(in higher dimension state ...)

- Degenerate Perturbation theory

Recall $\hat{H} = \hat{L}^2/(2I)$: rigid rotation.

$$\hat{H}|E\rangle = E|E\rangle \rightarrow E = \frac{\hbar^2}{2I} l(l+1) \qquad |E\rangle = |l,m\rangle$$

When $l \neq 0$, we have degeneracy $l=1 \rightarrow E_1, E_2, E_3$

$$\psi = a_1|E_1\rangle + a_2|E_2\rangle + a_3|E_3\rangle \text{ is also a eigenstate.}$$

"Generalization"

"K" degenerate states. $\{|E_i^{(0)}\rangle\}$ (for $i = 1 \sim k$)

$\Rightarrow E^{(0)}$ under $\hat{H}_0$

$\Rightarrow \hat{H} = \hat{H}_0 + \underline{\hat{H}_p} \rightarrow \boxed{\hat{H}_p|E^{(1)}\rangle = E^{(1)}|E^{(1)}\rangle}$

$$\Rightarrow \underbrace{\begin{bmatrix} \langle E_1^{(0)}|\hat{H}_p|E_1^{(0)}\rangle & \cdots & \langle E_1^{(0)}|\hat{H}_p|E_k^{(0)}\rangle \\ \vdots & & \\ \langle E_k^{(0)}|\hat{H}_p|E_1^{(0)}\rangle & \cdots & \langle E_k^{(0)}|\hat{H}_p|E_k^{(0)}\rangle \end{bmatrix}}_{\text{matrix } A} |E^{(1)}\rangle = E^{(1)}|E^{(1)}\rangle$$

$$\Rightarrow A|E^{(1)}\rangle = E^{(1)}|E^{(1)}\rangle$$

Time dependent pert. theory.

$\hat{H}(t) = \hat{H}_0 + \underbrace{\hat{H}_p(t)}_{\text{External stimulus.}}$ → How electrons change state under time.

↓

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

$\hat{H}_0 |E_n\rangle = E_n |E_n\rangle$ is fixed where $|\psi(t)\rangle = \sum_n C_n(t) |E_n\rangle$

We can't do $C_n(t) = C_n(0)\, e^{-j E_n/\hbar \cdot t}$

↓ can't be constant.

$\Rightarrow |\psi(t)\rangle = \sum_n a_n(t)\, e^{-j \frac{E_n}{\hbar} t} |E_n\rangle$

$LHS = j\hbar \frac{d}{dt} \left(\sum_n a_n(t)\, e^{-j w_n t} |E_n\rangle \right)$

$= \sum_n \left(j\hbar \dot{a}_n(t) + a_n(t) E_n \right) e^{-j w_n t} |E_n\rangle$

$RHS = \{ \hat{H}_0 + \hat{H}_p(t) \} \left(\sum_n a_n(t)\, e^{-j w_n t} |E_n\rangle \right)$

$= \sum_n a_n(t)\, e^{-j w_n t} \left(E_n + \hat{H}_p \right) |E_n\rangle$

$LHS = RHS \Rightarrow \langle E_k | LHS = \langle E_k | RHS$

$\Rightarrow j\hbar \dot{a}_k(t)\, e^{-j w_k t} = \langle E_k | LHS$

$\sum_n a_n(t)\, e^{-j w_n t} \langle E_k | \hat{H}_p | E_n\rangle = \langle E_k | RHS$

Thus we have, ...

$$|E\rangle = \sum_n a_n(t) \exp(-j E_n t/\hbar) |E_n\rangle$$

$$a_q^{(0)}(t) = 0 \rightarrow \text{Unperturbed solution.}$$

$$\dot{a}_q^{(1)}(t) = \frac{1}{j\hbar} \sum_n a_n^{(0)} \exp(j\omega_{qn} t) \langle E_q^{(0)} | \hat{H_p}(t) | E_n^{(0)} \rangle$$

$$\omega_{qn} = (E_q - E_n)/\hbar$$

$$\Rightarrow a_q = \underbrace{a_q^{(0)}}_{\text{constants}} + a_q^{(1)}(t) + \cdots$$

$$\Rightarrow \dot{a}_q^{(p+1)}(t) = \frac{1}{j\hbar} \sum_n a_n^{(p)} \exp(j\omega_{qn} t) \langle E_q^{(0)} | \hat{H_p} | E_n^{(0)} \rangle$$

(successive)

$$\frac{n^2 h^2}{8mL^2} = \frac{(2\pi\hbar)^2 n^2}{8mL^2}$$

$$= \frac{4\pi^2 \cdot \hbar^2 n^2}{8mL^2}$$

$$= \frac{n^2\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2.$$

$$= \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2.$$

2023/12/07.
12/7/23.

