1D Quantum System

1D Schrödinger Equation

we can set boundary condition for wavefunc. $\psi(x,t)$

In Schrödinger Picture, $\hat{H} = \frac{\hat{P}^2}{2\mu} + V(x)$

In position representation, $i\hbar\frac{\partial}{\partial t}\psi(x,t) = [-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2} + V(x)]\psi(x,t)$

$\xrightarrow{\text{stationary solution}}$ $\psi_E(x,t) = \psi_E(x)\exp(-iEt/\hbar)$

$$[-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2} + V(x)]\psi_E(x) = E\psi_E(x)$$ Stationary State Schrödinger Equation

Bound State Restriction: $\psi(x)\big|_{x\to\pm\infty} = 0$, $\forall |\psi\rangle \in \mathcal{H}$
束缚态

$$\int_{-\infty}^{+\infty}|\psi(x)|^2dx = 1 \rightsquigarrow E = E\int_{-\infty}^{+\infty}|\psi(x)|^2dx = \int_{-\infty}^{+\infty}\psi_E^*(x)[E\psi_E(x)]dx$$
$$= \frac{\hbar^2}{2\mu}\int_{-\infty}^{+\infty}\left|\frac{d\psi_E(x)}{dx}\right|^2dx + \int_{-\infty}^{+\infty}V(x)|\psi_E(x)|^2dx$$
$$\geq V_{min}\int_{-\infty}^{+\infty}|\psi_E(x)|^2dx$$

In bound state, we have $E \geq V_{min}$

Free Particle

For free particle, $V(x) = 0$

$$-\frac{\hbar^2}{2\mu}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \sim \psi(x) = A(k)\exp(ikx) + A(-k)\exp(-ikx) \qquad k = \sqrt{\frac{2\mu E}{\hbar^2}}$$
$-\infty < x < +\infty$

$\psi(x)|_{x\to\pm\infty}$ doesn't divergent, $k \in \mathbb{R}^+$

eigenvalue spectrum

$$E = \frac{\hbar^2k^2}{2\mu} \geq 0 \quad (\text{continuous}) \xrightarrow{p=\hbar k} \psi(x) = A(p)\exp(ipx/\hbar) \qquad E = \frac{p^2}{2\mu}$$

For CSCO $\{\hat{H}, \hat{P}\}$ $\Rightarrow$ $\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}}\exp(ipx/\hbar)$, $\int_{-\infty}^{+\infty}\psi_{p'}^*(x)\psi_p(x)dx = \delta(p-p')$

$\hat{H} = -\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2} + V(x)$
$\hat{P} = -i\hbar\frac{d}{dx}$

time-dependant free particle

$$\psi_p(x,t) = \psi_p\exp(-iEt/\hbar) = \frac{1}{\sqrt{2\pi\hbar}}\exp[ipx/\hbar - i(p^2/2\mu\hbar)t] \qquad (p=\hbar k)$$

for $\Delta p = 0$ (stationary state), $P(x,t) = |\psi_p(x,t)|^2 = \frac{1}{2\pi\hbar} \rightsquigarrow \Delta x = \infty$

$\boxed{p = \hbar k \ , \ E = \frac{\hbar^2 k^2}{2\mu}}$

for superposition $\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} dp\, A(p) \exp[ipx/\hbar - i(p^2/2\mu\hbar)t]$

$$\not= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dk\, A(k) \exp[ikx - i\underbrace{\omega(k)}_{\frac{k^2\hbar}{2\mu}}t]$$

The particle is at De Broglie wave packet

While $\psi(x,t)$ mainly focus nearby $k = k_0$, then

$$\psi(x,t) \approx \frac{1}{\sqrt{2\pi}} \int_{k_0-\Delta k}^{k_0+\Delta k} dk\, A(k) \exp(ikx - i\omega(k)t)$$

$$\approx 2A(k_0) \frac{\sin\{[x - (\frac{d\omega}{dk})_0 t]\Delta k\}}{[x - (\frac{d\omega}{dk})_0 t]} \exp[i(k_0x - \omega t)]$$

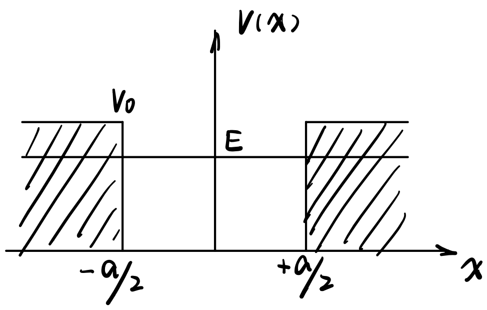
center place $x - (\frac{d\omega}{dk})_0 t = 0$

group velocity

$v_g = (\frac{d\omega}{dk})_0 = \frac{k_0\hbar}{\mu} = \frac{p_0}{\mu}$

$\sim$ the velocity of the particle

Finate Square Potential Well



def. $V(x) = \begin{cases} 0, & -\frac{a}{2} < x < \frac{a}{2} \\ V_0, & \text{otherwise} \end{cases}$

$\boxed{\text{bound state}}$

$$\frac{d^2\psi^{(2)}(x)}{dx^2} + k^2\psi^{(2)}(x) = 0, \quad k = \sqrt{\frac{2\mu E}{\hbar^2}}, \quad x < \left|\frac{a}{2}\right|$$

$$\frac{d^2\psi^{(1,3)}(x)}{dx^2} + K^2\psi^{(1,3)}(x) = 0, \quad K = \sqrt{\frac{2\mu}{\hbar^2}(V_0 - E)}, \quad x > \left|\frac{a}{2}\right|$$

$E \geq V_{min} = 0$, $k^2 \geq 0$, $k \in \mathbb{R}$

bound state condition

$\psi^{(1,3)}(x) = C\exp(Kx) + D\exp(-Kx)$, $\psi(x)|_{x\to\pm\infty} = 0$

$\to K > 0$, $\psi^{(1)}(x) = C\exp(Kx)$, $\psi^{(3)}(x) = D\exp(-Kx)$

For discontinued point: $\psi^{(1)}(-\frac{a}{2}) = \psi^{(2)}(-\frac{a}{2})$, $\psi^{(2)}(\frac{a}{2}) = \psi^{(3)}(\frac{a}{2})$

$$V(x) = V_0[\theta(x - a/2) + \theta(-x - a/2)]$$

$$-\frac{\hbar^2}{2\mu}\frac{d^2\psi(x)}{dx^2} + V_0[\theta(x - a/2) + \theta(-x - a/2)]\psi(x) = E\psi(x)$$

$$\to \left.\frac{d\psi^{(1)}(x)}{dx}\right|_{x=-a/2} = \left.\frac{d\psi^{(2)}(x)}{dx}\right|_{x=-a/2} \quad \left.\frac{d\psi^{(2)}(x)}{dx}\right|_{x=a/2} = \left.\frac{d\psi^{(3)}(x)}{dx}\right|_{x=a/2}$$

* For 1D quantum system, the energetic eigenvalue in bound state aren't degenerate

for finite square potential well:

$$-\frac{\hbar^2}{2\mu}\frac{d^2\psi(x)}{dx^2}+V_0[\theta(x-a/2)+\theta(-x-a/2)]\psi(x)=E\psi(x)$$

$$-\frac{\hbar^2}{2\mu}\frac{d^2\psi(-x)}{dx^2}+V_0[\theta(x-a/2)+\theta(-x-a/2)]\psi(-x)=E\psi(-x)$$

($\psi(x)$ & $\psi(-x)$ are eigenstates of E)

Nonedegeneracy request: $\psi(x)=c\psi(-x) \rightsquigarrow \psi(x)=c^2\psi(x)$ $\quad c=\pm 1$

$$\begin{cases}\text{odd parity} & \psi(x)=-\psi(-x)\\ \text{even parity} & \psi(x)=\psi(-x)\end{cases}$$

△

even parity $\Rightarrow \psi^{(1)}(x)=c\exp(\kappa x)$, $\psi^{(3)}(x)=C\exp(-\kappa x)$

$\psi^{(2)}(x)=A\cos(kx)$

continuity condition: $Ak\sin(ka/2)=C\kappa\exp(-\kappa a/2)$, $A\cos(ka/2)=C\exp(-\kappa x)$

$\Rightarrow \psi^{(1)}(x)=c\exp(\kappa x)$, $\psi^{(3)}(x)=C\exp(-\kappa x)$, $\quad \tan\left(\frac{ka}{2}\right)=\sqrt{\frac{2\mu V_0}{\hbar^2k^2}-1}$

$\psi^{(2)}(x)=C\sqrt{\frac{2\mu V_0}{\hbar^2k^2}}\exp(-\kappa a/2)\cos(kx)$ eigenstates

energetic eigenvalue spectrum described as the equation: $\begin{cases}\tan\left(\frac{ka}{2}-p\pi\right)=\sqrt{\frac{2\mu V_0}{\hbar^2k^2}-1}\\ k=\sqrt{\frac{2\mu E}{\hbar^2}}\end{cases}$

assume: $0\le\frac{ka}{2}-p\pi<\frac{\pi}{2} \Rightarrow p\pi\le\frac{ka}{2}<(p+\frac{1}{2})\pi$

$\Rightarrow \cos\left(\frac{ka}{2}-p\pi\right)=\frac{\hbar k}{\sqrt{2\mu V_0}}$

$$\frac{ka}{2}=p\pi+\arccos\frac{\hbar k}{\sqrt{2\mu V_0}}, \quad p=0,1,2,\cdots$$

if $V_0\to+\infty$, the particle will be bounded inside the potential well

$$\frac{ka}{2}=(p+\frac{1}{2})\pi, \quad k=(2p+1)\frac{\pi}{a}, \quad p=0,1,2,\cdots$$

$$E_p^{(\text{Even Parity})}=\frac{\pi^2\hbar^2}{2\mu a^2}(2p+1)^2, \quad p=0,1,2$$

energetic eigenfuction

$$\psi_p^{(\text{Even Parity})}=\sqrt{\frac{2}{a}}\cos\left[(2p+1)\frac{\pi x}{a}\right]\theta\left(\frac{a}{2}-x\right)\theta\left(x+\frac{a}{2}\right)$$

△ odd parity ⇒ $\psi^{(1)}(x) = -C\exp(\kappa x)$, $\psi^{(3)}(x) = C\exp(-\kappa x)$

$\psi^{(2)}(x) = B\sin(kx)$

continuity condition : $Bk\sin(ka/2) = -C\kappa\exp(-\kappa a/2)$, $B\sin(ka/2) = C\exp(-\kappa a/2)$

$\Rightarrow \psi^{(1)}(x) = -C\exp(\kappa x)$, $\psi^{(3)}(x) = C\exp(-\kappa x)$

$\psi^{(2)}(x) = C\sqrt{\frac{2\mu V_0}{\hbar^2 k^2}}\exp(-\kappa a/2)\sin kx$, $\cot\left(\frac{ka}{2}\right) = -\sqrt{\frac{2\mu V_0}{\hbar^2 k^2} - 1}$

$$\frac{ka}{2} = \left(p+\frac{1}{2}\right)\pi + \arccos\frac{\hbar k}{\sqrt{2\mu V_0}}, \quad p = 0, 1, 2, \cdots$$

if $V_0 \to +\infty$, the particle will be bounded inside the potential well , then

$$\frac{ka}{2} = (p+1)\pi \quad , k = 2(p+1)\frac{\pi}{a} \quad , p = 0, 1, 2, \cdots$$

$$E_p^{(\text{Odd Parity})} = \frac{2\pi^2\hbar^2}{\mu a^2}(p+1)^2 \quad , p = 0, 1, 2$$

energetic eigen-fuction

$$\psi_p^{(\text{Odd Parity})} = \sqrt{\frac{2}{a}}\sin\left[(p+1)\frac{2\pi x}{a}\right]\theta\left(\frac{a}{2}-x\right)\theta\left(x+\frac{a}{2}\right)$$

$\boxed{\text{unbound state}} \longrightarrow$ scattering state

$E > V_0 > 0$, common solution :

$\psi^{(1)}(x) = A\exp(i\tilde{k}x) + B\exp(-i\tilde{k}x)$

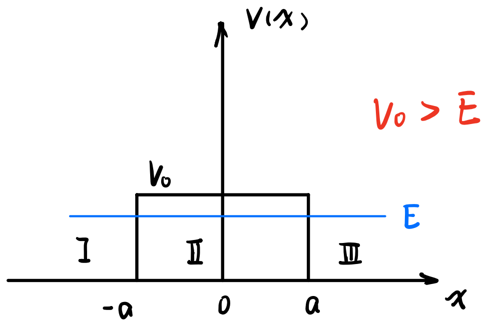
$\psi^{(2)}(x) = F\exp(ikx) + G\exp(-ikx)$

$\psi^{(3)}(x) = C\exp(i\tilde{k}x) + D\exp(-i\tilde{k}x)$

Law of conservation of probability : $\left|\frac{B}{A}\right|^2 + \left|\frac{C}{A}\right|^2 = 1$

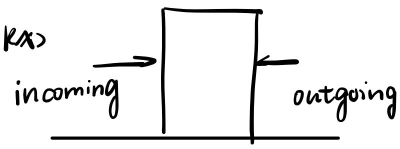
Square Potential Barrier

Def $V(x) = \begin{cases} V_0 , & -a < x < a \\ 0 , & \text{otherwise} \end{cases}$



$V_0 > E > 0$

For Region I, III. Scattering Solution $\begin{cases} \psi^{(1)}(x) = A\exp(ikx) + B\exp(-ikx) \\ \psi^{(3)}(x) = C\exp(ikx) + D\exp(-ikx) \end{cases}$



$$\frac{dJ(x)}{dx} = 0 \Rightarrow |A|^2 - |B|^2 = |C|^2 - |D^2| \rightarrow |A|^2 + |D|^2 = |B|^2 + |C|^2$$

for region II, $\psi^{(2)}(x) = E\exp(\kappa x) + G\exp(-\kappa x)$ $\quad \kappa = \sqrt{\frac{2\mu(V_0-E)}{\hbar^2}} > 0$

Continuity Condition (wavefunc. & its first differential):

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} \xrightarrow{\text{properties}} \begin{array}{l} M_{11}^* = M_{22} \\ M_{12}^* = M_{21} \\ \det M = 1 \end{array}$$

Def. M matrix consist of κ, k, a.

left-incident particle. $D = 0$, then

$$\psi(x) = \begin{cases} M_{11}C\exp(ikx) + M_{21}C\exp(-ikx) \\ C\exp(ikx) \end{cases}$$

possibility of crossing the barrier.