- Fermi's golden rule.

T.D.S.E $\quad i\hbar \, \partial/\partial t \, |\psi(t)\rangle = \hat{H}(t) \, |\psi(t)\rangle$ —— ①

$\hat{H}(t) = \hat{H}_0(t) + \hat{H}_p(t)$. with perturbation.

$|\psi(t)\rangle = \sum_n a_n(t) \, e^{-i\omega_n t} \, |E_n\rangle \quad (\omega_n = E_n/\hbar)$ —— ②

~~$c_n(t) \rightarrow$ expansion coefficient.~~

$H_0 |E_n\rangle = E_n |E_n\rangle$

② → ①

$\Rightarrow \sum_n i\hbar \, \dot{a}_n(t) \, e^{-i\omega_n t} \, |E_n\rangle = \sum_n a_n(t) \, e^{-i\omega_n t} \, \hat{H}_p |E_n\rangle$

$\downarrow \langle E_k|$

$\Rightarrow i\hbar \, \dot{a}_k(t) \, e^{-i\omega_k t} = \sum_n a_n(t) \, e^{-i\omega_n t} \, \langle E_k | \hat{H}_p | E_n \rangle$ —— ③

$a_n(t) = \underset{\propto \gamma}{a_n^{(0)}(t)} + \underset{\propto \gamma^2}{a_n^{(1)}(t)} + \cdots + \cdots \Rightarrow \gamma = \|\hat{H}_p\| / \|\hat{H}_0\|$ —— ④

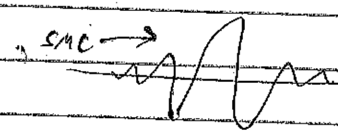
④ → ③ and perform order by order comparison.

$$\Rightarrow \begin{cases} \dot{a}_k^{(1)}(t') = \frac{1}{i\hbar} \sum_n a_n^{(0)} \, e^{i\omega_{kn} t'} \, \langle E_k | \hat{H}_p | E_n \rangle \\ \qquad\qquad (\omega_{km} = \omega_k - \omega_m) \\ \dot{a}_k^{(2)}(t') = \frac{1}{i\hbar} \sum_n a_n^{(1)}(t') \, e^{i\omega_{kn} t'} \, \langle E_k | \hat{H}_p | E_n \rangle \end{cases}$$

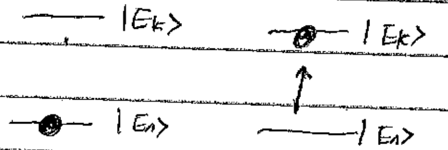
(5) $a_k(t) = a_k^{(0)} + a_k^{(1)}(t) = a_k^{(0)} + \int_0^t t' \; \dot{a}_k^{(0)}(t')$

$$|\psi(t)\rangle = e^{-i\omega_n t}|E_n\rangle + \sum_k \left(\int_0^t dt' \; \dot{a}_k^{(1)}(t')\right) e^{-i\omega_k t}|E_k\rangle$$

$\omega = \omega_{kn}$: "absorption" > 0



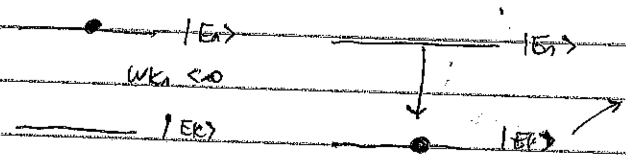
(1)



$$a_k^{(1)}(t) = t \cdot \left(\frac{A_{kn}}{i\hbar}\right) e^{i\left(\frac{\omega_{kn}-\omega}{2}\right)t} \, \mathrm{sinc}\left(\frac{\omega_{kn}-\omega}{2}t\right)$$

As $t \to \infty$ more population!

(2) $\omega_{kn} = \omega_k - \omega_n < 0$ "Emission"



$\omega = -\omega_{kn}$

$$a_k^{(1)}(t) = t\left(\frac{A_{kn}}{i\hbar}\right) e^{\left(i\,\frac{\omega_{kn}+\omega}{2}\,t\right)} \cdot \mathrm{sinc}\left(\frac{\omega_{kn}+\omega}{2}\,t\right)$$

As time evolves, more $t\uparrow$ → population increases!

2023 / 12 / 07.

- Fermi's golden rule.

Born's rule.

$$P_k(t) = |a_k(t)|^2 \simeq |a_k^{(0)} + a_k^{(1)}(t)|^2 = |a_k^{(1)}(t)|^2 \ (\text{when } k > 1)$$

$$P_k(t) = t^2/\hbar^2 \cdot |A_{k1}|^2 \operatorname{sinc}^2\left(\frac{\omega_{k1} - \omega}{2} t\right)$$

↓ $m=1$ → starting from ground state.

Total absorption probability

$$P_{total} = \sum_{k>1} P_k(t) = \sum_{k>1} t^2/\hbar^2 \cdot |A_{k1}|^2 \cdot \operatorname{sinc}^2\left\{\frac{\omega_{k1} - \omega}{2} \cdot t\right\}.$$

$$\simeq t^2/\hbar^2 |A_{m1}|^2 \operatorname{sinc}^2\left\{\frac{\omega_{m1} - \omega}{2} t\right\}.$$

for specific states 'm'

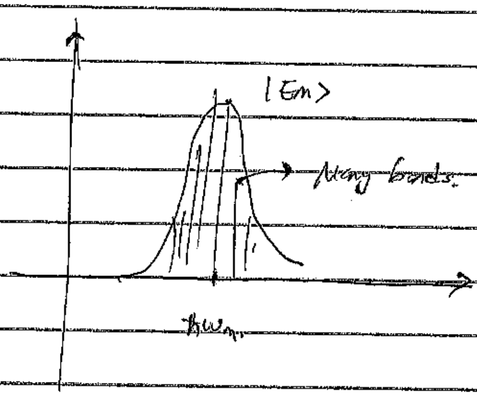
Reality) → Density of states.

$|E_m\rangle$ $\quad P_{total} \simeq t^2/\hbar^2 \, |A_{m1}|^2 \int_{-\infty}^{\infty} d(\hbar\omega_{m}) \, \underbrace{g(\hbar\,\omega_{m1})}_{\text{Density of states.}} \operatorname{sinc}^2\left(\frac{\omega_{m1} - \omega}{2} t\right)$

$\sim \omega_{m1}$

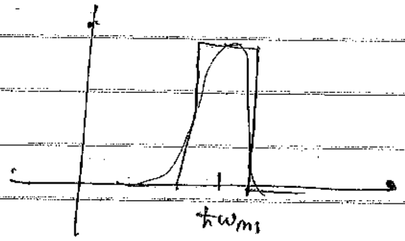
$|E_1\rangle$

(work with energy units?)



EE223.

Approximate to



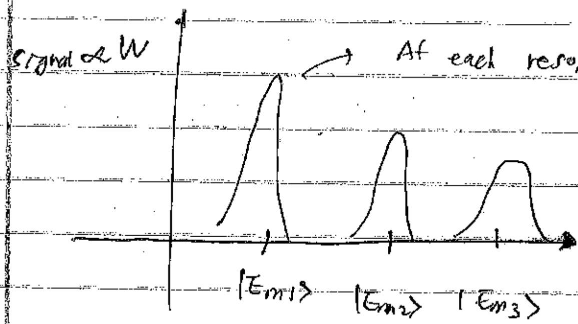
Assume $\hbar\omega_{m1}$ does not influence a lot.

$$\Rightarrow \frac{t^2}{\hbar^2} |A_{m1}|^2 \, g(\hbar\omega_{m1}) \underbrace{\int_{-\infty}^{\infty} d(\hbar\omega_{m1}) \, \mathrm{sinc}^2(X)}_{= \frac{2\pi\hbar}{t}}$$

$$= \frac{2\pi t}{\hbar} \cdot |A_{m1}|^2 \cdot g(\hbar\omega_{m1}) = a$$

$$W = \text{prob. change} / \text{unit time} = \frac{P_{pt}}{t}$$

$$= \underline{\frac{2\pi}{\hbar} \cdot |A_{m1}|^2 \cdot g(\hbar\omega_{m1})}$$; Fermi's golden rule.