Def. Reflection Coefficient : $\mathcal{R} = \frac{|B|^2}{|A|^2} = \frac{|M_{21}|^2}{|M_{11}|^2}$

Transmission Coefficient : $\mathcal{T} = \frac{|C|^2}{|A|^2} = \frac{1}{|M_{11}|^2}$

$\mathcal{R} + \mathcal{T} = 1$

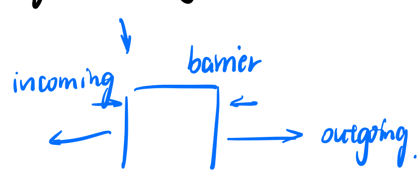
$\boxed{\mathcal{T} \neq 0 : \text{Tenneling effect}}$

隧穿效应

while $\kappa a \gg 1$, then $\mathcal{T} = 16\left(\frac{k\kappa}{k+\kappa}\right)^2 \exp(-4\kappa a) \rightarrow 0$.

Transfer the relationship from Region I & III to outgoing/incoming waves

$$\begin{pmatrix} B \\ C \end{pmatrix} = S \begin{pmatrix} A \\ D \end{pmatrix}$$



Properties : $* \; |B|^2 + |C|^2 = |A|^2 + |D|^2 \rightarrow S^\dagger S = I$

$* \; S^T = S \rightsquigarrow S_{12} = S_{21}$

$* \; S_{11} = S_{22}$

} symmetry restriction : $S = \begin{pmatrix} u & i\sqrt{1-u^2} \\ i\sqrt{1-u^2} & u \end{pmatrix} \exp(i\beta)$

Delta Function Potential Well

Def. $V(x) = -g\delta(x)$ (* $g = e^2$, 1D Hydrogen atom)

$$-\frac{\hbar^2}{2\mu}\frac{d^2\psi(x)}{dx^2} - g\delta(x)\psi(x) = E\psi(x)$$

→ continuity : $\psi(0) = \psi(0+) = \psi(0-)$

→ $\int_{-\varepsilon}^{+\varepsilon} E\psi(x)\,dx \approx 2\varepsilon\psi(0)E \approx 0 \rightarrow \left.\frac{d\psi(x)}{dx}\right|_{x=\varepsilon} - \left.\frac{d\psi(x)}{dx}\right|_{x=-\varepsilon} = -\frac{2\mu g}{\hbar^2}\psi(0)$

restriction

* For bound state , $E<0$

common solution : $\psi(x) = A\theta(x)\exp(-\kappa x) + B\theta(-x)\exp(\kappa x)$

$$\begin{cases} A = B, \quad -\kappa(A+B) + \frac{2\mu g}{\hbar^2}A = 0 \end{cases}$$

bound state energy $E = -\frac{\mu g^2}{2\hbar^2}$

$$\psi(x) = \sqrt{\kappa}\,\theta(x)\exp(-\kappa x) + \sqrt{\kappa}\,\theta(-x)\exp(\kappa x)$$

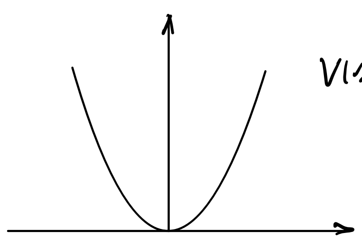
* Scattering State . $E>0$

$$\psi(x) = \theta(-x)\left[A\exp(ikx) + B\exp(-ikx)\right] + \theta(x)\left[C\exp(ikx)\right] \qquad k = \sqrt{\frac{2\mu E}{\hbar^2}} > 0$$

$|A^2| - |B^2| = |C|^2 \rightsquigarrow \mathcal{R} = \frac{\mu g^2}{2E\hbar^2 + \mu g^2}$, $\mathcal{T} = \frac{2E\hbar^2}{2E\hbar^2 + \mu g^2}$

reflected by delta potential

Harmonic Oscillator



$V(x) = \frac{1}{2}m\omega^2x^2$

$$-\frac{\hbar^2}{2m}\psi''(x) + \frac{1}{2}m\omega^2x^2\psi(x) = E\psi(x)$$

Nondimentionalization ↓ $\xi = \sqrt{\frac{m\omega}{\hbar}}x$, $\lambda = \frac{2E}{\hbar\omega}$

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

For bound state , $\xi \rightarrow \pm\infty$, $\psi(\xi) \rightarrow 0$

$$\left(\frac{d}{d\xi} - \xi\right)\left(\frac{d}{d\xi} + \xi\right)\psi(\xi) + (\lambda - 1)\psi(\xi) = 0 \rightsquigarrow \psi(\xi) \approx e^{-\xi^2/2}$$

meet bound state restriction .

set $\psi(\xi) = e^{-\xi^2/2} u(\xi)$, then $\underline{\dfrac{d^2u}{d\xi^2} - 2\xi \dfrac{du}{d\xi} + (\lambda - 1) u = 0}$ Hermite Equation.

$$\downarrow$$

$$u(\xi) = \sum_{k=0}^{+\infty} C_k \xi^k, \quad |\xi| < \infty$$

$$C_{k+2} = \frac{2k - \lambda + 1}{(k+1)(k+2)} C_k, \quad k = 0, 1, 2, \cdots$$

two linearly independent solutions: $u_1(\xi) = \sum_{k=0}^{+\infty} C_{2k} \xi^{2k}$ $\quad u_2(\xi) = \sum_{k=0}^{+\infty} C_{2k+1} \xi^{2k+1}$

$$\left(k \to +\infty : \ C_{k+2}/C_k \sim 2/k \right)$$

$$\Rightarrow \ u_1(\xi)\big|_{\xi \to \infty} = \sum_{\underset{\substack{\uparrow \\ \text{a large number}}}{m=M}}^{\infty} \frac{\xi^{2m}}{m!} \sim e^{\xi^2} \qquad u_2(\xi)\big|_{\xi \to \infty} = \xi e^{\xi^2}$$

$\star$ $\psi(x) = u(\xi) e^{-\xi^2/2} \sim e^{\xi^2/2} \ \Rightarrow$ divergence

$\star$ To create an appropriate wave function, $u_1(\xi) / u_2(\xi)$ should be polynom

$$\downarrow n \in \mathbb{N}$$

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

Hermitian Polynomial.

Hermitian Polynomial

$$e^{-s^2 + 2\xi s} = \sum_{n=0}^{\infty} \frac{H_n(\xi)}{n!} s^n$$

$$\Rightarrow H_n(\xi) = \frac{\partial^n}{\partial s^n} e^{-s^2 + 2\xi s} \Big|_{s=0} = (-1)^n e^{\xi^2} \frac{\partial^n e^{-\xi^2}}{\partial \xi^n}$$

$$\begin{cases} H_0(\xi) = 1 \\ H_1(\xi) = 2\xi \\ H_2(\xi) = 4\xi^2 - 2 \\ H_3(\xi) = 8\xi^3 - 12\xi \end{cases}$$

$$\int_{-\infty}^{+\infty} H_m(\xi) H_n(\xi) \underset{\substack{\uparrow \\ \text{weight coefficient}}}{e^{-\xi^2}} d\xi = \sqrt{\pi}\, 2^n \cdot n!\, \delta_{mn} \quad [\text{orthodox}]$$

$\star$ Energetic Eigenfunction: $\psi_n(x) = \sqrt{\dfrac{\alpha}{\sqrt{\pi}\, 2^n \cdot n!}}\, e^{-\alpha^2 x^2/2} H_n(\alpha x)$, $n = 0, 1, 2, \cdots$

$$\left(\alpha = \sqrt{\frac{m\omega}{\hbar}} \right)$$

$$\int_{-\infty}^{+\infty} dx\, \psi_m(x) \psi_n(x) = \delta_{mn}$$

Ground State.
$$\begin{cases} \text{zero-point energy} \quad E_0 = \frac{1}{2}\hbar\omega \neq 0 \\ \text{wave function} \quad \psi_0(x) = \dfrac{\sqrt{\alpha}}{\pi^{1/4}} e^{-\alpha^2 x^2/2} \\ \rho_0(x) = |\psi_0(x)|^2 = \dfrac{\alpha}{\sqrt{\pi}} e^{-\alpha^2 x^2} \quad \text{Gaussian Distribution} \end{cases}$$

eigen-length $\alpha^{-1} = \sqrt{\frac{\hbar}{m\omega}} \longrightarrow V(x)\Big|_{x=\pm\frac{1}{\alpha}} = \frac{\hbar\omega}{2} = E_0$

* In quantum mechanics, the prob. for the particle to exist in region $|x| > |\pm\frac{1}{\alpha}|$

$$P = 2\int_{\alpha^{-1}}^{+\infty} dx\, |\psi(x)|^2 = \frac{2\alpha}{\sqrt{\pi}} \int_{\alpha^{-1}}^{+\infty} dx\, e^{-\alpha^2 x^2} \approx 0.157$$

Dirac's Solution for Harmonic Oscillator

$$\hat{H} = \frac{1}{2\mu}\hat{P}^2 + \frac{1}{2}m\omega^2\hat{x}^2 , \quad [\hat{x}, \hat{p}] = i\hbar$$

guarentee the Schrödinger Equation

$$\hat{H} = \left(\frac{1}{\sqrt{2}}\right)^2 \underbrace{\left[\frac{\hat{p}}{\sqrt{m\hbar\omega}} + i\sqrt{\frac{m\omega}{\hbar}}\hat{x}\right]}_{\hat{a}^+} \underbrace{\left[\frac{\hat{p}}{\sqrt{m\hbar\omega}} - i\sqrt{\frac{m\omega}{\hbar}}\hat{x}\right]}_{\hat{a}} \hbar\omega + \frac{1}{2}\hbar\omega$$

$$[\hat{a}, \hat{a}^+] = \frac{i}{\hbar}[\hat{p}, \hat{x}] = \hat{I} \qquad [\hat{a}, \hat{a}] = [\hat{a}^+, \hat{a}^+] = 0$$

$$\hat{H} = [\hat{a}^+\hat{a} + \tfrac{1}{2}]\hbar\omega \triangleq [\hat{N} + \tfrac{1}{2}]\hbar\omega \quad (\hat{N} = \hat{a}^+\hat{a})$$

properties:
* $\hat{N}^+ = \hat{N}$, $[\hat{N}, \hat{H}] = 0$
* $[\hat{N}, \hat{a}] = -\hat{a}$, $[\hat{N}, \hat{a}^+] = \hat{a}^+$
* If eigenstates $\{|n\rangle\}$, $\hat{N}|n\rangle = n|n\rangle$, $\langle n|n\rangle = 1$

  $n = n\langle n|n\rangle = \langle n|\hat{N}|n\rangle = \langle n|\hat{a}^+\hat{a}|n\rangle = |\hat{a}|n\rangle|^2$

$\boxed{\text{Physical Meanings}}$

$[\hat{N}, \hat{a}] = -\hat{a}^+$, $[\hat{N}, \hat{a}^+] = -\hat{a}$

$|\lambda(n)|^2 = \langle n|\hat{a}^+\hat{a}|n\rangle = \langle n|\hat{N}|n\rangle = n$, $\lambda(n) = \sqrt{n}$

$$\begin{cases} \hat{N}\hat{a}|n\rangle = (n-1)\hat{a}|n\rangle \\ \hat{N}\hat{a}^+|n\rangle = (n+1)\hat{a}^+|n\rangle \end{cases} \longrightarrow \begin{cases} \hat{a}|n\rangle = \lambda(n)|n-1\rangle \\ \hat{a}^+|n\rangle = \nu(n)|n+1\rangle \end{cases}$$