Some notes 12/08/23.

- Transition dipole moment (from $|\psi_a\rangle$ to $|\psi_b\rangle$)

$$\langle \psi_b | (q\vec{r}) | \psi_a \rangle = \underline{q\int \psi_b^*(\vec{r})\cdot\vec{r}\cdot\psi_a(\vec{r})\, d^3\vec{r}}$$

note that if $\psi_b(\vec{r})$ and $\psi_a(\vec{r})$ has (opposite parity regarding $\vec{r}$,

$\psi_b^*(\vec{r})\ \vec{r}\ \psi_a(\vec{r})$ is ~~odd~~ even function $\rightarrow \langle \psi_b | (q\vec{r}) | \psi_a \rangle \neq 0$

If they have same parity. $\rightarrow \langle \psi_b | (q\vec{r}) | \psi_a \rangle = 0$

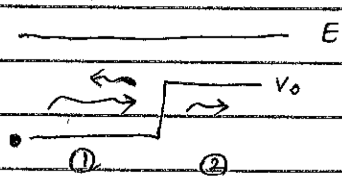
Transition matrix.

- $|E_n\rangle = |E_n^{(0)}\rangle + \underline{\delta |E_n\rangle}$

$\qquad = E_n^{(1)} + E_n^{(2)} + \cdots$ (not multiplied!)

↳ atleast here...

- Note that.



Region ① has reflected part where

" ② has only propagation..

10/29/23.

Midterm

- De Broglie's formula.

$$\lambda = \frac{h}{p}$$

- Time - Independent Schrödinger Equation (T.I.S.E)

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\psi = E\psi \Rightarrow \hat{H}\psi = E\psi$$

(Eigenvalue problem)

- Normalization

$$\int |\psi_n(\vec{r})|^2 d^3\vec{r} = 1$$

- Solving equation + Boundary Condition.

$$\psi = A\sin(kz) + B\cos(kz) \text{ form} \Rightarrow \psi(0) = \psi(L_z) = 0 \quad \left(k = \sqrt{2mE/\hbar^2}\right)$$

$$\Rightarrow k_z = n\pi/L_z$$

$$\Rightarrow \underline{E_n = \frac{\hbar^2}{2m}\left(n\pi/L_z\right)^2}$$

- Orthonormality

$$\int_0^{L_z} \psi_n^* \psi_m \, dz = \delta_{nm} \rightarrow \text{This says } \begin{cases} ① \text{ orthogonality} \\ ② \ \psi \text{ are normalized} \end{cases}$$

- Complete form

Already Normalized.

$$f(x) = \sum_n C_n \psi_n(x). \text{ Note } \int \psi_m^* f(x)\,dx = \int \psi_m^* \sum_n C_n \psi_n(x)\,dx$$

$$= C_m \quad (\text{only } m=n \text{ survives})$$

- Harmonic oscillator → next page

- Harmonic oscillator Note: $\nabla V = -\vec{F}$

$$F = m\, \partial^2 z / \partial t^2 = -\underbrace{s}_{\text{spring constant}} z \rightarrow V(z) = \int_0^z -F\,dz = \frac{1}{2} s z^2 = \frac{1}{2} m \omega^2 z^2$$

$$\rightarrow -\frac{\hbar^2}{2m} \cdot \frac{\partial^2 \psi}{\partial z^2} + \frac{1}{2} m\omega^2 z^2 \psi = E\psi \rightarrow \text{Define } \xi = \sqrt{\frac{m\omega}{\hbar}} \cdot z$$

$$\rightarrow \partial^2\psi / \partial\xi^2 - \xi^2 \psi = -\frac{2E}{\hbar\omega}\psi \rightsquigarrow \boxed{\psi \propto e^{-\xi^2/2}} \longrightarrow (1)$$

$$\Rightarrow \psi(\xi) = e^{-\xi^2/2} \cdot \underbrace{H_n(\xi)}_{\text{to be determined}} \Rightarrow \text{Plug in to } (1)$$

$$\Rightarrow \frac{\partial^2 H_n(\xi)}{\partial \xi^2} - 2\xi \cdot \frac{\partial H_n(\xi)}{\partial \xi} + \left(\frac{2E}{\hbar\omega} - 1\right) H_n(\xi) = 0 \rightarrow \text{known solution.}$$

$$\Rightarrow \frac{2E}{\hbar\omega} - 1 = 2n \quad \underbrace{(n = 0, 1, 2, \ldots)}_{\text{starts from zero!}} \Rightarrow \boxed{E_n = \left(n + \frac{1}{2}\right)\hbar\omega}$$

- Energy - Frequency

$$E = \hbar\omega$$

- Time Dependent Schrödinger Equation (T.D.S.E) No time dependent term ↳ Not a solution of T.D.S.E

$$-\frac{\hbar^2}{2m} \cdot \nabla^2 \psi(\vec{r},t) + V(\vec{r},t)\psi(\vec{r},t) = j\hbar \frac{\partial}{\partial t}\psi(\vec{r},t)$$

- Expansion (eigenstates and eigenvalues)

$$\psi(\vec{r},t) = \sum_n a_n \cdot \psi_n(\vec{r},t) = \sum_n a_n \cdot e^{-j E_n t/\hbar} \underbrace{\psi_n(\vec{r})}_{\text{Time independent}}$$

At $t=0 \rightarrow \psi(\vec{r})$

- Group Velocity.

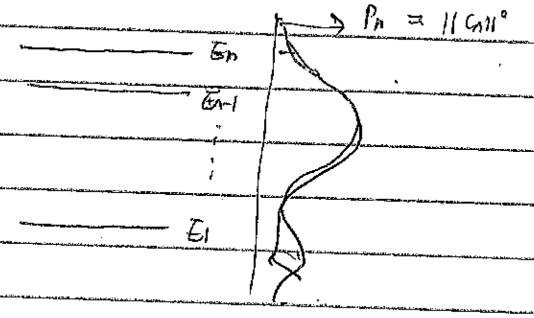
$v_p = w/k$ and $v_g = \partial w/\partial k$.

- Measurement. (Quantum Collapse)

$$\psi(\vec{r},t) = \sum_n c_n(t)\,\psi_n(\vec{r}) = \sum_n c_n\, e^{-jE_n/\hbar \cdot t} \cdot \psi_n(\vec{r},0)$$

In measurement, $P_n = \|c_n\|^2$

* system collapses into an eigenstate of the quantity being measured.



- Expectation

$$\langle E\rangle = \sum_n E_n P_n = \sum_n E_n |c_n|^2 \quad \text{(if we measure)} \qquad (1)$$

Now, consider. $I = \int \psi^*(\vec{r},t)\cdot \hat{H}\,\psi(\vec{r},t)\, d^3\vec{r}$.

$$\psi(\vec{r},t) = \sum_n c_n(t)\,\psi_n(\vec{r}). \Rightarrow \hat{H}\psi(\vec{r},t) = \sum_n c_n \hat{H}\psi_n(\vec{r}) = \sum_n c_n(t) E_n \psi_n(\vec{r})$$

$$\Rightarrow I = \int \left[\sum_m c_m^*(t)\,\psi_m^*(\vec{r})\right]\cdot\left[\sum_n c_n(t)\,\psi_n(\vec{r})\cdot E_n\right] d^3\vec{r}.$$

since $\psi_n(\vec{r})$ is orthonormal (i.e., $\int \psi_n \psi_m = \delta_{nm}$),

$$I = \int \psi^*(\vec{r},t)\,\hat{H}\,\psi(\vec{r},t)\, d^3\vec{r} = \sum_n E_n |c_n|^2$$

From (1), we know $\langle E\rangle = \int \psi^*(\vec{r},t)\,\hat{H}\,\psi(\vec{r},t)\, d^3\vec{r}$

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EE222 - Notes. (Final)