$|\nu(n)|^2 = \langle n|\hat{a}\hat{a}^+|n\rangle = \langle n|\hat{N} + \hat{I}|n\rangle = n+1$, $\nu(n) = \sqrt{n+1}$

* $\hat{a}$ is the annihilation operator for $\hat{N}$

  $\hat{a}^+$ is the creation operator for $\hat{N}$

* $\rightsquigarrow$ $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$, $\hat{a}^+|n\rangle = \sqrt{n+1}\,|n+1\rangle$

for $(\hat{a})^i|n\rangle = \sqrt{n(n-1)\cdots(n-i+1)}\,|n-i\rangle$, the operation should be finite $(n=0)$

$\hat{N}$: Occupation Number Operator $\quad \hat{N}|n\rangle = n|n\rangle$, $n = 0, 1, 2, \cdots$ $\left[|n\rangle = \frac{1}{\sqrt{n!}}(\hat{a}^+)^n|0\rangle\right]$

$\rightsquigarrow$ $\hat{H}|n\rangle = E_n|n\rangle$, $E_n = [n + \tfrac{1}{2}]\hbar\omega$

Ground State $|0\rangle$: $\hat{N}|0\rangle = 0|0\rangle$ $\begin{cases} \hat{a}|0\rangle = 0 \\ \hat{H}|0\rangle = \frac{1}{2}\hbar\omega|0\rangle \end{cases}$

$\hat{x} = i\sqrt{\frac{\hbar}{2m\omega}}(\hat{a} - \hat{a}^{\dagger})$, $\hat{p} = \sqrt{\frac{\hbar m\omega}{2}}(\hat{a} + \hat{a}^{\dagger})$

* Properties : $\langle m|n\rangle = \delta_{mn}$

$\langle n|\hat{x}|n\rangle = \langle n|\hat{p}|n\rangle = 0$

$\langle n|\hat{x}^2|n\rangle = \frac{\hbar}{2m\omega}(2n+1)$

$\langle n|\hat{p}^2|n\rangle = \frac{m\hbar\omega}{2}(2n+1)$

$\rightsquigarrow$ $(\Delta x)_0 = \sqrt{\frac{\hbar}{2m\omega}}$, $(\Delta p)_0 = \sqrt{\frac{m\hbar\omega}{2}}$

$(\Delta x)_0 (\Delta p)_0 = \frac{\hbar}{2}$

★ $|0\rangle$ is coherent state ★

In Position Representation : $\psi_0(x) = \langle x|0\rangle = N e^{-\frac{1}{2}\alpha^2 x^2} = \sqrt{\frac{\alpha}{\sqrt{\pi}}}\, e^{-\frac{1}{2}\alpha^2 x^2}$

$\psi_n(x) = \langle x|n\rangle = \sqrt{\frac{\alpha}{2^n i^n n! \sqrt{\pi}}}\, H_n(\alpha x) \exp(-\frac{1}{2}\alpha^2 x^2)$

Rotation Transformation & Angular Momentum Operator

Angular Momentum of Particles

* Assumption: Angular Momentum is $\begin{cases}\text{Observable} \\ \text{Generators of rotation transformation in } \mathcal{H}\end{cases}$

Rotation Transformation in E^3

transformation matrix

For $V = v_i \vec{e_i}$, $V' = v_i' \vec{e_i}$, we have $\begin{cases} V' = RV, & v_i' = R_{ij} v_j \\ |V| = |V'|, & v_i v_i = v_i' v_i' \end{cases}$

$$\delta_{jk} v_j v_k = v_i' v_i' = R_{ij} R_{ik} v_j v_k \Rightarrow \delta_{jk} = R_{ij} R_{ik}$$

$$[(AB)_{ij}] = \sum_m A_{im} B_{mj} = A_{im} B_{mj}$$

$$R^T R = I, \quad \det R = \pm 1$$

(R: orthogonal matrix)

$\begin{cases} \det R = 1 \Rightarrow \text{real rotation} \\ \det R = -1 \Rightarrow \text{counterfeit rotation} \end{cases}$ 包含空间反射变换

For infinitesimal ϕ, $R(\phi, e_a) = I - i\phi \chi_a \quad (a = 1, 2, 3)$ $\quad (\chi_a)_{bc} = -i\varepsilon_{abc}$

generator 生成元

$$[\chi_a, \chi_b]_{ij} = (\chi_a)_{ik}(\chi_b)_{kj} - (\chi_b)_{ik}(\chi_a)_{kj} = -\varepsilon_{aik}\varepsilon_{bkj} + \varepsilon_{bik}\varepsilon_{akj}$$

$$= i\varepsilon_{abc}(\chi_c)_{ij} \quad \rightsquigarrow \quad [\chi_a, \chi_b] = i\varepsilon_{abc}\chi_c$$

(The order of rotations in different directions is irreversable)

$$R(\theta, e_a) R(\phi, e_b) = (I - i\theta\chi_a)(I - i\phi\chi_b) \neq R(\phi, e_b) R(\theta, e_a)$$

Rotation Transformation in $\mathcal{H}$

Def. Linear Operator: $\hat{D}(R): |\psi\rangle \longrightarrow |\psi_R\rangle = \hat{D}(R)|\psi\rangle$

$$\langle\psi|\psi\rangle = \langle\psi_R|\psi_R\rangle = \langle\psi|\hat{D}^\dagger \hat{D}|\psi\rangle, \quad \hat{D}^\dagger \hat{D} = \hat{I}$$

$\rightsquigarrow \hat{D}(R)$ is unitary operator (contrast with $R(d\phi, \vec{n}) \approx I - id\phi\,\vec{n}\cdot\mathcal{X}$)

infinatesimal interval $\rightsquigarrow$ $\hat{D}(\delta\phi, n) = \hat{I} - i\frac{\delta\phi}{\hbar}\, n\cdot\hat{J}$

generators for states in $\mathcal{H}$

Def. describe $\hat{J}$ as the angular momentum operator

properties: * $\hat{J}^\dagger = \hat{J}$

* Commute Relationship $[\hat{J}_a, \hat{J}_b] = i\hbar\varepsilon_{abc}\hat{J}_c$

Eigenvalue of Angular Momentum Operator

$\hat{J}^2 = \hat{J}_1^2 + \hat{J}_2^2 + \hat{J}_3^2 = \hat{J}_i\hat{J}_i$, $\underline{[\hat{J}_i, \hat{J}^2] = [\hat{J}_i, \hat{J}_k\hat{J}_k] = i\hbar\varepsilon_{ikl}(\hat{J}_k\hat{J}_l + \hat{J}_l\hat{J}_k) = 0}$

$\sim$ $\hat{J}_3$ & $\hat{J}^2$ have the common eigenstate base. ★ $\begin{cases} \hat{J}^2|a,m\rangle = a\hbar^2|a,m\rangle \\ \hat{J}_3|a,m\rangle = m\hbar|a,m\rangle \end{cases}$

Introduce the ladder operator: $\hat{J}_\pm = \hat{J}_1 \pm i\hat{J}_2$, $(\hat{J}_\pm)^\dagger = \hat{J}_\mp$

$\sim$ $[\hat{J}_+, \hat{J}_-] = 2\hbar\hat{J}_3$, $[\hat{J}_3, \hat{J}_\pm] = \pm\hbar\hat{J}_\pm$, $[\hat{J}^2, \hat{J}_\pm] = 0$

$J_3|a,m\rangle = m\hbar|a,m\rangle \xrightarrow{\text{yields}} \hat{J}_3[\hat{J}_\pm|a,m\rangle] = [\hat{J}_3, \hat{J}_\pm]|a,m\rangle + \hat{J}_\pm[\hat{J}_3|a,m\rangle]$

$= (m\pm1)\hbar[\hat{J}_\pm|a,m\rangle]$

★ 即 $\hat{J}_\pm$ 为 $\hat{J}_3$ 本征值的升降算符

$\hat{J}^2[\hat{J}_\pm|a,m\rangle] = \hat{J}_\pm\hat{J}^2|a,m\rangle = a\hbar^2[\hat{J}_\pm|a,m\rangle]$

★ $\hat{J}_\pm$不改变$\hat{J}^2$本征值

$\Rightarrow$ $\hat{J}_\pm|a,m\rangle = \hat{N}_\pm|a,m\pm1\rangle$

normalization

$\langle\hat{J}^2\rangle_\psi \geq \langle\hat{J}_3^2\rangle_\psi$: $a \geq m^2$ restriction: $j' \leq m \leq j$, $a \geq j^2$, $a \geq j'^2$

$j' = -j$, $a = j(j+1)$

CSCO $\{\hat{J}^2, \hat{J}_3\}$ common base: $|a,m\rangle = |j(j+1), m\rangle \xrightarrow{\Delta} |j,m\rangle$

★ $\hat{J}^2|j,m\rangle = j(j+1)\hbar^2|j,m\rangle$, $\hat{J}_3|j,m\rangle = m\hbar|j,m\rangle$, $-j \leq m \leq j$

we could use operator $\hat{J}_-$: $\hat{J}_-$: $|j,j\rangle \to |j,j-1\rangle \to \cdots \to |j,-j\rangle$ $j = -j+n$, $j = \frac{n}{2}$

Matrix Element of Angular Momentum Operator in J_3 Representation

Choose $|j,m\rangle$ as the base of $\mathcal{H}$

Def. J_3 Representation
$$\begin{cases} \langle j',m'|\hat{J}^2|j,m\rangle = j(j+1)\hbar^2\delta_{jj'}\delta_{mm'} \\ \langle j',m'|\hat{J}_3|j,m\rangle = m\hbar\delta_{jj'}\delta_{mm'} \end{cases}$$

$$\boxed{\hat{J}_\pm|j,m\rangle = N_\pm|j,m\pm1\rangle,\ \langle j,m\pm1|N_\pm^* = \langle j,m|\hat{J}_\mp \rightsquigarrow N_\pm = \hbar\sqrt{j(j+1)-m(m\pm1)}}$$

$$\hat{J}_\pm|j,m\rangle = \hbar\sqrt{j(j+1)-m(m\pm1)}\ |j,m\pm1\rangle$$

$$\langle j',m'|\hat{J}_\pm|j,m\rangle = \hbar\sqrt{j(j+1)-m(m\pm1)}\ \delta_{j'j}\delta_{m'm-1}$$

$$\Big\downarrow\ \hat{J}_1 = \frac{1}{2}[\hat{J}_+ + \hat{J}_-]\ ,\ \hat{J}_2 = \frac{1}{2i}[\hat{J}_+ - \hat{J}_-]$$

$$\langle j',m'|\hat{J}_1|j,m\rangle = \langle j',m'|\frac{1}{2}[\hat{J}_+ + \hat{J}_-]|j,m\rangle$$
$$\langle j'm'|\hat{J}_2|j,m\rangle = \langle j',m'|\frac{1}{2i}[\hat{J}_+ - \hat{J}_-]|j,m\rangle$$

for $j=\frac{1}{2}$, $J = \frac{\hbar}{2}\sigma = \frac{\hbar}{2}\sigma_a e_a$, Pauli Matrix : σ_a ($a=1,2,3$)

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\sigma_a\sigma_b = \delta_{ab} + i\varepsilon_{abc}\sigma_c \quad \Rightarrow \quad \{\sigma_a, \sigma_b\} = 2\delta_{ab}$$

Orbital Angular Moment

Def. $\hat{L} = \hat{r}\times\hat{p}$: orbital angular momentum

$\downarrow$ position representation

$\hat{L} = -i\hbar r\times\nabla$ (we prefer <u>spherical coordinate</u> frame)

$$\begin{cases} r = r\vec{e}_r \\ \vec{e}_r = \vec{e}_3 C_\theta + \vec{e}_2 S_\theta S_\varphi + \vec{e}_1 S_\theta C_\varphi \\ \vec{e}_\theta = \partial_\theta \vec{e}_r\ ,\ \vec{e}_\phi = \frac{1}{S_\theta}\partial_\phi \vec{e}_\phi \end{cases}$$

$$L = -i\hbar r\times\nabla = -i\hbar\left[e_\phi\partial_\theta - e_\theta\frac{1}{S_\theta}\partial_\phi\right]$$

$$\begin{cases} \hat{L}_1 = i\hbar(S_\varphi\partial_\theta + \cot\theta C_\varphi\partial_\varphi) \\ \hat{L}_2 = -i\hbar(C_\varphi\partial_\theta - \cot\theta S_\varphi\partial_\varphi) \\ \hat{L}_3 = -i\hbar\partial_\varphi \end{cases}$$

* $\hat{L}$ only depend on polar coordinates (θ,ϕ)

similarly $\hat{L}^2 = \hat{L}\cdot\hat{L} = -\hbar^2 [\frac{1}{\sin\theta}\partial_\theta(\sin\theta\,\partial_\theta) + \frac{1}{\sin^2\theta}\partial_\phi^2]$ ✶ $[\hat{L}^2, \hat{L}_a] = 0,\ a = 1, 2, 3$