- Schrodinger equations $\begin{cases} \text{T.I.S.E} : -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x), & \hat{H}|\psi\rangle = E|\psi\rangle \\ \text{T.D.S.E} : -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = j\hbar\frac{\partial}{\partial t}\psi(t), & \hat{H}(t)|\psi(t)\rangle = j\hbar\frac{\partial}{\partial t}|\psi(t)\rangle \end{cases}$

In 1D, we have $\psi(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right)$ $\left(\because \psi(0)=0,\ \psi(L)=0,\ \frac{n\pi}{L}=k\right)$ $E_n = \frac{n^2h^2}{8mL^2} = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2$

In 3D, $\psi(x,y,z) = \left(\sqrt{\frac{2}{L}}\right)^3 \sin\left(\frac{n_x\pi}{L}x\right)\sin\left(\frac{n_y\pi}{L}y\right)\sin\left(\frac{n_z\pi}{L}z\right)$ $(L_x=L_y=L_z=L)$

→ particle in a box (if $(x,y,z)=(0,0,0)$ is center) ⇒ $\psi_1 = A\cos\left(\frac{\pi}{L}x\right)$, $\psi_2 = A\sin\left(\frac{2\pi x}{L}\right)$

- Born's rule : $\psi(r,t) = \sum_n c_n(t)\psi_n(\vec{r}) \to P_n = \|c_n\|^2$ (measurement), $c_n(t) = \exp\left(-j\frac{E_n}{\hbar}\cdot t\right)$ ($\frac{E_n}{\hbar} = w_n$)

$\langle E\rangle = \sum_n E_nP_n = \sum_n E_n|c_n|^2 = \langle\psi|\hat{H}|\psi\rangle = \int\psi^*(r,t)\hat{H}\psi(r,t)\,d^3\vec{r}$

- Phase velocity $v_p = w/k$, group velocity $= \partial w/\partial k = v_g = \frac{1}{\hbar}\cdot\partial E/\partial k$.
- Orthogonal : $\int\bar{f}g\,dx = 0$ (remember conjugate), Hermitian : $H^\dagger = H$, Unitary : $U^\dagger U = I = UU^\dagger$
- Dirac notation : ① state overlap : $\langle\phi|\psi\rangle = \int_{-\infty}^{\infty}dx\,\phi^*(x)\psi(x)$. ② TDSE : $|\psi(t)\rangle = \sum_n a_n(t)\exp(-jE_n/\hbar\,t)|E_n\rangle$.

③ Expectation : $\langle z\rangle = \langle E|z|E\rangle$ (variable value at certain state $|E\rangle$) ④ Transition : $\langle \underset{\text{end}}{2,1,0}|z|\underset{\text{start}}{1,0,0}\rangle$

- spherical harmonics $Y_l^m(\theta,\phi) = (-1)^m\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}\cdot P_l^m(\cos\theta)e^{jm\phi}$,

$Y_0^0 = 1/\sqrt{4\pi}$ | $Y_1^1 = -\sqrt{\frac{3}{8\pi}}\sin\theta e^{j\phi}$ | $Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$ | $Y_2^2 = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta e^{2j\phi}$ | $Y_2^1 = -\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{j\phi}$ | $Y_2^0 = \frac{1}{2}\sqrt{\frac{5}{4\pi}}(3\cos^2\theta-1)$

$R_{nl}(r)$ in transition with z, which is $z = r\cos\theta$, $y = r\sin\theta\sin\phi$, $x = r\sin\theta\cos\phi$.

$Y_l^{-m}(\theta,\phi) = (-1)^m\cdot Y_l^m(\theta,\phi)^*$ (for negative m) $(m>0)$

- Independence of $\sum_{ij}|a_{ij}|^2 = \sum_{mn}|\langle\psi_m|\hat{A}|\psi_n\rangle|^2 = \sum_{mn}\langle\psi_n|\hat{A}^\dagger|\psi_m\rangle\langle\psi_m|\hat{A}|\psi_n\rangle$ $(m,n)\to(p,q)$

$\hat{W} = \sum_{ij}a_{ij}|\phi_i\rangle\langle\psi_j|$, $\sum_i a_{iq}^*a_{ij} = \delta_{qj} \Rightarrow \hat{W}^\dagger W = I$ $\sum_p|\phi_p\rangle\langle\phi_p|$ $\sum_q|\phi_q\rangle\langle\phi_q|$