Orbital Angular Momentum Operator's Eigenvalue Equation:

$$\begin{cases} \hat{L}_3 Y_{l,m} = m\hbar Y_{l,m} \\ \hat{L}^2 Y_{lm} = l(l+1)\hbar^2 Y_{l,m} \end{cases}$$

$$\rightsquigarrow \begin{cases} \partial_\phi Y = imY \\ S_\theta\partial_\theta(S_\theta\partial_\theta)Y + [S_\theta^2 l(l+1) - m^2]Y = 0 \end{cases} \rightsquigarrow Y(\theta,\phi) = \Theta(\theta)e^{im\phi}$$

* because of the single value of $Y(\theta,\varphi)$, $Y(\theta,\varphi+2\pi) = Y(\theta,\varphi)$,

m can only be integars $m \in \mathbb{N}$

dem. In rectangular frame, $\hat{L} = -i\hbar r\times\nabla = -i\hbar\varepsilon_{abc}x_b\partial_{x_c}$

$\rightsquigarrow \hat{L}_3 = -i\hbar(x_1\partial_{x_2} - x_2\partial_{x_1})$

introduce several operators;

$$\hat{q}_1 = \frac{1}{\sqrt{2}}(x_1 - i\hbar\partial_{x_2}) \qquad \hat{p}_1 = -\frac{1}{\sqrt{2}}(x_2 + i\hbar\partial_{x_1})$$

$$\hat{q}_2 = \frac{1}{\sqrt{2}}(x_1 + i\hbar\partial_{x_2}) \qquad \hat{p}_2 = \frac{1}{\sqrt{2}}(x_2 - i\hbar\partial_{x_1})$$

Compared with position & momentum operators

$$[\hat{q}_a, \hat{q}_b] = [\hat{p}_a, \hat{p}_b] = 0, \quad [\hat{q}_a, \hat{p}_b] = i\hbar\delta_{ab}$$

use them to redescribe the $\hat{L}_3$:

$$\hat{L}_3 = \frac{1}{2}[(\hat{q}_1^2 + \hat{p}_1^2) - (\hat{q}_2^2 + \hat{p}_2^2)] \triangleq \frac{1}{2}[\hat{H}_1 - \hat{H}_2]$$

which $\hat{H}_a = \frac{1}{2}(\hat{q}_a^2 + \hat{p}_a^2)$. we could explain $\hat{H}_a$ as Hamiltian Operator of a harmonic oscillator. whose $\mu = 1$, $\omega = 1$, Then eigenvalue of $\hat{L}_3$ should be the minus of two harmonic oscillators' eigenvalues.

$$\Rightarrow m\hbar = [(n_1 + \tfrac{1}{2}) - (n_2 + \tfrac{1}{2})]\hbar\cdot 1 = (n_1 - n_2)\hbar$$

✶ m can only be integars.

Conclusion: for orbital AMO, $\hat{L}_3 = -i\hbar\frac{\partial}{\partial\phi}$, $\hat{L}^2 = -\hbar[\partial_\theta^2 + \cot\theta\,\partial_\theta + \frac{1}{S_\theta^2}\partial_\varphi^2]$

$$\hat{L}_3 \xrightarrow{\text{eigenvalue}} m\hbar \qquad \hat{L}^2 \rightarrow l(l+1)\hbar^2$$

$m = 0, \pm1, \pm2, \cdots, \pm l$; $l \in \mathbb{Z}$

their common eigenvalue function : $Y_{lm}(\theta,\phi) = (-1)^m \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}\, P_l^m(\cos\theta)\, e^{im\phi}$

(Spherical harmonics)

eg. $Y_{00} = \frac{1}{\sqrt{4\pi}}$, $Y_{10} = \sqrt{\frac{3}{4\pi}}\cos\theta$, $Y_{1,\pm1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\pm i\phi}$

Spin Angular Momentum of Electron

☆ Cannot regard electron spin as its rotation around spinning axis

* Velocity on the surface of electron $u \sim 205c$

☆ spin angular momentum / spin magnetic moment : intrinsic properties

Silver atom across S-G experiment device: two split lines

$$F = -\nabla U = \vec{e_z}\,\mu_z \frac{\partial B}{\partial z}$$

In contrast we adopt the quantum number $\underline{s}$. SAM's projection on z

$$S_3 = m_s\hbar \ , \ m_s = -s, -s+1, \cdots, s-1, s$$

$\Rightarrow$ electron spin : $s = \frac{1}{2}$ $\quad m_s = \pm\frac{1}{2}$

$$\hat{S}^2 = s(s+1)\hbar^2 = \frac{3}{4}\hbar^2$$

Electron has more than 3 DOFs : including spin , then the wave func:

Spinor Wavefunc. $\psi(r, S_3) = \begin{pmatrix} \psi(r, +\frac{\hbar}{2}) \\ \psi(r, -\frac{\hbar}{2}) \end{pmatrix}$ 旋量波函数

Explaination : $\int d^3x\, |\psi(r, +\frac{\hbar}{2})|^2$: prob. desity of particle at $\vec{r}$ with $S_3 = \frac{\hbar}{2}$

$\int d^3x\, |\psi(r, -\frac{\hbar}{2})|^2$: prob. desity of particle at $\vec{r}$ with $S_3 = -\frac{\hbar}{2}$

Normalization :

$$\int d^3x\, [\psi^*(r, +\tfrac{\hbar}{2}), \psi^*(r, -\tfrac{\hbar}{2})] \begin{bmatrix} \psi(r, +\frac{\hbar}{2}) \\ \psi(r, -\frac{\hbar}{2}) \end{bmatrix} = \int d^3x\, \psi^\dagger\psi = 1$$

In some occasion, variables seperation : $\psi(r, S_3, t) = \varphi(r, t)\,\chi(S_3)$

Description of $\chi(S_3)$

Normal form : $\chi(S_3) = \begin{bmatrix} a \\ b \end{bmatrix}$ $\quad |a|^2 = P(S_3 = \frac{\hbar}{2})$, $\quad |b|^2 = P(S_3 = -\frac{\hbar}{2})$ $\qquad \chi^\dagger\chi = |a|^2 + |b|^2 = 1$

Spin Angular Momentum Operator $\hat{S}$

* $\hat{S}$ is observable, $\hat{S}^\dagger = \hat{S}$
* $[\hat{S}_i, \hat{S}_j] = i\hbar\varepsilon_{ijk}\hat{S}_k$

$\Rightarrow$ introduce pauli operator $\hat{\sigma}$: $\hat{S} = \frac{\hbar}{2}\hat{\sigma}$

$\left.\begin{array}{l} \star\ [\hat{\sigma}_i, \hat{\sigma}_j] = 2i\varepsilon_{ijk}\hat{\sigma}_k \\ \text{eigenvalue for } \hat{\sigma}_i \text{ is } \pm 1: \quad \hat{\sigma}_i^2 = \hat{I} \end{array}\right\} \{\hat{\sigma}_i, \hat{\sigma}_j\} = \hat{\sigma}_i\hat{\sigma}_j + \hat{\sigma}_j\hat{\sigma}_i = 2\delta_{ij}$

$\rightarrow \hat{\sigma}_i\hat{\sigma}_j = \delta_{ij} + i\varepsilon_{ijk}\hat{\sigma}_k$, $\hat{\sigma}_i^\dagger = \hat{\sigma}_i$

Pauli Representation

In Pauli Representation, we described $\hat{\sigma}_3$ as a 2x2 matrix $\sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

$\hat{\sigma}_i\hat{\sigma}_j = \delta_{ij} + i\varepsilon_{ijk}\hat{\sigma}_k \rightarrow \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

Eigenvalue Equation: $\sigma_J \chi_\lambda = \lambda \chi_\lambda \quad (J = 1, 2, 3)$

$\chi_\lambda = \sigma_J^2 \chi_\lambda = \lambda^2 \chi_\lambda$, $\lambda = \pm 1$

For $\hat{\sigma}_3$ $\begin{cases} \lambda = 1 \rightarrow \alpha = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, & \hat{\sigma}_3\alpha = \alpha \\ \lambda = -1 \rightarrow \beta = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, & \hat{\sigma}_3\beta = -\beta \end{cases}$, $\alpha^\dagger\alpha = \beta^\dagger\beta = I$, $\alpha^\dagger\beta = \beta^\dagger\alpha = 0$

For $\hat{\sigma}_1$ & $\hat{\sigma}_2$

$\hat{\sigma}_1: \begin{cases} \lambda = 1, \psi = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \\ \lambda = -1, \psi = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \end{cases}$ $\quad \hat{\sigma}_2: \begin{cases} \lambda = 1, \psi = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix} \\ \lambda = -1, \psi = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix} \end{cases}$

Photon Spin

$\mu = 0$ for photon

$i\hbar\frac{\partial}{\partial t}\psi = [-\frac{\hbar^2}{2\mu}\nabla^2 + V(r)]\psi$ cannot describe the motion of a photon.

时空地位不等

Maxwell Equation $\begin{cases} \nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \\ \nabla \times \vec{B} = \mu_0\varepsilon_0\frac{\partial \vec{E}}{\partial t} \\ \nabla \cdot \vec{E} = 0 \\ \nabla \cdot \vec{B} = 0 \end{cases}$

* Def. complex field

$\vec{\psi} = \sqrt{\frac{\varepsilon_0}{2}}\vec{E} + i\frac{\vec{B}}{\sqrt{2\mu_0}}$

energy density

$|\vec{\psi}|^2 = \frac{1}{2}\varepsilon_0\vec{E}^2 + \frac{1}{2\mu_0}\vec{B}^2$

Maxwell Equation: $\begin{cases} i\hbar \frac{\partial \vec{\psi}}{\partial t} = \hbar c \nabla \times \vec{\psi} \\ \nabla \cdot \vec{\psi} = 0 \end{cases}$

Def. $S_i \ (i = 1, 2, 3)$, $(S_i)_{ab} = -i\varepsilon_{iab}$

$$i\hbar \frac{\partial \psi_a}{\partial t} = -i\hbar c (S_i)_{ab} \partial_i \psi_b = -i\hbar c (S \cdot \nabla)_{ab} \psi_b$$

$$\rightsquigarrow \quad i\hbar \frac{\partial \psi}{\partial t} = -i\hbar c (S \cdot \nabla) \psi$$

properties:

* Hamiltonian Operator: $\hat{H} = -i\hbar c S \cdot \nabla = c S \cdot \hat{p}$
* Wavefun represents the electromagnetic field not possibility wave.
* ψ and $\psi e^{i\alpha}$ are completely different photon state

△ For single photon, $\int |\psi(\vec{r}, t)|^2 d^3x$ represents energy of the photon, possibility of finding the photon at $\vec{r}$:

$$\rho(\vec{r}, t) = \frac{|\psi(\vec{r}, t)|^2}{\int d^3x \, |\psi(\vec{r}, t)|^2}$$

★ Photon Angular Momentum: $S\hbar$ $\quad [S_i, S_j] = i\varepsilon_{ijk} S_k$, $\quad S^2 = 2 \Rightarrow s = 1$

The wave function for photon is essentially field strength

$$\vec{\psi} = \sqrt{\frac{\varepsilon_0}{2}} \vec{E} + i \frac{\vec{B}}{\sqrt{2\mu_0}} \quad \rightsquigarrow \nabla \cdot \vec{\psi} = 0$$

we use $\vec{r}(x)$ to operate on $\vec{\psi}$, then

$$\vec{\psi}' = \vec{r} \vec{\psi} \quad \Rightarrow \nabla \cdot \vec{\psi}' = (\nabla \cdot \vec{r}) \cdot \vec{\psi}' \neq 0$$

$\vec{\psi}'$ doesn't meet Gaussian Law, such $\vec{\psi}'$ isn't wave function for photon

$\Rightarrow$ $\vec{r}$ isn't qualified to represent the position of photon. *

Photon	relativistic particle with $\mu = 0$	unrelativistic particle with μ	unrelativistic electron with μ
$\hat{H} = cS \cdot \hat{p}$ $\longrightarrow$	$\hat{H} = c\lvert\hat{p}\rvert$ $\longrightarrow$	$\hat{H} = \frac{\hat{p}^2}{2\mu}$ $\longrightarrow$	$\hat{H} = \frac{1}{2\mu}(\sigma \cdot \hat{p})^2$

Sum of Angular Momentum Operator

independent

Def. Total angular momentum $\hat{J} = \hat{L} + \hat{S}$, $[\hat{L}_i, \hat{S}_j] = 0$

for any system with $\hat{J}_1$ & $\hat{J}_2$, its total angular momentum $\hat{J} = \hat{J}_1 + \hat{J}_2$

$$\begin{cases} [\hat{J}_{1i}, \hat{J}_{1j}] = i\hbar\varepsilon_{ijk}\hat{J}_{1k} \\ [\hat{J}_{2i}, \hat{J}_{2j}] = i\hbar\varepsilon_{ijk}\hat{J}_{2k} \\ [\hat{J}_{1i}, \hat{J}_{2j}] = 0 \end{cases} \quad \text{seperate} \quad \rightsquigarrow \quad \begin{aligned} &[\hat{J}_i, \hat{J}_j] = i\hbar\varepsilon_{ijk}\hat{J}_k \\ &[J_i, \hat{J}^2] = 0 \end{aligned} \quad \text{total}$$

$\hat{J}_3$ & $\hat{J}^2$ have the common eigenstate base $\begin{cases} \hat{J}_3 |j,m\rangle = m\hbar |j,m\rangle \\ \hat{J}^2 |j,m\rangle = j(j+1)\hbar^2 |j,m\rangle \end{cases}$

$(m = -j, -j+1, \cdots, j-1, j)$

Components J_a $(a = 1, 2)$ $\begin{cases} \hat{J}_{a3} |j_a, m_a\rangle = m_a\hbar |j_a, m_a\rangle \\ \hat{J}_a^2 |j_a, m_a\rangle = j_a(j_a+1)\hbar^2 |j_a, m_a\rangle \end{cases}$

when j_1, j_2 are confirmed, the dimension for $\mathcal{H}_{j_1 j_2}$ is $(2j_1+1)(2j_2+1)$

Set the base for CSCO $\{\hat{J}_{13}, \hat{J}_1^2, \hat{J}_{23}, \hat{J}_2^2\}$ in $\mathcal{H}_{j_1 j_2}$ as:

$$|j_1, j_2; m_1, m_2\rangle :\overset{\Delta}{=} |j_1, m_1\rangle \otimes |j_2, m_2\rangle = |j_1, m_1\rangle |j_2, m_2\rangle$$

As for CSCO $\{\underbrace{\hat{J}_1^2, \hat{J}_2^2}_{\text{components}}, \underbrace{\hat{J}^2, \hat{J}_3}_{\text{total}}\}$, we assume their common base $|j_1, j_2, j, m\rangle$

* Conditions: $\begin{cases} \hat{J}_1^2 |j_1, j_2, j, m\rangle = j_1(j_1+1)\hbar^2 |j_1, j_2, j, m\rangle \\ \hat{J}_2^2 |j_1, j_2, j, m\rangle = j_2(j_2+1)\hbar^2 |j_1, j_2, j, m\rangle \\ \hat{J}^2 |j_1, j_2, j, m\rangle = j(j+1)\hbar^2 |j_1, j_2, j, m\rangle \\ \hat{J}_3 |j_1, j_2, j, m\rangle = m\hbar |j_1, j_2, j, m\rangle \end{cases}$

* $|j_1, j_2; j, m\rangle = \hat{I}\, |j_1, j_2; j, m\rangle$

$$= \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} |j_1, j_2; m_1, m_2\rangle \underline{\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle}$$

$\Downarrow$

Clebsch - Gordan (C-G) Coordinate

Properties about C-G coordinate

same dimension

$$\hat{J}_3 = \hat{J}_{13} + \hat{J}_{23} = \hat{J}_{13} \otimes \hat{I}_2 + \hat{I}_1 \otimes \hat{J}_{23}$$

Thus $\hat{J}_3 |j_1, j_2; m_1, m_2\rangle = [\hat{J}_{13} \otimes \hat{I}_2 + \hat{I}_1 \otimes \hat{J}_{23}] |j_1, m_1\rangle \otimes |j_2, m_2\rangle$

$$= [\hat{J}_{13} |j_1, m_1\rangle] \otimes |j_2, m_2\rangle + |j_1, m_1\rangle \otimes [\hat{J}_{23} |j_2, m_2\rangle]$$

$$= [m_1\hbar |j_1, m_1\rangle] \otimes |j_2, m_2\rangle + |j_1, m_1\rangle \otimes [m_2\hbar |j_2, m_2\rangle]$$

$$= (m_1 + m_2)\hbar |j_1, m_1\rangle \otimes |j_2, m_2\rangle$$

$$= (m_1 + m_2)\hbar |j_1, j_2; m_1, m_2\rangle$$

In another hand $\hat{J}_3 |j_1, j_2; j, m\rangle = m\hbar |j_1, j_2; j, m\rangle$

* $|j_1, j_2, j, m\rangle$ & $|j_1, j_2, m_1, m_2\rangle$ are both eigenstates for $\hat{J}_3$, while C-G coordinate $\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle \neq 0$, they're not orthodox : $m = m_1 + m_2$

* $(m - m_1 - m_2) \langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle = 0$

$$\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle \propto \delta_{m, m_1+m_2}$$

$$\rightsquigarrow |j_1, j_2; j, m\rangle = \sum_{m_1=-j_1}^{j_1} |j_1, j_2; m_1, m-m_1\rangle \underbrace{\langle j_1, j_2; m_1, m-m_1 | j_1, j_2; j, m\rangle}_{(C-G)}$$

Conclusions :

$$\boxed{|j_1, j_2, j, j\rangle = |j_1, j_2; j_1, j_2\rangle = |j_1, j_1\rangle \otimes |j_2, j_2\rangle \quad j_{max} = j_1 + j_2}$$

* $\hat{J}_3 |j_1, j_2; m_1, m_2\rangle = (m_1 + m_2)\hbar |j_1, j_2; m_1, m_2\rangle \rightsquigarrow \hat{J}_3$ is linear Hermitian Operator in $\mathcal{H}_{j_1 j_2}$

* $\hat{J}^2$ is linear Hermitian Operator in $\mathcal{H}_{j_1 j_2}$ as well.

* Dimension of base in $\mathcal{H}_{j_1 j_2}$ ($|j_1, m_1\rangle \otimes |j_2, m_2\rangle$) : $(2j_1+1)(2j_2+1)$

$$\rightsquigarrow (2j_1+1)(2j_2+1) = \sum_{j_{min}}^{j_{max} = j_1+j_2} (2j+1) \rightsquigarrow j_{min} = |j_1 - j_2|$$

Calculation of C-G coordinates

Ladder operator : $\hat{J}_\pm = \hat{J}_{1\pm} + \hat{J}_{2\pm}$

Highest eigenstate $|j_1, j_2; j, j\rangle = \delta_{j, j_1+j_2} |j_1, j_1\rangle \otimes |j_2, j_2\rangle$

$$\rightsquigarrow |j_1, j_2; j, j-1\rangle = \hat{J}_- |j_1, j_2; j, j\rangle = \delta_{j, j_1+j_2} [\hat{J}_{1-} + \hat{J}_{2-}] |j_1, j_2; j_1, j_2\rangle$$

$$= \delta_{j, j_1+j_2} \left[\sqrt{\frac{j_1}{j}} |j_1, j_2; j_1 - 1, j_2\rangle + \sqrt{\frac{j_2}{j}} |j_1, j_2; j_1, j_2 - 1\rangle \right]$$

Sum of Orbital & Spin Angular Momentum Operator for Electron

For electron Def. $\hat{J} = \hat{L} + \hat{S}$ (Total Angular Momentum Operator)

Proper CSCO: $\{\hat{L}^2, \hat{L}_3, \hat{S}_3\}$ $\left(\hat{S}^2 = \frac{3}{4}\hbar^2 = const\right)$

$/ \{\hat{L}^2, \hat{J}^2, \hat{J}_3\}$

$$\hat{J}^2 = (\hat{L} + \hat{S})^2 = \hat{L}^2 + \hbar \hat{L}\cdot\hat{\sigma} + \frac{3}{4}\hbar^2$$

$[\hat{J}^2, \hat{L}_3] \neq 0$, $[\hat{J}^2, \hat{\sigma}_3] \neq 0$

$[\hat{J}^2, \hat{L}^2] = [\hat{J}^2, \hat{J}_3] = 0$

Common base for $\{\hat{J}^2, \hat{J}_3, \hat{L}^2\}$ in (L_3, S_3) representation:

$$\psi(\theta, \phi, S_3) = \begin{bmatrix} \psi_1(\theta,\phi) \\ \psi_2(\theta,\phi) \end{bmatrix}$$

properties:

* $\hat{L}^2 \psi_1 = l(l+1)\hbar^2 \psi_1$, $\hat{L}^2 \psi_2 = l(l+1)\hbar^2 \psi_2$
* $\hat{J}_3 \psi = m_j \hbar \psi$
* $\hat{L}_3 \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} + \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = m_j \hbar \psi \rightsquigarrow \begin{cases} \hat{L}_3 \psi_1 = (m_j - \frac{1}{2})\hbar \psi_1 \\ \hat{L}_3 \psi_2 = (m_j + \frac{1}{2})\hbar \psi_2 \end{cases}$

$\downarrow$ transform

* Demand ψ to be eigenstate of $\hat{J}^2$: $\psi = \begin{bmatrix} a Y_{l,m}(\theta,\phi) \\ b Y_{l,m+1}(\theta,\phi) \end{bmatrix}$ $m = m_j - \frac{1}{2}$

$$\hat{J}^2 = \begin{bmatrix} \hat{L}^2 + \frac{3}{4}\hbar^2 + \hbar \hat{L}_3 & \hbar \hat{L}_- \\ \hbar \hat{L}_+ & \hat{L}^2 + \frac{3}{4}\hbar^2 - \hbar \hat{L}_3 \end{bmatrix}$$

$\hat{L}_\pm = \hat{L}_1 \pm i \hat{L}_2$

$[\hat{L}_3, \hat{L}_\pm] = \pm \hat{L}_\pm$

$$\hat{L}_3 \hat{L}_\pm Y_{l,m} = [\hat{L}_3, \hat{L}_\pm] Y_{l,m} + \hat{L}_\pm \hat{L}_3 Y_{l,m} = \pm \hat{L}_\pm Y_{l,m} + m \hat{L}_\pm Y_{l,m} = (m \pm 1)\hat{L}_\pm Y_{l,m}$$

$\hat{L}_\pm Y_{l,m} \sim Y_{l,m\pm1}$

$$\hat{L}_\pm Y_{lm} = \hbar\sqrt{(l \pm m + 1)(l \mp m)}\, Y_{l,m\pm1}$$

* $j(j+1)\hbar^2 \psi = \hat{J}^2 \psi = \begin{bmatrix} \hat{L}^2 + \frac{3}{4}\hbar^2 + \hbar \hat{L}_3 & \hbar \hat{L}_- \\ \hbar \hat{L}_+ & \hat{L}^2 + \frac{3}{4}\hbar^2 - \hbar \hat{L}_3 \end{bmatrix}\begin{bmatrix} a Y_{l,m}(\theta,\phi) \\ b Y_{l,m+1}(\theta,\phi) \end{bmatrix}$

$$\rightsquigarrow [l(l+1) + \tfrac{3}{4} + m - j(j+1)]\, a + \sqrt{(l-m)(l+m+1)}\, b = 0$$

$$\sqrt{(l-m)(l+m+1)}\, a + [l(l+1) - \tfrac{1}{4} - m - j(j+1)]\, b = 0$$

$\rightsquigarrow j = l \pm \frac{1}{2}$

$j = l + \frac{1}{2}$, $\frac{a}{b} = \sqrt{\frac{l+m+1}{l-m}}$ $\psi(\theta,\phi,S_3) = \frac{1}{\sqrt{2l+1}}\begin{bmatrix} \sqrt{l+m+1}\, Y_{l,m} \\ \sqrt{l-m}\, Y_{l,m+1} \end{bmatrix} \Big/ \frac{1}{\sqrt{2j}}\begin{bmatrix} \sqrt{j+m_j}\, Y_{j-\frac{1}{2}, m_j - \frac{1}{2}} \\ \sqrt{j-m_j}\, Y_{j-\frac{1}{2}, m_j+\frac{1}{2}} \end{bmatrix}$

$j = l - \frac{1}{2}$, $\frac{a}{b} = -\sqrt{\frac{l-m}{l+m+1}}$ $\psi(\theta,\phi,S_3) = \frac{1}{\sqrt{2l+1}}\begin{bmatrix} -\sqrt{l-m}\, Y_{l,m} \\ \sqrt{l+m+1}\, Y_{l,m+1} \end{bmatrix} \Big/ \frac{1}{\sqrt{2j+2}}\begin{bmatrix} -\sqrt{j-m_j+1}\, Y_{j-\frac{1}{2}, m_j-\frac{1}{2}} \\ \sqrt{j+m_j+1}\, Y_{j-\frac{1}{2}, m_j+\frac{1}{2}} \end{bmatrix}$

Quantum Mechanics in 3D Space System

Central Field

$V = V(\vec{r})$ Constant in classical mechanics : $\frac{d\vec{L}}{dt} = \frac{d\vec{r}}{dt} \times \vec{p} + \vec{r} \times \frac{d\vec{p}}{dt} = 0$

Hamiltian Operator in central field : $\hat{H} = \frac{\hat{\vec{p}}^2}{2\mu} + V(r) = -\frac{\hbar^2}{2\mu}\nabla^2 + V(r)$

$$\begin{cases} [\hat{L}_i, \hat{\vec{p}}^2] = 2i\hbar\varepsilon_{ijn}\hat{p}_j\hat{p}_n = 0 \\ [\hat{\vec{L}}, V(r)] = \vec{e}_i\varepsilon_{ijk}x_j[p_k, V(r)] = \vec{e}_i\varepsilon_{ijk}x_j p_k(-i\hbar\partial_k V(r)) = -i\hbar\vec{r}\times\nabla V(r) = 0 \end{cases}$$