→ Basis independence of $\|\hat{A}\|_F = \left(\sum_{ij}|a_{ij}|^2\right)$ $E_2 = E_2^{(0)} + E_2^{(1)}$

- Coherent state : $\hat{a}|\alpha\rangle = \alpha|\alpha\rangle$ where $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}mw^2x^2$, $\hat{H} = \hbar w\left(\hat{n}+\frac{1}{2}\right)$, $\hat{a} = \frac{1}{\sqrt{2m\hbar w}}(j\hat{p} + mw\hat{x})$

$\hat{H}|n\rangle = E_n|n\rangle$ where $E_n = \hbar w\left(n+\frac{1}{2}\right)$ $(n=0,1,2,\dots,n)$ $\hat{H}|n\rangle = \hbar w\left(n+\frac{1}{2}\right)|n\rangle$. (oscillatory potential)

$n = \bar{n} = |\alpha|^2 \to$ (max) probability.

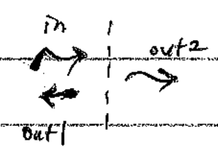
$P_k(t) = \|a_k(t)\|^2 = \|a_k^{(0)} + a_k^{(1)}(t)\|^2$

$a_k^{(1)}(t) = t\left(\frac{A_{kn}}{j\hbar}\right)e^{\left(j\frac{w_{kn}+w}{2}t\right)}\operatorname{sinc}\left(\frac{w_{kn}+w}{2}t\right)$

$t\uparrow$, population $\uparrow$

$\hat{H}|n,l,m\rangle = -\frac{E_1}{n^2}\cdot|n,l,m\rangle$

- $\hat{A} = \begin{pmatrix}\langle 1|A|1\rangle & \cdots & \langle 1|\hat{A}|n\rangle \\ \vdots & & \vdots \\ \langle n|A|1\rangle & \cdots & \langle n|A|n\rangle\end{pmatrix}$ $A_{ij} = \langle i|A|j\rangle$



formulation : reflection exists at starting region.

• T.I.P.T. : $\hat{H}_0 |E_0\rangle = E_0|E_0\rangle \Rightarrow (\hat{H}_0+\hat{H}_p)|E\rangle = E|E\rangle$ (where $\|\hat{H}_p\| / \|\hat{H}_0\| = \alpha \ll 1$)

$|E_n\rangle = |E_n^{(0)}\rangle + \delta|E_n\rangle \rightarrow$ ① Value corrections : $E_n^{(1)} = \langle E_n^{(0)}|\hat{H}_p|E_n^{(0)}\rangle$

② State corrections : $|E_n^{(1)}\rangle = \sum_{i\neq n} a_i^{(1)} |E_i^{(0)}\rangle$ $\qquad E_n^{(2)} = \sum_{i\neq n} \frac{|\langle E_i^{(0)}|\hat{H}_p|E_n^{(0)}\rangle|^2}{E_i^{(0)} - E_n^{(0)}}$

$|E_n^{(2)}\rangle = \sum_{i\neq n} a_i^{(2)} |E_i^{(0)}\rangle$.

• $a_i^{(1)} = -\frac{\langle E_i^{(0)}|H_p|E_n^{(0)}\rangle}{E_i^{(0)} - E_n^{(0)}}$, $a_i^{(2)} = \frac{E_n^{(1)} a_i^{(1)} - \langle E_i^{(0)}|H_p|E_n^{(1)}\rangle}{E_i^{(0)} - E_n^{(0)}}$.

$|E_n\rangle = |E_n^{(0)}\rangle + |E_n^{(1)}\rangle + |E_n^{(2)}\rangle + \cdots$, as $E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)} + \cdots$

• Degenerate Perturbation : If we have r degenerate states, $|E\rangle = \sum_{i=0} |E_i^{(0)}\rangle$ in matrix form,