$\rightsquigarrow$ orbital angular momentum is constant operator $[\hat{\vec{L}}, \hat{H}] = 0$

Also $[\hat{\vec{L}}^2, \hat{H}] = [\hat{L}_i\hat{L}_i, \hat{H}] = \hat{L}_i[\hat{L}_i, \hat{H}] + [\hat{L}_i, \hat{H}]\hat{L}_i = 0$

$\rightsquigarrow$ CSCO : $\{\hat{L}_3, \hat{\vec{L}}^2, \hat{H}\}$

☆ energetic eigenfunction can be eigenfuction of $\hat{L}_3$ & $\hat{\vec{L}}^2$ ($Y_{l,m}$)

$\hat{\vec{p}}^2 = -\frac{\hbar^2}{r}\partial_r^2 r + \frac{\hat{\vec{L}}^2}{r^2}$

eigenvalue equation in spheric frame :

$$\left[-\frac{\hbar^2}{2\mu r}\partial_r^2 r + \frac{\hat{\vec{L}}^2}{2\mu r^2} + V(r)\right]\psi_E(r,\theta,\phi) = E\psi_E(r,\theta,\phi)$$

Contrifugal potential (离心势能)

should be $\psi_E(r,\theta,\phi) = R_l(r)Y_{lm}(\theta,\phi)$ $\quad l = 0, 1, 2\cdots$; $m = 0, \pm1, \cdots \pm l$

☆ Radial Wavefunc. $R_l(r)$: $\left[\frac{1}{r}\frac{d^2}{dr^2}r + \frac{2\mu}{\hbar^2}(E - V(r)) - \frac{l(l+1)}{r^2}\right]R(r) = 0$

$$R_l(r) = \frac{\chi_l(r)}{r}$$

$$\chi_l''(r) + \left[\frac{2\mu}{\hbar^2}(E - V(r)) - \frac{l(l+1)}{r^2}\right]\chi_l(r) = 0$$

☆ $\begin{cases}\text{radial wave function depend on specific } V(r) \text{ eg. } V(r) = \frac{\alpha}{r},\ V(r) = \frac{1}{2}\mu\omega^2 r^2 \\ \text{irrelated to } m, \text{ the degeneracy : } 2l+1\end{cases}$

when $r \longrightarrow 0$ = $\lim_{r\to0} r^2V(r) = 0$, then $R_l''(r) + \frac{2}{r}R_l'(r) - \frac{l(l+1)}{r^2}R_l(r) = 0$

assume $R_l(r) = r^s$, we have $s(s+1) - l(l+1) = 0$ $\quad s = l \,/\, -(l+1)$

$R_l(r) \sim r^l$ / $R_l(r) \sim \frac{1}{r^{l+1}}$

physically accepted.

Hydrogen Atom

$$V(r) = -\frac{e}{r} \rightsquigarrow \chi''_l(r) + \left[\frac{2\mu}{\hbar^2}\left(E+\frac{e^2}{r}\right) - \frac{l(l+1)}{r^2}\right]\chi_l(r) = 0$$

$\downarrow$ atomic units $\hbar = e = \mu = 1$

$$\chi_l''(r) + \left[2E + \frac{2}{r} - \frac{l(l+1)}{r^2}\right]\chi_l(r) = 0$$

while $r \to 0$, $\chi_l(r) \sim r^{l+1}$

bound state restriction : $E<0$

while $r \to \infty$, $\chi_l''(r) + 2E\chi_l(r) = 0$ $\nearrow$ $\chi_l(r) \sim e^{-\beta r}$, $\beta = \sqrt{-2E} > 0$

* To meet bound state restriction : Def. Principle quantum number $n = 1, 2, 3, \cdots$

* Energetic Eigenvalues $E_n = -\frac{1}{2n^2} \left(= -\frac{e^2}{2a}\frac{1}{n^2}\right)$, $n = 1, 2, 3, \cdots$

* Degeneracy of each energy level : for E_n, angular quantum number l

$l = 0, 1, \cdots, n-1$

eigenstate for energy E_n : $\psi_{nlm}(r,\theta,\phi) = R_{nl}(r)Y_{lm}(\theta,\phi)$, degenracy $d_n = 2\sum_{l=0}^{n-1}(2l+1) = 2n^2$

Conclusions : For CSCO $\{\hat{L}^2, \hat{L}_3, \hat{H}\}$, eigenfunction $\psi_{nlm}(r,\theta,\phi)$:
$$\begin{cases} \hat{L}^2\psi_{nlm} = l(l+1)\hbar^2\psi_{nlm} \\ \hat{L}_3\psi_{nlm} = m\hbar\psi_{nlm} \\ \hat{H}\psi_{nlm} = -\frac{\mu e^4}{2\hbar^2}\frac{1}{n^2}\psi_{nlm} \end{cases}$$

Current density vector & magnetic moment

when the atom is at ψ_{nlm}, then $\vec{j} = \frac{ie\hbar}{2\mu}\left[\psi^*_{nlm}\nabla\psi_{nlm} - \psi_{nlm}\nabla\psi^*_{nlm}\right]$

in spheric frame, $j_r = j_\theta = 0$

$$j_\phi = \frac{ie\hbar}{2\mu r\sin\theta}\, 2im\,|\psi_{nlm}|^2$$

The magnetic moment of electron :

transform to $(\vec{i},\vec{j},\vec{k})$

$$\vec{M} = \frac{1}{2c}\int d^3x\, \vec{r}\times\vec{j}(\vec{r}) = \frac{e\hbar m}{2\mu c}\int d^3x\, \frac{\vec{e}_\theta}{\sin\theta}|\psi_{nlm}|^2 = -\frac{e\hbar m}{2\mu c}\vec{k}$$

[$\mu_B = \frac{e\hbar}{2\mu c}$: Bohr magnetron], then we have

$$M_3 = -\frac{e\hbar m}{2\mu c} = -\mu_B m$$

when $l = m = 0$, $M_3 = 0$

Hamiltonian of Charged Particles in Electromagnetic Field.

Gauge Potential : $(\varphi, \vec{A})$ Hamiltonian $H = \frac{1}{2\mu}(\underbrace{\vec{P}}_{\text{canonical momentum (正则动量)}} - \frac{q}{c}\vec{A})^2 + q\varphi$

Canonical Equation : $\begin{cases} \underline{v_i = \dot{x}_i = \partial_{p_i} H = \frac{1}{\mu}(P_i - \frac{q}{c}A_i)} \rightsquigarrow \vec{P} = \mu\vec{v} + \frac{q}{c}\vec{A} \\ \dot{P}_i = -\partial_{x_i} H = \frac{q}{\mu c}(P_j - \frac{q}{c}A_j)\partial_i A_j - q\partial_i\varphi = \frac{q}{c}v_j\partial_i A_j - q\partial_i\varphi \\ / \ \dot{P}_i = \mu\dot{v}_i + \frac{q}{c}\dot{A}_i = \mu\dot{v}_i + \frac{q}{c}(\partial_t A_i + v_j\partial_j A_i) \end{cases}$

$$\rightsquigarrow \mu\dot{v}_i = -\frac{q}{c}(\partial_t A_i + v_j\partial_j A_i) + \frac{q}{c}v_j\partial_i A_j - q\partial_i\varphi$$

$$= q(-\partial_i\varphi - \frac{1}{c}\partial_t A_i) + \frac{q}{c}v_j(\underbrace{\partial_i A_j - \partial_j A_i}_{\nabla\times\vec{A}}) = q(E_i + \frac{1}{c}\varepsilon_{ijk}v_j B_k)$$

$$\rightsquigarrow \mu\ddot{x} = q\vec{E} + \frac{q}{c}\vec{v}\times\vec{B} \quad \star$$

Quantilization 正则量子化

canonical momentum

$$\vec{P} \rightsquigarrow \hat{p} = -i\hbar\nabla$$

势-流耦合项

Thus Hamiltonian Operator $\hat{H} = \frac{1}{2\mu}(-i\hbar\nabla - \frac{q}{c}\vec{A})^2 + q\varphi$

Schrödinger Equation $i\hbar\partial_t\psi = [-\frac{\hbar}{2\mu}(\nabla - \frac{iq}{\hbar c}\vec{A})^2 + q\varphi]\psi$

Schrödinger Equation in Coulumb Gauge

$$[\hat{\vec{P}}, \vec{A}] = [\hat{p}_i, A_i] = -i\hbar\partial_i A_i = -i\hbar\nabla\cdot\vec{A} \xrightarrow{\text{attach } \nabla\cdot\vec{A}=0} = 0$$

In Coulumb Gauge $\rightsquigarrow i\hbar\partial_t\psi = [\frac{1}{2\mu}\hat{\vec{P}}^2 - \frac{q}{\mu c}\vec{A}\cdot\hat{\vec{P}} + \frac{q^2}{2\mu c^2}\vec{A}^2 + q\varphi]\psi$

$\star$ Check that ψ meet the conservation of prob. $\begin{cases} \rho \geq 0 \\ \partial_t\rho + \nabla\cdot\vec{j} = 0 \end{cases}$

$\rho = |\psi|^2 = \psi\psi^*$

$$i\hbar\partial_t|\psi|^2 = \frac{1}{2\mu}(\psi^*\hat{P}^2\psi - \psi\hat{P}^2\psi^*) - \frac{q}{\mu c}(\psi^* A\cdot\hat{P}\psi - \psi A\cdot\hat{P}\psi^*)$$

$$= -\frac{i\hbar}{2\mu}\nabla\cdot[\psi^*(\hat{\vec{P}} - \frac{q}{c}\vec{A})\psi + \psi(\hat{\vec{P}} - \frac{q}{c}\vec{A})^*\psi^*]$$

$$\Rightarrow \partial_t\rho + \nabla\cdot\vec{J} = 0$$

$\rho = \psi^*\psi$

def. velocity operator. $\hat{\vec{v}} = \frac{1}{\mu}(\hat{\vec{P}} - \frac{q}{c}\vec{A})$

$\vec{J} = \frac{1}{2}(\psi^*\hat{\vec{v}}\psi + \psi\hat{\vec{v}}\psi^*) = \mathrm{Re}(\psi\hat{\vec{v}}\psi^*)$

☆ Check that ψ meet Gauge Symmetry (规范变换)

When gauge potential do the transformation $\begin{cases} \vec{A}' = \vec{A} + \nabla \cdot \chi(\vec{r},t) \\ \varphi' = \varphi - \frac{1}{c}\partial_t \chi(\vec{r},t) \end{cases}$ ($\vec{E}, \vec{B}$) shouldn't change.

Gauge Transformation: $\psi' = \exp[\frac{iq}{\hbar c}\chi(\vec{r},t)]\psi$

$$\downarrow \quad \hat{M} = e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{B} + [\hat{A},\hat{B}] + \frac{1}{2!}[\hat{A},[\hat{A},\hat{B}]] + \frac{1}{3!}[\hat{A},[\hat{A},[\hat{A},\hat{B}]]] + \cdots$$

$$i\hbar\frac{\partial}{\partial t}\psi' = [-\frac{\hbar^2}{2\mu}(\nabla - \frac{iq}{\hbar c}\vec{A}')^2 + q\varphi']\psi'$$

Schrödinger Equation meet Gauge Inviariance (规范不变性) in EM field

(规范原理：概率诠释允许的规范变换导致电磁相互作用的存在)

Motion of Charged Particles in Electromagnetic Field.

Intrinsic magnetic moment of electron

Hamiltonian for free electron (considering spin) $\hat{H} = \frac{1}{2\mu}(\sigma\cdot\hat{\vec{P}})^2$

$(\sigma\cdot\hat{\vec{P}})^2 = \sigma_i\hat{P}_i\sigma_j\hat{P}_j = (\delta_{ij} + i\varepsilon_{ijk}\sigma_k)\hat{P}_i\hat{P}_j = \hat{P}_i\hat{P}_i = \hat{P}_i^2$

$\downarrow$ attach the field $\vec{B} = \nabla\times\vec{A}$

$\vec{P} \rightsquigarrow \vec{P} - \frac{q}{c}\vec{A}$ $\qquad [(\sigma\cdot\vec{A})(\sigma\cdot\vec{B})] = \vec{A}\cdot\vec{B} + i\sigma(\vec{A}\times\vec{B})$

$$\hat{H} = \frac{1}{2\mu}[\sigma\cdot(\hat{\vec{P}} + \frac{e}{c}\vec{A})]^2$$

$$= \frac{1}{2\mu}(\hat{\vec{P}} + \frac{e}{c}\vec{A})^2 + \underline{\frac{i}{2\mu}\sigma\cdot[(\hat{\vec{P}} + \frac{e}{c}\vec{A})\times(\hat{\vec{P}} + \frac{e}{c}\vec{A})]}$$

$$\Downarrow$$

$$\frac{ie}{2\mu c}\sigma\cdot(\hat{\vec{P}}\times\hat{\vec{A}} + \hat{\vec{A}}\times\hat{\vec{P}})$$

$$= \frac{ie}{2\mu c}\varepsilon_{ijk}\sigma_i[\hat{P}_j, \hat{A}_k] = \frac{ie}{2\mu c}\varepsilon_{ijk}\sigma_i(-i\hbar)\frac{\partial A_k}{\partial x_j}$$

$$= \frac{e\hbar}{2\mu c}\sigma\cdot(\nabla\times\vec{A}) = \frac{e\hbar}{2\mu c}\sigma\cdot\vec{B} := -\vec{\mu}_s\vec{B}$$

where $\mu_s = -\frac{e\hbar}{2\mu c}\sigma = -\frac{e}{\mu c}\hat{\vec{S}}$ $\qquad (\mu_l = -\frac{e}{2\mu c}\hat{\vec{L}})$

$\uparrow$ Spin magnetic momentum $\rightsquigarrow g_s = -2$

Normal Zeeman Effect

Def. Atomic Spectrum splited triple

☆ Energy level degeracy eliminated by interaction with outter field

In uniform magnetic field : $\vec{A} = \alpha \vec{r} \times \vec{B}$

$$\vec{B} = \alpha \nabla \times (\vec{r} \times \vec{B}) = -2\alpha \vec{B} \Rightarrow \alpha = -\frac{1}{2}$$

$$\vec{B} = B\vec{e_z} \rightsquigarrow A_x = -\frac{1}{2} yB, \quad A_y = \frac{1}{2} xB, \quad A_z = 0$$

Considering Alkali Atom 屏蔽库伦场 $e\phi = V(r)$

$$\hat{H} = \frac{1}{2\mu}\left[(\hat{P}_x - \frac{eB}{2c} y)^2 + (\hat{P}_y - \frac{eB}{2c} x)^2 + \hat{P}_z^2 \right] + V(r)$$

$$= \frac{1}{2\mu}\left[\hat{\vec{P}}^2 + \frac{eB}{c} \underbrace{(x\hat{P}_y - y\hat{P}_x)}_{= \hat{L}_3} + \frac{e^2B^2}{4c^2}(x^2+y^2) \right] + V(r)$$

$\frac{e^2B^2(x^2+y^2)/4c^2}{\frac{eB}{c}\hbar} < 10^{-4}$ (B^2 term leave out)

$$\rightsquigarrow \hat{H} = \frac{1}{2\mu}\hat{\vec{P}}^2 + V(r) + \frac{eB}{2\mu c}\hat{L}_3$$

describe as $-\hat{\vec{\mu}} \cdot \vec{B}$ ($\hat{\vec{\mu}} = -\frac{1}{2\mu c}\hat{\vec{L}}$)

* $[\hat{L}_x, \hat{H}] \neq 0$, $[\hat{L}_y, \hat{H}] \neq 0$
* For CSCO $\{\hat{L}_3, \hat{\vec{L}}^2, \hat{H}\}$, $\Upsilon_{nlm} = R_{n,l}(r) Y_{lm}(\theta, \varphi)$

energetic eigenvalue $E_{n,l,m} = E_{n,l} + m\frac{eB\hbar}{2\mu c}$ (elemination of degenracy)

$\omega_L = \frac{eB}{2\mu c}$ Lamor Frequency

Landau Level

Free electron in $\vec{B} = \vec{B_z}$, $\vec{A} = -\frac{1}{2}\vec{r} \times \vec{B}$

Hamiltonian : $\hat{H} = \frac{1}{2\mu}(\hat{P}_x^2 + \hat{P}_y^2) + \frac{e^2B^2}{8\mu c^2}(x^2+y^2) + \frac{eB}{2\mu c}(x\hat{P}_y - y\hat{P}_x) + \frac{1}{2\mu}P_z^2$

z direction : $\hat{H}_1 = \frac{\hat{\vec{P}}_z^2}{2\mu}$, $\psi(z) \sim e^{ip_0 z/\hbar}$

(x, y) direction : $\hat{H}_2 = \hat{H}_0 + \hat{H}'$

$\hat{H}' = \frac{e^2B^2}{8\mu c^2}\hat{L}_z \sim \omega_L \hat{L}_z \xrightarrow{\text{polar coordinate}} \hat{H}' = -i\hbar\omega_L \partial_\varphi$

$$\hat{H}_0 = \frac{1}{2M}(\hat{\vec{P}}_x^2 + \hat{\vec{P}}_y^2) + \frac{e^2B^2}{8\mu c^2}(x^2+y^2)$$

(2D Harmonic Oscillator)

$[\hat{H}_0, \hat{H}'] = 0$

$$\xrightarrow{\text{polar coordinate}} \hat{H}_0 = -\frac{\hbar^2}{2\mu}\left[\frac{1}{\rho}\partial_\rho(\rho\partial_\rho) + \frac{1}{\rho^2}\partial_\varphi^2\right] + \frac{1}{2}\mu\omega_L^2\rho^2$$

Bound State in uniform magnetic field :

合流超几何函数

eigenfunction : $R_{n_\rho,|m|}(\xi) \sim \xi^{|m|} e^{-\xi^2/2} F(-n_\rho, |m|+1, \xi^2)$ $\quad (\rho = \sqrt{\frac{\hbar}{\omega_L \mu}}\,\xi)$

Landau level : $E_{n_\rho, m} = (2n_\rho + m + |m| + 1)\hbar\omega_L$

* $-\vec{\mu}\cdot\vec{B} = (2n_\rho + m + |m| + 1)\hbar\omega_L \rightsquigarrow \mu_z < 0$: anti-magnetic

Hamiltonian of electron considering spin-orbit coupling

* Spin-orbit Coupling item : $\hat{H}' = \xi(r)\hat{S}\cdot\hat{L}$ $\quad (\xi(r) = \frac{1}{2\mu^2c^2r}\frac{dV(r)}{dr})$

While outer magnetic field is essentially strong, spin-orbit coupling can be neglected.

$[\hat{L}, \hat{S}\cdot\hat{L}] \neq 0$

$[\hat{S}, \hat{S}\cdot\hat{L}] \neq 0$ $\rightsquigarrow [\hat{J}, \hat{S}\cdot\hat{L}] = 0 \rightsquigarrow [\hat{J}, \hat{H}] = 0$

$\hat{J}$ is constant

Choose CSCO $\{\hat{H}, \hat{J}^2, J_3, \hat{L}^2\}$

$$\{\hat{J}^2, \hat{J}_3, \hat{L}^2\} \rightarrow \psi_{ljm_j} = \frac{1}{\sqrt{2}}\begin{bmatrix} \sqrt{j+m_j}\, Y_{j-1/2,\, m_j-1/2} \\ \sqrt{j-m_j}\, Y_{j-1/2,\, m_j+1/2} \end{bmatrix} \quad (j = l \pm \tfrac{1}{2})$$

For $H' = \hat{S}\cdot\hat{L}$, $\hat{S}\cdot\hat{L} = \frac{1}{2}[\hat{J}^2 - \hat{L}^2 - \frac{3}{4}\hbar^2]$

depend on j / l

$$\rightsquigarrow \hat{S}\cdot\hat{L}\,\psi_{ljm_j} = \frac{\hbar^2}{2}[j(j+1) - l(l+1) - \tfrac{3}{4}]\psi_{ljm_j}$$

eg. Alkali Atom $\xi(r) = \frac{1}{2\mu^2c^2r}\frac{dV(r)}{dr}$, $E_{nlj=l+1/2} > E_{nlj=l-1/2}$

Abnormal Zeeman Effect

$\vec{B} = B\vec{e}_z$

In weak outer field : $\hat{H} = \frac{\hat{P}^2}{2\mu} + V(r) + \xi(r)\hat{S}\cdot\hat{L} + \frac{e}{2\mu c}\vec{B}(\hat{L} + 2\hat{S})$

$$= \frac{\hat{P}^2}{2\mu} + V(r) + \xi(r)\hat{S}\cdot\hat{L} + \frac{eB}{2\mu c}\hat{J}_3 + \underline{\frac{eB}{2\mu c}}\hat{S}_3$$

$[\hat{S}_3, \hat{J}^2] \neq 0$

in weak field $\rightarrow$ $\hat{H} = \frac{\hat{P}^2}{2\mu} + V(r) + \xi(r)\hat{S}\cdot\hat{L} + \frac{eB}{2\mu c}\hat{J}_3$

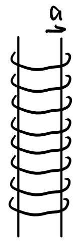
CSCO $\{\hat{H}, \hat{L}^2, \hat{J}^2, \hat{J}_3\}$

Energe Enginvalue : $E = E_{nlj} + m_j\frac{e\hbar B}{2\mu c}$

Aharonov - Bohm Effect

$$i\hbar\partial_t\psi = \left[-\frac{\hbar^2}{2\mu}\left(\nabla - \frac{iq}{\hbar c}\vec{A}\right)^2 + q\phi\right]\psi \qquad \begin{cases} \vec{A} \rightsquigarrow \vec{A}' = \vec{A} + \nabla\chi(\vec{r},t) \\ \phi \rightsquigarrow \phi' = \phi - \frac{1}{c}\partial_t\chi(\vec{r},t) \\ \psi \rightsquigarrow \psi' = \exp\left[\frac{iq}{\hbar c}\chi(\vec{r},t)\right] \end{cases}$$

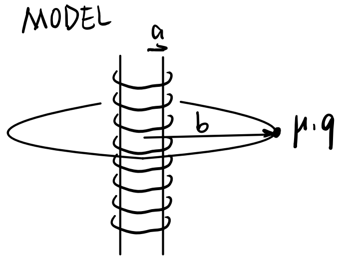
★ Even in an empty field ($\vec{B}=0$) whose vector-potential $\vec{A}\neq 0$, $\vec{A}$ could impact the behavior of a particle



Uniform field $\vec{B} = B\vec{e}_3\,\theta(r-a) \rightsquigarrow \vec{A} = \frac{B\vec{e}_\phi}{2r}\left[r^2\theta(a-r) + a^2\theta(r-a)\right]$

Outta Space $(\vec{B}=0) \rightsquigarrow \vec{A} = \frac{Ba^2}{2r}\vec{e}_\phi = \frac{\Phi}{2\pi r}\vec{e}_\phi$

MODEL



Sch Equ :

磁通量

$$\left[-\frac{\hbar^2}{2\mu b^2}\frac{d^2}{d\varphi^2} + \frac{i\hbar q\Phi}{2\pi b^2\mu c}\frac{d}{d\varphi} + \frac{q^2\Phi^2}{8\pi^2 b^2\mu c^2}\right]\psi = E\psi$$

$$\psi(\varphi) = A\exp\left[i\left(\beta \pm \frac{b}{\hbar}\sqrt{2\mu E}\right)\phi\right] \qquad \left(\beta = \frac{q\Phi}{2\pi\hbar c}\right)$$

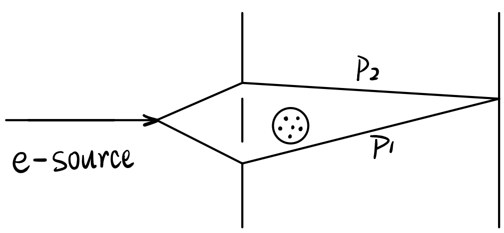
$\psi(\varphi+2\pi) = \psi(\varphi) \rightsquigarrow \quad \beta \pm \frac{b}{\hbar}\sqrt{2\mu E} = n \in \mathbb{N}$

$$E = E_n = \frac{\hbar^2}{2\mu b^2}\left(n - \frac{q\Phi}{2\pi\hbar c}\right)^2, \quad n = 0, \pm1, \pm2, \cdots$$

★ Eigenvalues different appears from magnetic flux Φ

$$\Phi = \oint_{r=b}\vec{A}\cdot dl$$

origin A-B effect experiement



$$i\hbar\partial_t\psi = \left[-\frac{\hbar^2}{2\mu}\left(\nabla - \frac{iq}{\hbar c}\vec{A}\right)^2 + q\phi\right]\psi$$

$\downarrow$ Gauge Trans.

$$\vec{A}' = \vec{A} + \nabla\chi(\vec{r},t)$$

$$\phi' = \phi - \frac{1}{c}\partial_t\chi(\vec{r},t)$$

* If we find specific $\chi(\vec{r})$ to make $\vec{A}' = 0$, then $i\hbar\partial_t\psi' = -\frac{\hbar^2}{2\mu}\nabla^2\psi'$

$$\nabla\chi(\vec{r}) = -\vec{A} \quad \rightarrow \quad \chi(\vec{r}) = -\int_p \vec{A}\cdot d\vec{r}$$

thus $\psi' = \psi\exp\left[-\frac{iq}{\hbar c}\int_p \vec{A}\cdot d\vec{r}\right]$