④ $\begin{bmatrix} \langle E_1^{(0)}|\hat{H}_p|E_1^{(0)}\rangle & \cdots & \langle E_1^{(0)}|\hat{H}_p|E_k^{(0)}\rangle \\ \vdots & & \vdots \\ \langle E_k^{(0)}|\hat{H}_p|E_1^{(0)}\rangle & \cdots & \langle E_k^{(0)}|\hat{H}_p|E_k^{(0)}\rangle \end{bmatrix} \begin{bmatrix} |E_1^{(1)}\rangle \\ \vdots \\ |E_k^{(1)}\rangle \end{bmatrix} = E^{(1)} \begin{bmatrix} |E_1^{(1)}\rangle \\ \vdots \\ |E_k^{(1)}\rangle \end{bmatrix}$ $\quad |E^{(1)}\rangle = E_1^{(1)} + \cdots + E_k^{(1)}$

Degeneracy is lifted by $E_k^{(1)}$

* Note that total state is given as $|E_n\rangle = |E_n^{(0)}\rangle + |E_n^{(1)}\rangle + \cdots$ and value, $E_n = E_n^{(0)} + E_n^{(1)} + \cdots$

• TDPT : $|E\rangle = \sum_n a_n(t) \exp(-jE_n t/\hbar)|E_n\rangle$, $a_q^{(0)}(t) = 0$ (at initial ground state, $a_1^{(0)} = 1$, all others zero)

$\dot{a}_q^{(1)}(t) = \frac{1}{j\hbar}\sum_n a_n^{(0)} \exp(j\omega_{qn}t)\langle E_q|\hat{H}_p(t)|E_n\rangle \Rightarrow a_q^{(1)}(t) = \int_0^t \dot{a}_q^{(1)}(\tau)\,d\tau$.

→ Use this when external "perturbation" is given → not in static state!

Probability of finding at a_q is $\|a_q^{(0)} + a_q^{(1)}\|^2$ when $a_q^{(1)}$ is sufficient approximation.

• Operators : $[\hat{p}_x, \hat{p}_y] = 0$, $[\hat{L}_x, \hat{L}_y] = j\hbar\hat{L}_z$, K.E. $= \frac{\hat{L}^2}{2I} \Rightarrow |l,m\rangle \Rightarrow$ ① $\frac{\hat{L}^2}{2I}|l,m\rangle = \frac{\hbar^2}{2I} l(l+1)|l,m\rangle$

also, since $[\hat{L}^2, L_z] = 0$, ② $\hat{L}_z|l,m\rangle = \hbar m\,|l,m\rangle$, $|l,m\rangle = I|l,m\rangle = \left(\int d\Omega\,|\theta,\phi\rangle\langle\theta,\phi|\right)|l,m\rangle = \int d\Omega\, Y_{lm}(\theta,\phi)|\theta,\phi\rangle$

$Y_{l,m} = A_{l,m} P_l^m(\cos\theta) e^{jm\phi}$, Degeneracy : n, l, m $(-l \le m \le l,\ l = 0, 1, \cdots, n-1)$ $\sum_{l=0}^{n-1}(2l+1) = n(n-1) + n = n^2$

• Useful operators : $\hat{A} = \sum_i \alpha_i |\psi_i\rangle\langle\psi_i|$ where $A|\psi_i\rangle = \alpha_i|\psi_i\rangle$ (direct substitution).

$\hat{A}^{-1} = \sum_i (1/\alpha_i)|\psi_i\rangle\langle\psi_i|$

• Uncertainty principle : $\sigma_A^2 = Var(\hat{A}) = \sum_i = \langle\psi|(\hat{A} - \langle\hat{A}\rangle)^2|\psi\rangle = \langle(\hat{A} - \langle\hat{A}\rangle)^2\rangle$

• Angular momentum operation. $\hat{p}_x = -j\hbar\,\partial/\partial x \Rightarrow [\hat{L}_x, \hat{L}_y] \neq 0$, $[\hat{L}^2, \hat{L}_x] = [\hat{L}^2, \hat{L}_y] = [\hat{L}^2, \hat{L}_z] = 0$.

$[\hat{x}, \hat{p}_x] \Rightarrow [\hat{x}, \hat{p}_x]\psi(x) = j\hbar\psi(x) \Rightarrow [\hat{x}, \hat{p}_x] = j\hbar$.

• Degeneracy : H's entries $\begin{pmatrix} A & 0 & 0 \\ 0 & A & 0 \\ 0 & 0 & B \end{pmatrix} \rightarrow$ $\underline{\uparrow A}$ $\underline{\uparrow A}$ $\underline{\uparrow B}$ (degeneracy changes!)