Consider the situation without solenoid, the prob. amplitude

$$\psi' = \psi_1' + \psi_2' \quad \text{(paths combine)}$$

with solenoid, the prob. amplitude

$$\psi = \psi_1 + \psi_2 = \psi_1' \exp\left[\frac{iq}{\hbar c}\int_{p_1}\vec{A}\cdot d\vec{r}\right] + \psi_2' \exp\left[\frac{iq}{\hbar c}\int_{p_2}\vec{A}\cdot d\vec{r}\right] \quad \{P_1 - P_2 \text{ 闭合}\}$$

$$= \underbrace{\exp\left[\frac{iq}{\hbar c}\int_{p_1}\vec{A}\cdot d\vec{r}\right]}_{\text{unrelated}} \left\{\psi_1' + \psi_2' \exp\left[\frac{iq}{\hbar c}\oint_c \vec{A}\cdot d\vec{r}\right]\right\}$$

$$= \psi_1' + \psi_2' \exp\left[\frac{iq}{\hbar c}\Phi\right]$$

Existance of vector-potential change the phase difference between two splits

$\Rightarrow$ the inteference stripe would move

Energy Level of Hydrogen Atom (Algebra Solution by Pauli)

In central field $\quad F(\vec{r}) = -\nabla V(\vec{r}) = -\frac{e}{r^3}\vec{r}$

$$\vec{L} = \vec{r}\times\vec{p} = \vec{r}\times(\mu\dot{\vec{r}}) = \mu r^2 \vec{e_r}\times\dot{\vec{e_r}}$$

Spotted: $\quad \frac{d}{dt}(\vec{p}\times\vec{L}) = \dot{\vec{p}}\times\vec{L} + \vec{p}\times\dot{\vec{L}} = \mu e^2\dot{\vec{e_r}}$

$$\Rightarrow \frac{d}{dt}\underbrace{\left(\frac{1}{\mu e^2}\vec{p}\times\vec{L} - \vec{e_r}\right)}_{\vec{A}} = 0$$

$\vec{A}$ (Runge – Lenz vector : constant vector)

In QM: $(\hat{\vec{p}}\times\hat{\vec{L}})^\dagger = -(\hat{\vec{L}}\times\hat{\vec{p}})$

Pauli defind Runge - Lenz Vector Operator $\quad \hat{A} = \frac{1}{2\mu e^2}(\hat{\vec{p}}\times\hat{\vec{L}} - \hat{\vec{L}}\times\hat{\vec{p}}) - \frac{\hat{\vec{r}}}{r}$

properties : * $\hat{\vec{A}}^\dagger = \hat{\vec{A}}$, * $[\hat{\vec{A}}, \hat{H}] = 0$

In QM, the <u>vector operator</u> $\hat{V}$ is defined by

$$[\hat{J}_i, \hat{V}_j] = i\hbar\varepsilon_{ijk}\hat{V}_k$$, where $\hat{J}_i$ is angular moment operator

$$[\hat{L}_i, \hat{n}_j] = i\hbar\varepsilon_{ijk}\hat{n}_k \quad \left(\hat{\vec{n}} = \frac{\hat{\vec{r}}}{r}\right)$$

$$[\hat{L}_i, \hat{p}_j] = i\hbar\varepsilon_{ijk}\hat{p}_k, \quad [\hat{L}_i, \hat{L}_j] = i\hbar\varepsilon_{ijk}\hat{L}_k$$

$\boxed{\text{Theorem: } \vec{\alpha}, \vec{\beta} \text{ are vector operator} \rightarrow \vec{\alpha}\times\vec{\beta} \text{ is vector operator}}$

* $[\hat{L}_i, \hat{A}_j] = i\hbar \varepsilon_{ijk} \hat{A}_k \Rightarrow \vec{A}$ is vector operator.
* $\hat{\vec{A}} \cdot \hat{\vec{L}} = \hat{\vec{L}} \cdot \hat{\vec{A}} = 0$
* commuting relationship between each components

$$[\hat{A}_i, \hat{A}_j] = i\hbar \left(-\frac{2\hat{H}}{\mu e^4}\right) \varepsilon_{ijk} \hat{L}_k, \quad \hat{H} = \frac{\hat{\vec{P}}^2}{2\mu} - \frac{e^2}{r}$$

while the electron is at energetic eigenstate: $\hat{H} \to E$ (<0: bound state)

introduce Runge - Lenz operator

$$\hat{M} = \sqrt{-\frac{\mu e^4}{2E}} \hat{A} \Rightarrow [\hat{M}_i, \hat{M}_j] = i\hbar \varepsilon_{ijk} \hat{L}_k$$

* Calculate $\hat{\vec{A}}^2 = \frac{2}{\mu e^4} \hat{H} (\hat{\vec{L}}^2 + \hbar^2) + \hat{I}$

$$\underline{\underline{\hat{H} \to E}} \quad \frac{2}{\mu e^4} E (\hat{\vec{L}}^2 + \hbar^2) + \hat{I}$$

$$\Rightarrow -\frac{\mu e^4}{2E} = \hat{\vec{M}}^2 + \hat{\vec{L}}^2 + \hbar^2$$

introduce $\hat{\vec{J}}_\pm = \frac{1}{2}(\hat{\vec{M}} \pm \hat{\vec{L}})$, $\hat{\vec{J}}_+^2 = \hat{\vec{J}}_-^2 = \frac{1}{4}(\hat{\vec{M}}^2 + \hat{\vec{L}}^2)$

$$-\frac{\mu e^4}{2E} = 4\hat{\vec{J}}_+^2 + \hbar^2$$

$$\rightsquigarrow E(j) = -\frac{\mu e^4}{\hbar^2} \frac{1}{2(2j+1)^2} = -\frac{\mu e^4}{\hbar^2} \frac{1}{2n^2}$$

Identical Particle

Def. Particles which have the exact same intrinsic properties.

propertity: * any observables for any two particles obey exchange inviarence

* two electrons system (Gaussian Frame)

$$\hat{H} = \frac{\hat{\vec{p}}_1^2}{2m} + \frac{\hat{\vec{p}}_2^2}{2m} - \frac{2e^2}{r_1} - \frac{2e^2}{r_2} + \frac{e^2}{|r_1 - r_2|} \qquad \hat{P}_{12} \hat{H} \hat{P}_{12}^{-1} = \hat{H}$$

* N particles system:

$$\hat{P}_{ij} \psi(q_1, \cdots, q_i, \cdots, q_j, \cdots, q_N) = \psi(q_1, \cdots, q_j, \cdots q_i, \cdots q_N)$$

identical particles $\Rightarrow \hat{P}_{ij} \psi = c\psi$, $c^2 = \pm 1$

symmetry: $\hat{P}_{ij} \psi = \psi$ / dissymmetry $\hat{P}_{ij} \psi = -\psi$

Experiment indicate :

particles whose Spin = $n\hbar$ $\xrightarrow{\text{consist}}$ Boson System : wave func. are symmetry for arbitrary dual-particles

particles whose Spin = $(\frac{1}{2}+n)\hbar$ $\xrightarrow{\text{consist}}$ Fermion System : wave func. are dissymmetry for arbitrary dual-particles

★ Ignore the interaction between two particles.

Double Identical Particles System :

$$\hat{H} = \underbrace{\hat{h}(q_1) + \hat{h}(q_2)}_{\text{formatively similar}} \Rightarrow [\hat{P}_{12}, \hat{H}] = 0$$

assume : $\hat{h}(q)\varphi_k(q) = \underbrace{\varepsilon_k}_{\text{energy for single particle}}\varphi_k(q)$: k (complete quantum number set)

when two particles are at different states ($\varphi_{k_1}, \varphi_{k_2}$)

Boson : system made of boson : symmetry wavefunc.

if $k_1 = k_2 = k$ $\quad \psi^{S}_{kk}(q_1, q_2) = \varphi_k(q_1)\varphi_k(q_2)$ $\quad$ ← symmetry

$k_1 \neq k_2$ $\quad \psi^{S}_{k_1k_2}(q_1, q_2) = \frac{1}{\sqrt{2}}[\varphi_{k_1}(q_1)\varphi_{k_2}(q_2) + \varphi_{k_2}(q_1)\varphi_{k_1}(q_2)]$

Fermion : system made of Fermion : Anti-Symmetry WF

$k_1 \neq k_2$, $\psi^{A}_{k_1k_2}(q_1, q_2) = \frac{1}{\sqrt{2}}[\varphi_{k_1}(q_1)\varphi_{k_2}(q_2) - \varphi_{k_2}(q_1)\varphi_{k_1}(q_2)]$

$$= \frac{1}{\sqrt{2}}\begin{vmatrix} \varphi_{k_1}(q_1) & \varphi_{k_1}(q_2) \\ \varphi_{k_2}(q_1) & \varphi_{k_2}(q_2) \end{vmatrix}$$

$k_1 = k_2$, $\psi^{A}_{kk} = 0$: Pauli

N Fermion System △

when each particle is at $k_1 < k_2 < \cdots < k_N$ state, their normalized wave func.

$$\psi^{A}_{k_1k_2\cdots k_N}(q_1, q_2, \cdots, q_N) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \varphi_{k_1}(q_1) & \varphi_{k_1}(q_2) & \cdots & \varphi_{k_N}(q_N) \\ \varphi_{k_2}(q_1) & \varphi_{k_2}(q_2) & \cdots & \varphi_{k_N}(q_N) \\ \vdots & \vdots & & \vdots \\ \varphi_{k_N}(q_1) & \varphi_{k_2}(q_N) & \cdots & \varphi_{k_N}(q_N) \end{vmatrix}$$

N Boson System △

set particles which are at φ_{k_i} : n_i $\quad (\sum_i n_i = N)$

$$\hookrightarrow \psi^{S}_{n_1n_2\cdots n_N}(q_1, q_2, \cdots, q_N) = \sqrt{\frac{\prod_i n_i!}{N!}}\sum_P P[\varphi_{k_1}(q_1)\cdots\varphi_{k_N}(q_N)]$$

Single State & Triple State

CSCO : $\{\hat{S}_{1z}, \hat{S}_{2z}\}$: $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ $\begin{cases} \hat{S}_{1z} = \frac{\hbar}{2}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix} \otimes \hat{I}_2 \\ \hat{S}_{2z} = \hat{I}_1 \otimes \frac{\hbar}{2}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix} \end{cases}$

For $\hat{S}_{1z}$, $\hat{S}_{2z}$, eigenstates $\alpha(1)/\alpha(2) = \begin{bmatrix}1\\0\end{bmatrix}$, $\beta(1)/\beta(2) = \begin{pmatrix}0\\1\end{pmatrix}$

Possible Choices : $\alpha(1)\otimes\alpha(2)$; $\alpha(1)\otimes\beta(2)$; $\beta(1)\otimes\alpha(2)$; $\beta(1)\otimes\beta(2)$

Spin State which meet identical principle :

exchange symmetry : $\alpha(1)\otimes\alpha(2)$; $\frac{1}{\sqrt{2}}[\alpha(1)\otimes\beta(2) + \beta(1)\otimes\alpha(2)]$, $\beta(1)\otimes\beta(2)$

exchange antisymmetry : $\frac{1}{\sqrt{2}}[\alpha(1)\otimes\beta(2) - \alpha(2)\otimes\beta(1)]$

Not eigenstates

if the state cannot be described as direct product of single particle's state we call it entangled state.

choose $\{\hat{S}^2, \hat{S}_z\}$ as CSCO

$$\begin{cases} \hat{S}_z\,\alpha(1)\otimes\alpha(2) = \hbar\,\alpha(1)\otimes\alpha(2) \\ \hat{S}_z\frac{1}{\sqrt{2}}[\alpha(1)\otimes\beta(2) + \beta(1)\otimes\alpha(2)] = 0 \\ \hat{S}_z\,\beta(1)\otimes\beta(2) = -\hbar\,\beta(1)\otimes\beta(2) \end{cases}$$

$$\hat{S}_z\frac{1}{\sqrt{2}}[\alpha(1)\otimes\beta(2) - \beta(1)\otimes\alpha(2)] = 0$$

$$\hat{S}^2 = \frac{3}{2}\hbar^2 + \frac{\hbar^2}{2}\sigma_1\cdot\sigma_2 \Rightarrow \begin{cases} \hat{S}^2\,\alpha(1)\otimes\alpha(2) = 2\hbar^2\alpha(1)\otimes\alpha(2) \\ \hat{S}^2\frac{1}{\sqrt{2}}[\alpha(1)\otimes\beta(2) + \beta(1)\otimes\alpha(2)] = 2\hbar\frac{1}{\sqrt{2}}[\alpha(1)\otimes\beta(2) + \beta(1)\otimes\alpha(2)] \\ \hat{S}^2\beta(1)\otimes\beta(2) = 2\hbar^2\beta(1)\otimes\beta(2) \end{cases}$$

$$\hat{S}^2\frac{1}{\sqrt{2}}[\alpha(1)\otimes\beta(2) - \beta(1)\otimes\alpha(2)] = 0$$

☆ symmetry wave function : triple state χ_{1m_s} $\begin{cases} \chi_{11} = \alpha(1)\otimes\alpha(2) \\ \chi_{10} = \frac{1}{\sqrt{2}}[\alpha(1)\otimes\beta(2) + \beta(1)\otimes\alpha(2)] \\ \chi_{1,-1} = \beta(1)\otimes\beta(2) \end{cases}$

anti-symmetry wave function : single state $\chi_{00} = \frac{1}{\sqrt{2}}[\alpha(1)\otimes\beta(2) - \beta(1)\otimes\alpha(2)]$